wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 01:59 pm BST

PDB ID	:	2YCP
Title	:	F448H mutant of tyrosine phenol-lyase from Citrobacter freundii in complex with quinonoid intermediate formed with 3-fluoro-L-tyrosine
Authors	:	Milic, D.; Demidkina, T.V.; Faleev, N.G.; Phillips, R.S.; Matkovic-Calogovic, D.; Antson, A.A.
Deposited on	:	2011-03-16
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references ⓘ) were used in the production of this report:

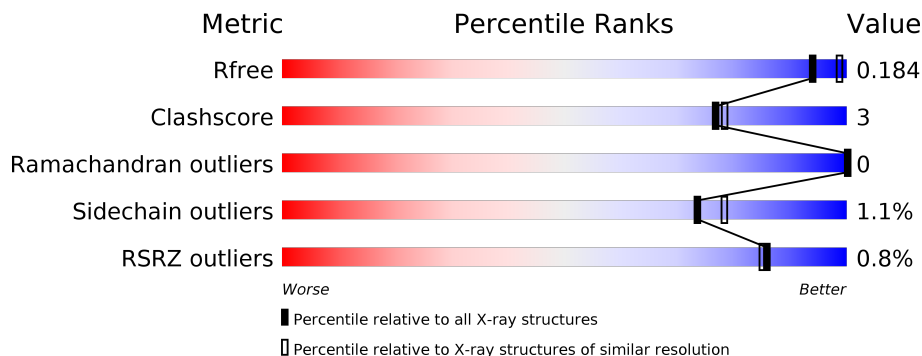|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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	Percentile Ranks	Value
Rfree		0.184
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		0.8%

Worse — *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	456	92% · 8%
1	B	456	92% · 7%
1	C	456	95% · 5%
1	D	456	94% · 6%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16890 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.
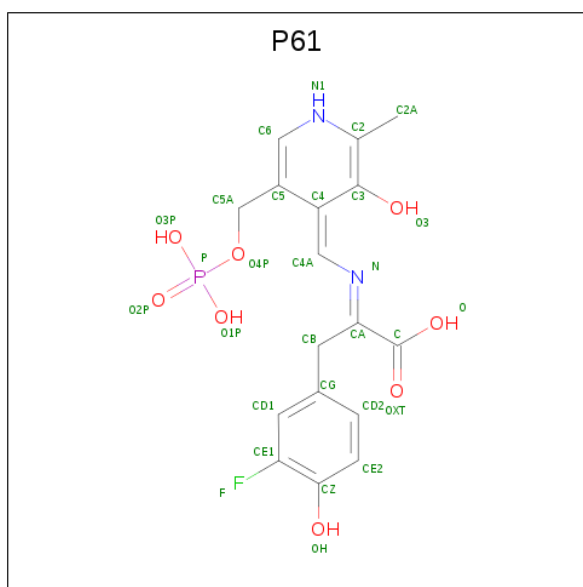
- Molecule 1 is a protein called TYROSINE PHENOL-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total 3661	C 2317	N 638	O 679	S 27	0	8	0
1	B	456	Total 3652	C 2312	N 633	O 680	S 27	0	7	0
1	C	456	Total 3672	C 2326	N 637	O 682	S 27	0	10	0
1	D	456	Total 3651	C 2312	N 635	O 677	S 27	0	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	448	HIS	PHE	engineered mutation	UNP P31013
B	448	HIS	PHE	engineered mutation	UNP P31013
C	448	HIS	PHE	engineered mutation	UNP P31013
D	448	HIS	PHE	engineered mutation	UNP P31013

- Molecule 2 is (2E)-3-(3-fluoro-4-hydroxyphenyl)-2-{[(Z)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4(1H)-ylidene}methyl]imino}propanoic acid (three-letter code: P61) (formula: $C_{17}H_{18}FN_2O_8P$).

