Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2025 – 11:26 AM EDT

PDB ID	:	2O4M / pdb_00002o4m
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

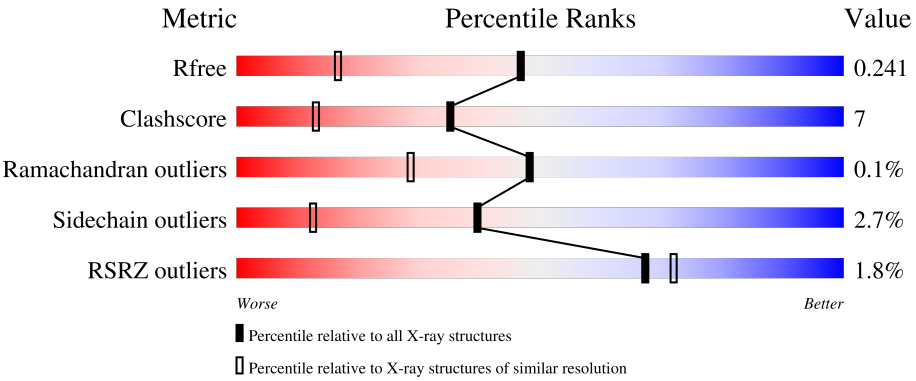
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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}	164625	1015 (1.64-1.64)
Clashscore	180529	1093 (1.64-1.64)
Ramachandran outliers	177936	1077 (1.64-1.64)
Sidechain outliers	177891	1077 (1.64-1.64)
RSRZ outliers	164620	1015 (1.64-1.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	86% 13%
1	B	331	2% 87% 11%
1	C	331	2% 87% 12%
1	P	331	3% 84% 14%

2 Entry composition (i)

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 mutation	UNP P0A434
A	132	GLY	PHE	engineered mutation	UNP P0A434
A	257	TYR	HIS	engineered mutation	UNP P0A434
B	106	GLY	ILE	engineered mutation	UNP P0A434
B	132	GLY	PHE	engineered mutation	UNP P0A434
B	257	TYR	HIS	engineered mutation	UNP P0A434
C	106	GLY	ILE	engineered mutation	UNP P0A434
C	132	GLY	PHE	engineered mutation	UNP P0A434
C	257	TYR	HIS	engineered mutation	UNP P0A434
P	106	GLY	ILE	engineered mutation	UNP P0A434
P	132	GLY	PHE	engineered mutation	UNP P0A434
P	257	TYR	HIS	engineered mutation	UNP P0A434

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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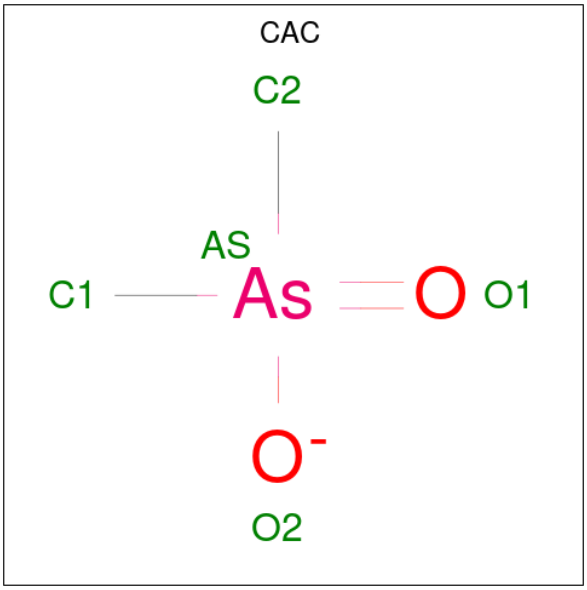
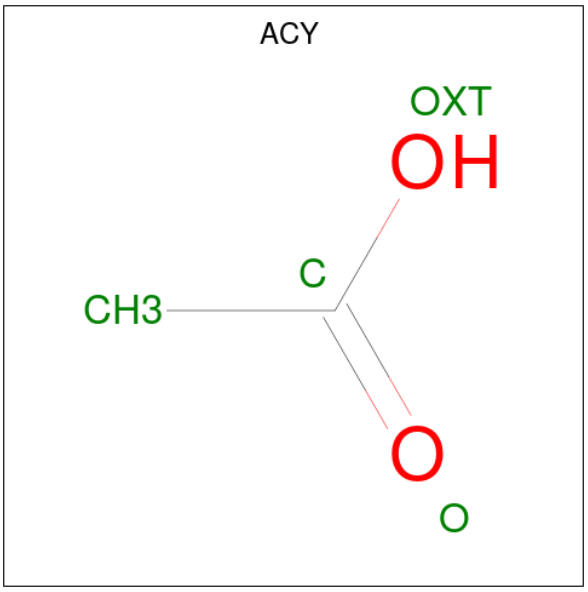
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	6	Total Zn 6 6	0	0
2	P	6	Total Zn 6 6	0	0

