



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:46 AM GMT

PDB ID : 2O4M  
Title : Structure of Phosphotriesterase mutant I106G/F132G/H257Y  
Authors : Kim, J.; Ramagopal, U.A.; Tsai, P.; Raushel, F.M.; Almo, S.C.  
Deposited on : 2006-12-04  
Resolution : 1.64 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

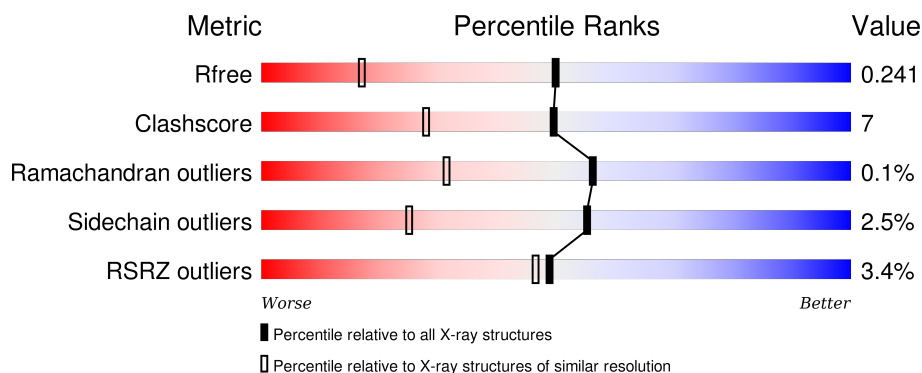
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	331	<div> <div>87%</div> <div>12%</div> <div>•</div> </div>
1	B	331	<div> <div>5%</div> <div>88%</div> <div>12%</div> <div>•</div> </div>
1	C	331	<div> <div>5%</div> <div>87%</div> <div>12%</div> <div>•</div> </div>
1	P	331	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>•</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
4	GOL	C	5005	-	-	-	X
4	GOL	P	5003	-	-	-	X
5	ACY	A	6003	-	-	-	X
5	ACY	B	6002	-	-	-	X
5	ACY	C	6001	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11956 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	9	0
			2571	1624	457	483	7			
1	B	331	Total	C	N	O	S	0	8	0
			2561	1616	462	476	7			
1	C	331	Total	C	N	O	S	0	11	0
			2574	1630	457	480	7			
1	P	331	Total	C	N	O	S	0	7	0
			2571	1620	462	482	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	ILE	ENGINEERED	UNP P0A434
A	132	GLY	PHE	ENGINEERED	UNP P0A434
A	257	TYR	HIS	ENGINEERED	UNP P0A434
B	106	GLY	ILE	ENGINEERED	UNP P0A434
B	132	GLY	PHE	ENGINEERED	UNP P0A434
B	257	TYR	HIS	ENGINEERED	UNP P0A434
C	106	GLY	ILE	ENGINEERED	UNP P0A434
C	132	GLY	PHE	ENGINEERED	UNP P0A434
C	257	TYR	HIS	ENGINEERED	UNP P0A434
P	106	GLY	ILE	ENGINEERED	UNP P0A434
P	132	GLY	PHE	ENGINEERED	UNP P0A434
P	257	TYR	HIS	ENGINEERED	UNP P0A434

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

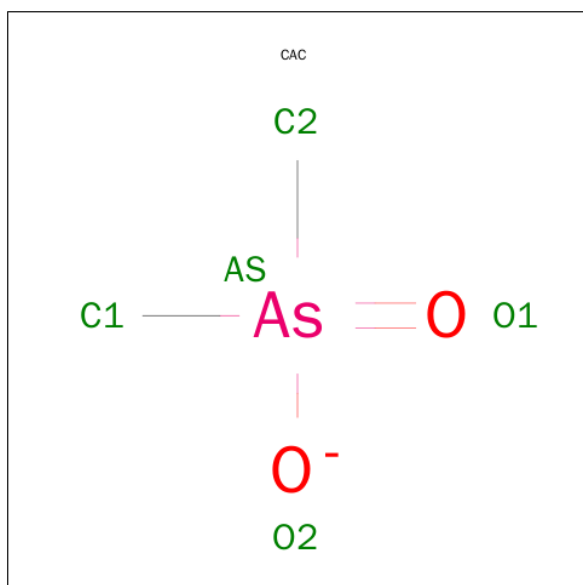
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	6	Total	Zn	0	0
			6	6		
2	B	5	Total	Zn	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Zn	0	0
			6	6		
2	C	6	Total	Zn	0	0
			6	6		

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula:  $\text{C}_2\text{H}_6\text{AsO}_2$ ).



