Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 07:23 pm BST

PDB ID	:	2IZ0
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 (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 (i)) were used in the production of this report:

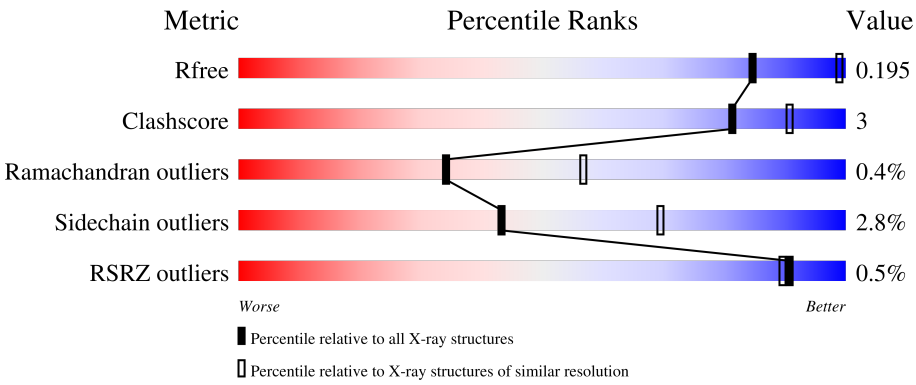
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

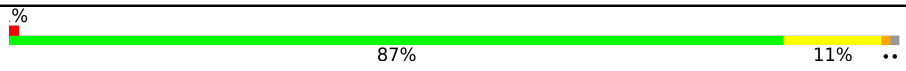
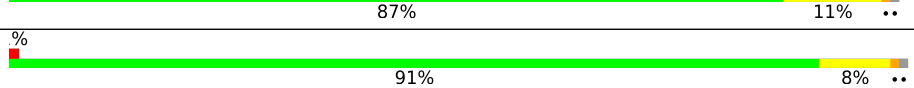
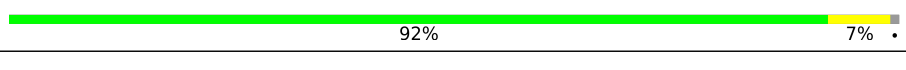
The reported resolution of this entry is 2.60 Å.

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	
1	B	474	
1	C	474	

2 Entry composition (i)

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.

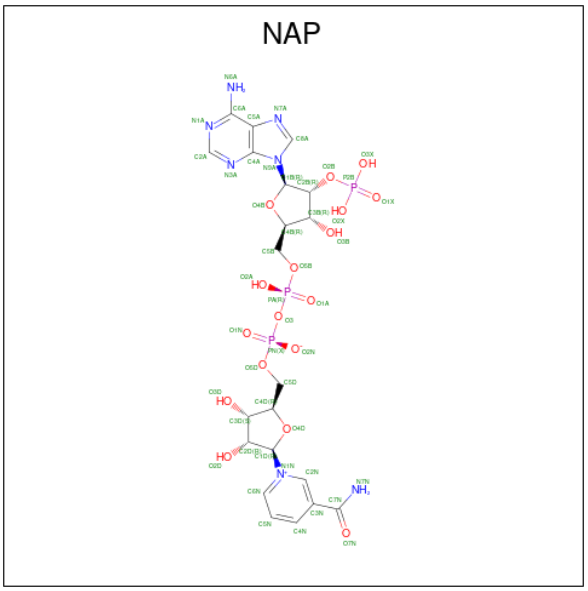
- Molecule 1 is a protein called 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING.

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

There are 9 discrepancies between the modelled and reference sequences:

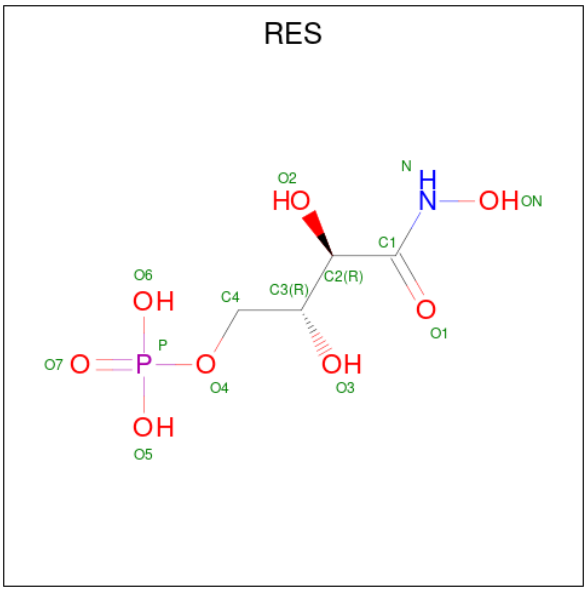
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP P96789
A	0	HIS	-	expression tag	UNP P96789
A	43	PHE	TYR	conflict	UNP P96789
B	-1	HIS	-	expression tag	UNP P96789
B	0	HIS	-	expression tag	UNP P96789
B	43	PHE	TYR	conflict	UNP P96789
C	-1	HIS	-	expression tag	UNP P96789
C	0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

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



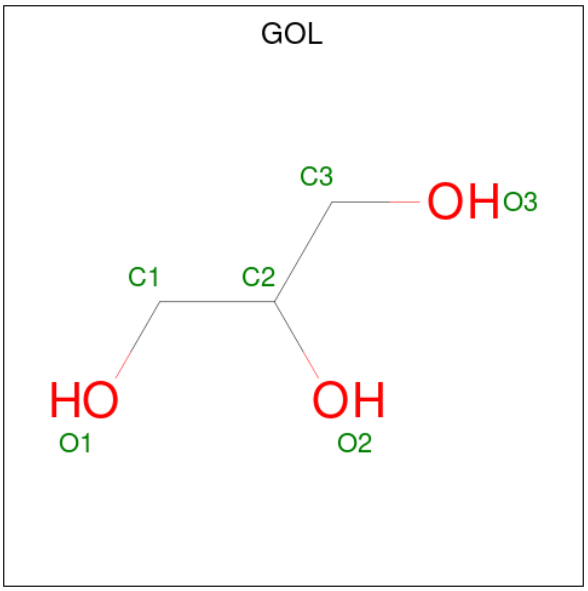
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is 4-PHOSPHO-D-ERYTHRONOHYDROXAMIC ACID (three-letter code: RES) (formula: $C_4H_{10}NO_8P$).



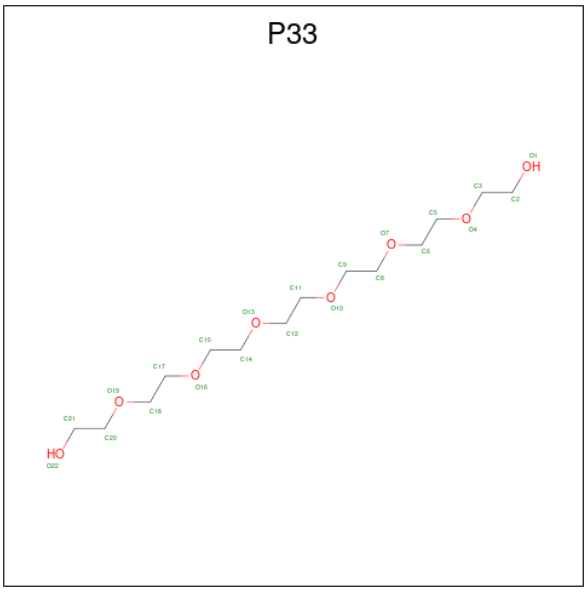
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	14	4	1	8	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