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



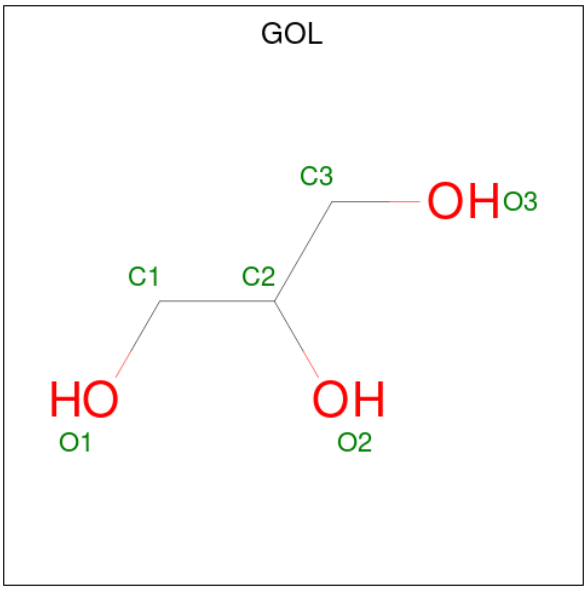
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total As C O 5 1 2 2	0	0
3	B	1	Total As C O 5 1 2 2	0	0
3	C	1	Total As C O 5 1 2 2	0	0
3	P	1	Total As C O 5 1 2 2	0	0

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

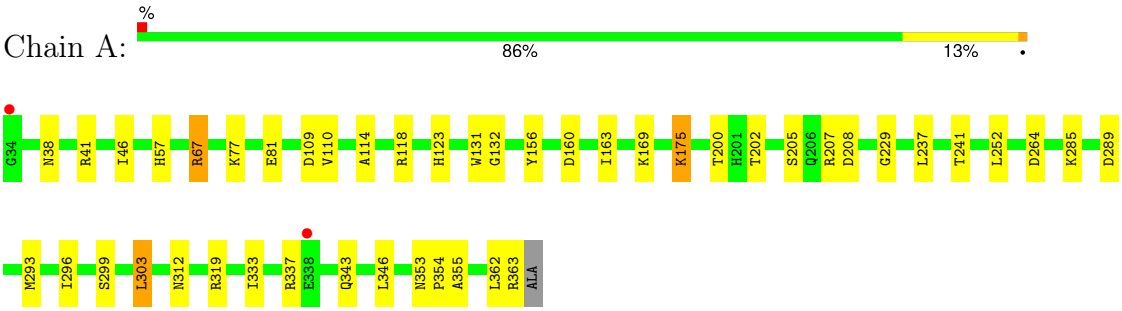
- Molecule 6 is water.