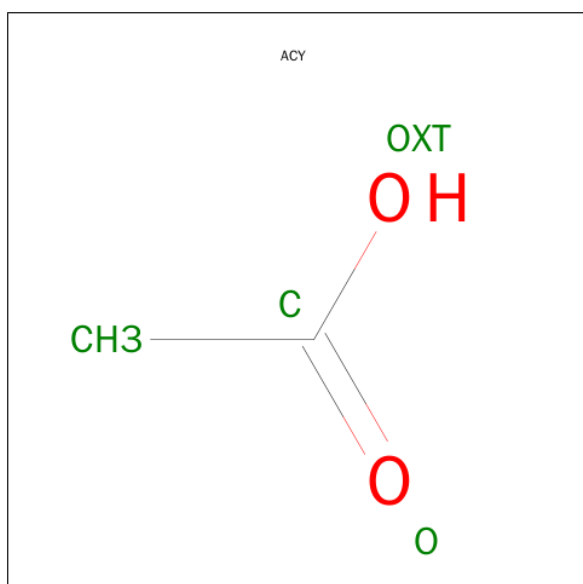
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	C	1	Total	As	C	O	0	0
			5	1	2	2		
3	P	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	P	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

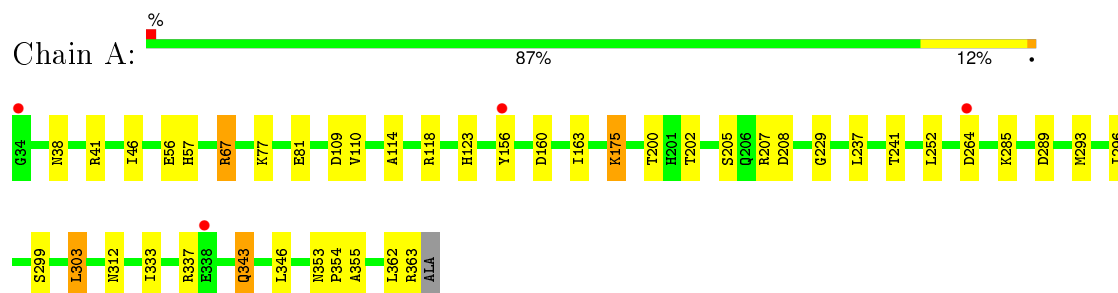
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	414	Total O 414 414	0	0
6	B	395	Total O 395 395	0	0
6	C	408	Total O 408 408	0	0
6	P	377	Total O 377 377	0	0

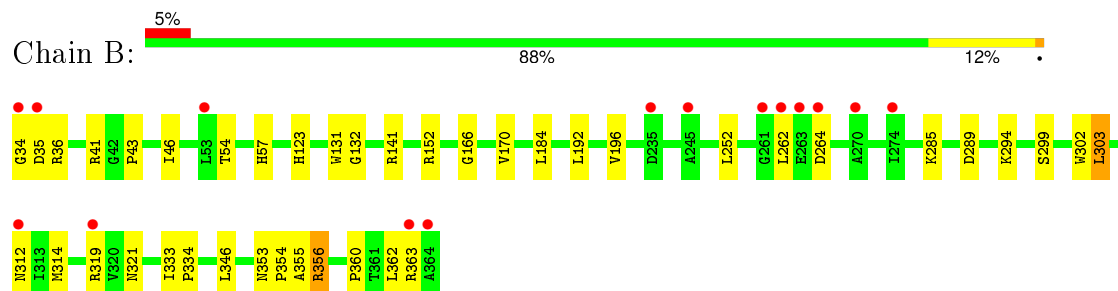
### 3 Residue-property plots [i](#)

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.

