



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:22 PM GMT

PDB ID : 4LE6
Title : Crystal structure of the phosphotriesterase OPHC2 from *Pseudomonas pseudoalcaligenes*
Authors : Gotthard, G.; Hiblot, J.; Chabriere, E.; Elias, M.
Deposited on : 2013-06-25
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

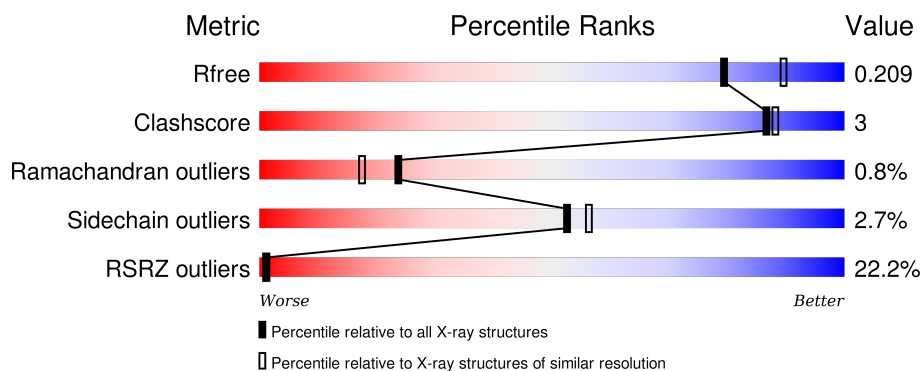
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	324	<div> <div>4%</div> <div>74%</div> <div>5%</div> <div>21%</div> </div>
1	B	324	<div> <div>3%</div> <div>73%</div> <div>5%</div> <div>21%</div> </div>
1	C	324	<div> <div>3%</div> <div>73%</div> <div>•</div> <div>22%</div> </div>
1	D	324	<div> <div>30%</div> <div>73%</div> <div>•</div> <div>23%</div> </div>
1	E	324	<div> <div>47%</div> <div>65%</div> <div>12%</div> <div>23%</div> </div>

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
2	GOL	A	402	-	-	-	X
2	GOL	B	401[A]	-	-	-	X
2	GOL	B	401[B]	-	-	-	X
2	GOL	B	402[A]	-	-	-	X
2	GOL	B	402[B]	-	-	-	X
2	GOL	C	401	-	-	-	X
2	GOL	C	402	-	-	-	X
3	EDO	A	403	-	-	-	X
3	EDO	A	407	-	-	-	X
3	EDO	B	404	-	-	-	X
3	EDO	C	403	-	-	-	X
4	PGE	A	404[A]	-	-	-	X
4	PGE	A	404[B]	-	-	-	X

2 Entry composition [i](#)

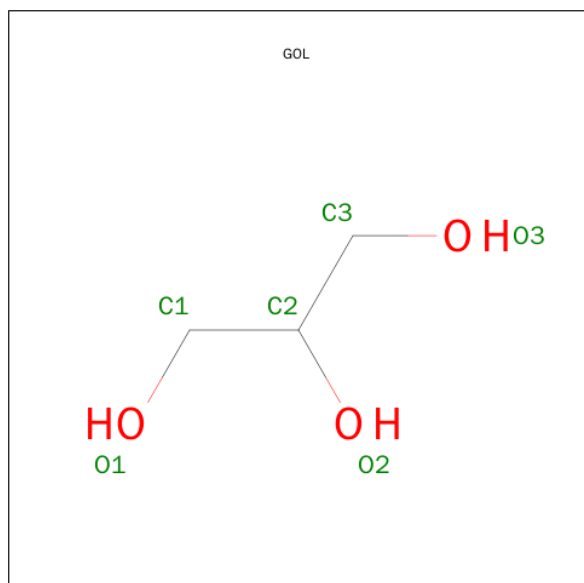
There are 6 unique types of molecules in this entry. The entry contains 20066 atoms, of which 9617 are hydrogens and 0 are deuteriums.