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

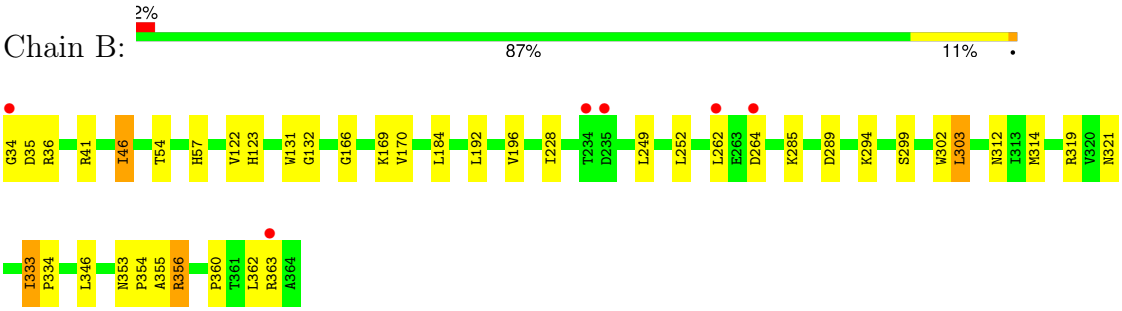
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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.

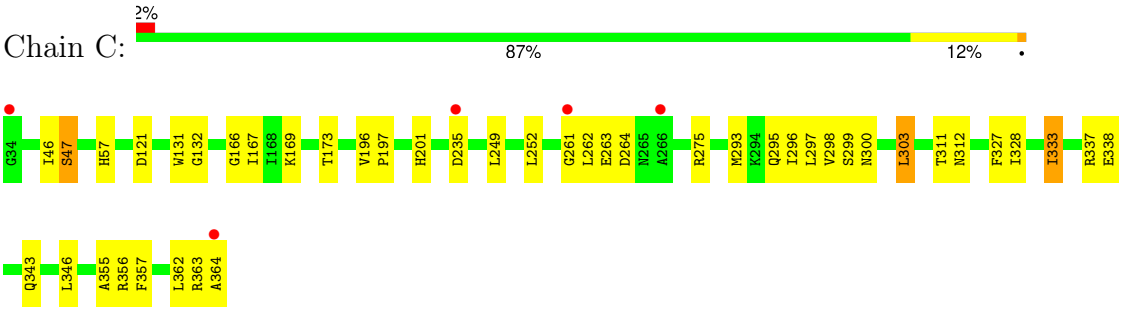
• Molecule 1: Parathion hydrolase



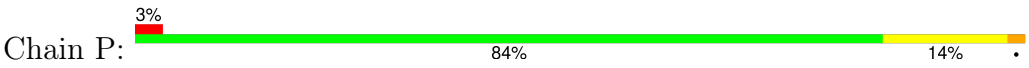
• Molecule 1: Parathion hydrolase

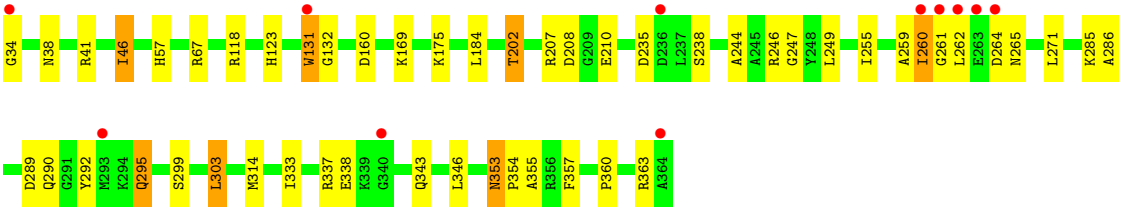


• Molecule 1: Parathion hydrolase



• Molecule 1: Parathion hydrolase




G34
N38
R41
I46
H57
R67
R118
H123
W131
G132
D160
K169
K175
L184
T202
R207
D208
G209
E210
D235
D236
L237
S238
A244
A245
R246
G247
Y248
L249
I255
A259
I260
G261
L262
E263
D264
N265
L271
K285
A286
D289
Q290
G291
Y292
M293
K294
Q295
S299
L303
M314
I333
R337
E338
K339
G340
Q343
L346
N353
P354
A355
H356
F357
P360
R363
A364