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

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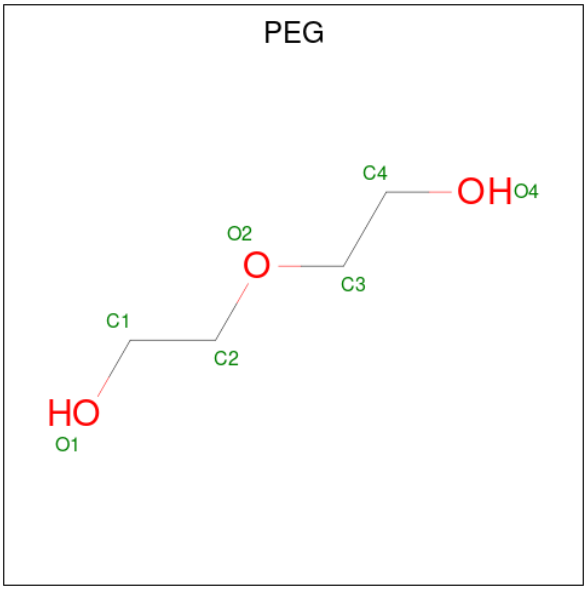
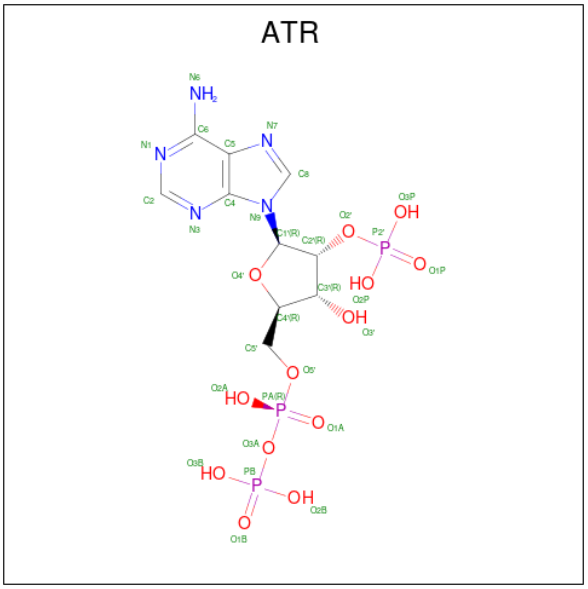
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	19	12	7	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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

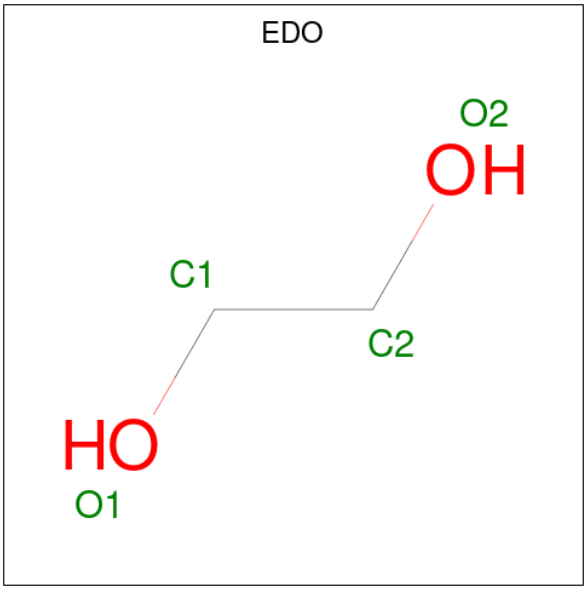


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	42	12	5	20	5	0	1
7	C	1	42	12	5	20	5	0	1

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 10 is water.

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

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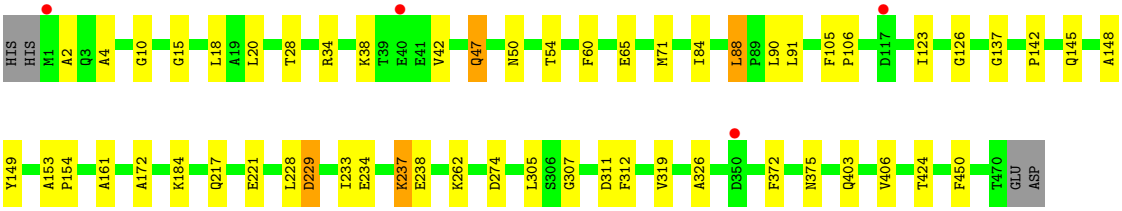
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	C	584	584	584	0	0

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.

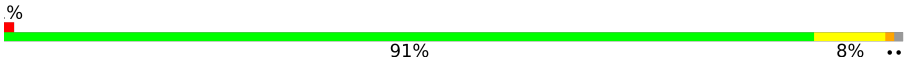
• Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING

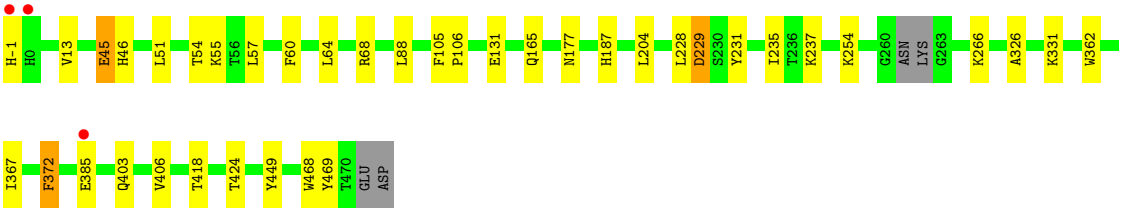
Chain A:



• Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING

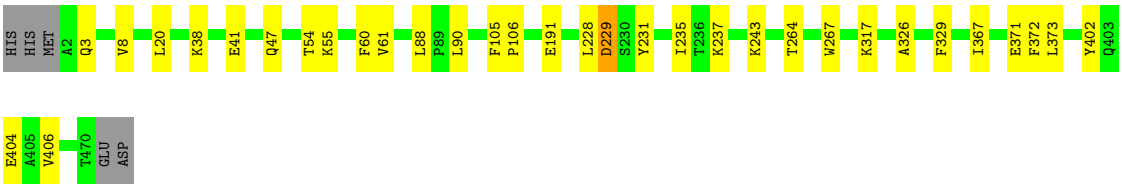
Chain B:





• Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING

Chain C:



4 Data and refinement statistics (i)

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 44.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (235.70-2.60) 97.5 (44.47-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.07%)	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)	0.34 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, RES, CL, EDO, ATR, P33, GOL, NAP

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	0.44	0/3946	0.56	0/5329
1	B	0.43	0/3933	0.55	3/5314 (0.1%)
1	C	0.43	0/3953	0.55	0/5337
All	All	0.44	0/11832	0.55	3/15980 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	-1[A]	HIS	CB-CA-C	5.42	121.24	110.40
1	B	-1[B]	HIS	CB-CA-C	5.42	121.24	110.40
1	B	469	TYR	O-C-N	-5.21	114.37	122.70

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 (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	3802	0	3818	28	0
1	B	3793	0	3776	18	0
1	C	3803	0	3846	17	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	3	0
All	All	13264	0	11582	59	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 (59) 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	0.68
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
1:A:142:PRO:HD2	1:A:172:ALA:O	2.02	0.59
1:B:449:TYR:HA	1:B:468:TRP:CD1	2.39	0.58
1:A:274[A]:ASP:OD1	1:B:266:LYS:NZ	2.36	0.56
1:C:38[B]:LYS:CE	1:C:41[B]:GLU:OE1	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
9:B:1473:EDO:H12	10:B:2567:HOH:O	2.13	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:A:228:LEU:HB3	1:A:233:ILE:HD13	1.98	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:B:54:THR:HG21	1:B:60:PHE:HA	2.00	0.43
1:C:228:LEU:O	1:C:229:ASP:C	2.56	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:A:126:GLY:HA3	1:A:184:LYS:HB2	2.00	0.43
1:A:153:ALA:N	1:A:154:PRO:CD	2.81	0.43
1:B:228:LEU:O	1:B:229:ASP:C	2.58	0.42
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:123[B]:ILE:HD11	1:A:149:TYR:HA	2.03	0.40
1:A:228:LEU:O	1:A:229:ASP:C	2.59	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: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 (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	491/474 (104%)	478 (97%)	11 (2%)	2 (0%)	34	57
1	B	487/474 (103%)	470 (96%)	15 (3%)	2 (0%)	34	57
1	C	493/474 (104%)	476 (97%)	15 (3%)	2 (0%)	34	57
All	All	1471/1422 (103%)	1424 (97%)	41 (3%)	6 (0%)	34	57