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 Organophosphorus hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total	C	H	N	O	S	0	3	0
			3903	1253	1936	336	374	4			
1	B	255	Total	C	H	N	O	S	0	1	0
			3850	1237	1908	333	368	4			
1	C	254	Total	C	H	N	O	S	0	1	0
			3831	1233	1896	329	369	4			
1	D	251	Total	C	H	N	O	S	0	1	0
			3792	1221	1879	325	363	4			
1	E	251	Total	C	H	N	O	S	0	0	0
			3770	1215	1866	323	362	4			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

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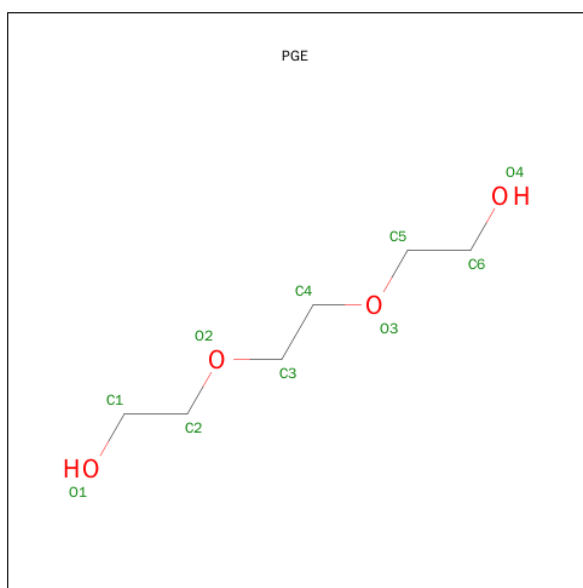
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	1
			28	6	16	6		
2	B	1	Total	C	H	O	0	1
			28	6	16	6		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	1
			48	12	28	8		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		
5	A	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		
5	E	2	Total	Zn	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	325	Total	O	0	0
			325	325		
6	B	167	Total	O	0	0
			167	167		
6	C	136	Total	O	0	0
			136	136		

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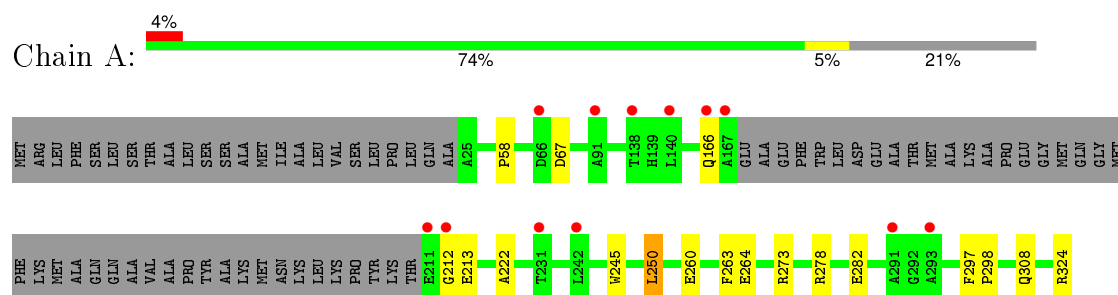
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	43	Total 43	O 43	0	0
6	E	11	Total 11	O 11	0	0

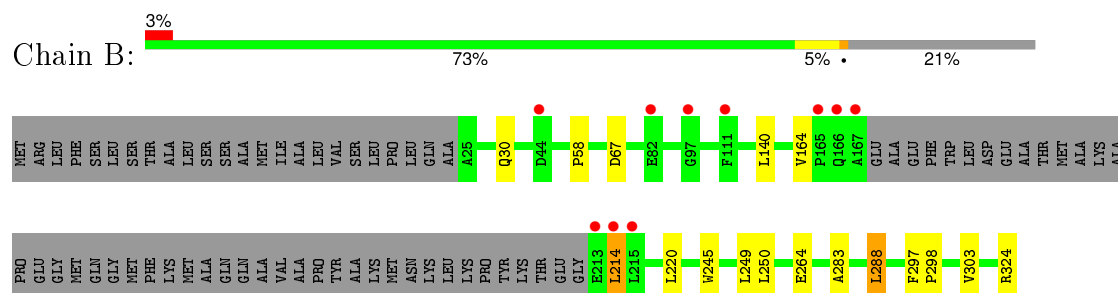
3 Residue-property plots [i](#)

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

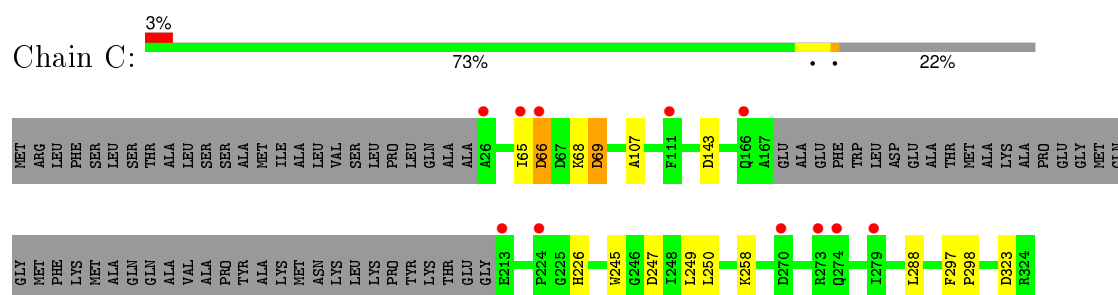
- Molecule 1: Organophosphorus hydrolase



