



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:11 AM UTC

PDB ID : 2IZ0 / pdb_00002iz0
Title : PEX inhibitor-home data
Authors : Sundaramoorthy, R.; Iulek, J.; Hunter, W.N.
Deposited on : 2006-07-23
Resolution : 2.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

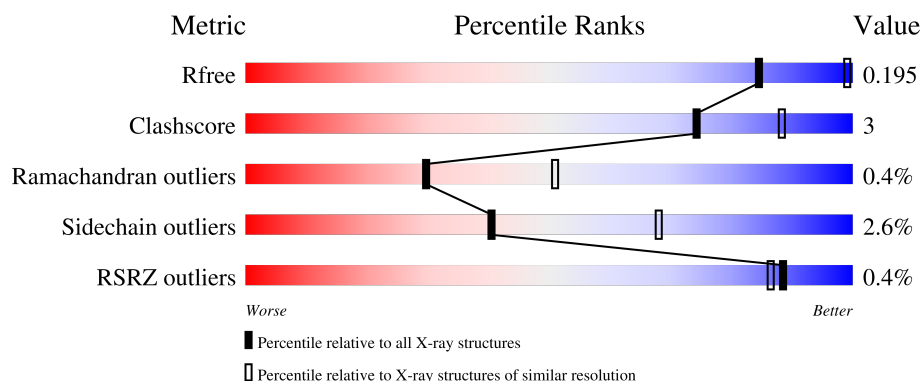
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

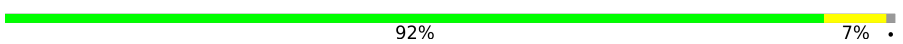
The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	474	 86% 13% ..
1	B	474	 89% 9% ..
1	C	474	 92% 7% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13264 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 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	24	1
			3802	2433	617	737	15			
1	B	470	Total	C	N	O	S	0	22	1
			3793	2423	618	737	15			
1	C	469	Total	C	N	O	S	0	26	1
			3803	2440	620	730	13			

There are 9 discrepancies between the modelled and reference sequences:

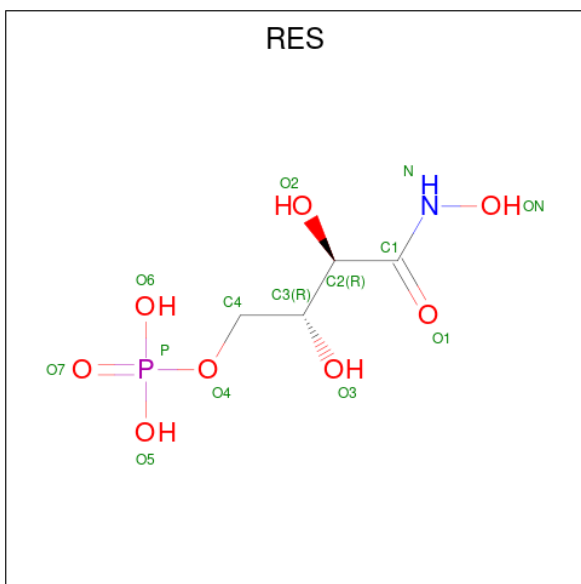
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP P96789
A	0	HIS	-	expression tag	UNP P96789
A	43	PHE	TYR	conflict	UNP P96789
B	-1	HIS	-	expression tag	UNP P96789
B	0	HIS	-	expression tag	UNP P96789
B	43	PHE	TYR	conflict	UNP P96789
C	-1	HIS	-	expression tag	UNP P96789
C	0	HIS	-	expression tag	UNP P96789
C	43	PHE	TYR	conflict	UNP P96789

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



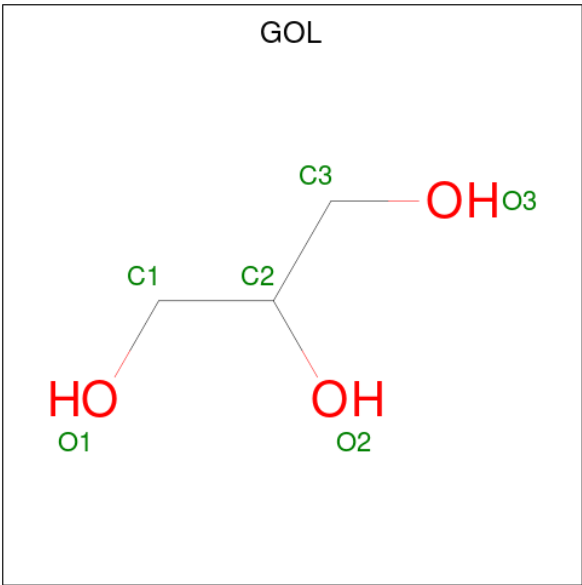
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is 4-PHOSPHO-D-ERYTHRONOXYHYDROXYAMIC ACID (CCD ID: RES) (formula: $C_4H_{10}NO_8P$).



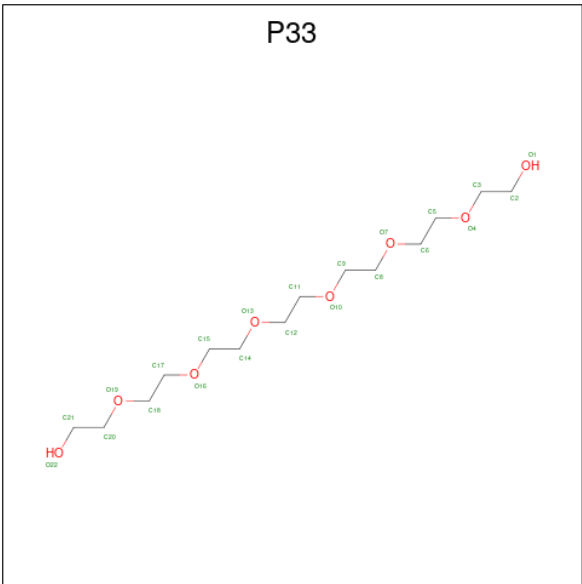
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			14	4	1	8	1		

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



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

- Molecule 5 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: C₁₄H₃₀O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	14	8		

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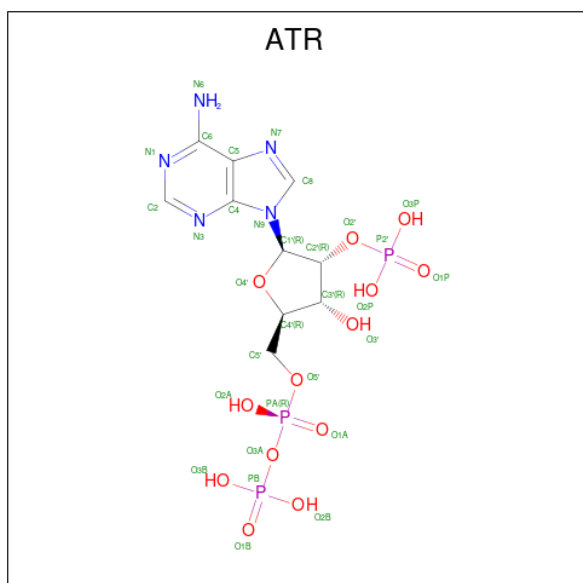
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 2'-MONOPHOSPHOADENOSINE-5'-DIPHOSPHATE (CCD ID: ATR) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

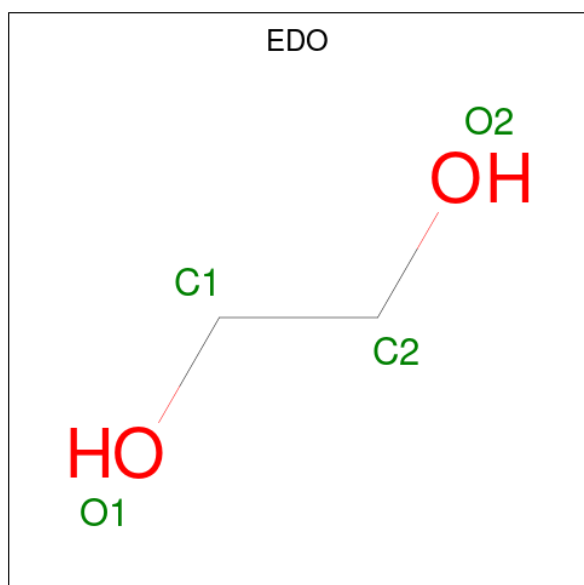


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	1
			42	12	5	20	5		
7	C	1	Total	C	N	O	P	0	1
			42	12	5	20	5		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Cl	0	0
			2	2		
8	C	2	Total	Cl	0	0
			2	2		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	500	Total	O	0	0
			500	500		
10	B	568	Total	O	0	0
			568	568		