All (6) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	B	177	ASN
1	C	229	ASP
1	B	229	ASP

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	409/390 (105%)	394 (96%)	15 (4%)	34	60
1	B	407/390 (104%)	396 (97%)	11 (3%)	44	71
1	C	410/390 (105%)	400 (98%)	10 (2%)	49	74
All	All	1226/1170 (105%)	1190 (97%)	36 (3%)	43	68

All (36) 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	47[A]	GLN
1	A	47[B]	GLN
1	A	88	LEU
1	A	90	LEU
1	A	91	LEU
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

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Mol	Chain	Res	Type
1	B	88	LEU
1	B	165	GLN
1	B	237	LYS
1	B	254	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	237	LYS
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	375	ASN
1	C	47	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 monosaccharides 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	0.38	0	5,5,5	0.26	0
3	RES	A	1471	-	12,13,13	0.56	0	14,18,18	0.86	0
6	PEG	A	1474	-	6,6,6	0.39	0	5,5,5	0.31	0
7	ATR	C	1470[A]	-	27,33,33	0.95	1 (3%)	35,52,52	1.25	2 (5%)
2	NAP	A	1470	-	45,52,52	1.71	4 (8%)	56,80,80	1.15	2 (3%)
7	ATR	C	1470[B]	-	27,33,33	0.96	1 (3%)	35,52,52	1.25	3 (8%)
5	P33	C	1474	-	18,18,21	0.55	0	17,17,20	0.48	0
7	ATR	B	1470[A]	-	27,33,33	0.94	2 (7%)	35,52,52	1.26	2 (5%)
9	EDO	B	1473	-	3,3,3	0.41	0	2,2,2	0.34	0
7	ATR	B	1470[B]	-	27,33,33	0.92	2 (7%)	35,52,52	1.26	2 (5%)
5	P33	A	1473	-	21,21,21	0.57	0	20,20,20	0.62	0
4	GOL	C	1473	-	5,5,5	0.39	0	5,5,5	0.37	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
4	GOL	A	1472	-	-	2/4/4/4	-
3	RES	A	1471	-	-	5/16/16/16	-
6	PEG	A	1474	-	-	0/4/4/4	-
7	ATR	C	1470[A]	-	-	7/17/37/37	0/3/3/3
2	NAP	A	1470	-	-	6/31/67/67	0/5/5/5
7	ATR	C	1470[B]	-	-	6/17/37/37	0/3/3/3
5	P33	C	1474	-	-	12/16/16/19	-
7	ATR	B	1470[A]	-	-	5/17/37/37	0/3/3/3
9	EDO	B	1473	-	-	0/1/1/1	-
7	ATR	B	1470[B]	-	-	2/17/37/37	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	P33	A	1473	-	-	11/19/19/19	-
4	GOL	C	1473	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1470	NAP	O7N-C7N	8.91	1.41	1.24
2	A	1470	NAP	C2A-N3A	3.88	1.38	1.32
2	A	1470	NAP	C2A-N1A	2.55	1.38	1.33
7	B	1470[A]	ATR	O4'-C1'	2.47	1.44	1.41
7	B	1470[B]	ATR	O4'-C1'	2.47	1.44	1.41
2	A	1470	NAP	C2N-N1N	2.37	1.37	1.35
7	B	1470[A]	ATR	C2-N3	2.17	1.35	1.32
7	B	1470[B]	ATR	C2-N3	2.17	1.35	1.32
7	C	1470[A]	ATR	O4'-C1'	2.07	1.44	1.41
7	C	1470[B]	ATR	O4'-C1'	2.07	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1470	NAP	N3A-C2A-N1A	-5.62	119.89	128.68
7	B	1470[A]	ATR	N3-C2-N1	-4.88	121.05	128.68
7	B	1470[B]	ATR	N3-C2-N1	-4.88	121.05	128.68
7	C	1470[A]	ATR	N3-C2-N1	-4.40	121.80	128.68
7	C	1470[B]	ATR	N3-C2-N1	-4.40	121.80	128.68
7	C	1470[B]	ATR	O3B-PB-O2B	2.13	115.77	107.64
7	B	1470[A]	ATR	C4-C5-N7	-2.09	107.22	109.40
7	B	1470[B]	ATR	C4-C5-N7	-2.09	107.22	109.40
7	C	1470[A]	ATR	C3'-C2'-C1'	-2.05	99.03	102.89
7	C	1470[B]	ATR	C3'-C2'-C1'	-2.05	99.03	102.89
2	A	1470	NAP	C6N-N1N-C2N	-2.03	120.12	121.97

There are no chirality outliers.

All (58) 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

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

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Mol	Chain	Res	Type	Atoms
7	B	1470[A]	ATR	C2'-O2'-P2'-O2P
7	B	1470[A]	ATR	C2'-O2'-P2'-O3P
7	B	1470[B]	ATR	C2'-O2'-P2'-O2P
7	B	1470[B]	ATR	C2'-O2'-P2'-O3P
7	C	1470[A]	ATR	C2'-O2'-P2'-O3P
7	C	1470[B]	ATR	C2'-O2'-P2'-O3P
5	C	1474	P33	C21-C20-O19-C18
2	A	1470	NAP	PN-O3-PA-O1A
7	C	1470[B]	ATR	PB-O3A-PA-O2A
5	A	1473	P33	C14-C15-O16-C17
7	C	1470[B]	ATR	C5'-O5'-PA-O1A

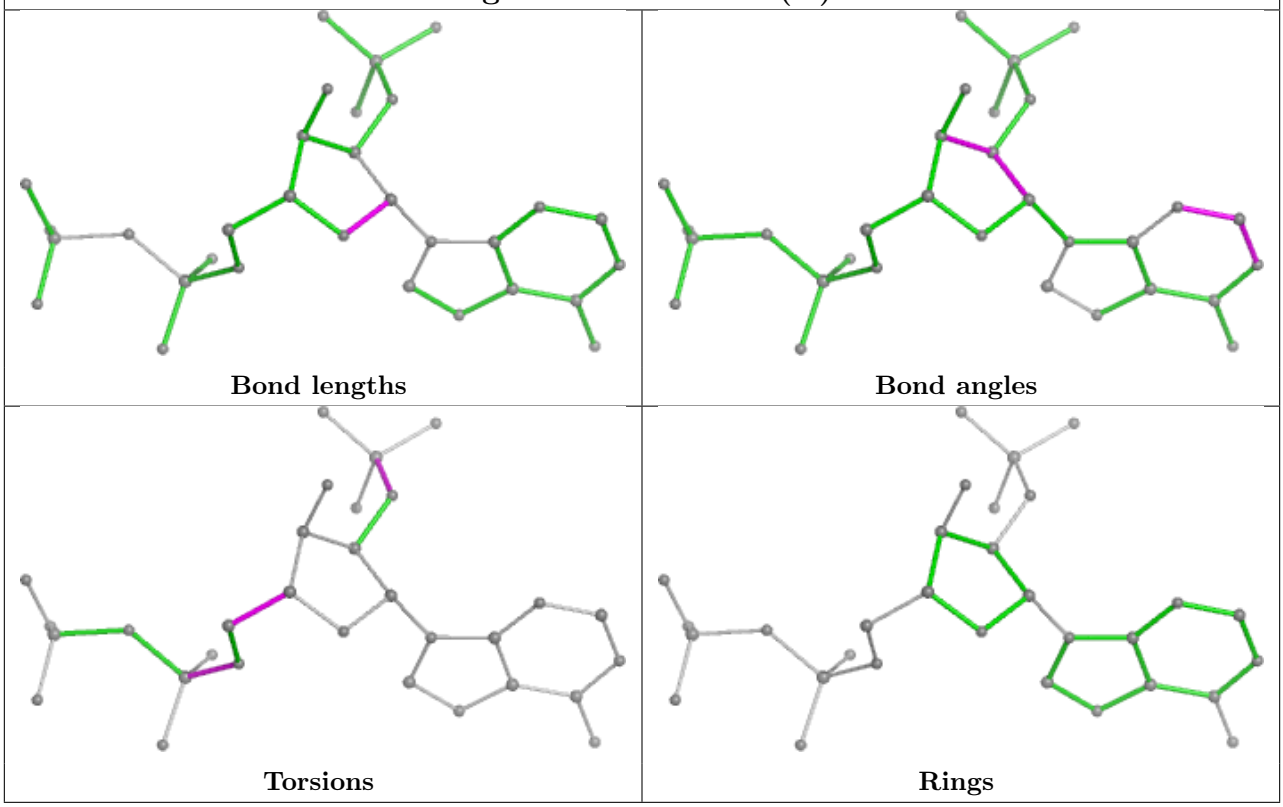
There are no ring outliers.