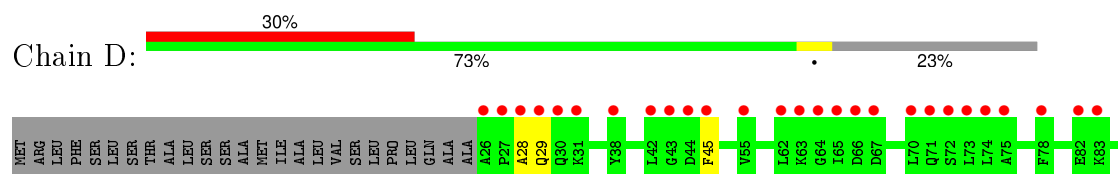
- Molecule 1: Organophosphorus hydrolase

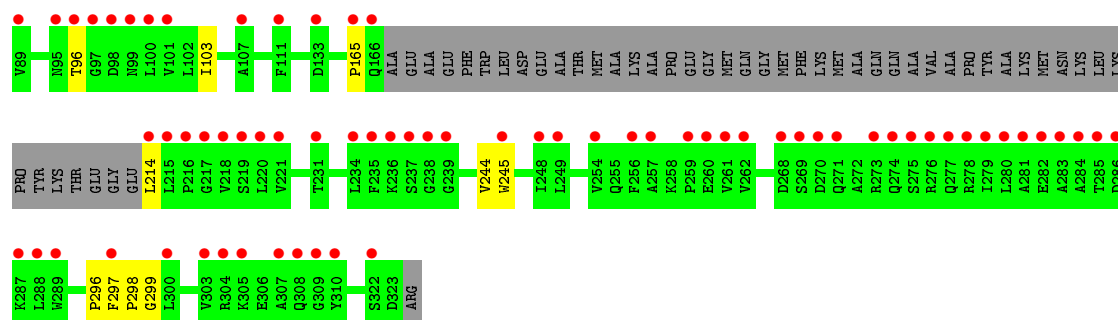


- Molecule 1: Organophosphorus hydrolase

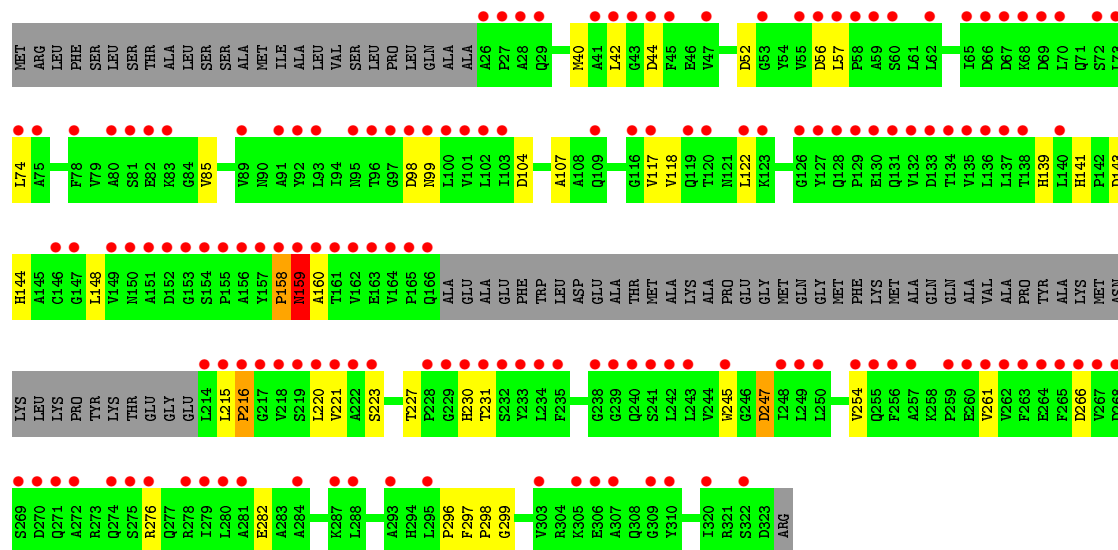


- Molecule 1: Organophosphorus hydrolase





• Molecule 1: Organophosphorus hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.91 Å 63.85 Å 221.26 Å 90.00° 101.85° 90.00°	Depositor
Resolution (Å)	42.80 – 2.10 48.12 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (42.80-2.10) 93.7 (48.12-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.10 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1352)	Depositor
R, R_{free}	0.173 , 0.210 0.172 , 0.209	Depositor DCC
R_{free} test set	4125 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.1	EDS
Estimated twinning fraction	0.016 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.016 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 82530 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20066	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ZN, PGE, EDO

