



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 05:08 AM BST

PDB ID : 1W2Z
Title : PSAO and Xenon
Authors : Duff, A.P.; Trambaiolo, D.M.; Cohen, A.E.; Ellis, P.J.; Juda, G.A.; Shepard, E.M.; Langley, D.B.; Dooley, D.M.; Freeman, H.C.; Guss, J.M.
Deposited on : 2004-07-11
Resolution : 2.24 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

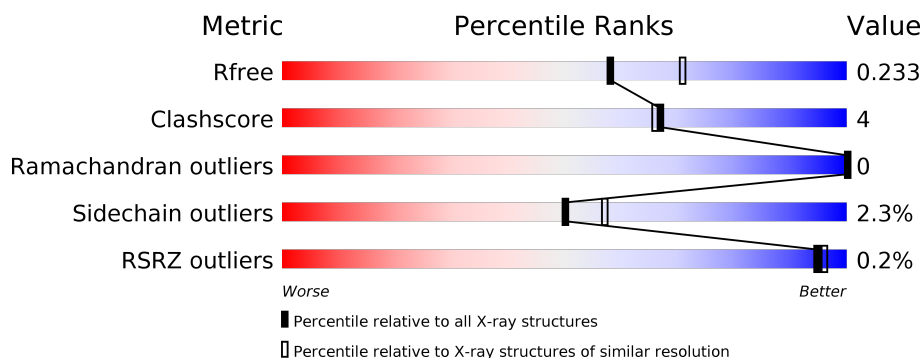
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	649	 90% 9% .
1	B	649	 89% 9% ..
1	C	649	 89% 9% ..
1	D	649	 90% 8% .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	IOD	A	1667	-	-	X	-
6	IOD	A	1674	-	-	X	-
6	IOD	A	1677	-	-	X	-
6	IOD	A	1683	-	-	X	-
6	IOD	A	1687	-	-	X	-
6	IOD	A	1688	-	-	X	-
6	IOD	A	1692	-	-	X	-
6	IOD	B	1666	-	-	X	-
6	IOD	B	1675	-	-	X	-
6	IOD	B	1678	-	-	X	-
6	IOD	B	1684	-	-	X	-
6	IOD	B	1686	-	-	X	-
6	IOD	B	1687	-	-	X	-
6	IOD	C	1663	-	-	X	-
6	IOD	C	1668	-	-	X	-
6	IOD	C	1669	-	-	X	-
6	IOD	C	1686	-	-	X	-
6	IOD	C	1687	-	-	X	-
6	IOD	D	1652	-	-	X	-
6	IOD	D	1659	-	-	X	-
6	IOD	D	1662	-	-	X	-
6	IOD	D	1676	-	-	X	-
6	IOD	D	1680	-	-	X	-
6	IOD	D	1686	-	-	X	-
6	IOD	D	1689	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 40764 atoms, of which 19073 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 AMINE OXIDASE, COPPER CONTAINING.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	642	Total	C	H	N	O	S	9	7	0
			9956	3343	4750	879	972	12			
1	B	642	Total	C	H	N	O	S	4	8	0
			9948	3338	4748	879	971	12			
1	C	642	Total	C	H	N	O	S	4	7	0
			9942	3336	4746	879	969	12			
1	D	642	Total	C	H	N	O	S	6	8	0
			9941	3338	4741	879	971	12			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

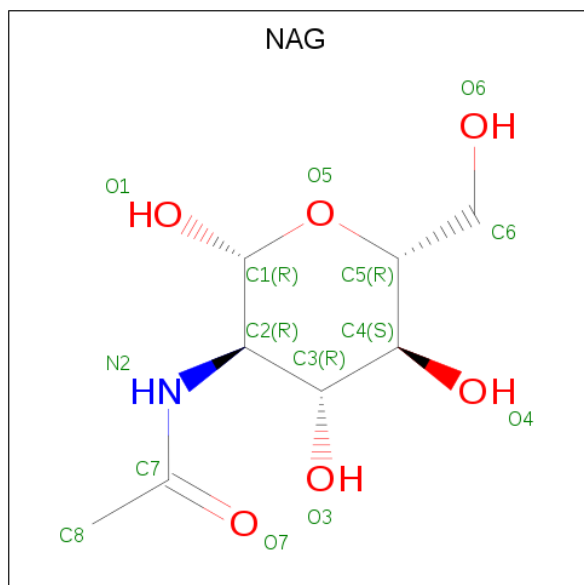
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Xe	0	0
			2	2		
4	A	2	Total	Xe	0	0
			2	2		
4	D	2	Total	Xe	0	0
			2	2		
4	C	2	Total	Xe	0	0
			2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	A	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	B	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	B	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	C	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	C	1	Total	C	H	N	O	0	0
			25	8	11	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
5	D	1	Total	C	H	N	O	0	0
			25	8	11	1	5		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	48	Total	I	0	0
			48	48		
6	A	46	Total	I	0	0
			46	46		
6	D	42	Total	I	0	0
			42	42		
6	C	40	Total	I	0	0
			40	40		