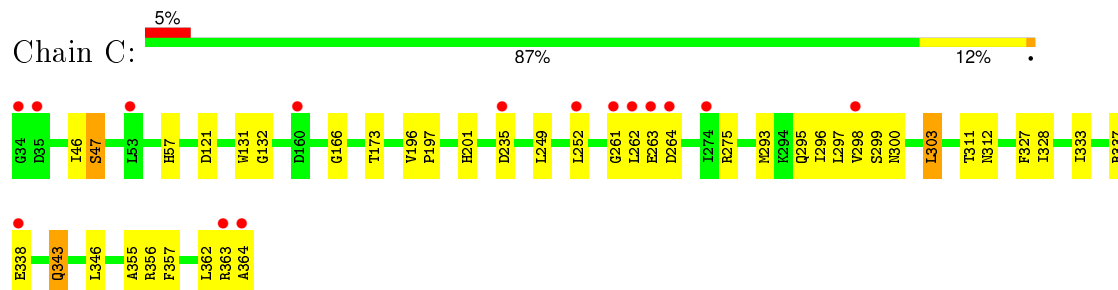
#### • Molecule 1: Parathion hydrolase



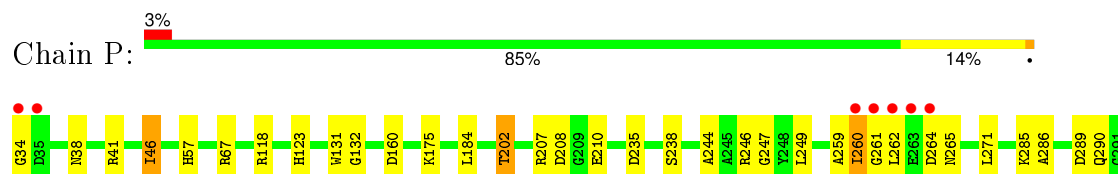
#### • Molecule 1: Parathion hydrolase



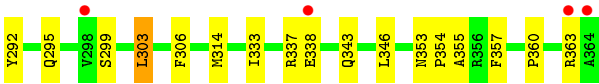
#### • Molecule 1: Parathion hydrolase



#### • Molecule 1: Parathion hydrolase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.76Å 68.91Å 89.67Å 90.03° 100.29° 94.12°	Depositor
Resolution (Å)	28.33 – 1.64 28.33 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.3 (28.33-1.64) 94.9 (28.33-1.64)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.189 , 0.244 0.187 , 0.241	Depositor DCC
$R_{free}$ test set	7763 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 155682 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: CAC, GOL, ZN, ACY, KCX

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	0.79	1/2621 (0.0%)	0.78	0/3557
1	B	0.73	0/2610	0.77	2/3540 (0.1%)
1	C	0.73	0/2638	0.78	0/3583
1	P	0.76	0/2612	0.78	0/3544
All	All	0.75	1/10481 (0.0%)	0.78	2/14224 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	P	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	CB-CG	5.15	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	152	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	LEU	Peptide
1	B	252	LEU	Peptide
1	C	252	LEU	Peptide
1	P	202	THR	Peptide
1	P	235	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2571	0	2596	44	0
1	B	2561	0	2593	29	0
1	C	2574	0	2624	33	0
1	P	2571	0	2585	47	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
2	C	6	0	0	0	0
2	P	6	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	P	5	0	0	0	0
4	B	6	0	8	1	0
4	C	12	0	14	1	0
4	P	12	0	15	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
6	A	414	0	0	14	0
6	B	395	0	0	17	0
6	C	408	0	0	4	0
6	P	377	0	0	14	0
All	All	11956	0	10444	147	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 7.