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 95.2 (28.33-1.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.64Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.244 0.187 , 0.241	Depositor DCC
R_{free} test set	7763 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11956	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 12.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, KCX, ACY, ZN, CAC

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	0.96	0/2621	1.00	0/3557
1	B	0.93	1/2610 (0.0%)	0.94	0/3540
1	C	0.91	1/2638 (0.0%)	0.94	0/3583
1	P	0.96	0/2612	0.98	5/3544 (0.1%)
All	All	0.94	2/10481 (0.0%)	0.97	5/14224 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	ILE	CA-CB	5.29	1.59	1.53
1	C	167	ILE	N-CA	5.02	1.51	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	131	TRP	N-CA-C	-6.98	99.45	109.29
1	P	353	ASN	CA-C-N	-5.78	112.92	119.28
1	P	353	ASN	C-N-CA	-5.78	112.92	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	255	ILE	CA-C-N	-5.07	114.83	120.45
1	P	255	ILE	C-N-CA	-5.07	114.83	120.45

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 (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	2571	0	2597	45	0
1	B	2561	0	2594	31	0
1	C	2574	0	2624	35	0
1	P	2571	0	2586	48	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	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
5	B	6	0	8	1	0
5	C	12	0	14	1	0
5	P	12	0	15	1	0
6	A	414	0	0	14	0
6	B	395	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	408	0	0	5	0
6	P	377	0	0	14	0
All	All	11956	0	10447	153	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 (153) 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:P:131:TRP:CG	1:P:132:GLY:H	2.05	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
1:B:46:ILE:HG23	1:B:355:ALA:HB1	1.78	0.66
5:B:5002:GOL:H2	6:B:6138:HOH:O	1.95	0.66
1:P:286:ALA:O	1:P:290:GLN:HG2	1.98	0.64
1:C:131:TRP:CG	1:C:132:GLY:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:ILE:HG23	1:P:355:ALA:HB1	1.84	0.60
1:P:337[B]:ARG:HD2	1:P:343:GLN:OE1	2.01	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	5:P:5003:GOL:H31	1.82	0.59
1:B:131:TRP:CG	1:B:132:GLY:H	2.21	0.58
1:P:337[B]:ARG:NH1	1:P:343:GLN:HB2	2.19	0.58
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:B:41[A]:ARG:NH2	6:B:6138:HOH:O	2.39	0.56
1:C:293:MET:HE3	6:C:6378:HOH:O	2.06	0.56
1:C:356[B]:ARG:HG3	6:C:6196:HOH:O	2.05	0.56
1:P:184:LEU:HD13	6:P:5259:HOH:O	2.04	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:A:131:TRP:CG	1:A:132:GLY:H	2.26	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:A:264:ASP:OD2	1:A:264:ASP:N	2.42	0.53
1:P:246:ARG:HD2	6:P:5321:HOH:O	2.07	0.53
1:C:262:LEU:O	1:C:264:ASP:N	2.42	0.53
1:C:262:LEU:C	1:C:264:ASP:N	2.65	0.52
1:C:121:ASP:OD1	5:C:5004:GOL:H2	2.09	0.52
1:C:298[B]:VAL:CG1	1:C:328:ILE:HD12	2.38	0.52
1:A:57:HIS:O	1:A:303:LEU:HA	2.09	0.52
1:P:264:ASP:OD2	1:P:264:ASP:N	2.32	0.52
1:A:41[B]:ARG:CD	1:A:118:ARG:HG2	2.35	0.52