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	0.40	0/2023	0.57	0/2760
1	B	0.32	0/1992	0.52	0/2720
1	C	0.30	0/1985	0.51	0/2711
1	D	0.26	0/1960	0.46	0/2678
1	E	0.26	0/1951	0.46	0/2666
All	All	0.31	0/9911	0.51	0/13535

There are no bond length outliers.

There are no bond angle outliers.

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	1967	1936	1933	12	0
1	B	1942	1908	1905	9	0
1	C	1935	1896	1893	7	0
1	D	1913	1879	1876	5	0
1	E	1904	1866	1863	20	0
2	A	12	16	16	1	0
2	B	30	40	40	2	0
2	C	12	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	8	8	0	0
3	A	8	12	12	1	0
3	B	4	6	6	0	0
3	C	4	6	6	0	0
4	A	20	28	28	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
6	A	325	0	0	5	0
6	B	167	0	0	2	0
6	C	136	0	0	1	0
6	D	43	0	0	0	0
6	E	11	0	0	3	0
All	All	10449	9617	9602	52	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 3.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLN:NE2	1:E:44:ASP:O	2.17	0.77
1:A:278[B]:ARG:NH2	6:A:783:HOH:O	2.18	0.76
1:E:261:VAL:O	1:E:276:ARG:NH1	2.26	0.68
1:E:158:PRO:O	1:E:160:ALA:N	2.28	0.66
1:E:221:VAL:O	1:E:231:THR:OG1	2.16	0.63
1:E:247:ASP:OD1	1:E:247:ASP:N	2.33	0.61
1:A:67:ASP:OD1	6:A:761:HOH:O	2.16	0.59
1:E:57:LEU:O	1:E:85:VAL:N	2.34	0.59
1:E:98:ASP:O	1:E:99:ASN:ND2	2.37	0.57
1:E:104:ASP:OD2	1:E:144:HIS:ND1	2.40	0.54
1:E:223:SER:OG	6:E:511:HOH:O	2.18	0.54
1:B:283:ALA:HB3	1:B:303:VAL:HG11	1.90	0.53
1:A:297:PHE:CD1	1:A:298:PRO:HA	2.44	0.53
1:B:30:GLN:OE1	6:B:629:HOH:O	2.19	0.52
1:C:69:ASP:OD2	1:C:258:LYS:NZ	2.43	0.52
2:A:402:GOL:O3	2:B:401[A]:GOL:H11	2.10	0.52
1:A:264:GLU:HG2	1:B:58:PRO:HG3	1.93	0.50
1:D:297:PHE:CD1	1:D:298:PRO:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ASP:OD2	1:E:107:ALA:N	2.47	0.47
1:E:143:ASP:OD2	6:E:510:HOH:O	2.20	0.47
1:B:297:PHE:CD1	1:B:298:PRO:HA	2.50	0.46
1:C:65:ILE:O	1:C:66:ASP:CB	2.63	0.46
1:E:118:VAL:O	1:E:122:LEU:N	2.49	0.46
1:A:260:GLU:HA	1:A:273:ARG:HD3	1.98	0.45
1:C:297:PHE:CD1	1:C:298:PRO:HA	2.52	0.45
2:B:402[A]:GOL:O1	6:B:603:HOH:O	2.10	0.45
1:C:323:ASP:OD2	6:C:594:HOH:O	2.21	0.45
1:A:324:ARG:NH1	6:A:752:HOH:O	2.50	0.44
1:A:58:PRO:HG3	1:B:264:GLU:HG2	1.99	0.44
1:A:222:ALA:HB1	3:A:403:EDO:H22	1.99	0.43
1:C:226:HIS:CD2	1:C:247:ASP:HB2	2.53	0.43
1:A:250:LEU:HD22	1:A:263:PHE:CE1	2.54	0.43
1:B:140:LEU:HD21	1:B:164:VAL:HG13	2.00	0.43
1:A:250:LEU:HD22	1:A:263:PHE:CD1	2.54	0.43
1:E:296:PRO:O	1:E:299:GLY:N	2.49	0.43
1:D:45:PHE:CD1	1:D:96:THR:HA	2.54	0.42
1:E:297:PHE:CD1	1:E:298:PRO:HA	2.54	0.42
1:C:107:ALA:HB2	1:C:143:ASP:HA	2.01	0.42
1:E:215:LEU:HB3	1:E:216:PRO:HD2	2.02	0.42
1:E:139:HIS:CD2	1:E:141:HIS:CG	3.08	0.42
1:A:166:GLN:N	6:A:723:HOH:O	2.52	0.42
1:D:296:PRO:O	1:D:299:GLY:N	2.53	0.42
1:D:103:ILE:HG21	1:D:244:VAL:HG11	2.02	0.41
1:E:227:THR:H	1:E:230:HIS:HB2	1.85	0.41
1:E:159:ASN:N	1:E:159:ASN:OD1	2.54	0.41
1:B:283:ALA:HA	1:B:288:LEU:HD11	2.02	0.41
1:B:214:LEU:HD12	1:B:220:LEU:HD11	2.03	0.41
1:A:282:GLU:OE2	6:A:788:HOH:O	2.22	0.41
1:E:266:ASP:N	6:E:508:HOH:O	2.54	0.40
1:C:65:ILE:O	1:C:66:ASP:HB2	2.21	0.40
1:E:52:ASP:OD1	1:E:117:VAL:N	2.50	0.40
1:B:283:ALA:CB	1:B:288:LEU:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/324 (79%)	249 (97%)	5 (2%)	2 (1%)	24	17
1	B	252/324 (78%)	247 (98%)	5 (2%)	0	100	100
1	C	251/324 (78%)	240 (96%)	10 (4%)	1 (0%)	39	37
1	D	248/324 (76%)	233 (94%)	13 (5%)	2 (1%)	24	17
1	E	247/324 (76%)	204 (83%)	38 (15%)	5 (2%)	9	4
All	All	1254/1620 (77%)	1173 (94%)	71 (6%)	10 (1%)	24	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	ASP
1	E	158	PRO
1	E	159	ASN
1	E	74	LEU
1	E	216	PRO
1	A	212	GLY
1	A	213	GLU
1	D	28	ALA
1	D	165	PRO
1	E	254	VAL