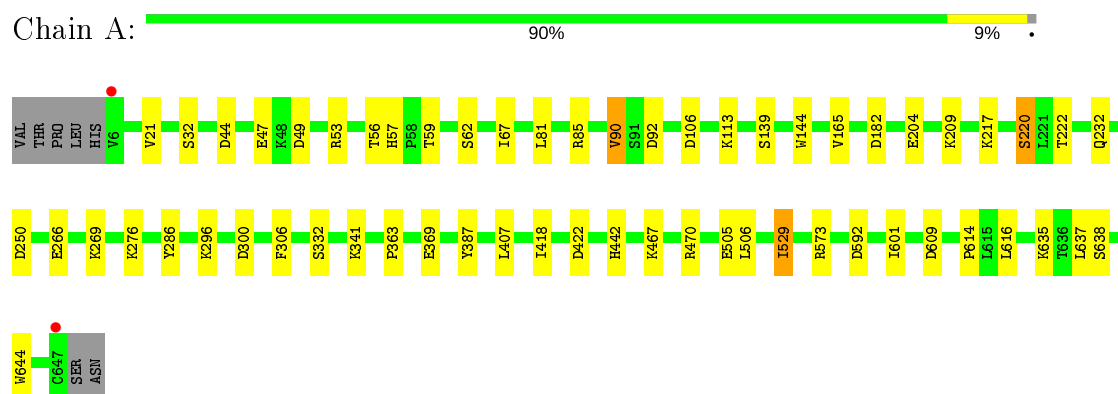
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	174	Total	O	0	0
			174	174		
7	B	141	Total	O	0	0
			141	141		
7	C	125	Total	O	0	0
			125	125		
7	D	145	Total	O	0	0
			145	145		

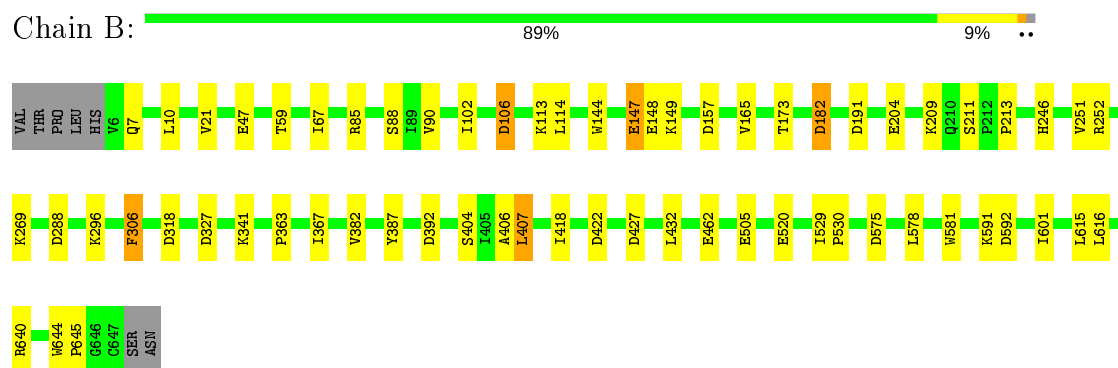
3 Residue-property plots [i](#)

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.

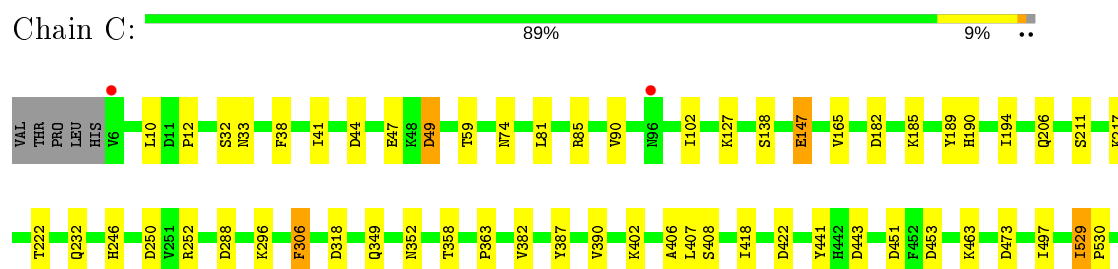
- Molecule 1: AMINE OXIDASE, COPPER CONTAINING