All (147) 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:A:109:ASP:HB2	6:A:6151:HOH:O	1.54	1.07
1:A:207:ARG:HD2	6:A:6310:HOH:O	1.54	1.04
1:A:114:ALA:O	1:A:118:ARG:HG3	1.70	0.91
1:P:160:ASP:HB3	6:P:5135:HOH:O	1.69	0.91
1:C:249[B]:LEU:HD13	1:C:297:LEU:HD11	1.56	0.87
1:C:249[B]:LEU:HD12	1:C:357:PHE:CD1	2.12	0.84
1:P:41[A]:ARG:HD3	1:P:118:ARG:HG2	1.58	0.82
1:A:41[B]:ARG:HD2	1:A:118:ARG:HG2	1.64	0.78
1:A:175[A]:LYS:HA	1:A:175[A]:LYS:HE2	1.67	0.76
1:A:285:LYS:HE2	6:A:6278:HOH:O	1.84	0.75
1:P:41[A]:ARG:HD3	1:P:118:ARG:CG	2.16	0.75
1:C:173[B]:THR:HG21	6:C:6348:HOH:O	1.86	0.74
1:C:333[A]:ILE:HG23	1:C:346:LEU:HD13	1.70	0.72
1:A:312:ASN:HA	6:A:6119:HOH:O	1.91	0.71
1:P:184:LEU:CD1	6:P:5259:HOH:O	2.38	0.70
1:A:175[A]:LYS:HE2	1:A:175[A]:LYS:CA	2.21	0.69
1:A:77:LYS:HD3	6:A:6152:HOH:O	1.92	0.69
1:P:67:ARG:HD3	6:P:5231:HOH:O	1.93	0.69
1:B:285:LYS:HE3	6:B:6360:HOH:O	1.94	0.67
1:C:333[A]:ILE:CG2	1:C:346:LEU:HD13	2.25	0.66
1:P:333:ILE:HG23	1:P:346:LEU:HD13	1.77	0.66
4:B:5002:GOL:H2	6:B:6138:HOH:O	1.95	0.66
1:B:46:ILE:HG23	1:B:355:ALA:HB1	1.78	0.66
1:P:286:ALA:O	1:P:290:GLN:HG2	1.98	0.64
1:A:337:ARG:HD3	1:A:343:GLN:OE1	1.97	0.64
1:P:265:ASN:HB2	6:P:5238:HOH:O	1.99	0.62
1:P:244:ALA:O	1:P:295[B]:GLN:NE2	2.33	0.62
1:B:264:ASP:HA	6:B:6235:HOH:O	1.98	0.62
1:A:160:ASP:O	1:P:337[B]:ARG:NH1	2.33	0.61
1:A:175[A]:LYS:HG2	6:A:6200:HOH:O	2.01	0.61
1:B:34:GLY:HA3	1:B:360:PRO:O	2.02	0.60
1:P:337[B]:ARG:HD2	1:P:343:GLN:OE1	2.01	0.60
1:P:46:ILE:HG23	1:P:355:ALA:HB1	1.84	0.60
1:C:249[B]:LEU:HD23	1:C:295:GLN:HA	1.82	0.60
1:B:363:ARG:HD2	6:B:6041:HOH:O	2.01	0.60
1:A:156[A]:TYR:OH	1:P:343:GLN:HG3	2.02	0.60
1:B:333:ILE:HG23	1:B:346:LEU:HD13	1.83	0.60
1:P:264:ASP:HB2	6:P:5309:HOH:O	2.02	0.59
1:A:156[A]:TYR:CZ	1:P:343:GLN:HG3	2.38	0.59
1:P:271:LEU:HD12	4:P:5003:GOL:H31	1.82	0.59
1:P:337[B]:ARG:NH1	1:P:343:GLN:HB2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:SER:HB3	6:C:6177:HOH:O	2.04	0.57
1:B:363:ARG:HG2	6:B:6119:HOH:O	2.05	0.57
1:P:249:LEU:HD22	1:P:357:PHE:CD1	2.39	0.57
1:P:184:LEU:HD13	6:P:5259:HOH:O	2.04	0.56
1:B:41[A]:ARG:NH2	6:B:6138:HOH:O	2.39	0.56
1:C:356[B]:ARG:HG3	6:C:6196:HOH:O	2.05	0.56