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	208/258 (81%)	205 (99%)	3 (1%)	74	80
1	B	205/258 (80%)	198 (97%)	7 (3%)	44	45
1	C	205/258 (80%)	199 (97%)	6 (3%)	50	53
1	D	203/258 (79%)	201 (99%)	2 (1%)	82	87
1	E	202/258 (78%)	193 (96%)	9 (4%)	34	32
All	All	1023/1290 (79%)	996 (97%)	27 (3%)	52	58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	TRP
1	A	250	LEU
1	A	308	GLN
1	B	67	ASP
1	B	214	LEU
1	B	245	TRP
1	B	249	LEU
1	B	250	LEU
1	B	288	LEU
1	B	324	ARG
1	C	68	LYS
1	C	69	ASP
1	C	245	TRP
1	C	249	LEU
1	C	250	LEU
1	C	288	LEU
1	D	214	LEU
1	D	245	TRP
1	E	40	MET
1	E	42	LEU
1	E	56	ASP
1	E	148	LEU
1	E	159	ASN
1	E	220	LEU
1	E	245	TRP
1	E	247	ASP
1	E	282	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	$\# Z > 2$
2	GOL	A	401	-	5,5,5	0.37	0	5,5,5	0.25	0
2	GOL	A	402	-	5,5,5	0.22	0	5,5,5	0.61	0
3	EDO	A	403	-	3,3,3	0.42	0	2,2,2	0.35	0
4	PGE	A	404[A]	-	9,9,9	0.30	0	8,8,8	0.29	0
4	PGE	A	404[B]	-	9,9,9	0.31	0	8,8,8	0.35	0
3	EDO	A	407	-	3,3,3	0.45	0	2,2,2	0.57	0
2	GOL	B	401[A]	-	5,5,5	0.34	0	5,5,5	0.25	0
2	GOL	B	401[B]	-	5,5,5	0.33	0	5,5,5	0.27	0
2	GOL	B	402[A]	-	5,5,5	0.26	0	5,5,5	0.24	0
2	GOL	B	402[B]	-	5,5,5	0.32	0	5,5,5	0.31	0
2	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.24	0
3	EDO	B	404	-	3,3,3	0.31	0	2,2,2	0.26	0
2	GOL	C	401	-	5,5,5	0.37	0	5,5,5	0.51	0
2	GOL	C	402	-	5,5,5	0.35	0	5,5,5	0.37	0
3	EDO	C	403	-	3,3,3	0.50	0	2,2,2	0.25	0
2	GOL	D	401	-	5,5,5	0.36	0	5,5,5	0.19	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
2	GOL	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	PGE	A	404[A]	-	-	0/7/7/7	0/0/0/0
4	PGE	A	404[B]	-	-	0/7/7/7	0/0/0/0
3	EDO	A	407	-	-	0/1/1/1	0/0/0/0
2	GOL	B	401[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401[B]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	402[B]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	402	-	-	0/4/4/4	0/0/0/0
3	EDO	C	403	-	-	0/1/1/1	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GOL	1	0
3	A	403	EDO	1	0
2	B	401[A]	GOL	1	0
2	B	402[A]	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	257/324 (79%)	0.68	12 (4%) 35 44	16, 27, 46, 122	3 (1%)
1	B	255/324 (78%)	0.44	10 (3%) 43 52	27, 42, 68, 147	1 (0%)
1	C	254/324 (78%)	0.51	11 (4%) 39 48	30, 50, 78, 106	1 (0%)
1	D	251/324 (77%)	2.04	96 (38%) 0 0	48, 81, 119, 142	2 (0%)
1	E	251/324 (77%)	2.94	153 (60%) 0 0	64, 115, 149, 168	5 (1%)
All	All	1268/1620 (78%)	1.32	282 (22%) 1 1	16, 56, 130, 168	12 (0%)