1:A:205:SER:HB2	6:A:6382:HOH:O	2.09	0.51
1:C:196:VAL:HG13	1:C:197:PRO:HD2	1.92	0.51
1:A:156[A]:TYR:CZ	1:P:343:GLN:CG	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:262:LEU:C	1:C:264:ASP:H	2.20	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:173[B]:THR:HG23	6:C:6099:HOH:O	2.11	0.49
1:C:261:GLY:H	1:C:263:GLU:CD	2.20	0.48
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:B:333:ILE:HB	1:B:334:PRO:HD3	1.95	0.48
1:P:67:ARG:NH1	6:P:5271:HOH:O	2.46	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:B:35:ASP:OD2	1:B:36:ARG:NH1	2.47	0.47
1:C:166:GLY:O	1:C:196:VAL:HG13	2.14	0.47
1:C:298[B]:VAL:HG12	1:C:328:ILE:HD12	1.95	0.47
1:A:109:ASP:OD1	1:A:109:ASP:C	2.57	0.47
1:A:67:ARG:HG3	6:B:6264:HOH:O	2.14	0.47
1:A:110:VAL:CG2	1:A:163:ILE:HG21	2.45	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:363:ARG:HD2	6:A:6398:HOH:O	2.15	0.47
1:A:202:THR:HB	1:A:208:ASP:HB2	1.95	0.46
1:P:285:LYS:NZ	1:P:289:ASP:OD2	2.42	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:B:170:VAL:HG21	1:B:184:LEU:HD23	1.99	0.45
1:P:337[B]:ARG:HH11	1:P:343:GLN:HB2	1.80	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:259:ALA:O	1:P:260:ILE:C	2.59	0.45
1:P:338:GLU:HB3	6:P:5313:HOH:O	2.17	0.45
1:A:175[A]:LYS:HG2	1:A:175[A]:LYS:H	1.60	0.45
1:C:131:TRP:CG	1:C:132:GLY:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:HIS:O	1:B:303:LEU:HA	2.17	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:A:237:LEU:O	1:A:241:THR:HG23	2.18	0.43
1:B:319:ARG:HG3	6:B:6182:HOH:O	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: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
1:A:175[A]:LYS:NZ	1:A:175[A]:LYS:HB3	2.35	0.42
1:A:353:ASN:HB2	1:A:354:PRO:HD3	2.01	0.42
1:P:290:GLN:HB2	1:P:292:TYR:HD1	1.85	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: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:A:333:ILE:HG23	1:A:346:LEU:HD13	2.02	0.41
1:B:34:GLY:HA2	6:B:6159:HOH:O	2.19	0.41
1:A:81:GLU:HG3	6:A:6304:HOH:O	2.20	0.41
1:A:285:LYS:NZ	1:A:289:ASP:OD2	2.54	0.41
1:B:302:TRP:CH2	1:B:321:ASN:HB3	2.56	0.41
1:C:298[B]:VAL:HG12	1:C:328:ILE:CD1	2.51	0.41
1:C:311:THR:O	1:C:312:ASN:HB2	2.21	0.41
1:P:46:ILE:N	1:P:46:ILE:CD1	2.84	0.41
1:B:356[A]:ARG:NE	6:B:6189:HOH:O	2.54	0.40
1:C:249[A]:LEU:HD22	1:C:297:LEU:HD11	2.02	0.40
1:B:41[A]:ARG:HH21	1:B:122:VAL:C	2.29	0.40
1:P:363:ARG:CZ	6:P:5343:HOH:O	2.69	0.40
1:A:46:ILE:HG22	1:A:355:ALA:HB1	2.04	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

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	100	100
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%)	37	19
All	All	1344/1324 (102%)	1300 (97%)	43 (3%)	1 (0%)	48	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	260	ILE

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	271/262 (103%)	264 (97%)	7 (3%)	41	13
1	B	268/262 (102%)	258 (96%)	10 (4%)	29	5
1	C	273/262 (104%)	266 (97%)	7 (3%)	41	13
1	P	269/262 (103%)	261 (97%)	8 (3%)	36	10
All	All	1081/1048 (103%)	1049 (97%)	32 (3%)	40	10