2 monomers are involved in 2 short contacts:

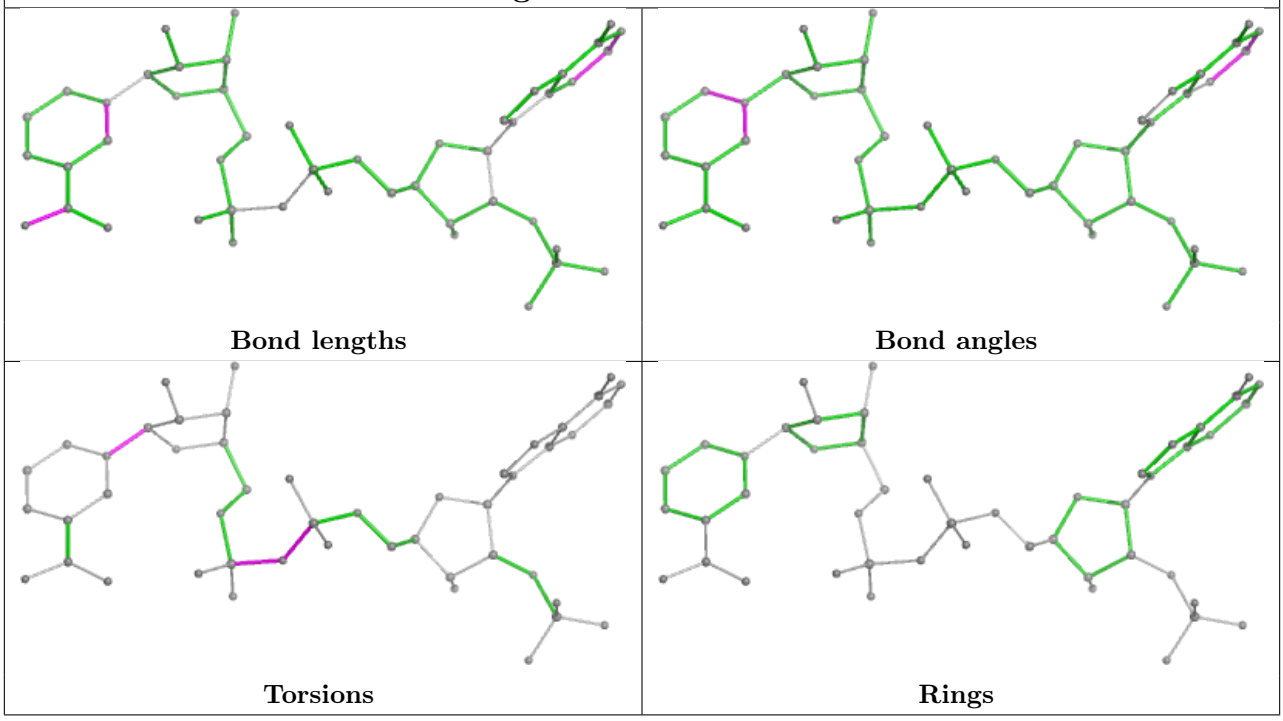
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1473	EDO	1	0
5	A	1473	P33	1	0

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 then 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.

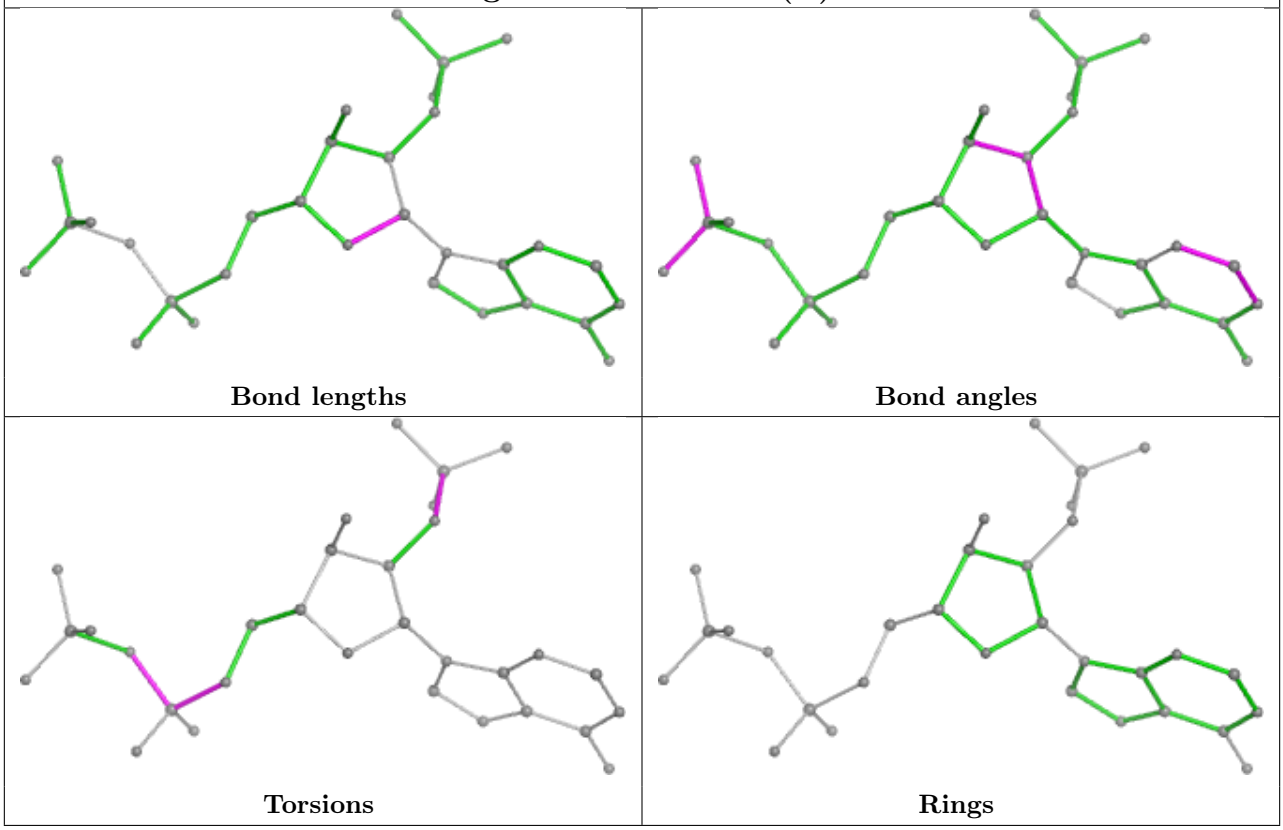
Ligand ATR C 1470 (A)