- Molecule 1: AMINE OXIDASE, COPPER CONTAINING

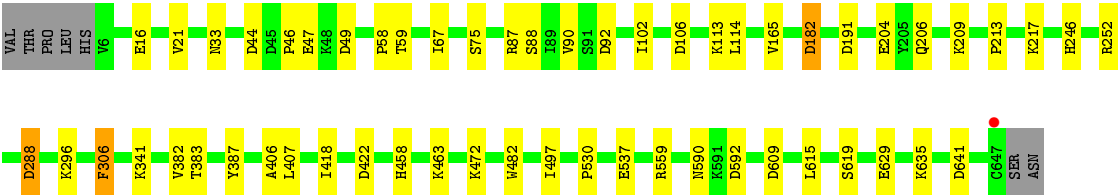
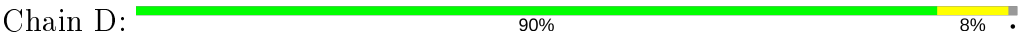


- Molecule 1: AMINE OXIDASE, COPPER CONTAINING





● Molecule 1: AMINE OXIDASE, COPPER CONTAINING



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.51Å 196.27Å 89.67Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	29.88 – 2.24 29.82 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.88-2.24) 99.3 (29.82-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.224 0.194 , 0.233	Depositor DCC
R_{free} test set	13962 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 16.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.249 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40764	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MN, XE, TPQ, IOD, 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	0.58	0/5340	0.77	9/7270 (0.1%)
1	B	0.61	1/5347 (0.0%)	0.79	12/7280 (0.2%)
1	C	0.57	0/5339	0.78	13/7269 (0.2%)
1	D	0.58	0/5347	0.77	9/7280 (0.1%)
All	All	0.58	1/21373 (0.0%)	0.78	43/29099 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	GLU	CB-CG	-12.28	1.28	1.52

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	592	ASP	CB-CG-OD2	7.25	124.82	118.30
1	A	592	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	318	ASP	CB-CG-OD2	6.46	124.12	118.30
1	B	147	GLU	CA-CB-CG	6.46	127.60	113.40
1	C	49	ASP	CB-CG-OD2	6.42	124.08	118.30

There are no chirality outliers.

There are no planarity outliers.

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	5206	4750	5098	39	1
1	B	5200	4748	5093	42	0
1	C	5196	4746	5092	43	0
1	D	5200	4741	5093	35	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
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
4	A	2	0	0	1	0
4	B	2	0	0	1	0
4	C	2	0	0	1	0
4	D	2	0	0	1	0
5	A	28	22	26	0	0
5	B	28	22	26	0	0
5	C	28	22	26	0	0
5	D	28	22	26	0	0
6	A	46	0	0	24	0
6	B	48	0	0	29	0
6	C	40	0	0	20	0
6	D	42	0	0	26	0
7	A	174	0	0	2	0
7	B	141	0	0	6	0
7	C	125	0	0	4	0
7	D	145	0	0	3	0
All	All	21691	19073	20480	162	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 162 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)
6:A:1692:IOD:I	6:B:1696:IOD:I	1.79	1.78
1:C:33:ASN:ND2	6:C:1686:IOD:I	2.27	1.37
1:C:613[B]:MET:HE2	7:C:2065:HOH:O	1.22	1.32
1:D:182[A]:ASP:OD2	6:D:1676:IOD:I	2.20	1.30
1:C:182[B]:ASP:OD2	6:C:1668:IOD:I	2.24	1.26

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:O	1:D:537:GLU:OE1[2_646]	2.18	0.02

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	645/649 (99%)	629 (98%)	16 (2%)	0	100	100
1	B	646/649 (100%)	628 (97%)	18 (3%)	0	100	100
1	C	645/649 (99%)	630 (98%)	15 (2%)	0	100	100
1	D	646/649 (100%)	627 (97%)	19 (3%)	0	100	100
All	All	2582/2596 (100%)	2514 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	581/582 (100%)	567 (98%)	14 (2%)	49	55
1	B	582/582 (100%)	571 (98%)	11 (2%)	57	64
1	C	581/582 (100%)	566 (97%)	15 (3%)	46	52
1	D	582/582 (100%)	569 (98%)	13 (2%)	52	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2326/2328 (100%)	2273 (98%)	53 (2%)	50 57