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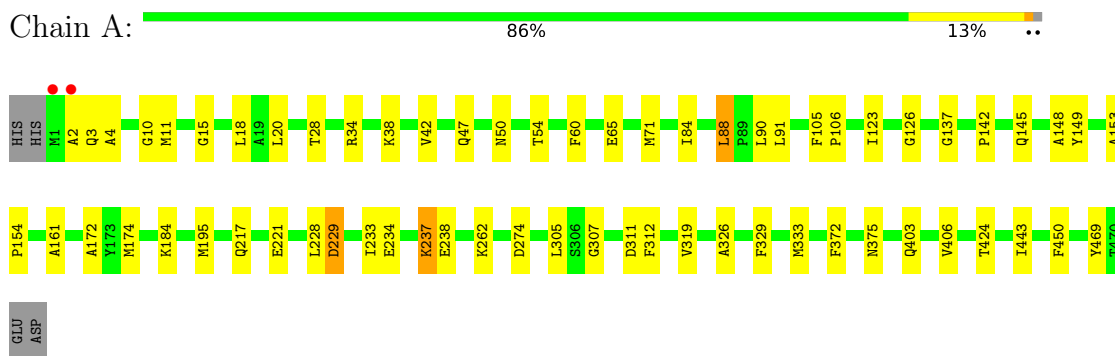
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	584	Total	O	0	0
			584	584		

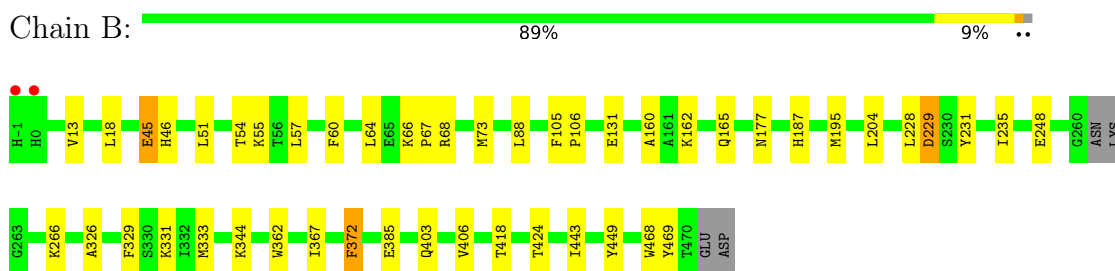
3 Residue-property plots

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.

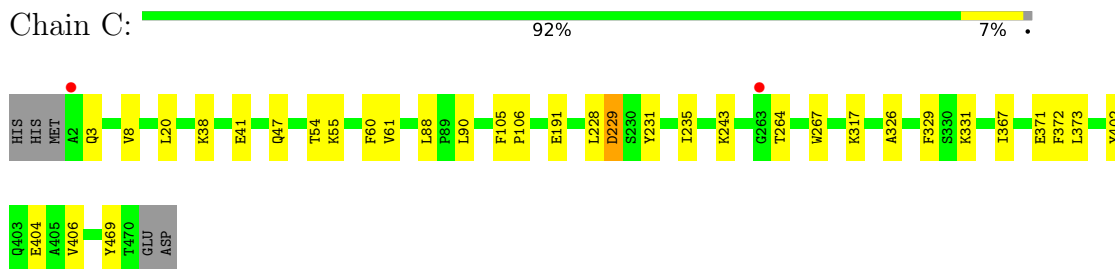
- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.96Å 104.46Å 241.48Å 90.00° 98.52° 90.00°	Depositor
Resolution (Å)	235.70 – 2.60 235.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (235.70-2.60) 97.5 (235.70-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.123 , 0.193 0.141 , 0.195	Depositor DCC
R_{free} test set	2659 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13264	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: P33, NAP, EDO, ATR, RES, CL, GOL, PEG

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	0.56	1/3946 (0.0%)	0.73	0/5329
1	B	0.55	1/3933 (0.0%)	0.73	1/5314 (0.0%)
1	C	0.54	1/3953 (0.0%)	0.74	0/5337
All	All	0.55	3/11832 (0.0%)	0.74	1/15980 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	469	TYR	C-N	-7.50	1.22	1.33
1	A	469	TYR	C-N	-6.72	1.24	1.33
1	C	469	TYR	C-N	-6.63	1.24	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	469	TYR	O-C-N	-5.39	114.37	123.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	LYS	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	3802	0	3818	34	0
1	B	3793	0	3776	24	0
1	C	3803	0	3846	18	0
2	A	48	0	25	0	0
3	A	14	0	10	0	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
5	A	22	0	30	1	0
5	C	19	0	25	0	0
6	A	7	0	10	0	0
7	B	42	0	10	0	0
7	C	42	0	10	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
9	B	4	0	6	1	0
10	A	500	0	0	0	0
10	B	568	0	0	1	1
10	C	584	0	0	4	0
All	All	13264	0	11582	70	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 3.

All (70) 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:C:317[B]:LYS:HE2	10:C:2412:HOH:O	1.64	0.94
1:C:231:TYR:CZ	1:C:235[B]:ILE:HD11	2.11	0.85
1:A:217:GLN:HE22	1:A:221:GLU:CD	1.97	0.72
1:C:38[B]:LYS:HE3	1:C:41[B]:GLU:OE1	2.00	0.61
1:A:234:GLU:O	1:A:237[A]:LYS:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PRO:HD2	1:A:172:ALA:O	2.02	0.59
1:A:274[A]:ASP:OD1	1:B:266:LYS:NZ	2.36	0.59
1:B:449:TYR:HA	1:B:468:TRP:CD1	2.39	0.58
1:A:174:MET:HA	1:A:174:MET:HE2	1.87	0.56
1:C:38[B]:LYS:CE	1:C:41[B]:GLU:OE1	2.54	0.56
1:C:231:TYR:CE2	1:C:235[A]:ILE:HD11	2.46	0.51
1:B:64:LEU:HB2	1:B:68[B]:ARG:HG2	1.91	0.51
1:A:326:ALA:HA	1:A:406:VAL:HG22	1.91	0.51
1:A:28[A]:THR:HG22	1:A:50:ASN:HB3	1.93	0.51
1:A:237[B]:LYS:NZ	1:A:238:GLU:OE2	2.42	0.51
1:A:450:PHE:CE2	1:B:367[B]:ILE:HD12	2.45	0.51
1:B:326:ALA:HA	1:B:406:VAL:HG22	1.93	0.51
1:A:47[A]:GLN:HE21	1:A:47[A]:GLN:HA	1.76	0.50
1:A:54:THR:HG21	1:A:60:PHE:HA	1.93	0.50
1:B:204:LEU:HD23	1:B:418:THR:HG21	1.93	0.50
1:C:329:PHE:CG	1:C:406:VAL:HG21	2.46	0.50
1:C:331:LYS:NZ	10:C:2431:HOH:O	2.44	0.49
1:B:231:TYR:CE2	1:B:235:ILE:HD11	2.47	0.49
1:A:10:GLY:O	1:A:15:GLY:HA3	2.13	0.49
1:A:18[A]:LEU:HD21	1:A:71:MET:SD	2.53	0.48
1:C:228:LEU:O	1:C:229:ASP:C	2.56	0.48
9:B:1473:EDO:H12	10:B:2567:HOH:O	2.13	0.47
1:A:195:MET:HE2	1:B:443:ILE:HG23	1.95	0.47
1:A:84:ILE:HG22	1:A:88:LEU:HD22	1.96	0.47
1:B:187:HIS:HB2	1:B:362:TRP:CZ2	2.50	0.47
1:B:105:PHE:CD1	1:B:106:PRO:HD3	2.50	0.46
1:C:231:TYR:CE2	1:C:235[B]:ILE:HD11	2.47	0.46
1:B:228:LEU:O	1:B:229:ASP:C	2.58	0.46
1:A:228:LEU:HB3	1:A:233:ILE:HD13	1.98	0.45
1:A:228:LEU:O	1:A:229:ASP:C	2.59	0.45
1:C:326:ALA:HA	1:C:406:VAL:HG22	1.98	0.45
1:C:54:THR:HG21	1:C:60:PHE:HA	1.99	0.45
1:A:450:PHE:CD2	1:B:367[B]:ILE:HD12	2.51	0.45
1:B:331:LYS:HE2	1:B:372:PHE:CE1	2.53	0.44
1:A:312:PHE:CZ	1:A:319:VAL:HG21	2.52	0.44
1:B:45:GLU:HG3	1:B:46:HIS:CD2	2.53	0.44
1:A:10:GLY:O	1:A:11:MET:HE2	2.17	0.43
1:B:54:THR:HG21	1:B:60:PHE:HA	2.00	0.43
1:A:105:PHE:CD1	1:A:106:PRO:HD3	2.53	0.43
1:B:64:LEU:CB	1:B:68[B]:ARG:HG2	2.48	0.43
1:B:66:LYS:HA	1:B:67:PRO:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLY:HA3	1:A:184:LYS:HB2	2.00	0.43
1:B:329:PHE:CZ	1:B:333:MET:HE3	2.54	0.43
1:A:153:ALA:N	1:A:154:PRO:CD	2.81	0.43
1:A:137:GLY:O	1:A:161:ALA:HB2	2.19	0.42
5:A:1473:P33:H32	1:C:47:GLN:HB2	2.02	0.42
1:B:18[B]:LEU:HD12	1:B:73:MET:HE2	2.01	0.42
1:A:372:PHE:HA	1:A:375:ASN:HD22	1.84	0.42
1:C:402:TYR:O	1:C:406:VAL:HG23	2.20	0.42
1:A:329:PHE:CZ	1:A:333:MET:HE3	2.54	0.41
1:A:4:ALA:O	1:A:65[A]:GLU:HG2	2.20	0.41
1:B:13[B]:VAL:HG11	1:B:131:GLU:OE2	2.20	0.41
1:C:404[B]:GLU:HG2	10:C:2218:HOH:O	2.20	0.41
1:A:307:GLY:HA2	1:B:403:GLN:OE1	2.21	0.41
1:C:105:PHE:N	1:C:106:PRO:CD	2.84	0.41
1:C:191:GLU:CG	1:C:367[A]:ILE:HD11	2.51	0.41
1:A:443:ILE:HG23	1:B:195:MET:HE2	2.03	0.41
1:A:123[B]:ILE:HD11	1:A:149:TYR:HA	2.03	0.40
1:C:61[A]:VAL:HG21	1:C:90:LEU:HB3	2.03	0.40
1:A:28[A]:THR:HG23	10:C:2247:HOH:O	2.20	0.40
1:C:264:THR:HG22	1:C:267:TRP:CZ2	2.56	0.40
1:A:123[A]:ILE:HD11	1:A:148:ALA:HB1	2.04	0.40
1:B:160:ALA:O	1:B:162:LYS:NZ	2.53	0.40
1:A:424:THR:HB	1:B:424:THR:HB	2.03	0.40