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	GLN	12.3
1	B	167	ALA	10.7
1	E	218	VAL	10.5
1	D	70	LEU	10.4
1	E	134	THR	10.4
1	D	27	PRO	10.0
1	E	100	LEU	9.9
1	D	215	LEU	9.9
1	D	28	ALA	9.3
1	E	140	LEU	8.8
1	E	165	PRO	7.6
1	E	257	ALA	7.6
1	E	75	ALA	7.5
1	E	166	GLN	7.4
1	E	67	ASP	7.4
1	D	220	LEU	7.3
1	D	307	ALA	7.2
1	E	72	SER	7.1
1	E	45	PHE	6.9
1	E	132	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
1	E	219	SER	6.9
1	E	220	LEU	6.9
1	E	26	ALA	6.8
1	E	99	ASN	6.7
1	E	128	GLN	6.5
1	E	217	GLY	6.5
1	D	285	THR	6.4
1	E	260	GLU	6.4
1	D	44	ASP	6.3
1	E	101	VAL	6.3
1	E	162	VAL	6.3
1	D	237	SER	6.2
1	D	308	GLN	6.1
1	E	272	ALA	6.1
1	E	274	GLN	6.0
1	E	28	ALA	6.0
1	E	214	LEU	6.0
1	E	155	PRO	6.0
1	D	216	PRO	6.0
1	E	70	LEU	6.0
1	D	279	ILE	5.9
1	E	157	TYR	5.9
1	E	161	THR	5.9
1	D	257	ALA	5.8
1	E	261	VAL	5.8
1	D	97	GLY	5.8
1	D	281	ALA	5.8
1	E	68	LYS	5.8
1	D	26	ALA	5.7
1	E	216	PRO	5.7
1	D	309	GLY	5.7
1	E	65	ILE	5.7
1	A	211	GLU	5.6
1	E	127	TYR	5.6
1	D	219	SER	5.6
1	D	287	LYS	5.5
1	E	215	LEU	5.4
1	E	160	ALA	5.4
1	E	275	SER	5.4
1	E	164	VAL	5.3
1	E	97	GLY	5.3
1	E	154	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	214	LEU	5.2
1	D	218	VAL	5.1
1	E	309	GLY	5.1
1	E	221	VAL	5.0
1	E	93	LEU	5.0
1	D	43	GLY	5.0
1	E	279	ILE	5.0
1	D	98	ASP	5.0
1	E	69	ASP	5.0
1	E	27	PRO	5.0
1	A	212	GLY	4.9
1	E	96	THR	4.9
1	E	222	ALA	4.9
1	E	263	PHE	4.8
1	E	310	TYR	4.8
1	D	283	ALA	4.8
1	D	65	ILE	4.8
1	E	280	LEU	4.8
1	D	284	ALA	4.7
1	D	96	THR	4.6
1	D	288	LEU	4.6
1	E	42	LEU	4.6
1	D	217	GLY	4.6
1	E	131	GLN	4.6
1	E	136	LEU	4.6
1	E	270	ASP	4.5
1	E	80	ALA	4.5
1	E	265	PHE	4.5
1	D	270	ASP	4.4
1	E	55	VAL	4.4
1	D	256	PHE	4.4
1	E	159	ASN	4.3
1	E	249	LEU	4.3
1	C	66	ASP	4.3
1	E	44	ASP	4.3
1	D	310	TYR	4.3
1	E	243	LEU	4.3
1	E	149	VAL	4.3
1	E	98	ASP	4.2
1	E	130	GLU	4.2
1	D	235	PHE	4.2
1	D	322	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	214	LEU	4.2
1	E	117	VAL	4.2
1	D	286	ASP	4.2
1	E	133	ASP	4.1
1	E	129	PRO	4.1
1	E	268	ASP	4.0
1	D	305	LYS	4.0
1	D	234	LEU	4.0
1	E	287	LYS	4.0
1	D	278	ARG	3.9
1	D	66	ASP	3.9
1	E	116	GLY	3.9
1	E	66	ASP	3.9
1	D	238	GLY	3.9