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	529	ILE
1	C	138	SER
1	D	472	LYS
1	B	591	LYS
1	C	32	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	A	519	ASN
1	B	316	ASN
1	D	227	GLN
1	D	316	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	D	387[A]	-	13,14,15	1.70	4 (30%)	15,19,21	1.46	2 (13%)
1	TPQ	B	387[B]	-	13,14,15	1.57	2 (15%)	15,19,21	1.72	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPQ	D	387[B]	-	13,14,15	1.61	2 (15%)	15,19,21	1.66	2 (13%)
1	TPQ	C	387[B]	-	13,14,15	1.51	2 (15%)	15,19,21	1.08	1 (6%)
1	TPQ	C	387[A]	-	13,14,15	1.73	4 (30%)	15,19,21	1.01	1 (6%)
1	TPQ	A	387[A]	-	13,14,15	1.57	2 (15%)	15,19,21	1.70	4 (26%)
1	TPQ	B	387[A]	-	13,14,15	1.75	4 (30%)	15,19,21	1.85	2 (13%)
1	TPQ	A	387[C]	-	13,14,15	1.57	2 (15%)	15,19,21	1.70	4 (26%)
1	TPQ	A	387[B]	-	13,14,15	1.47	2 (15%)	15,19,21	1.52	2 (13%)

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	D	387[A]	-	-	4/5/22/24	0/1/1/1
1	TPQ	B	387[B]	-	-	2/5/22/24	0/1/1/1
1	TPQ	D	387[B]	-	-	2/5/22/24	0/1/1/1
1	TPQ	C	387[B]	-	-	3/5/22/24	0/1/1/1
1	TPQ	C	387[A]	-	-	4/5/22/24	0/1/1/1
1	TPQ	A	387[A]	-	-	3/5/22/24	0/1/1/1
1	TPQ	B	387[A]	-	-	4/5/22/24	0/1/1/1
1	TPQ	A	387[C]	-	-	2/5/22/24	0/1/1/1
1	TPQ	A	387[B]	-	-	2/5/22/24	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387[B]	TPQ	O4-C4	-3.46	1.25	1.34
1	B	387[B]	TPQ	O4-C4	-3.44	1.25	1.34
1	C	387[B]	TPQ	O4-C4	-3.41	1.25	1.34
1	D	387[B]	TPQ	O4-C4	-3.29	1.25	1.34
1	B	387[A]	TPQ	O4-C4	-3.24	1.25	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387[B]	TPQ	CB-CA-C	-4.68	102.70	111.47
1	B	387[A]	TPQ	CB-CA-C	-4.68	102.70	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	387[A]	TPQ	CB-CA-C	-4.01	103.96	111.47
1	D	387[B]	TPQ	CB-CA-C	-4.01	103.96	111.47
1	B	387[A]	TPQ	CA-CB-C1	3.96	121.08	113.51

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	387[A]	TPQ	N-CA-CB-C1
1	D	387[A]	TPQ	C-CA-CB-C1
1	D	387[A]	TPQ	C2-C1-CB-CA
1	B	387[B]	TPQ	N-CA-CB-C1
1	D	387[B]	TPQ	N-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 200 ligands modelled in this entry, 192 are monoatomic - leaving 8 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	NAG	C	1558	1	14,14,15	0.37	0	17,19,21	1.50	3 (17%)
5	NAG	A	1131	1	14,14,15	0.67	0	17,19,21	1.14	1 (5%)
5	NAG	D	1558	1	14,14,15	0.57	0	17,19,21	1.04	2 (11%)
5	NAG	B	1131	1	14,14,15	0.56	0	17,19,21	1.40	3 (17%)
5	NAG	B	1558	1	14,14,15	0.51	0	17,19,21	1.61	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	1131	1	14,14,15	0.52	0	17,19,21	1.60	2 (11%)
5	NAG	C	1131	1	14,14,15	0.61	0	17,19,21	1.27	2 (11%)
5	NAG	A	1558	1	14,14,15	0.47	0	17,19,21	1.63	5 (29%)

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	NAG	C	1558	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1131	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1558	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1131	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1558	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1131	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1131	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1558	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1131	NAG	C1-O5-C5	4.80	118.70	112.19
5	B	1558	NAG	C1-O5-C5	4.39	118.14	112.19
5	A	1558	NAG	O5-C1-C2	-3.89	105.15	111.29
5	C	1558	NAG	C1-O5-C5	3.65	117.14	112.19
5	B	1131	NAG	O5-C1-C2	-3.37	105.96	111.29