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)
10:B:2017:HOH:O	10:B:2017:HOH:O[2_656]	0.58	1.62

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	491/474 (104%)	478 (97%)	11 (2%)	2 (0%)	30	51
1	B	487/474 (103%)	470 (96%)	15 (3%)	2 (0%)	30	51
1	C	493/474 (104%)	476 (97%)	15 (3%)	2 (0%)	30	51
All	All	1471/1422 (103%)	1424 (97%)	41 (3%)	6 (0%)	30	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	C	3	GLN
1	A	229	ASP
1	B	177	ASN
1	C	229	ASP
1	B	229	ASP

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	409/390 (105%)	396 (97%)	13 (3%)	34	62
1	B	407/390 (104%)	395 (97%)	12 (3%)	37	65
1	C	410/390 (105%)	401 (98%)	9 (2%)	45	72
All	All	1226/1170 (105%)	1192 (97%)	34 (3%)	40	66

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	34	ARG
1	A	38	LYS
1	A	42	VAL
1	A	88	LEU
1	A	90	LEU
1	A	91	LEU

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Mol	Chain	Res	Type
1	A	145	GLN
1	A	237[A]	LYS
1	A	237[B]	LYS
1	A	305	LEU
1	A	311	ASP
1	A	403	GLN
1	B	45	GLU
1	B	51	LEU
1	B	55	LYS
1	B	57	LEU
1	B	88	LEU
1	B	165	GLN
1	B	248[A]	GLU
1	B	248[B]	GLU
1	B	344	LYS
1	B	372	PHE
1	B	385[A]	GLU
1	B	385[B]	GLU
1	C	8	VAL
1	C	20	LEU
1	C	55	LYS
1	C	88	LEU
1	C	243	LYS
1	C	371[A]	GLU
1	C	371[B]	GLU
1	C	372	PHE
1	C	373	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	224	ASN
1	A	261	ASN
1	A	360	GLN
1	A	375	ASN
1	B	374	GLN
1	B	375	ASN
1	C	47	GLN
1	C	102	ASN
1	C	121	ASN
1	C	158	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 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	$\# Z > 2$
4	GOL	A	1472	-	5,5,5	0.39	0	5,5,5	0.28	0
5	P33	A	1473	-	21,21,21	0.57	0	20,20,20	0.61	0
7	ATR	B	1470[B]	-	32,33,33	0.93	1 (3%)	50,52,52	1.88	9 (18%)
4	GOL	C	1473	-	5,5,5	0.40	0	5,5,5	0.39	0
7	ATR	C	1470[A]	-	32,33,33	1.00	1 (3%)	50,52,52	1.74	8 (16%)
7	ATR	B	1470[A]	-	32,33,33	0.95	1 (3%)	50,52,52	1.89	9 (18%)
9	EDO	B	1473	-	3,3,3	0.38	0	2,2,2	0.37	0
7	ATR	C	1470[B]	-	32,33,33	1.00	1 (3%)	50,52,52	1.73	9 (18%)
5	P33	C	1474	-	18,18,21	0.55	0	17,17,20	0.48	0
6	PEG	A	1474	-	6,6,6	0.39	0	5,5,5	0.31	0
3	RES	A	1471	-	12,13,13	0.58	0	14,18,18	0.92	0
2	NAP	A	1470	-	50,52,52	1.75	7 (14%)	71,80,80	1.59	12 (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
4	GOL	A	1472	-	-	2/4/4/4	-
5	P33	A	1473	-	-	11/19/19/19	-
7	ATR	B	1470[B]	-	-	0/21/37/37	0/3/3/3
4	GOL	C	1473	-	-	2/4/4/4	-
7	ATR	C	1470[A]	-	-	6/21/37/37	0/3/3/3
7	ATR	B	1470[A]	-	-	3/21/37/37	0/3/3/3
9	EDO	B	1473	-	-	0/1/1/1	-
7	ATR	C	1470[B]	-	-	4/21/37/37	0/3/3/3
5	P33	C	1474	-	-	12/16/16/19	-
6	PEG	A	1474	-	-	0/4/4/4	-
3	RES	A	1471	-	-	5/16/16/16	-
2	NAP	A	1470	-	-	7/35/67/67	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1470	NAP	O7N-C7N	9.18	1.41	1.24
2	A	1470	NAP	PN-O3	2.83	1.62	1.59
2	A	1470	NAP	PA-O3	2.68	1.62	1.59
2	A	1470	NAP	C2A-N1A	2.65	1.38	1.33
2	A	1470	NAP	C2N-N1N	2.61	1.37	1.35
2	A	1470	NAP	C2A-N3A	2.49	1.38	1.33
2	A	1470	NAP	C8A-N7A	2.25	1.36	1.31
7	B	1470[A]	ATR	C5-N7	-2.11	1.35	1.39
7	B	1470[B]	ATR	C5-N7	-2.11	1.35	1.39
7	C	1470[A]	ATR	C5-N7	-2.09	1.35	1.39
7	C	1470[B]	ATR	C5-N7	-2.09	1.35	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1470[A]	ATR	C5-C4-N3	-6.09	118.33	126.72
7	B	1470[B]	ATR	C5-C4-N3	-6.09	118.33	126.72
2	A	1470	NAP	N3A-C2A-N1A	-5.74	119.89	128.58
7	B	1470[A]	ATR	N3-C2-N1	-4.98	121.05	128.58
7	B	1470[B]	ATR	N3-C2-N1	-4.98	121.05	128.58
2	A	1470	NAP	C5A-C4A-N3A	-4.90	119.97	126.72
7	C	1470[A]	ATR	C5-C4-N3	-4.68	120.27	126.72
7	C	1470[B]	ATR	C5-C4-N3	-4.68	120.27	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1470[A]	ATR	N3-C2-N1	-4.48	121.80	128.58
7	C	1470[B]	ATR	N3-C2-N1	-4.48	121.80	128.58
7	B	1470[A]	ATR	N3-C4-N9	4.10	134.15	127.17
7	B	1470[B]	ATR	N3-C4-N9	4.10	134.15	127.17
7	C	1470[A]	ATR	N9-C8-N7	-3.92	108.38	113.94
7	C	1470[B]	ATR	N9-C8-N7	-3.92	108.38	113.94
7	B	1470[A]	ATR	C2-N3-C4	3.74	120.97	111.83
7	B	1470[B]	ATR	C2-N3-C4	3.74	120.97	111.83
7	C	1470[A]	ATR	N3-C4-N9	3.73	133.52	127.17
7	C	1470[B]	ATR	N3-C4-N9	3.73	133.52	127.17
7	C	1470[A]	ATR	C4-N9-C8	3.71	109.64	105.74
7	C	1470[B]	ATR	C4-N9-C8	3.71	109.64	105.74
2	A	1470	NAP	N9A-C8A-N7A	-3.71	108.67	113.94
2	A	1470	NAP	C2A-N3A-C4A	3.62	120.68	111.83
7	B	1470[A]	ATR	N9-C8-N7	-3.60	108.83	113.94
7	B	1470[B]	ATR	N9-C8-N7	-3.60	108.83	113.94
2	A	1470	NAP	N3A-C4A-N9A	3.44	133.01	127.17
2	A	1470	NAP	C5A-N7A-C8A	3.38	108.76	103.45
7	C	1470[A]	ATR	C5-N7-C8	2.98	108.14	103.45
7	C	1470[B]	ATR	C5-N7-C8	2.98	108.14	103.45
7	B	1470[A]	ATR	C4-C5-N7	-2.94	107.22	110.58
7	B	1470[B]	ATR	C4-C5-N7	-2.94	107.22	110.58
7	B	1470[A]	ATR	C5-N7-C8	2.91	108.03	103.45
7	B	1470[B]	ATR	C5-N7-C8	2.91	108.03	103.45
7	C	1470[A]	ATR	C2-N3-C4	2.79	118.66	111.83
7	C	1470[B]	ATR	C2-N3-C4	2.79	118.66	111.83
7	C	1470[A]	ATR	C4-C5-N7	-2.59	107.63	110.58
7	C	1470[B]	ATR	C4-C5-N7	-2.59	107.63	110.58
7	B	1470[A]	ATR	C4-N9-C8	2.53	108.39	105.74
7	B	1470[B]	ATR	C4-N9-C8	2.53	108.39	105.74
2	A	1470	NAP	C2B-C1B-N9A	-2.43	109.75	113.75
2	A	1470	NAP	C6A-C5A-C4A	2.29	120.31	117.18
2	A	1470	NAP	O4B-C1B-N9A	2.24	112.39	108.09
2	A	1470	NAP	C4A-C5A-N7A	-2.21	108.05	110.58
2	A	1470	NAP	P2B-O2B-C2B	-2.13	117.75	123.43
7	C	1470[B]	ATR	O3B-PB-O2B	2.12	115.77	107.80
2	A	1470	NAP	C6N-N1N-C2N	-2.06	120.12	121.88
7	B	1470[A]	ATR	C2'-C1'-N9	-2.03	110.41	113.75
7	B	1470[B]	ATR	C2'-C1'-N9	-2.03	110.41	113.75