1:P:131:TRP:CG	1:P:132:GLY:N	2.74	0.55
1:B:285:LYS:NZ	1:B:289:ASP:OD2	2.39	0.55
1:P:38:ASN:ND2	6:P:5116:HOH:O	2.39	0.55
1:C:46:ILE:CG2	1:C:355:ALA:HB1	2.37	0.55
1:A:38:ASN:ND2	6:A:6105:HOH:O	2.39	0.54
1:A:293:MET:HA	1:A:296:ILE:HD12	1.90	0.54
1:C:173[B]:THR:HG22	1:C:201:HIS:HE2	1.73	0.53
1:C:249[B]:LEU:CD1	1:C:357:PHE:CD1	2.90	0.53
1:P:246:ARG:HD2	6:P:5321:HOH:O	2.07	0.53
1:A:264:ASP:OD2	1:A:264:ASP:N	2.42	0.53
1:C:262:LEU:O	1:C:264:ASP:N	2.42	0.53
1:C:298[B]:VAL:CG1	1:C:328:ILE:HD12	2.38	0.52
1:C:121:ASP:OD1	4:C:5004:GOL:H2	2.09	0.52
1:P:264:ASP:OD2	1:P:264:ASP:N	2.32	0.52
1:A:57:HIS:O	1:A:303:LEU:HA	2.09	0.52
1:A:41[B]:ARG:CD	1:A:118:ARG:HG2	2.35	0.52
1:C:196:VAL:HG13	1:C:197:PRO:HD2	1.92	0.51
1:A:205:SER:HB2	6:A:6382:HOH:O	2.09	0.51
1:A:156[A]:TYR:CZ	1:P:343:GLN:CG	2.93	0.51
1:C:249[B]:LEU:HD13	1:C:297:LEU:CD1	2.36	0.51
1:B:312:ASN:HA	6:B:6185:HOH:O	2.11	0.50
1:A:41[A]:ARG:NH2	6:A:6201:HOH:O	2.31	0.50
1:B:353:ASN:HB2	1:B:354:PRO:HD3	1.92	0.50
1:A:156[B]:TYR:O	1:P:343:GLN:NE2	2.45	0.50
1:C:262:LEU:C	1:C:264:ASP:N	2.65	0.49
1:C:173[B]:THR:HG23	6:C:6099:HOH:O	2.11	0.49
1:A:156[A]:TYR:CE2	1:P:343:GLN:HG2	2.49	0.48
1:P:363:ARG:NH2	6:P:5343:HOH:O	2.46	0.48
1:P:67:ARG:NH1	6:P:5271:HOH:O	2.46	0.48
1:B:333:ILE:HB	1:B:334:PRO:HD3	1.95	0.48
1:P:249:LEU:HD12	1:P:249:LEU:N	2.29	0.48
1:B:356[B]:ARG:NH2	6:B:6189:HOH:O	2.35	0.48
1:P:353:ASN:HB2	1:P:354:PRO:HD3	1.96	0.48
1:C:235:ASP:OD2	1:C:275:ARG:NE	2.43	0.47
1:C:298[B]:VAL:HG12	1:C:328:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLY:O	1:C:196:VAL:HG13	2.14	0.47
1:B:35:ASP:OD2	1:B:36:ARG:NH1	2.47	0.47
1:A:67:ARG:HG3	6:B:6264:HOH:O	2.14	0.47
1:A:343:GLN:HA	1:A:346:LEU:HD12	1.96	0.47
1:B:264:ASP:CA	6:B:6235:HOH:O	2.60	0.47
1:P:57:HIS:O	1:P:303:LEU:HA	2.14	0.47
1:A:110:VAL:CG2	1:A:163:ILE:HG21	2.45	0.47
1:A:363:ARG:HD2	6:A:6398:HOH:O	2.15	0.47
1:P:285:LYS:NZ	1:P:289:ASP:OD2	2.42	0.46
1:A:202:THR:HB	1:A:208:ASP:HB2	1.95	0.46
1:B:294:LYS:O	1:B:356[B]:ARG:NH1	2.48	0.46
1:P:41[A]:ARG:HD3	1:P:118:ARG:HG3	1.97	0.46
1:C:57:HIS:O	1:C:303:LEU:HA	2.16	0.46
1:P:337[B]:ARG:HH11	1:P:343:GLN:HB2	1.80	0.45
1:B:170:VAL:HG21	1:B:184:LEU:HD23	1.99	0.45