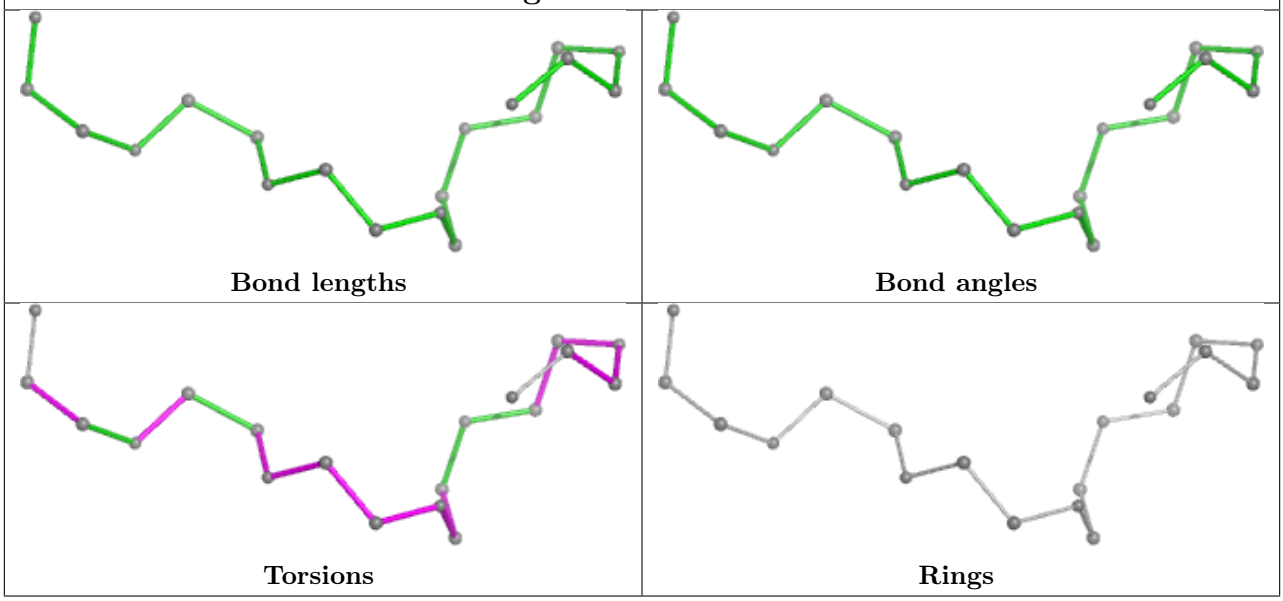
Ligand NAP A 1470



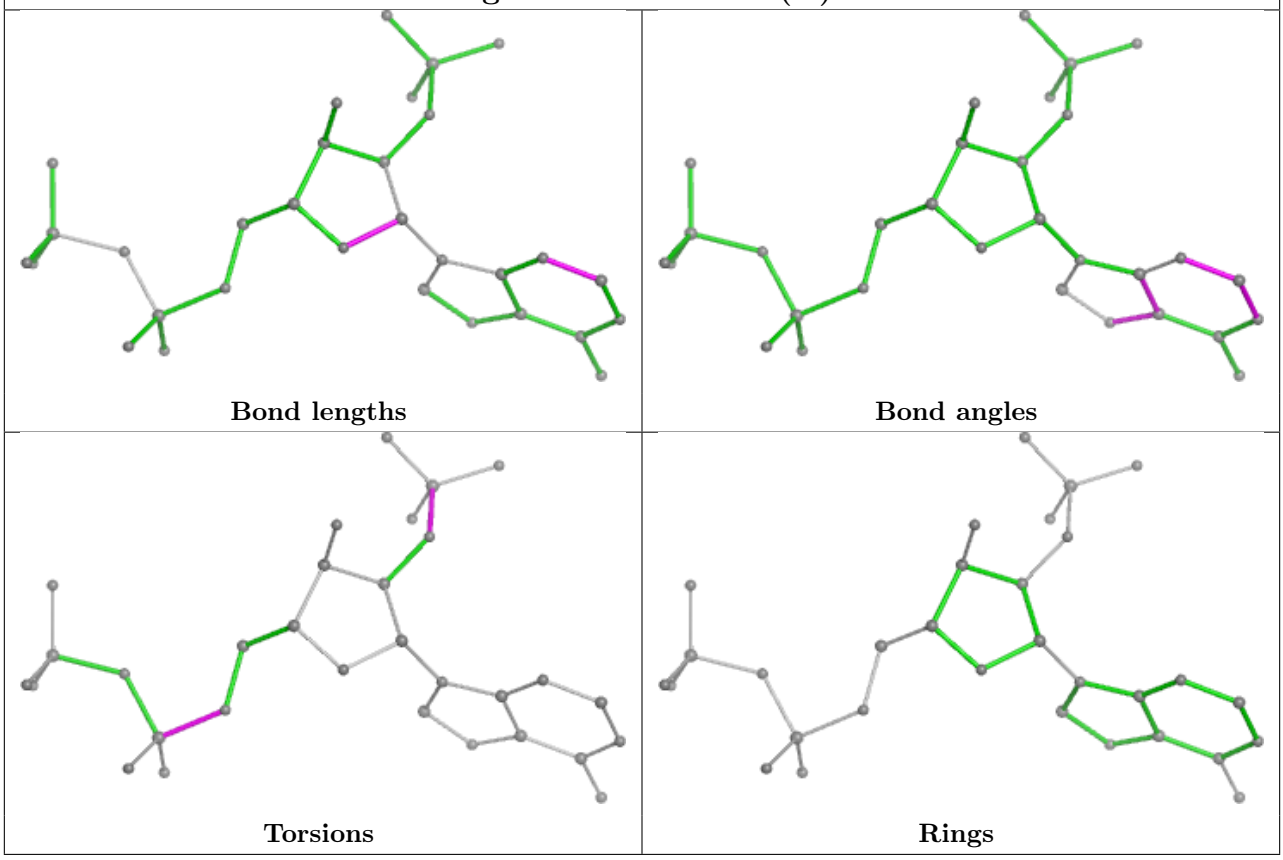
Ligand ATR C 1470 (B)