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1470	NAP	O4D-C1D-N1N-C2N
2	A	1470	NAP	O4D-C1D-N1N-C6N
2	A	1470	NAP	C2D-C1D-N1N-C2N
2	A	1470	NAP	C2D-C1D-N1N-C6N
3	A	1471	RES	C2-C1-N-ON
3	A	1471	RES	O1-C1-N-ON
4	A	1472	GOL	C1-C2-C3-O3
4	A	1472	GOL	O2-C2-C3-O3
4	C	1473	GOL	O1-C1-C2-C3
7	B	1470[A]	ATR	C5'-O5'-PA-O2A
7	C	1470[A]	ATR	C5'-O5'-PA-O1A
7	C	1470[A]	ATR	C5'-O5'-PA-O2A
5	A	1473	P33	C5-C6-O7-C8
5	C	1474	P33	O16-C17-C18-O19
5	C	1474	P33	O10-C11-C12-O13
5	A	1473	P33	O4-C5-C6-O7
5	A	1473	P33	O16-C17-C18-O19
5	A	1473	P33	O10-C11-C12-O13
5	C	1474	P33	O19-C20-C21-O22
4	C	1473	GOL	O1-C1-C2-O2
5	C	1474	P33	O4-C5-C6-O7
7	C	1470[A]	ATR	O4'-C4'-C5'-O5'
7	C	1470[A]	ATR	C2'-O2'-P2'-O2P
7	C	1470[B]	ATR	C2'-O2'-P2'-O2P
2	A	1470	NAP	PA-O3-PN-O5D
5	A	1473	P33	C9-C8-O7-C6
5	C	1474	P33	C12-C11-O10-C9
5	C	1474	P33	C8-C9-O10-C11
5	A	1473	P33	C17-C18-O19-C20
7	B	1470[A]	ATR	C5'-O5'-PA-O1A
7	B	1470[A]	ATR	C5'-O5'-PA-O3A
7	C	1470[A]	ATR	C5'-O5'-PA-O3A
7	C	1470[B]	ATR	C5'-O5'-PA-O1A
3	A	1471	RES	C3-C4-O4-P
5	C	1474	P33	C11-C12-O13-C14
5	A	1473	P33	C12-C11-O10-C9
7	C	1470[B]	ATR	PB-O3A-PA-O1A
5	C	1474	P33	O13-C14-C15-O16
5	C	1474	P33	C9-C8-O7-C6
5	A	1473	P33	O7-C8-C9-O10
5	A	1473	P33	C18-C17-O16-C15
5	A	1473	P33	C6-C5-O4-C3
3	A	1471	RES	C4-O4-P-O7

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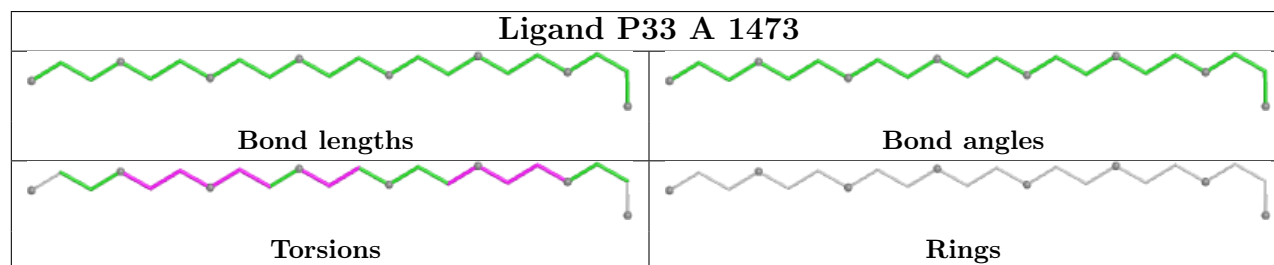
Mol	Chain	Res	Type	Atoms
3	A	1471	RES	C4-O4-P-O5
5	C	1474	P33	C17-C18-O19-C20
5	C	1474	P33	C15-C14-O13-C12
5	A	1473	P33	C14-C15-O16-C17
2	A	1470	NAP	PN-O3-PA-O1A
7	C	1470[B]	ATR	PB-O3A-PA-O2A
7	C	1470[A]	ATR	C3'-C4'-C5'-O5'
5	C	1474	P33	C21-C20-O19-C18
2	A	1470	NAP	PN-O3-PA-O2A

There are no ring outliers.