1:C:262:LEU:C	1:C:264:ASP:H	2.20	0.45
1:B:356[A]:ARG:HD3	6:B:6382:HOH:O	2.16	0.45
1:P:202:THR:HB	1:P:208:ASP:HB2	1.97	0.45
1:P:207:ARG:NH1	1:P:210:GLU:OE1	2.48	0.45
1:B:192:LEU:HD22	1:B:363:ARG:HD3	1.98	0.45
1:P:338:GLU:HB3	6:P:5313:HOH:O	2.17	0.45
1:A:175[A]:LYS:H	1:A:175[A]:LYS:HG2	1.60	0.45
1:C:131:TRP:CG	1:C:132:GLY:N	2.84	0.45
1:B:57:HIS:O	1:B:303:LEU:HA	2.17	0.44
1:C:261:GLY:H	1:C:263:GLU:CD	2.20	0.44
1:C:46:ILE:HG22	1:C:355:ALA:HB1	2.00	0.44
1:P:67:ARG:CD	6:P:5231:HOH:O	2.61	0.43
1:B:319:ARG:HG3	6:B:6182:HOH:O	2.18	0.43
1:A:237:LEU:O	1:A:241:THR:HG23	2.18	0.43
1:P:247:GLY:HA2	1:P:295[B]:GLN:HE22	1.83	0.43
1:A:175[A]:LYS:HD2	6:A:6301:HOH:O	2.17	0.43
1:A:156[A]:TYR:OH	1:P:343:GLN:CG	2.67	0.43
1:B:166:GLY:O	1:B:196:VAL:HG13	2.18	0.43
1:P:123:HIS:HD2	6:P:5042:HOH:O	2.01	0.43
1:B:356[A]:ARG:NH1	6:B:6095:HOH:O	2.52	0.43
1:C:337:ARG:NE	1:C:343:GLN:OE1	2.51	0.42
1:A:109:ASP:OD1	1:A:109:ASP:C	2.57	0.42
1:C:300:ASN:OD1	1:C:327:PHE:HB3	2.18	0.42
1:C:363:ARG:HD3	1:C:364:ALA:O	2.19	0.42
1:P:261:GLY:O	1:P:262:LEU:HD23	2.19	0.42
1:C:293:MET:HA	1:C:296:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175[A]:LYS:HB3	1:A:175[A]:LYS:NZ	2.35	0.42
1:P:290:GLN:HB2	1:P:292:TYR:HD1	1.85	0.42
1:A:353:ASN:HB2	1:A:354:PRO:HD3	2.01	0.42
1:A:77:LYS:HE3	6:A:6097:HOH:O	2.20	0.41
1:P:34:GLY:HA3	1:P:360:PRO:O	2.20	0.41
1:A:123:HIS:HD2	6:A:6044:HOH:O	2.03	0.41
1:B:54:THR:HG23	6:B:6127:HOH:O	2.20	0.41
1:A:333:ILE:HG23	1:A:346:LEU:HD13	2.02	0.41
1:A:67:ARG:HD3	1:A:67:ARG:HA	1.49	0.41
1:A:200:THR:O	1:A:229:GLY:HA3	2.20	0.41
1:B:34:GLY:HA2	6:B:6159:HOH:O	2.19	0.41
1:A:285:LYS:NZ	1:A:289:ASP:OD2	2.54	0.41
1:C:298[B]:VAL:HG12	1:C:328:ILE:CD1	2.51	0.41
1:B:302:TRP:CH2	1:B:321:ASN:HB3	2.56	0.41
1:C:311:THR:O	1:C:312:ASN:HB2	2.21	0.41
1:A:81:GLU:HG3	6:A:6304:HOH:O	2.20	0.41
1:P:46:ILE:CD1	1:P:46:ILE:N	2.84	0.41
1:C:249[A]:LEU:HD22	1:C:297:LEU:HD11	2.02	0.40
1:B:356[A]:ARG:NE	6:B:6189:HOH:O	2.54	0.40
1:P:259:ALA:O	1:P:260:ILE:C	2.59	0.40
1:P:363:ARG:CZ	6:P:5343:HOH:O	2.69	0.40
1:B:123:HIS:HD2	6:B:6038:HOH:O	2.04	0.40
1:B:131:TRP:CG	1:B:132:GLY:N	2.88	0.40
1:A:46:ILE:HG22	1:A:355:ALA:HB1	2.04	0.40