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1558	NAG	C8-C7-N2-C2
5	D	1558	NAG	O7-C7-N2-C2
5	D	1558	NAG	C4-C5-C6-O6
5	C	1131	NAG	C4-C5-C6-O6
5	D	1558	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	641/649 (98%)	-0.56	2 (0%) 94 94	10, 18, 31, 50	2 (0%)
1	B	641/649 (98%)	-0.58	0 100 100	9, 18, 32, 49	2 (0%)
1	C	641/649 (98%)	-0.53	2 (0%) 94 94	10, 18, 32, 50	2 (0%)
1	D	641/649 (98%)	-0.57	1 (0%) 95 96	9, 18, 32, 49	2 (0%)
All	All	2564/2596 (98%)	-0.56	5 (0%) 95 96	9, 18, 32, 50	8 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	VAL	4.0
1	A	6	VAL	2.2
1	C	96	ASN	2.1
1	A	647	CYS	2.1
1	D	647	CYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPQ	D	387[A]	14/15	0.93	0.17	12,26,32,35	11
1	TPQ	D	387[B]	14/15	0.93	0.17	12,24,30,32	11
1	TPQ	C	387[B]	14/15	0.93	0.19	13,23,30,32	11
1	TPQ	C	387[A]	14/15	0.93	0.19	13,25,32,35	11
1	TPQ	A	387[A]	14/15	0.93	0.15	13,26,30,35	11
1	TPQ	A	387[C]	14/15	0.93	0.15	0,0,20,21	9
1	TPQ	A	387[B]	14/15	0.93	0.15	13,24,30,32	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPQ	B	387[B]	14/15	0.95	0.15	13,24,30,32	11
1	TPQ	B	387[A]	14/15	0.95	0.15	13,26,31,35	11