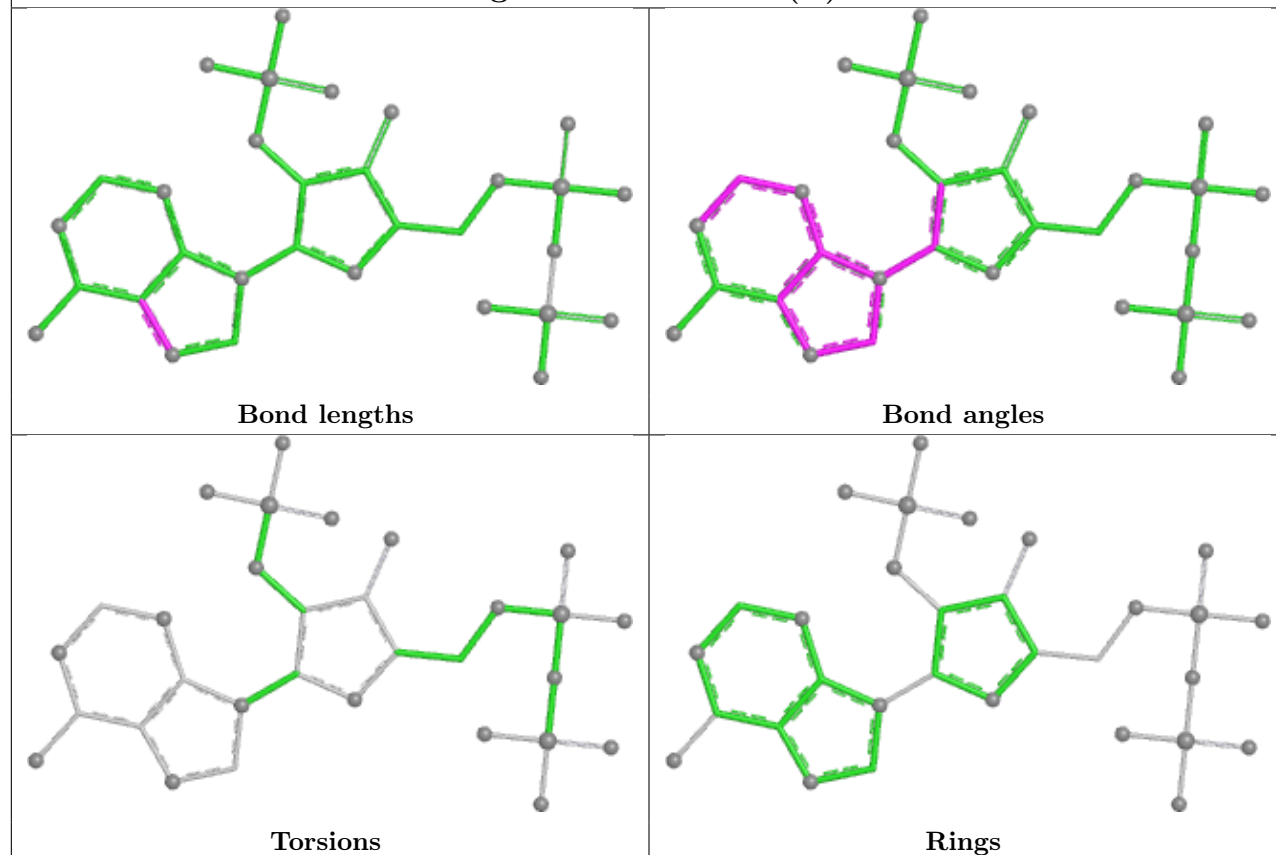
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1473	P33	1	0
9	B	1473	EDO	1	0

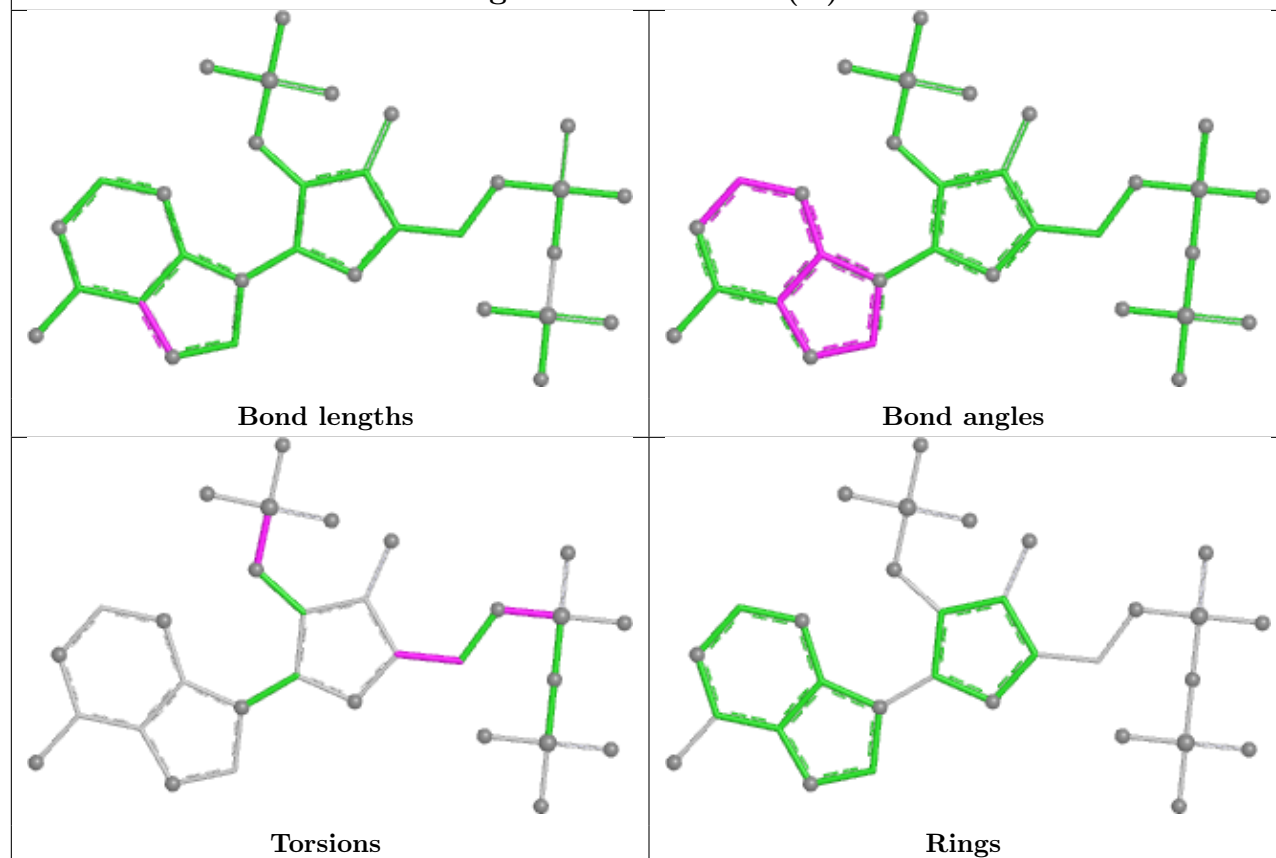
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



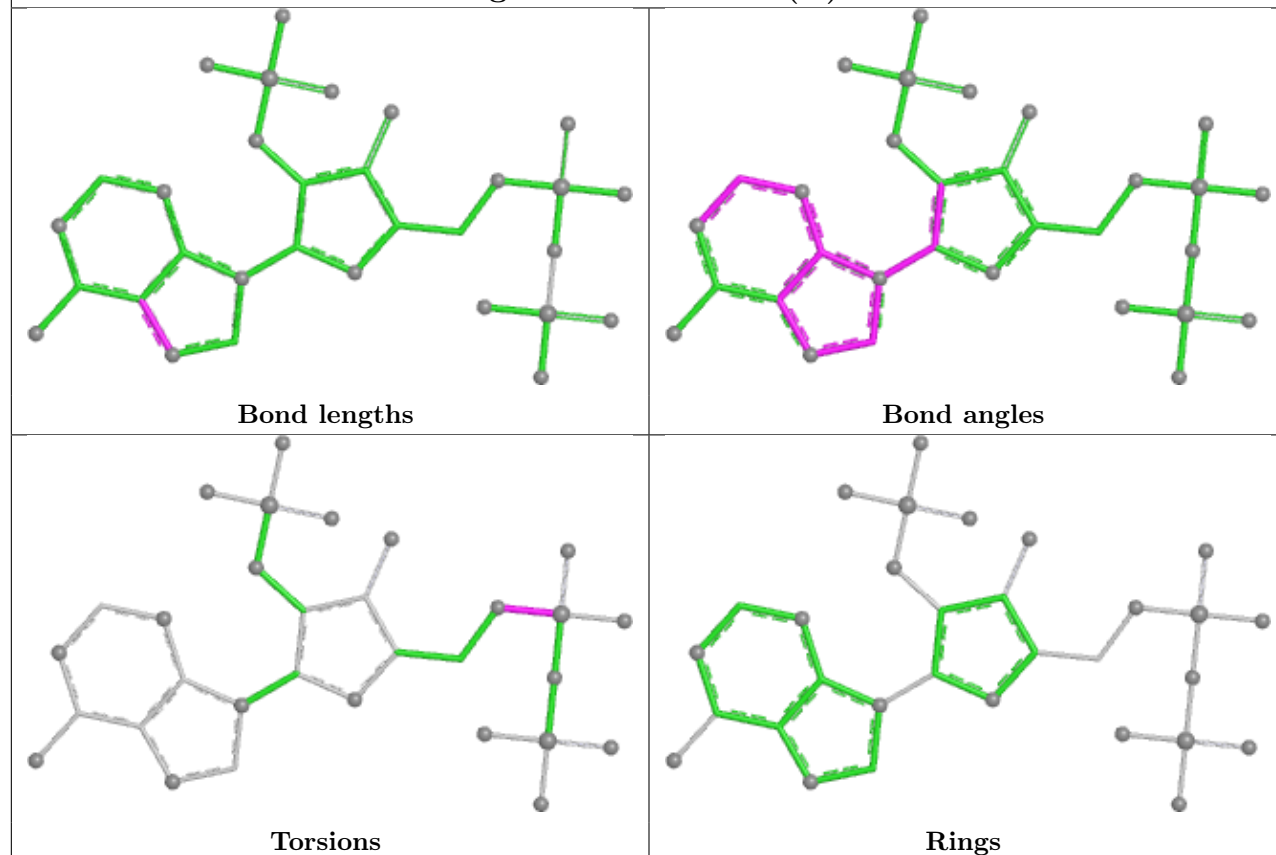
Ligand ATR B 1470 (B)