1	D	101	VAL	3.9
1	E	303	VAL	3.9
1	E	254	VAL	3.8
1	E	264	GLU	3.8
1	E	307	ALA	3.8
1	E	122	LEU	3.8
1	D	274	GLN	3.7
1	D	239	GLY	3.7
1	E	137	LEU	3.7
1	E	120	THR	3.7
1	E	248	ILE	3.7
1	D	42	LEU	3.7
1	D	280	LEU	3.7
1	E	238	GLY	3.6
1	E	102	LEU	3.6
1	D	268	ASP	3.6
1	D	221	VAL	3.6
1	E	234	LEU	3.6
1	D	277	GLN	3.6
1	D	236	LYS	3.5
1	E	138	THR	3.5
1	E	152	ASP	3.5
1	D	273	ARG	3.5
1	E	103	ILE	3.5
1	E	57	LEU	3.5
1	E	267	VAL	3.4
1	D	100	LEU	3.4
1	C	213	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	59	ALA	3.4
1	E	73	LEU	3.3
1	E	245	TRP	3.3
1	D	282	GLU	3.3
1	E	158	PRO	3.3
1	E	320	ILE	3.3
1	D	275	SER	3.3
1	C	166	GLN	3.3
1	D	74	LEU	3.2
1	C	274	GLN	3.2
1	D	289	TRP	3.2
1	E	262	VAL	3.2
1	D	45	PHE	3.2
1	E	228	PRO	3.2
1	E	60	SER	3.1
1	B	165	PRO	3.1
1	B	166	GLN	3.1
1	D	82	GLU	3.1
1	D	64	GLY	3.1
1	E	95	ASN	3.1
1	E	146	CYS	3.1
1	C	65	ILE	3.1
1	D	99	ASN	3.0
1	E	242	LEU	3.0
1	D	231	THR	3.0
1	E	153	GLY	3.0
1	E	58	PRO	3.0
1	E	83	LYS	3.0
1	E	278	ARG	3.0
1	E	232	SER	3.0
1	B	215	LEU	3.0
1	E	271	GLN	3.0
1	E	56	ASP	2.9
1	C	279	ILE	2.9
1	E	81	SER	2.9
1	D	262	VAL	2.9
1	B	111	PHE	2.9
1	E	82	GLU	2.9
1	A	167	ALA	2.9
1	E	240	GLN	2.9
1	E	233	TYR	2.9
1	D	29	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	259	PRO	2.8
1	D	303	VAL	2.8
1	D	276	ARG	2.8
1	D	133	ASP	2.8
1	C	26	ALA	2.8
1	E	288	LEU	2.8
1	D	63	LYS	2.8
1	E	89	VAL	2.8
1	D	271	GLN	2.7
1	E	123	LYS	2.7
1	E	156	ALA	2.7
1	E	255	GLN	2.7
1	E	230	HIS	2.7
1	E	150	ASN	2.7
1	D	75	ALA	2.7
1	E	41	ALA	2.7
1	E	92	TYR	2.7
1	C	273	ARG	2.6
1	A	291	ALA	2.6
1	E	147	GLY	2.6
1	E	109	GLN	2.6
1	D	78	PHE	2.5
1	E	78	PHE	2.5
1	E	126	GLY	2.5
1	D	72	SER	2.5
1	D	165	PRO	2.5
1	E	43	GLY	2.5
1	D	260	GLU	2.5
1	D	269	SER	2.5
1	E	322	SER	2.5
1	E	62	LEU	2.5
1	D	95	ASN	2.5
1	E	29	GLN	2.5
1	A	66	ASP	2.5
1	E	256	PHE	2.5
1	E	119	GLN	2.5
1	D	297	PHE	2.5
1	E	74	LEU	2.4
1	D	261	VAL	2.4
1	D	89	VAL	2.4
1	E	135	VAL	2.4
1	E	163	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	231	THR	2.4
1	B	97	GLY	2.4
1	E	223	SER	2.4
1	E	235	PHE	2.4
1	E	259	PRO	2.3
1	E	306	GLU	2.3
1	D	38	TYR	2.3
1	E	266	ASP	2.3
1	D	55	VAL	2.3
1	D	31	LYS	2.3