All (32) 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	319	ARG
1	A	362	LEU
1	B	46	ILE
1	B	249	LEU
1	B	262	LEU
1	B	299	SER
1	B	303	LEU
1	B	314	MET
1	B	333	ILE
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	333[A]	ILE
1	C	333[B]	ILE
1	C	338	GLU
1	C	362	LEU
1	P	46	ILE
1	P	175	LYS
1	P	238	SER
1	P	295[A]	GLN
1	P	295[B]	GLN
1	P	299	SER
1	P	303	LEU
1	P	314	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	C	169	2,1	10,11,12	0.81	0	6,12,14	1.69	1 (16%)
1	KCX	B	169	2,1	10,11,12	0.85	0	6,12,14	2.02	1 (16%)
1	KCX	A	169	2,1	10,11,12	1.17	1 (10%)	6,12,14	0.81	0
1	KCX	P	169	2,1	10,11,12	0.87	0	6,12,14	1.26	1 (16%)

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	C	169	2,1	-	0/9/10/12	-
1	KCX	B	169	2,1	-	0/9/10/12	-
1	KCX	A	169	2,1	-	0/9/10/12	-
1	KCX	P	169	2,1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	KCX	OQ1-CX	2.76	1.26	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	KCX	OQ1-CX-NZ	-4.66	117.85	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	KCX	OQ1-CX-NZ	-3.72	119.27	124.92
1	P	169	KCX	OQ1-CX-NZ	-2.39	121.29	124.92