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	A	1660	1/1	0.52	0.13	121,121,121,121	1
6	IOD	A	1687	1/1	0.74	0.16	78,78,78,78	1
5	NAG	A	1558	14/15	0.78	0.23	62,78,83,83	0
6	IOD	B	1682	1/1	0.79	0.15	72,72,72,72	1
5	NAG	C	1558	14/15	0.81	0.22	69,83,88,88	0
5	NAG	C	1131	14/15	0.81	0.17	54,64,70,79	0
6	IOD	D	1673	1/1	0.83	0.15	77,77,77,77	1
5	NAG	D	1131	14/15	0.83	0.20	58,66,76,77	0
5	NAG	B	1131	14/15	0.84	0.17	60,66,77,78	0
6	IOD	A	1692	1/1	0.84	0.11	48,48,48,48	1
6	IOD	C	1655	1/1	0.84	0.11	130,130,130,130	1
5	NAG	D	1558	14/15	0.85	0.22	71,84,87,88	0
5	NAG	B	1558	14/15	0.85	0.19	59,71,80,80	0
6	IOD	C	1660	1/1	0.86	0.07	103,103,103,103	1
6	IOD	B	1690	1/1	0.86	0.13	65,65,65,65	1
6	IOD	C	1683	1/1	0.87	0.10	55,55,55,55	1
4	XE	B	711	1/1	0.89	0.18	51,51,51,51	1
5	NAG	A	1131	14/15	0.89	0.13	48,58,68,68	0
6	IOD	A	1683	1/1	0.89	0.09	61,61,61,61	1
6	IOD	B	1685	1/1	0.90	0.08	66,66,66,66	1
6	IOD	C	1669	1/1	0.90	0.06	74,74,74,74	1
6	IOD	B	1696	1/1	0.90	0.16	64,64,64,64	1
6	IOD	D	1663	1/1	0.91	0.07	64,64,64,64	1
6	IOD	C	1658	1/1	0.91	0.06	68,68,68,68	1
6	IOD	A	1663	1/1	0.91	0.09	62,62,62,62	1
6	IOD	C	1675	1/1	0.91	0.06	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	B	1693	1/1	0.91	0.10	42,42,42,42	1
6	IOD	C	1677	1/1	0.92	0.11	78,78,78,78	1
6	IOD	A	1671	1/1	0.92	0.14	71,71,71,71	1
4	XE	A	711	1/1	0.92	0.14	47,47,47,47	1
6	IOD	C	1686	1/1	0.92	0.10	42,42,42,42	1
6	IOD	C	1676	1/1	0.93	0.11	57,57,57,57	1
6	IOD	A	1672	1/1	0.93	0.07	77,77,77,77	1
6	IOD	A	1680	1/1	0.93	0.08	60,60,60,60	1
6	IOD	A	1667	1/1	0.93	0.07	78,78,78,78	1
6	IOD	D	1687	1/1	0.93	0.10	59,59,59,59	1
6	IOD	B	1655	1/1	0.93	0.05	75,75,75,75	1
6	IOD	B	1684	1/1	0.93	0.07	66,66,66,66	1
6	IOD	B	1658	1/1	0.93	0.06	77,77,77,77	1
4	XE	D	711	1/1	0.93	0.16	55,55,55,55	1
6	IOD	C	1681	1/1	0.93	0.06	49,49,49,49	1
6	IOD	C	1679	1/1	0.93	0.06	67,67,67,67	1
6	IOD	A	1658	1/1	0.94	0.09	44,44,44,44	1
6	IOD	C	1656	1/1	0.94	0.12	48,48,48,48	1
6	IOD	C	1684	1/1	0.94	0.09	49,49,49,49	1
6	IOD	B	1662	1/1	0.94	0.07	68,68,68,68	1
6	IOD	A	1675	1/1	0.94	0.10	87,87,87,87	1
6	IOD	D	1681	1/1	0.94	0.11	64,64,64,64	1
6	IOD	D	1672	1/1	0.94	0.10	51,51,51,51	1
6	IOD	A	1653	1/1	0.94	0.12	78,78,78,78	1
6	IOD	B	1678	1/1	0.94	0.09	59,59,59,59	1
6	IOD	A	1690	1/1	0.94	0.11	55,55,55,55	1
6	IOD	B	1667	1/1	0.95	0.09	82,82,82,82	1
6	IOD	A	1685	1/1	0.95	0.09	55,55,55,55	1
6	IOD	B	1663	1/1	0.95	0.07	44,44,44,44	1
6	IOD	A	1670	1/1	0.95	0.06	63,63,63,63	1
6	IOD	C	1657	1/1	0.95	0.07	90,90,90,90	1
6	IOD	B	1657	1/1	0.95	0.06	74,74,74,74	1
6	IOD	D	1675	1/1	0.95	0.06	76,76,76,76	1
6	IOD	D	1677	1/1	0.95	0.12	53,53,53,53	1
6	IOD	B	1683	1/1	0.95	0.11	70,70,70,70	1
6	IOD	D	1659	1/1	0.95	0.10	92,92,92,92	1
6	IOD	A	1669	1/1	0.95	0.07	71,71,71,71	1
6	IOD	B	1692	1/1	0.95	0.15	59,59,59,59	1
6	IOD	C	1662	1/1	0.95	0.06	49,49,49,49	1
6	IOD	A	1654	1/1	0.95	0.06	83,83,83,83	1
6	IOD	A	1649	1/1	0.96	0.10	47,47,47,47	0