1	D	107	ALA	2.3
1	D	111	PHE	2.3
1	E	276	ARG	2.3
1	E	284	ALA	2.3
1	C	224	PRO	2.3
1	D	304	ARG	2.3
1	A	91	ALA	2.3
1	E	229	GLY	2.2
1	A	166	GLN	2.2
1	D	249	LEU	2.2
1	A	138	THR	2.2
1	E	47	VAL	2.2
1	D	62	LEU	2.2
1	C	111	PHE	2.2
1	E	281	ALA	2.2
1	B	44	ASP	2.2
1	D	73	LEU	2.2
1	E	250	LEU	2.2
1	B	213	GLU	2.2
1	E	151	ALA	2.2
1	D	300	LEU	2.2
1	E	295	LEU	2.2
1	D	245	TRP	2.2
1	D	67	ASP	2.1
1	E	241	SER	2.1
1	E	269	SER	2.1
1	A	242	LEU	2.1
1	C	270	ASP	2.1
1	D	30	GLN	2.1
1	D	71	GLN	2.1
1	D	83	LYS	2.1
1	A	140	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	305	LYS	2.0
1	A	293	ALA	2.0
1	E	293	ALA	2.0
1	A	231	THR	2.0
1	D	254	VAL	2.0
1	D	248	ILE	2.0
1	E	91	ALA	2.0
1	B	82	GLU	2.0
1	E	53	GLY	2.0
1	E	239	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	C	403	4/4	0.83	0.76	52.30	32,38,43,44	10
2	GOL	C	402	6/6	0.79	1.21	32.92	29,35,40,43	14
2	GOL	A	402	6/6	0.59	1.00	27.38	32,38,40,41	14
3	EDO	A	407	4/4	0.90	0.71	22.86	41,49,51,51	10
4	PGE	A	404[B]	10/10	0.80	0.90	21.66	31,38,44,45	24
4	PGE	A	404[A]	10/10	0.80	0.90	21.46	31,39,45,46	24
2	GOL	B	401[B]	6/6	0.65	0.69	15.10	35,42,46,49	14
2	GOL	B	401[A]	6/6	0.65	0.69	14.75	35,42,46,46	14
3	EDO	B	404	4/4	0.94	0.36	12.84	20,24,26,31	10
2	GOL	B	402[B]	6/6	0.66	0.55	10.33	38,49,56,59	14
2	GOL	B	402[A]	6/6	0.66	0.55	10.33	30,46,53,56	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	A	403	4/4	0.84	0.54	7.94	20,26,37,44	10
2	GOL	C	401	6/6	0.87	0.35	7.34	23,29,36,44	14
5	ZN	B	405	1/1	0.99	0.16	0.66	34,34,34,34	0
2	GOL	B	403	6/6	0.94	0.14	0.46	33,41,51,56	0
2	GOL	D	401	6/6	0.94	0.17	0.04	56,68,80,82	0
5	ZN	B	406	1/1	1.00	0.14	-0.00	31,31,31,31	0
2	GOL	A	401	6/6	0.96	0.14	-0.43	24,31,41,45	0
5	ZN	C	405	1/1	0.97	0.14	-0.89	42,42,42,42	0
5	ZN	C	404	1/1	0.99	0.13	-1.06	43,43,43,43	0
5	ZN	A	405	1/1	0.99	0.17	-2.19	24,24,24,24	0
5	ZN	E	401	1/1	0.78	0.10	-2.21	97,97,97,97	0
5	ZN	D	403	1/1	0.97	0.10	-2.24	56,56,56,56	0
5	ZN	E	402	1/1	0.96	0.10	-2.27	98,98,98,98	0
5	ZN	D	402	1/1	0.97	0.09	-3.00	53,53,53,53	0
5	ZN	A	406	1/1	1.00	0.15	-3.62	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.