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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	GOL	C	5005	2	5,5,5	0.29	0	5,5,5	0.68	0
3	CAC	P	4004	2	2,4,4	0.68	0	2,6,6	0.57	0
3	CAC	C	4003	2	2,4,4	0.55	0	2,6,6	2.71	2 (100%)
3	CAC	A	4001	2	2,4,4	0.79	0	2,6,6	0.98	0
4	ACY	A	6003	2	3,3,3	0.95	0	3,3,3	0.98	0
4	ACY	C	6001	2	3,3,3	0.84	0	3,3,3	0.96	0
5	GOL	C	5004	2	5,5,5	0.34	0	5,5,5	0.45	0
5	GOL	P	5003	2	5,5,5	0.24	0	5,5,5	1.57	1 (20%)
3	CAC	B	4002	2	2,4,4	0.82	0	2,6,6	0.32	0
4	ACY	B	6002	2	3,3,3	0.82	0	3,3,3	0.96	0
5	GOL	P	5001	-	5,5,5	0.35	0	5,5,5	0.91	0
5	GOL	B	5002	-	5,5,5	0.28	0	5,5,5	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	5005	2	-	0/4/4/4	-
5	GOL	P	5003	2	-	2/4/4/4	-
5	GOL	C	5004	2	-	2/4/4/4	-
5	GOL	P	5001	-	-	2/4/4/4	-
5	GOL	B	5002	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4003	CAC	O1-AS-C2	3.10	124.22	109.44
5	P	5003	GOL	C3-C2-C1	-2.50	102.64	111.80
3	C	4003	CAC	O1-AS-C1	-2.26	98.66	109.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5002	GOL	C1-C2-C3-O3
5	B	5002	GOL	O2-C2-C3-O3
5	C	5004	GOL	O1-C1-C2-C3
5	P	5001	GOL	O1-C1-C2-C3
5	P	5003	GOL	O1-C1-C2-C3
5	C	5004	GOL	O1-C1-C2-O2
5	P	5001	GOL	O1-C1-C2-O2
5	P	5003	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5004	GOL	1	0
5	P	5003	GOL	1	0
5	B	5002	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^{th} 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	329/331 (99%)	-0.21	2 (0%)	85	88	7, 15, 27, 40	9 (2%)
1	B	330/331 (99%)	-0.02	6 (1%)	67	72	7, 17, 29, 47	8 (2%)
1	C	330/331 (99%)	-0.07	5 (1%)	71	76	8, 17, 31, 44	11 (3%)
1	P	330/331 (99%)	-0.04	11 (3%)	49	53	6, 16, 29, 49	8 (2%)
All	All	1319/1324 (99%)	-0.08	24 (1%)	67	72	6, 16, 29, 49	36 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	34	GLY	6.1
1	C	235	ASP	4.1
1	P	261	GLY	3.7
1	B	235	ASP	3.3
1	P	262	LEU	3.1
1	P	263	GLU	3.0
1	P	364	ALA	3.0
1	C	34	GLY	2.9
1	C	364	ALA	2.7
1	B	262	LEU	2.7
1	B	234	THR	2.6
1	A	34	GLY	2.4
1	B	363	ARG	2.4
1	C	266	ALA	2.3
1	P	264	ASP	2.3
1	B	264	ASP	2.2
1	C	261	GLY	2.2
1	P	236	ASP	2.1
1	P	260	ILE	2.1
1	B	34	GLY	2.1
1	A	338	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	293[A]	MET	2.1
1	P	131	TRP	2.1
1	P	340	GLY	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. The B-factors column lists the minimum, median, 95^{th} 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	KCX	P	169	12/13	0.93	0.07	10,12,16,18	0
1	KCX	B	169	12/13	0.95	0.07	11,13,16,18	0
1	KCX	A	169	12/13	0.95	0.06	8,10,14,15	0
1	KCX	C	169	12/13	0.96	0.06	10,12,16,17	0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	C	5005	6/6	0.82	0.13	14,35,36,43	0
5	GOL	B	5002	6/6	0.84	0.11	30,33,35,39	0
5	GOL	C	5004	6/6	0.85	0.13	22,32,39,40	0
4	ACY	C	6001	4/4	0.85	0.18	35,37,38,38	0
5	GOL	P	5003	6/6	0.87	0.13	22,27,33,35	0
4	ACY	A	6003	4/4	0.88	0.16	18,24,25,26	4
5	GOL	P	5001	6/6	0.89	0.11	23,26,31,41	0
2	ZN	P	3022	1/1	0.90	0.22	18,18,18,18	1
4	ACY	B	6002	4/4	0.91	0.14	31,32,35,38	0
2	ZN	A	3024	1/1	0.92	0.13	20,20,20,20	1
2	ZN	P	3012	1/1	0.93	0.12	19,19,19,19	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	3019	1/1	0.94	0.05	21,21,21,21	1
2	ZN	C	3020	1/1	0.94	0.20	22,22,22,22	1
2	ZN	A	3018	1/1	0.94	0.06	23,23,23,23	1
2	ZN	A	3013	1/1	0.95	0.08	21,21,21,21	1
2	ZN	P	3021	1/1	0.96	0.10	12,12,12,12	1
2	ZN	B	3014	1/1	0.96	0.06	23,23,23,23	1
2	ZN	C	3015	1/1	0.97	0.07	21,21,21,21	1
3	CAC	C	4003	5/5	0.99	0.12	8,13,18,23	5
2	ZN	B	3010	1/1	0.99	0.05	18,18,18,18	1
2	ZN	P	3002	1/1	0.99	0.09	8,8,8,8	1
2	ZN	P	3004	1/1	0.99	0.07	10,10,10,10	1
2	ZN	P	3011	1/1	0.99	0.04	14,14,14,14	0
2	ZN	A	3009	1/1	0.99	0.06	16,16,16,16	0
2	ZN	C	3016	1/1	0.99	0.05	16,16,16,16	1
2	ZN	C	3017	1/1	0.99	0.06	15,15,15,15	1
3	CAC	B	4002	5/5	0.99	0.10	8,15,18,18	5
2	ZN	B	3006	1/1	1.00	0.04	14,14,14,14	0
2	ZN	A	3001	1/1	1.00	0.07	9,9,9,9	1
2	ZN	A	3003	1/1	1.00	0.06	10,10,10,10	1
2	ZN	B	3005	1/1	1.00	0.06	12,12,12,12	0
3	CAC	A	4001	5/5	1.00	0.10	7,10,14,15	5
2	ZN	C	3007	1/1	1.00	0.06	12,12,12,12	0
2	ZN	C	3008	1/1	1.00	0.05	14,14,14,14	0
3	CAC	P	4004	5/5	1.00	0.10	7,13,16,16	5

6.5 Other polymers (i)

There are no such residues in this entry.