6	IOD	B	1656	1/1	0.96	0.08	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	D	1671	1/1	0.96	0.09	37,37,37,37	1
6	IOD	D	1683	1/1	0.96	0.06	50,50,50,50	1
6	IOD	D	1658	1/1	0.96	0.10	50,50,50,50	1
6	IOD	B	1677	1/1	0.96	0.11	54,54,54,54	1
6	IOD	A	1688	1/1	0.96	0.09	47,47,47,47	1
6	IOD	A	1673	1/1	0.96	0.06	62,62,62,62	1
6	IOD	A	1691	1/1	0.96	0.05	65,65,65,65	1
6	IOD	A	1684	1/1	0.96	0.07	67,67,67,67	1
6	IOD	B	1650	1/1	0.96	0.09	82,82,82,82	1
6	IOD	B	1664	1/1	0.96	0.08	61,61,61,61	1
6	IOD	B	1673	1/1	0.96	0.10	56,56,56,56	1
6	IOD	D	1680	1/1	0.96	0.05	51,51,51,51	1
6	IOD	C	1651	1/1	0.96	0.08	82,82,82,82	0
6	IOD	B	1687	1/1	0.96	0.09	51,51,51,51	1
6	IOD	A	1682	1/1	0.96	0.07	55,55,55,55	1
6	IOD	B	1689	1/1	0.97	0.07	34,34,34,34	1
6	IOD	D	1654	1/1	0.97	0.06	52,52,52,52	1
6	IOD	B	1672	1/1	0.97	0.10	40,40,40,40	1
6	IOD	B	1653	1/1	0.97	0.08	55,55,55,55	1
6	IOD	A	1662	1/1	0.97	0.08	46,46,46,46	1
6	IOD	A	1676	1/1	0.97	0.06	55,55,55,55	1
6	IOD	D	1657	1/1	0.97	0.10	39,39,39,39	1
6	IOD	C	1667	1/1	0.97	0.09	61,61,61,61	1
3	MN	C	702	1/1	0.97	0.06	35,35,35,35	0
6	IOD	C	1674	1/1	0.97	0.08	57,57,57,57	1
6	IOD	C	1678	1/1	0.97	0.03	52,52,52,52	1
6	IOD	B	1679	1/1	0.97	0.07	37,37,37,37	1
6	IOD	B	1674	1/1	0.97	0.07	48,48,48,48	1
6	IOD	C	1653	1/1	0.97	0.07	45,45,45,45	1
6	IOD	C	1666	1/1	0.97	0.06	54,54,54,54	1
6	IOD	C	1659	1/1	0.97	0.08	51,51,51,51	1
6	IOD	D	1651	1/1	0.97	0.06	72,72,72,72	1
6	IOD	D	1667	1/1	0.97	0.05	58,58,58,58	1
6	IOD	B	1676	1/1	0.97	0.07	47,47,47,47	1
6	IOD	C	1682	1/1	0.97	0.08	41,41,41,41	1
6	IOD	D	1655	1/1	0.97	0.09	50,50,50,50	1
6	IOD	D	1682	1/1	0.97	0.09	47,47,47,47	1
6	IOD	A	1695	1/1	0.97	0.05	48,48,48,48	1
6	IOD	D	1665	1/1	0.97	0.08	45,45,45,45	1
6	IOD	D	1676	1/1	0.97	0.06	39,39,39,39	1
6	IOD	C	1671	1/1	0.97	0.10	67,67,67,67	1
6	IOD	D	1648	1/1	0.97	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	D	1664	1/1	0.97	0.06	50,50,50,50	1
6	IOD	D	1686	1/1	0.97	0.05	54,54,54,54	1
6	IOD	C	1654	1/1	0.97	0.05	51,51,51,51	1
6	IOD	D	1689	1/1	0.97	0.05	54,54,54,54	1
6	IOD	A	1689	1/1	0.97	0.10	50,50,50,50	1
6	IOD	C	1663	1/1	0.97	0.05	57,57,57,57	1
6	IOD	B	1669	1/1	0.98	0.06	66,66,66,66	1
6	IOD	C	1650	1/1	0.98	0.09	37,37,37,37	0
6	IOD	C	1664	1/1	0.98	0.09	43,43,43,43	1
6	IOD	B	1659	1/1	0.98	0.05	54,54,54,54	1
6	IOD	D	1666	1/1	0.98	0.06	61,61,61,61	1
6	IOD	C	1661	1/1	0.98	0.05	48,48,48,48	1
6	IOD	C	1672	1/1	0.98	0.04	50,50,50,50	1
6	IOD	B	1661	1/1	0.98	0.08	47,47,47,47	1
6	IOD	C	1670	1/1	0.98	0.08	55,55,55,55	1
6	IOD	A	1679	1/1	0.98	0.07	53,53,53,53	1
6	IOD	A	1659	1/1	0.98	0.06	51,51,51,51	1
6	IOD	D	1688	1/1	0.98	0.09	38,38,38,38	1
6	IOD	D	1685	1/1	0.98	0.04	40,40,40,40	1
6	IOD	A	1664	1/1	0.98	0.05	55,55,55,55	1
6	IOD	A	1657	1/1	0.98	0.05	48,48,48,48	1
6	IOD	A	1666	1/1	0.98	0.04	49,49,49,49	1
6	IOD	A	1686	1/1	0.98	0.04	43,43,43,43	1
6	IOD	C	1668	1/1	0.98	0.08	41,41,41,41	1