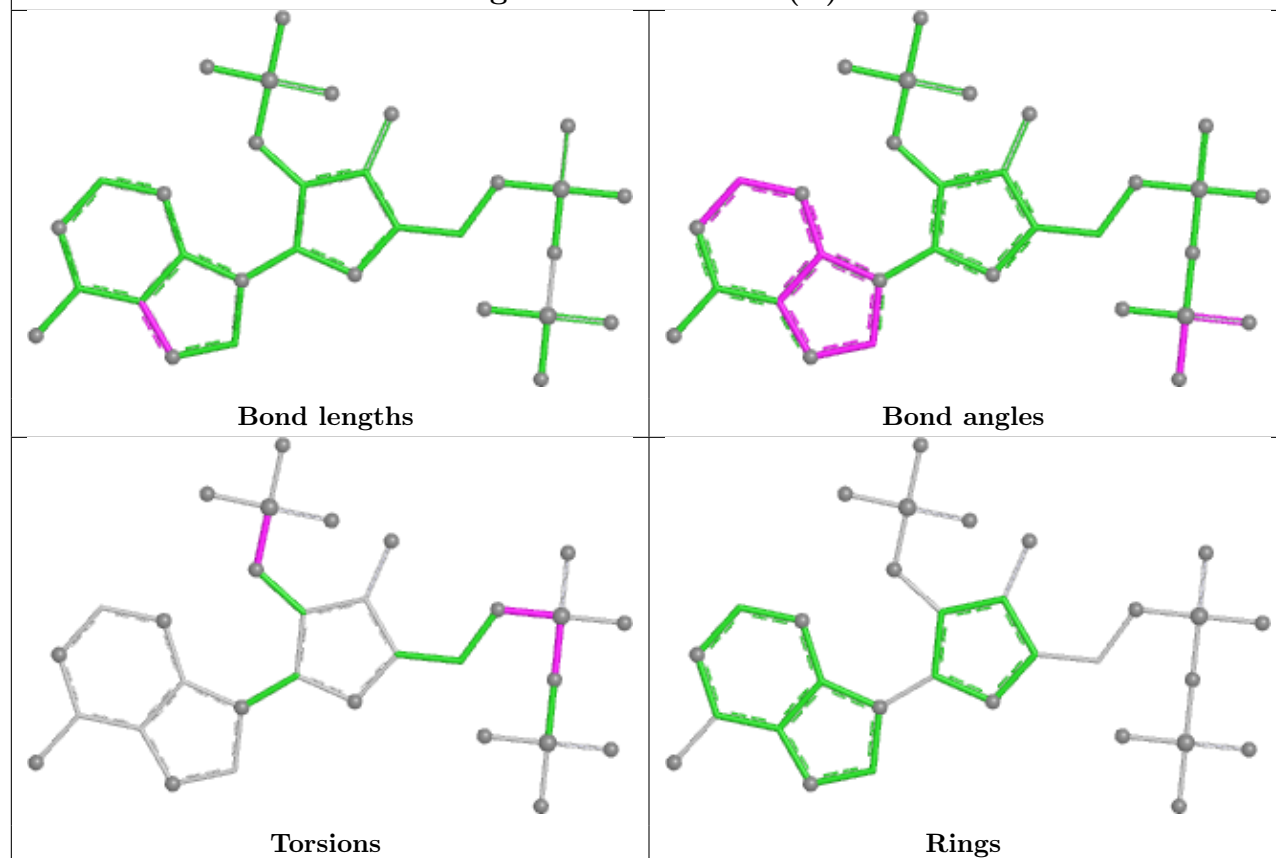
Ligand ATR C 1470 (A)

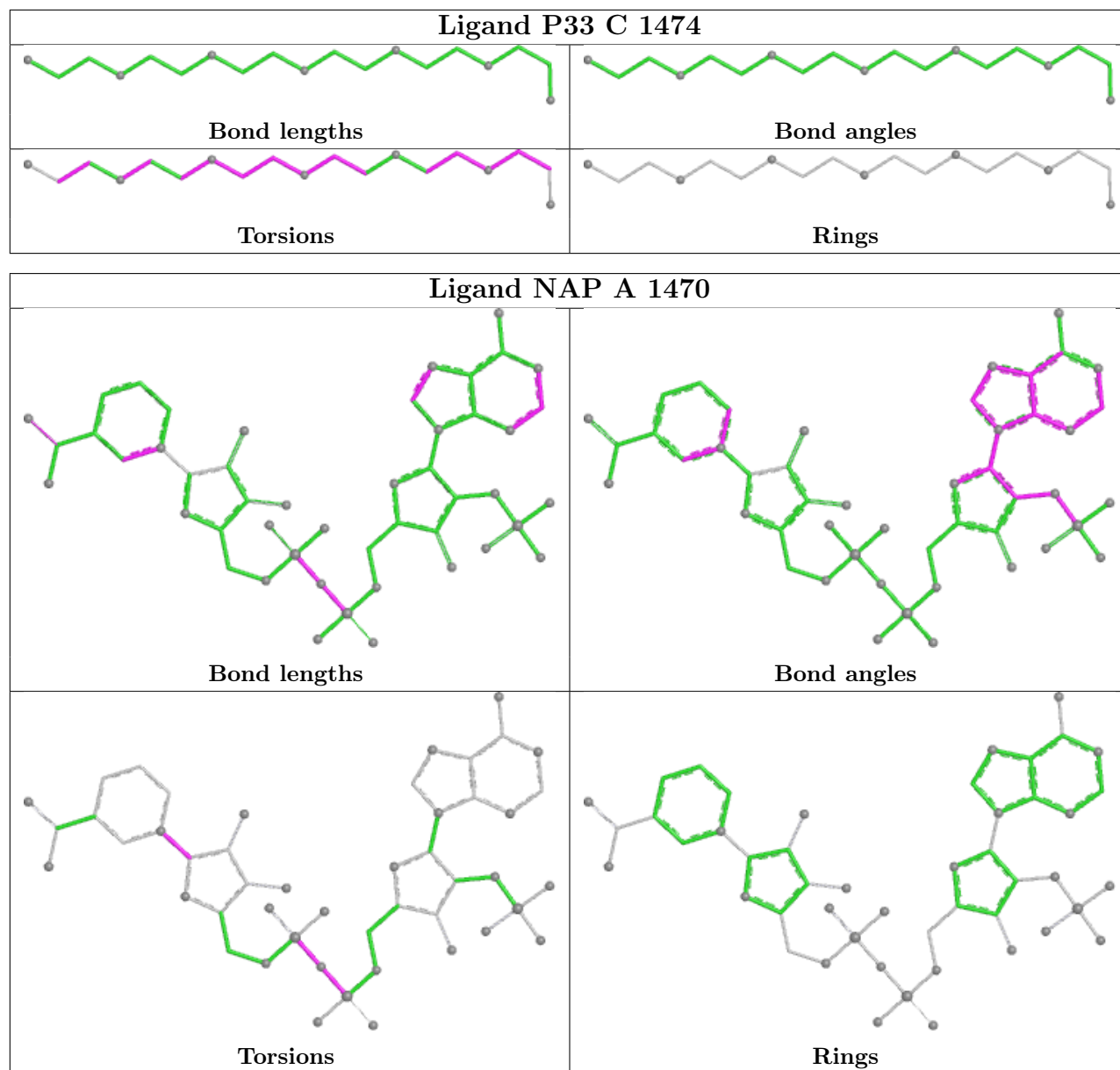


Ligand ATR B 1470 (A)