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	336/331 (102%)	325 (97%)	11 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	334/331 (101%)	321 (96%)	13 (4%)	0	100	100
1	C	339/331 (102%)	328 (97%)	11 (3%)	0	100	100
1	P	335/331 (101%)	326 (97%)	8 (2%)	1 (0%)	46	23
All	All	1344/1324 (102%)	1300 (97%)	43 (3%)	1 (0%)	56	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	260	ILE

### 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	271/262 (103%)	264 (97%)	7 (3%)	54	23
1	B	268/262 (102%)	260 (97%)	8 (3%)	48	17
1	C	273/262 (104%)	267 (98%)	6 (2%)	60	30
1	P	269/262 (103%)	262 (97%)	7 (3%)	54	23
All	All	1081/1048 (103%)	1053 (97%)	28 (3%)	55	23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	175[A]	LYS
1	A	175[B]	LYS
1	A	299	SER
1	A	303	LEU
1	A	343	GLN
1	A	362	LEU
1	B	43	PRO
1	B	262	LEU
1	B	299	SER

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Mol	Chain	Res	Type
1	B	303	LEU
1	B	314	MET
1	B	356[A]	ARG
1	B	356[B]	ARG
1	B	362	LEU
1	C	47	SER
1	C	299	SER
1	C	303	LEU
1	C	338	GLU
1	C	343	GLN
1	C	362	LEU
1	P	46	ILE
1	P	175	LYS
1	P	238	SER
1	P	299	SER
1	P	303	LEU
1	P	306	PHE
1	P	314	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	P	38	ASN
1	P	312	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	KCX	A	169	1,2	7,11,12	0.89	0	7,12,14	1.20	0
1	KCX	B	169	1,2	7,11,12	0.60	0	7,12,14	1.51	1 (14%)
1	KCX	C	169	1,2	7,11,12	0.57	0	7,12,14	1.51	1 (14%)
1	KCX	P	169	1,2	7,11,12	0.73	0	7,12,14	1.30	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
1	KCX	A	169	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	169	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	169	1,2	-	0/6/10/12	0/0/0/0
1	KCX	P	169	1,2	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	KCX	CE-NZ-CX	-3.32	119.73	123.49
1	B	169	KCX	CE-NZ-CX	-3.16	119.91	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 23 are monoatomic - leaving 12 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
3	CAC	A	4001	2	0,4,4	0.00	-	0,6,6	0.00	-
5	ACY	A	6003	2	1,3,3	1.67	0	0,3,3	0.00	-
3	CAC	B	4002	2	0,4,4	0.00	-	0,6,6	0.00	-
4	GOL	B	5002	-	5,5,5	0.22	0	5,5,5	0.22	0
5	ACY	B	6002	2	1,3,3	0.87	0	0,3,3	0.00	-
3	CAC	C	4003	2	0,4,4	0.00	-	0,6,6	0.00	-
4	GOL	C	5004	2	5,5,5	0.26	0	5,5,5	0.40	0
4	GOL	C	5005	2	5,5,5	0.22	0	5,5,5	0.58	0
5	ACY	C	6001	2	1,3,3	1.39	0	0,3,3	0.00	-
3	CAC	P	4004	2	0,4,4	0.00	-	0,6,6	0.00	-
4	GOL	P	5001	-	5,5,5	0.32	0	5,5,5	0.79	0
4	GOL	P	5003	2	5,5,5	0.25	0	5,5,5	1.42	1 (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
3	CAC	A	4001	2	-	0/0/0/0	0/0/0/0
5	ACY	A	6003	2	-	0/0/0/0	0/0/0/0
3	CAC	B	4002	2	-	0/0/0/0	0/0/0/0
4	GOL	B	5002	-	-	0/4/4/4	0/0/0/0
5	ACY	B	6002	2	-	0/0/0/0	0/0/0/0
3	CAC	C	4003	2	-	0/0/0/0	0/0/0/0
4	GOL	C	5004	2	-	0/4/4/4	0/0/0/0
4	GOL	C	5005	2	-	0/4/4/4	0/0/0/0
5	ACY	C	6001	2	-	0/0/0/0	0/0/0/0
3	CAC	P	4004	2	-	0/0/0/0	0/0/0/0
4	GOL	P	5001	-	-	0/4/4/4	0/0/0/0
4	GOL	P	5003	2	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	5003	GOL	C3-C2-C1	-2.16	102.64	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5002	GOL	1	0
4	C	5004	GOL	1	0