6	IOD	B	1652	1/1	0.98	0.05	57,57,57,57	1
6	IOD	B	1649	1/1	0.98	0.09	43,43,43,43	0
6	IOD	A	1665	1/1	0.98	0.07	53,53,53,53	1
3	MN	A	702	1/1	0.98	0.07	36,36,36,36	0
6	IOD	B	1681	1/1	0.98	0.10	40,40,40,40	1
6	IOD	C	1680	1/1	0.98	0.06	50,50,50,50	1
6	IOD	B	1651	1/1	0.98	0.07	47,47,47,47	1
6	IOD	B	1688	1/1	0.98	0.07	42,42,42,42	1
6	IOD	D	1668	1/1	0.98	0.07	76,76,76,76	1
6	IOD	B	1648	1/1	0.98	0.07	36,36,36,36	0
6	IOD	D	1674	1/1	0.98	0.12	40,40,40,40	1
6	IOD	C	1673	1/1	0.98	0.05	50,50,50,50	1
6	IOD	A	1668	1/1	0.98	0.06	62,62,62,62	1
6	IOD	C	1685	1/1	0.98	0.06	40,40,40,40	1
6	IOD	A	1651	1/1	0.98	0.09	52,52,52,52	0
6	IOD	B	1668	1/1	0.98	0.05	48,48,48,48	1
6	IOD	D	1653	1/1	0.98	0.08	45,45,45,45	1
6	IOD	D	1660	1/1	0.98	0.07	74,74,74,74	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	XE	C	711	1/1	0.98	0.10	49,49,49,49	1
6	IOD	A	1648	1/1	0.98	0.08	39,39,39,39	0
6	IOD	A	1655	1/1	0.99	0.04	47,47,47,47	1
6	IOD	B	1665	1/1	0.99	0.06	46,46,46,46	1
6	IOD	C	1652	1/1	0.99	0.10	44,44,44,44	1
4	XE	C	710	1/1	0.99	0.07	32,32,32,32	1
6	IOD	D	1678	1/1	0.99	0.09	40,40,40,40	1
6	IOD	B	1675	1/1	0.99	0.04	43,43,43,43	1
6	IOD	C	1648	1/1	0.99	0.09	47,47,47,47	0
2	CU	C	701	1/1	0.99	0.10	33,33,33,33	0
6	IOD	C	1665	1/1	0.99	0.06	49,49,49,49	1
6	IOD	D	1656	1/1	0.99	0.06	44,44,44,44	1
6	IOD	B	1670	1/1	0.99	0.09	42,42,42,42	1
6	IOD	A	1650	1/1	0.99	0.08	45,45,45,45	0
6	IOD	D	1670	1/1	0.99	0.08	47,47,47,47	1
6	IOD	B	1660	1/1	0.99	0.06	40,40,40,40	1
4	XE	A	710	1/1	0.99	0.08	32,32,32,32	1
4	XE	D	710	1/1	0.99	0.07	33,33,33,33	1
6	IOD	B	1686	1/1	0.99	0.07	50,50,50,50	1
6	IOD	C	1687	1/1	0.99	0.07	63,63,63,63	1
2	CU	A	701	1/1	0.99	0.09	34,34,34,34	0
4	XE	B	710	1/1	0.99	0.08	35,35,35,35	1
6	IOD	A	1674	1/1	0.99	0.12	53,53,53,53	1
3	MN	D	702	1/1	0.99	0.06	36,36,36,36	0
6	IOD	B	1694	1/1	0.99	0.06	52,52,52,52	1
6	IOD	D	1662	1/1	0.99	0.05	56,56,56,56	1
6	IOD	D	1652	1/1	0.99	0.04	53,53,53,53	1
3	MN	B	702	1/1	0.99	0.03	33,33,33,33	0
6	IOD	D	1649	1/1	0.99	0.06	52,52,52,52	0
6	IOD	D	1679	1/1	0.99	0.06	49,49,49,49	1
6	IOD	A	1681	1/1	0.99	0.05	50,50,50,50	1
6	IOD	B	1666	1/1	0.99	0.05	47,47,47,47	1
6	IOD	A	1656	1/1	0.99	0.07	45,45,45,45	1
6	IOD	A	1652	1/1	0.99	0.08	39,39,39,39	0
6	IOD	D	1669	1/1	0.99	0.07	68,68,68,68	1
6	IOD	B	1691	1/1	0.99	0.09	50,50,50,50	1
6	IOD	B	1680	1/1	0.99	0.04	41,41,41,41	1
6	IOD	A	1677	1/1	0.99	0.03	47,47,47,47	1
6	IOD	B	1671	1/1	0.99	0.06	49,49,49,49	1
6	IOD	B	1654	1/1	0.99	0.06	48,48,48,48	1
6	IOD	C	1649	1/1	0.99	0.07	42,42,42,42	0
6	IOD	D	1661	1/1	0.99	0.07	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	A	1661	1/1	0.99	0.10	51,51,51,51	1
6	IOD	A	1678	1/1	0.99	0.07	43,43,43,43	1
2	CU	B	701	1/1	1.00	0.08	31,31,31,31	0
2	CU	D	701	1/1	1.00	0.07	29,29,29,29	0
6	IOD	D	1650	1/1	1.00	0.07	37,37,37,37	0
6	IOD	D	1684	1/1	1.00	0.07	44,44,44,44	1

6.5 Other polymers [i](#)

There are no such residues in this entry.