Ligand ATR C 1470 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/474 (99%)	-0.62	2 (0%) 88 86	4, 15, 29, 41	25 (5%)
1	B	470/474 (99%)	-0.80	2 (0%) 88 86	3, 11, 26, 49	22 (4%)
1	C	469/474 (98%)	-0.75	2 (0%) 88 86	3, 13, 26, 41	26 (5%)
All	All	1409/1422 (99%)	-0.72	6 (0%) 88 86	3, 13, 28, 49	73 (5%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1[A]	HIS	4.7
1	A	1[A]	MET	4.6
1	C	2	ALA	2.6
1	A	2	ALA	2.6
1	B	0	HIS	2.4
1	C	263	GLY	2.2

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](#)

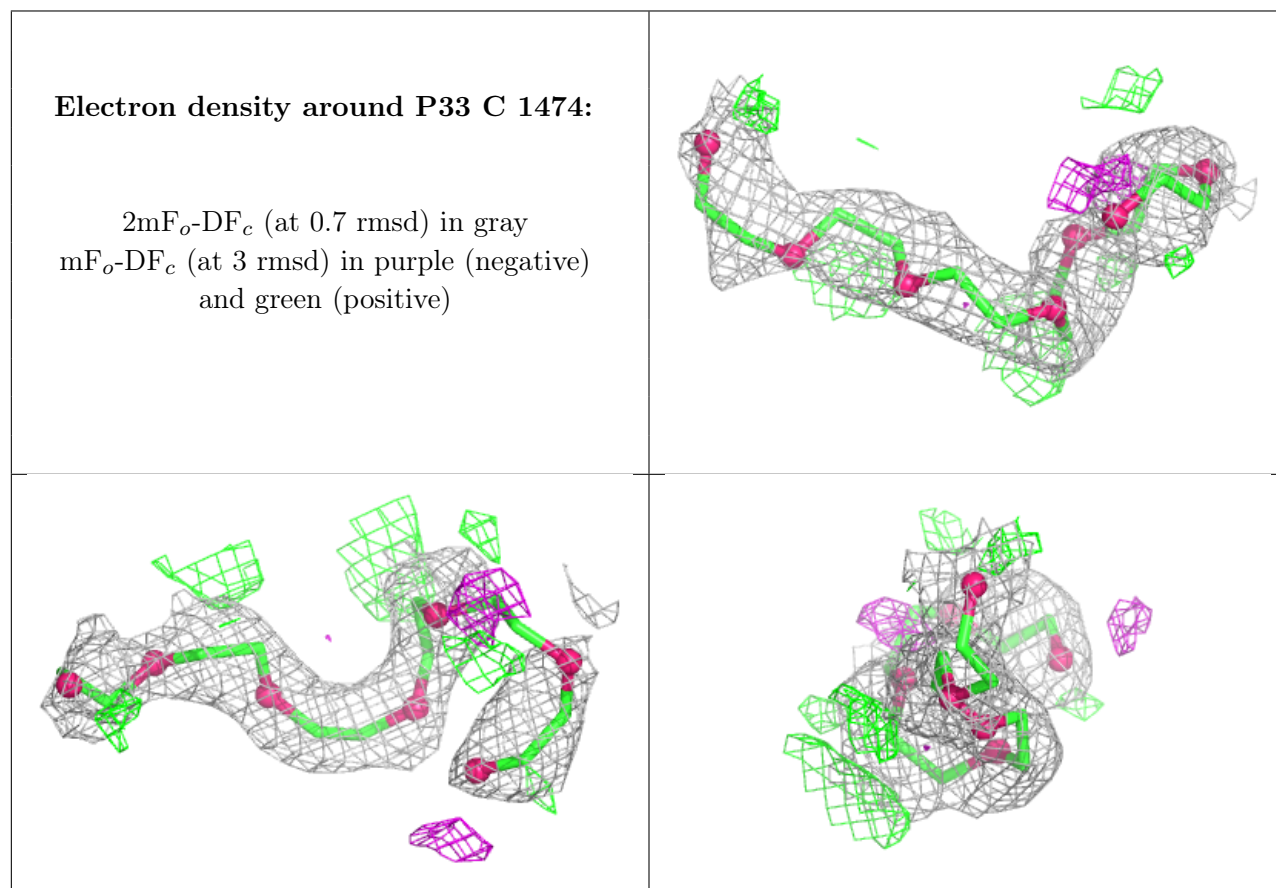
There are no oligosaccharides in this entry.

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.

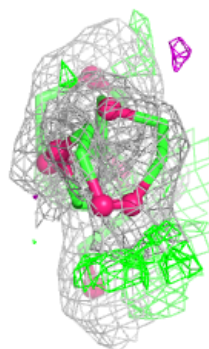
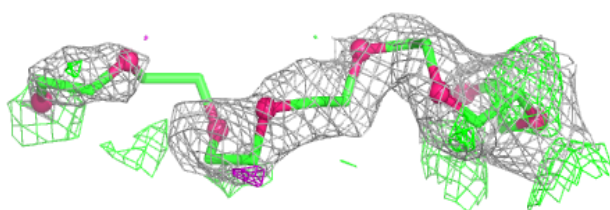
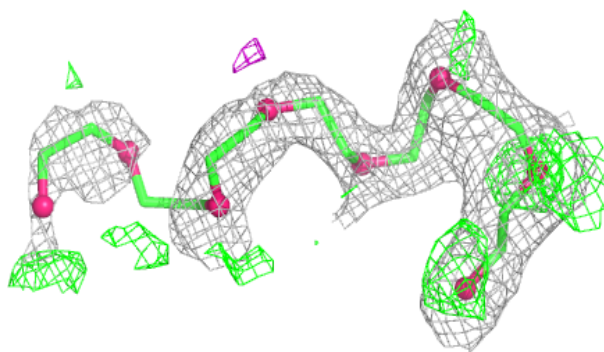
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	P33	C	1474	19/22	0.77	0.17	48,55,59,60	0
6	PEG	A	1474	7/7	0.79	0.13	57,58,59,59	0
5	P33	A	1473	22/22	0.80	0.19	41,57,64,64	0
9	EDO	B	1473	4/4	0.90	0.12	19,23,23,24	0
4	GOL	C	1473	6/6	0.91	0.13	35,36,38,39	0
8	CL	C	1471	1/1	0.92	0.14	55,55,55,55	0
4	GOL	A	1472	6/6	0.93	0.11	31,34,35,35	0
8	CL	B	1471	1/1	0.94	0.14	43,43,43,43	0
7	ATR	C	1470[B]	31/31	0.95	0.08	13,16,19,21	11
7	ATR	B	1470[A]	31/31	0.95	0.08	15,19,24,25	11
7	ATR	B	1470[B]	31/31	0.95	0.08	15,19,27,28	11
7	ATR	C	1470[A]	31/31	0.95	0.08	13,17,32,34	11
2	NAP	A	1470	48/48	0.96	0.07	15,20,24,25	0
8	CL	C	1472	1/1	0.98	0.16	28,28,28,28	0
3	RES	A	1471	14/14	0.98	0.06	6,10,11,12	1
8	CL	B	1472	1/1	0.99	0.15	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

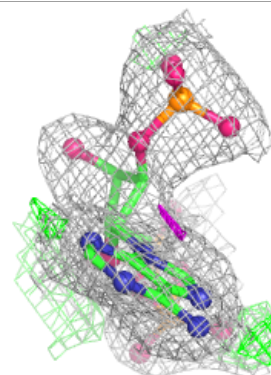
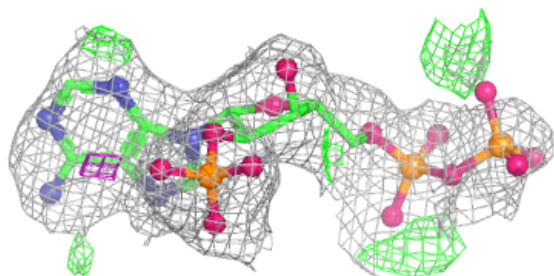
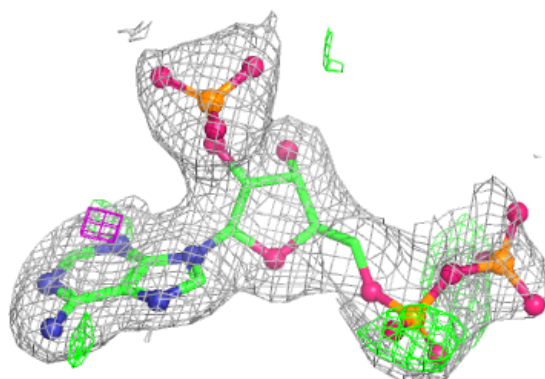