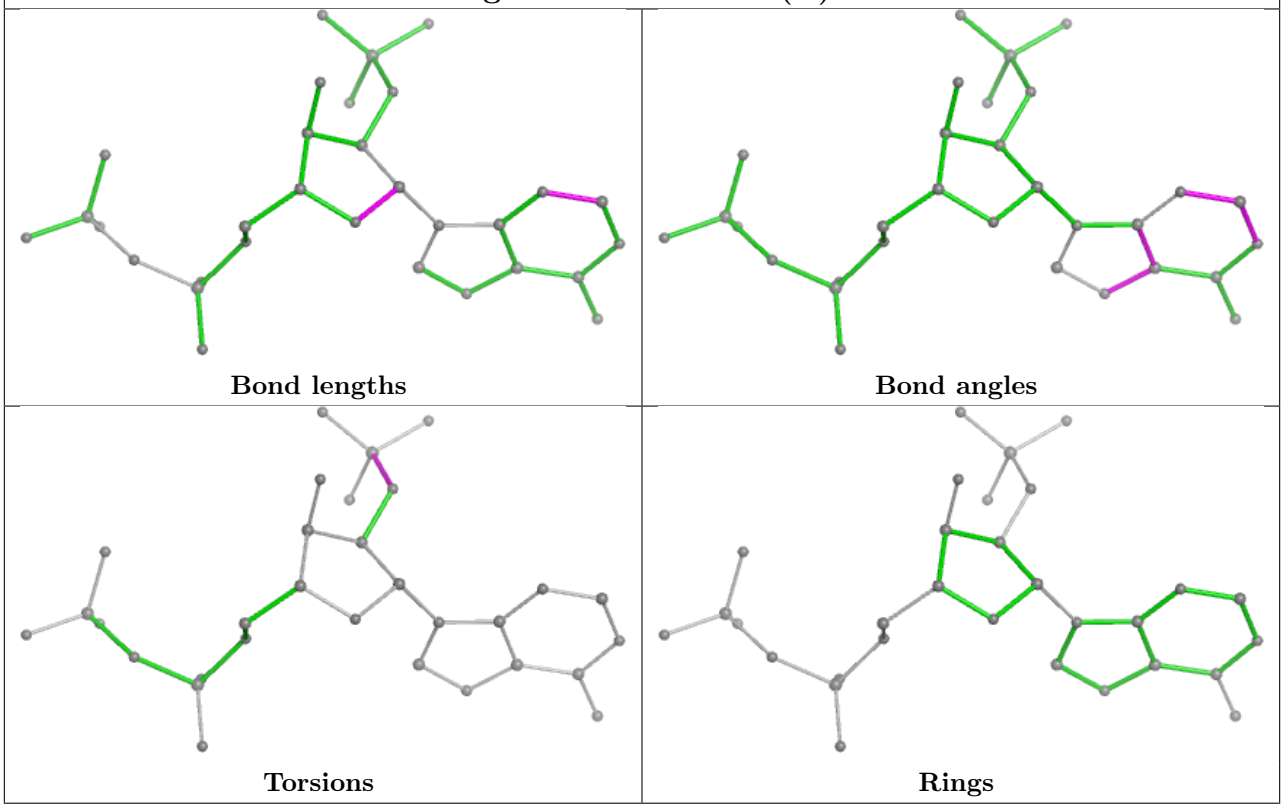
Ligand P33 C 1474



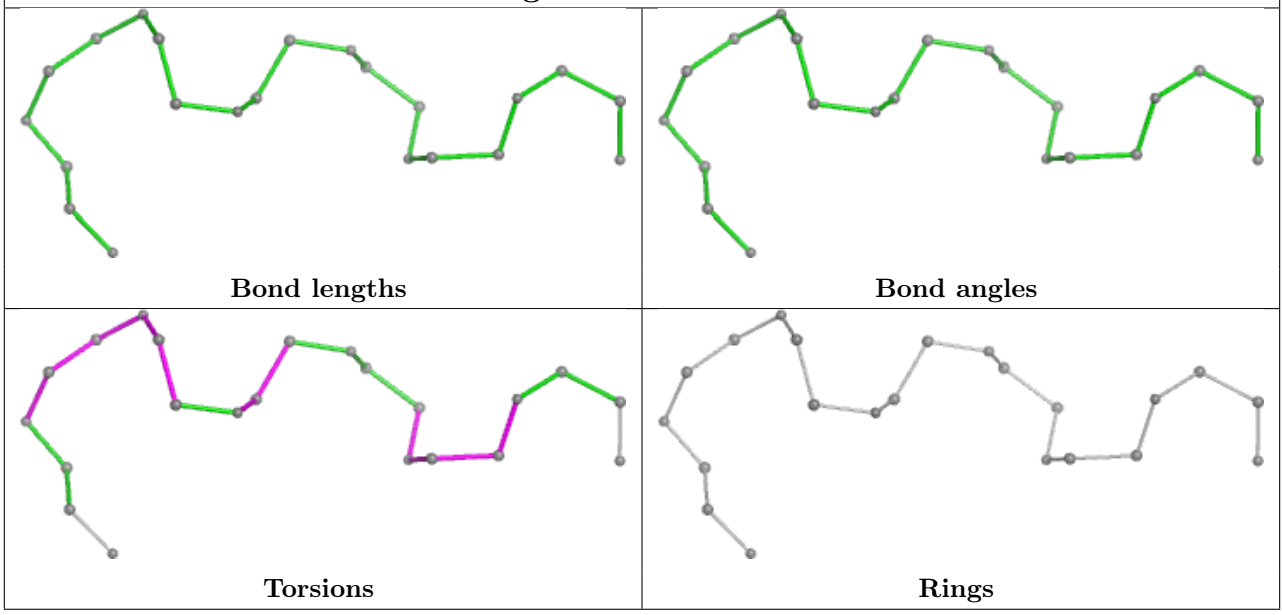
Ligand ATR B 1470 (A)



Ligand ATR B 1470 (B)



Ligand P33 A 1473



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%)	-0.37	4 (0%)	84	82	4, 15, 31, 42	2 (0%)
1	B	470/474 (99%)	-0.58	3 (0%)	89	88	3, 11, 27, 49	0
1	C	469/474 (98%)	-0.55	0	100	100	4, 13, 27, 41	0
All	All	1409/1422 (99%)	-0.50	7 (0%)	91	89	3, 13, 29, 49	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1[A]	MET	5.9
1	B	-1[A]	HIS	5.4
1	B	0	HIS	2.6
1	B	385[A]	GLU	2.5
1	A	117	ASP	2.3
1	A	350[A]	ASP	2.2
1	A	40	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

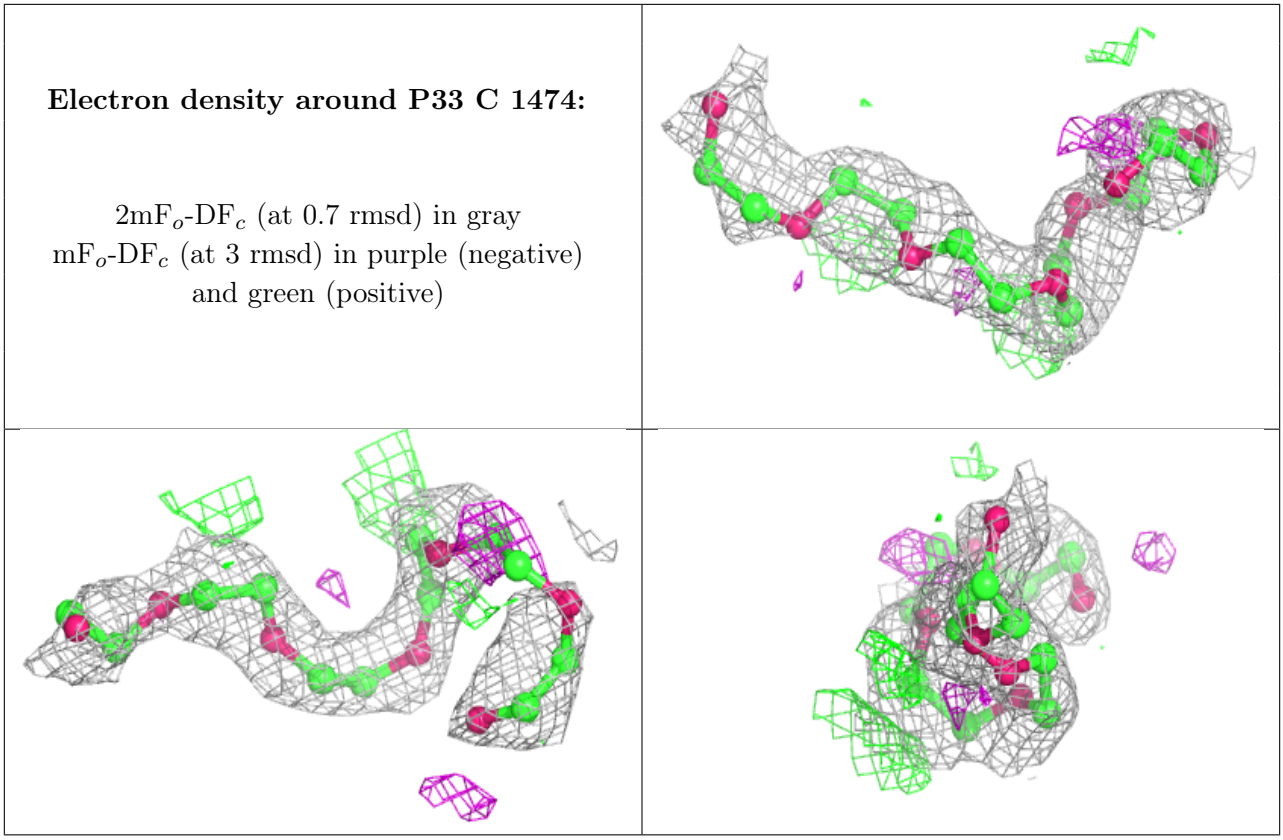
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	P33	C	1474	19/22	0.79	0.28	48,55,59,60	0
5	P33	A	1473	22/22	0.81	0.28	41,57,64,64	0
6	PEG	A	1474	7/7	0.81	0.35	57,58,59,59	0
8	CL	C	1471	1/1	0.91	0.13	55,55,55,55	0
4	GOL	C	1473	6/6	0.93	0.21	35,36,38,39	0
9	EDO	B	1473	4/4	0.93	0.18	19,23,23,24	0
7	ATR	B	1470[B]	31/31	0.94	0.19	15,19,27,28	11
7	ATR	C	1470[A]	31/31	0.94	0.16	13,17,32,34	11
7	ATR	C	1470[B]	31/31	0.94	0.16	13,16,19,21	11
4	GOL	A	1472	6/6	0.94	0.19	31,34,35,35	0
7	ATR	B	1470[A]	31/31	0.94	0.19	15,19,24,25	11
2	NAP	A	1470	48/48	0.96	0.14	15,20,24,25	0
8	CL	B	1471	1/1	0.97	0.10	43,43,43,43	0
3	RES	A	1471	14/14	0.98	0.09	6,10,11,12	1
8	CL	C	1472	1/1	0.99	0.25	28,28,28,28	0
8	CL	B	1472	1/1	0.99	0.27	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.