4	P	5003	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	329/331 (99%)	0.03	4 (1%) 81 82	9, 15, 27, 40	0
1	B	330/331 (99%)	0.26	15 (4%) 37 33	10, 17, 29, 47	2 (0%)
1	C	330/331 (99%)	0.21	15 (4%) 37 33	11, 17, 31, 44	0
1	P	330/331 (99%)	0.17	11 (3%) 50 48	9, 16, 29, 49	2 (0%)
All	All	1319/1324 (99%)	0.17	45 (3%) 49 46	9, 16, 29, 49	4 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	34	GLY	7.5
1	P	262	LEU	5.5
1	B	263	GLU	5.4
1	B	262	LEU	5.0
1	P	364	ALA	4.7
1	B	235	ASP	4.6
1	C	235	ASP	4.6
1	B	364	ALA	4.5
1	P	263	GLU	4.3
1	C	34	GLY	4.1
1	B	264	ASP	4.1
1	B	363	ARG	4.0
1	A	264	ASP	3.9
1	P	261	GLY	3.9
1	A	34	GLY	3.7
1	A	156[A]	TYR	3.6
1	B	34	GLY	3.6
1	C	364	ALA	3.6
1	C	363	ARG	3.5
1	P	264	ASP	3.4
1	C	263	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	P	35	ASP	3.0
1	C	261	GLY	2.9
1	A	338	GLU	2.8
1	P	363	ARG	2.8
1	C	274	ILE	2.7
1	B	53	LEU	2.7
1	C	298[A]	VAL	2.6
1	C	264	ASP	2.6
1	B	319	ARG	2.6
1	B	274	ILE	2.5
1	C	35	ASP	2.4
1	B	312	ASN	2.4
1	B	261	GLY	2.4
1	C	338	GLU	2.3
1	P	338	GLU	2.3
1	C	53	LEU	2.3
1	B	270	ALA	2.3
1	B	35	ASP	2.3
1	P	298[A]	VAL	2.2
1	C	160	ASP	2.1
1	B	245	ALA	2.1
1	P	260	ILE	2.0
1	C	252	LEU	2.0
1	C	262	LEU	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	A	169	12/13	0.95	0.09	-	8,10,14,15	0
1	KCX	C	169	12/13	0.95	0.12	-	10,12,16,17	0
1	KCX	P	169	12/13	0.94	0.13	-	10,12,16,18	0
1	KCX	B	169	12/13	0.95	0.10	-	11,13,16,18	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACY	C	6001	4/4	0.70	0.22	8.28	35,37,38,38	0
5	ACY	A	6003	4/4	0.84	0.18	7.02	18,24,25,26	4
4	GOL	P	5003	6/6	0.87	0.13	3.12	22,27,33,35	0
4	GOL	C	5005	6/6	0.87	0.20	2.32	14,35,36,43	0
5	ACY	B	6002	4/4	0.90	0.13	2.19	31,32,35,38	0
3	CAC	C	4003	5/5	1.00	0.15	1.77	8,13,18,23	5
3	CAC	P	4004	5/5	1.00	0.14	1.56	7,13,16,16	5
4	GOL	B	5002	6/6	0.79	0.16	1.41	30,33,35,39	0
3	CAC	B	4002	5/5	0.99	0.13	1.41	8,15,18,18	5
3	CAC	A	4001	5/5	1.00	0.14	1.41	7,10,14,15	5
4	GOL	P	5001	6/6	0.87	0.14	1.25	23,26,31,41	0
4	GOL	C	5004	6/6	0.81	0.12	-0.52	22,32,39,40	0
2	ZN	A	3024	1/1	0.89	0.09	-	20,20,20,20	1
2	ZN	P	3011	1/1	1.00	0.06	-	14,14,14,14	0
2	ZN	P	3002	1/1	1.00	0.12	-	8,8,8,8	1
2	ZN	C	3007	1/1	1.00	0.09	-	12,12,12,12	0
2	ZN	B	3005	1/1	1.00	0.09	-	12,12,12,12	0
2	ZN	C	3020	1/1	0.95	0.05	-	22,22,22,22	1
2	ZN	P	3021	1/1	0.98	0.12	-	12,12,12,12	1
2	ZN	A	3018	1/1	0.97	0.05	-	23,23,23,23	1
2	ZN	B	3019	1/1	0.94	0.07	-	21,21,21,21	1
2	ZN	A	3003	1/1	1.00	0.08	-	10,10,10,10	1
2	ZN	A	3013	1/1	0.97	0.06	-	21,21,21,21	1
2	ZN	A	3009	1/1	0.99	0.07	-	16,16,16,16	0
2	ZN	B	3006	1/1	1.00	0.06	-	14,14,14,14	0
2	ZN	P	3022	1/1	0.83	0.15	-	18,18,18,18	1
2	ZN	B	3010	1/1	0.99	0.06	-	18,18,18,18	1
2	ZN	C	3017	1/1	0.99	0.04	-	15,15,15,15	1
2	ZN	P	3004	1/1	1.00	0.09	-	10,10,10,10	1
2	ZN	C	3008	1/1	1.00	0.06	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	3014	1/1	0.98	0.03	-	23,23,23,23	1
2	ZN	C	3016	1/1	0.99	0.06	-	16,16,16,16	1
2	ZN	A	3001	1/1	1.00	0.10	-	9,9,9,9	1
2	ZN	C	3015	1/1	0.97	0.04	-	21,21,21,21	1
2	ZN	P	3012	1/1	0.98	0.07	-	19,19,19,19	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.