Electron density around P33 A 1473:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

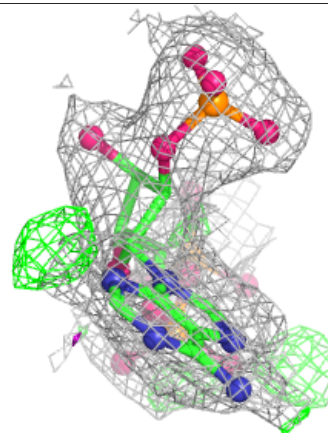
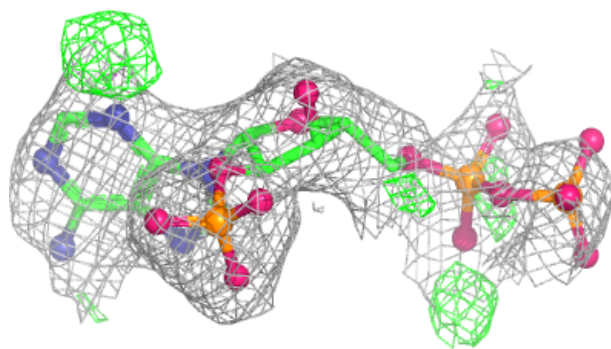
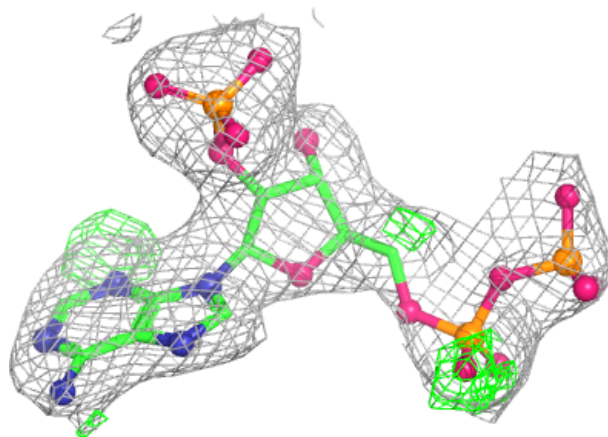
**Electron density around ATR C 1470 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



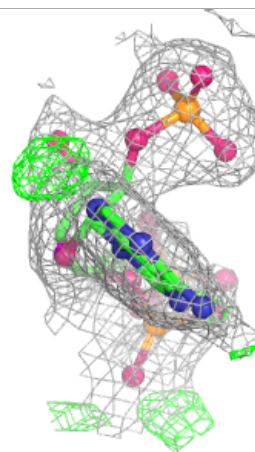
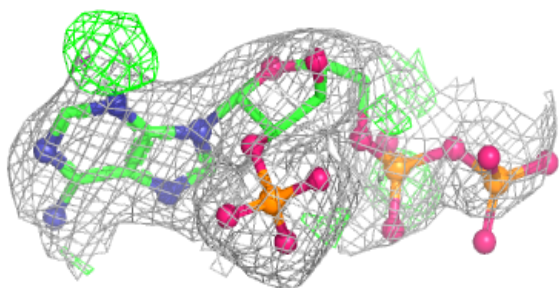
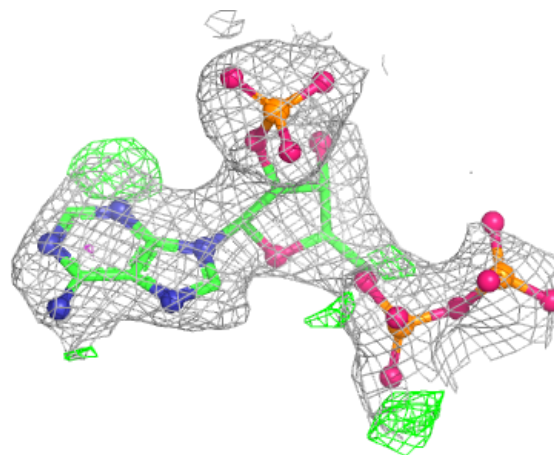
Electron density around ATR B 1470 (A):

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



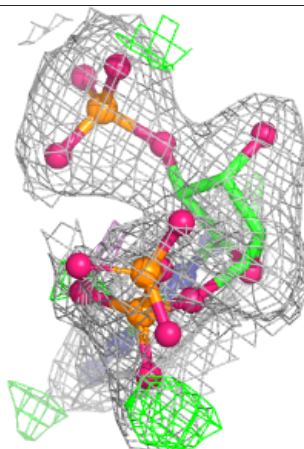
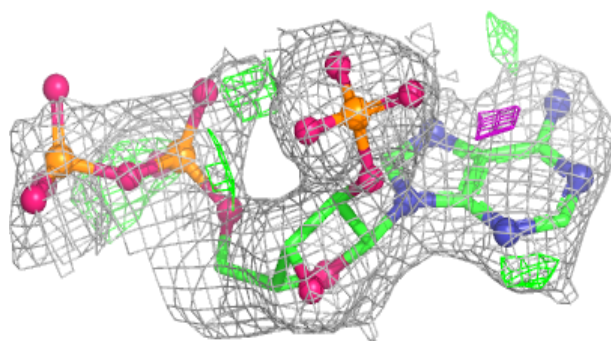
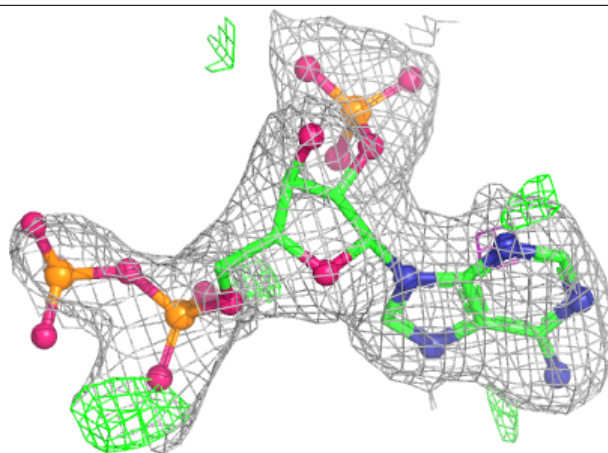
Electron density around ATR B 1470 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

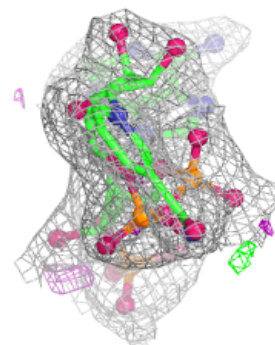
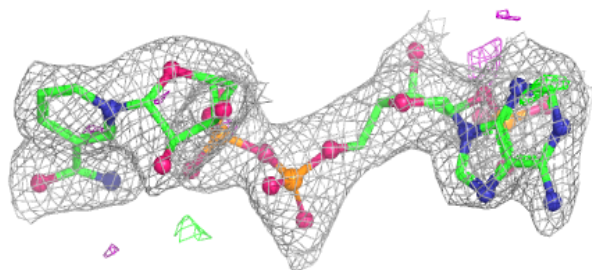
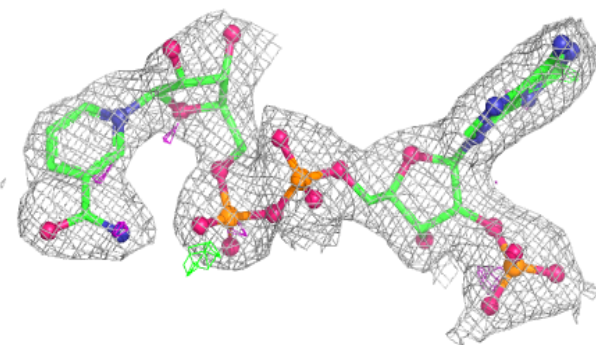


Electron density around ATR C 1470 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAP A 1470:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.