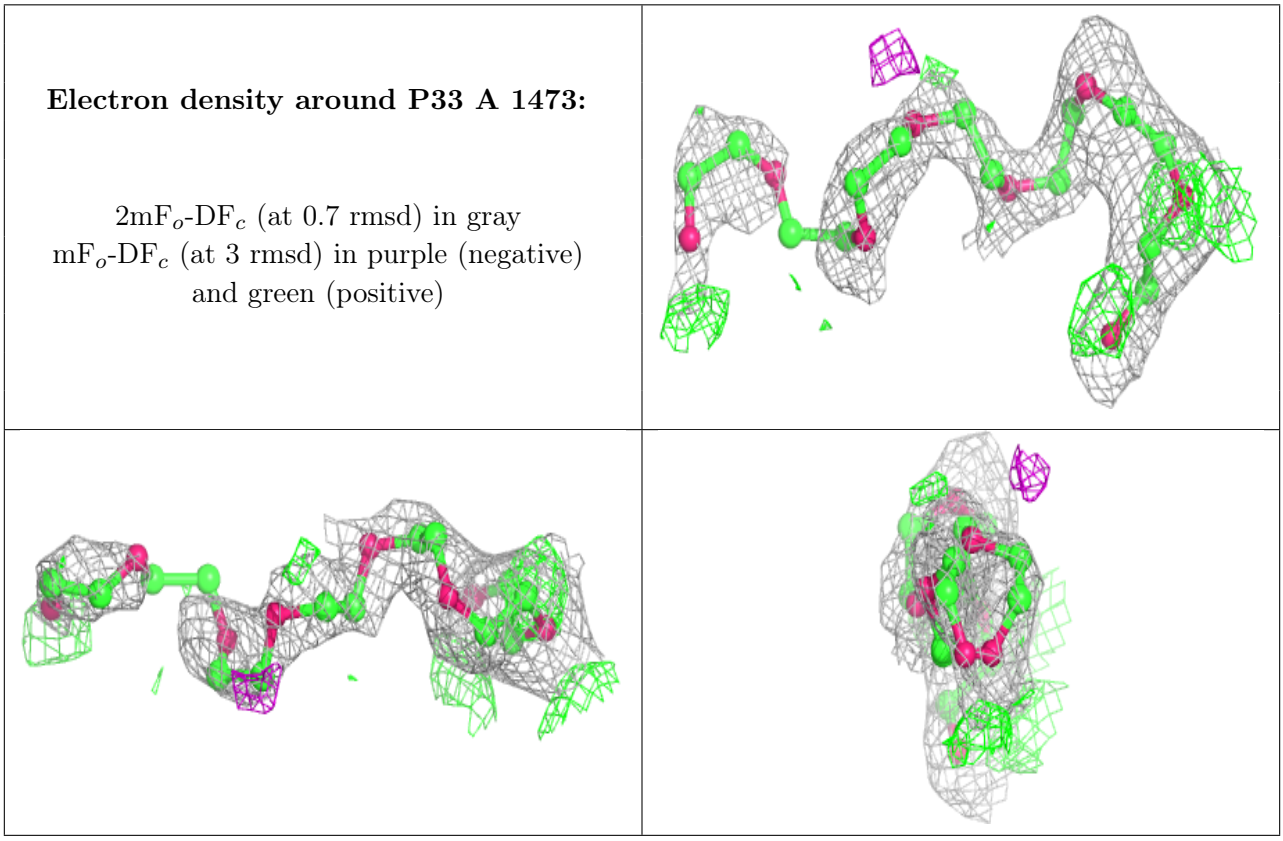
Electron density around P33 C 1474:

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



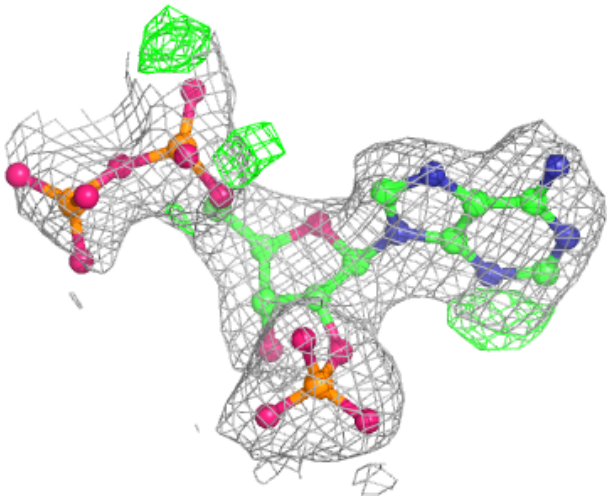
Electron density around P33 A 1473:

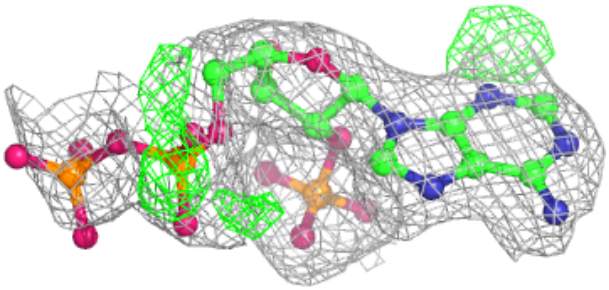
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

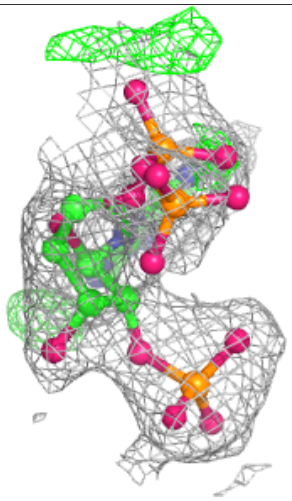


Electron density around ATR B 1470 (B):

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

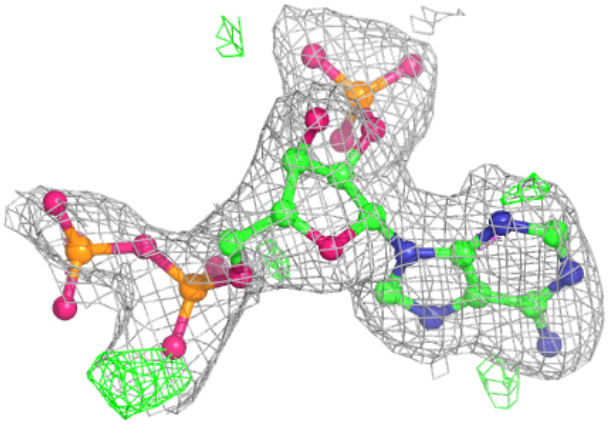


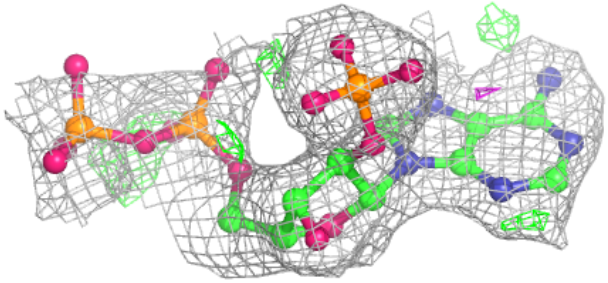


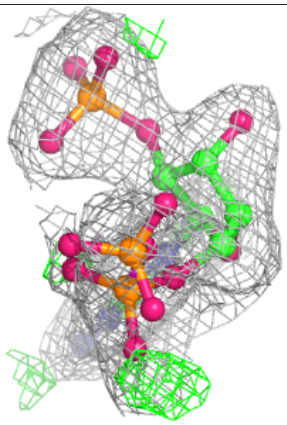


Electron density around ATR C 1470 (A):

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

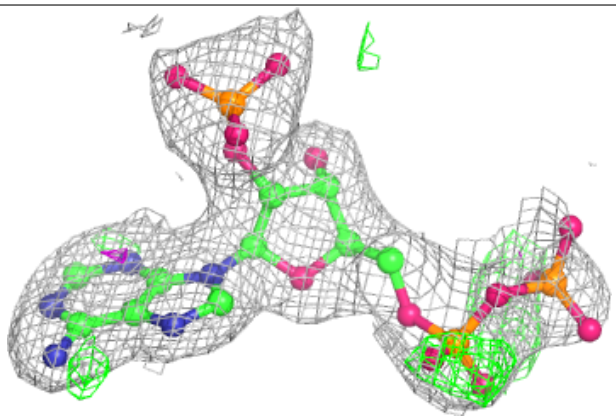


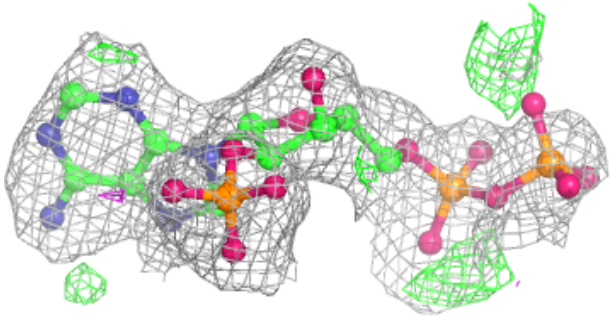


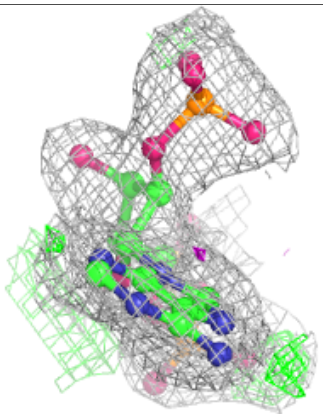


Electron density around ATR C 1470 (B):

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

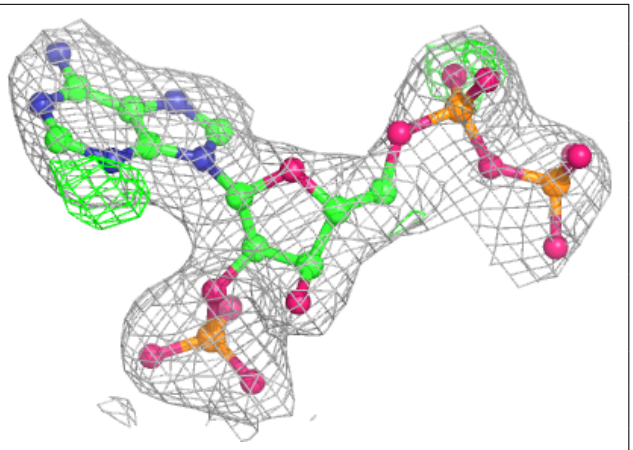


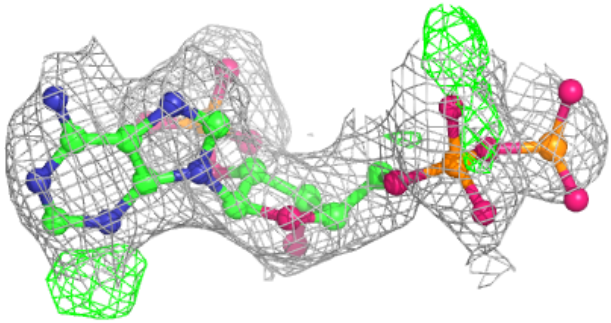


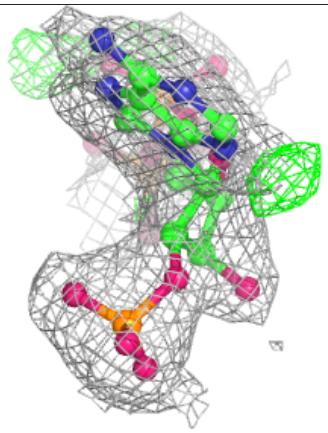


Electron density around ATR B 1470 (A):

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

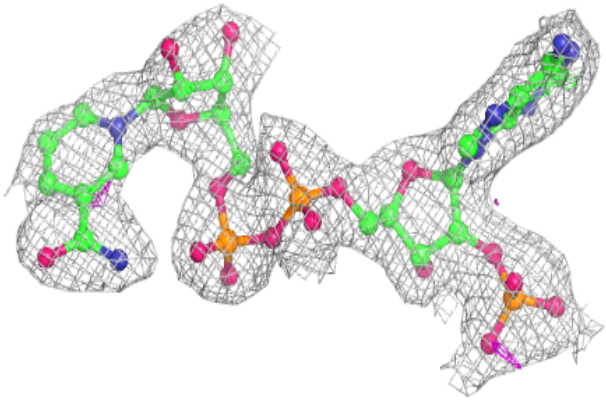


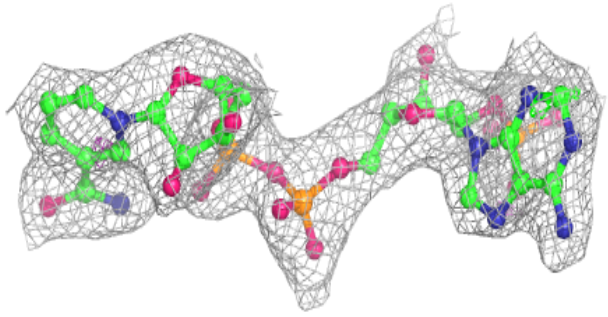


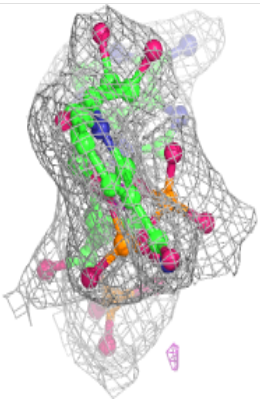


Electron density around NAP A 1470:

$2mF_o$-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 (i)

There are no such residues in this entry.