P61

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			29	17	1	2	8	1		
2	B	1	Total	C	F	N	O	P	0	0
			29	17	1	2	8	1		
2	C	1	Total	C	F	N	O	P	0	0
			29	17	1	2	8	1		
2	D	1	Total	C	F	N	O	P	0	0
			29	17	1	2	8	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE
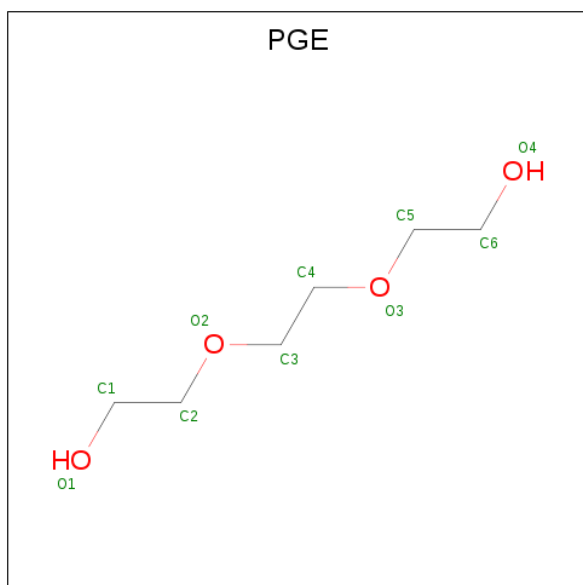
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4
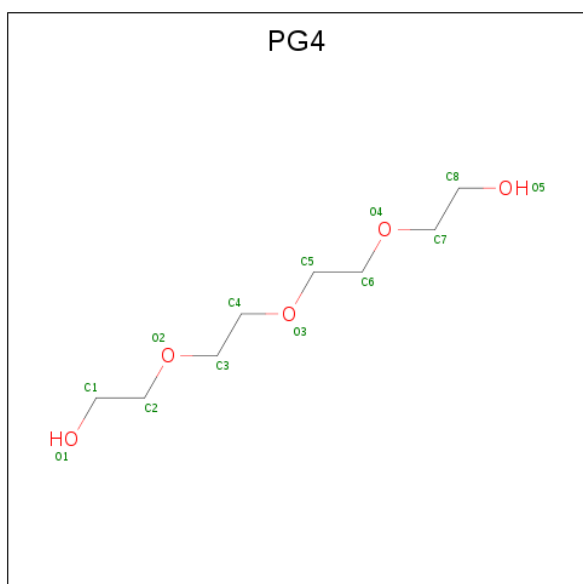
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 8	O 5	0	0
4	A	1	Total 13	C 8	O 5	0	0
4	B	1	Total 13	C 8	O 5	0	0
4	B	1	Total 13	C 8	O 5	0	0
4	D	1	Total 13	C 8	O 5	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	K 2	0	0
5	C	2	Total 2	K 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
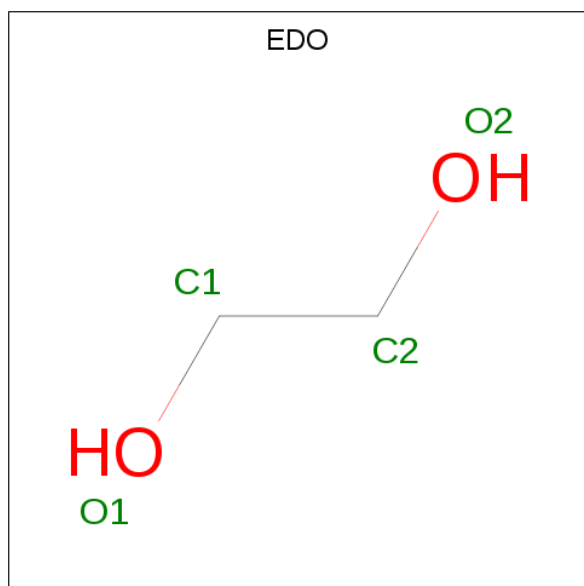
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 2	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
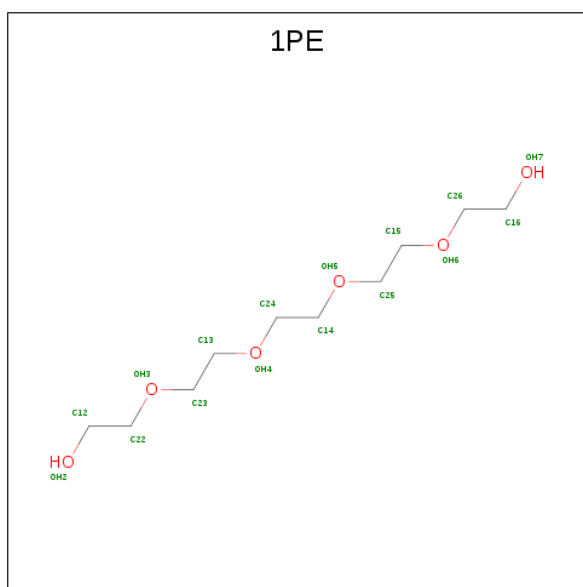
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 16	C 10	O 6	0	0

- Molecule 8 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).
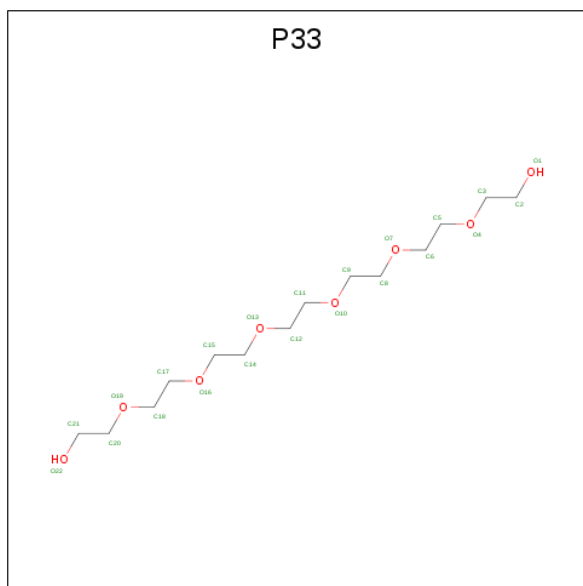
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 22	C 14	O 8	0	0
8	D	1	Total 22	C 14	O 8	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG
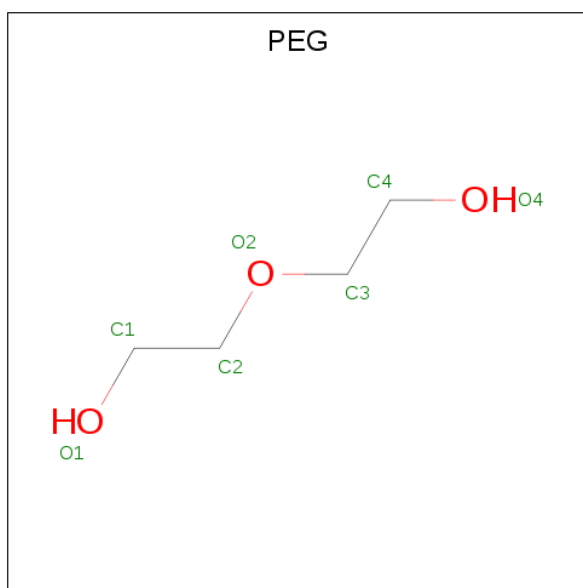
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total 7	C 4	O 3	0	0
9	D	1	Total 7	C 4	O 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	484	Total 484	O 484	0	0
10	B	454	Total 454	O 454	0	0
10	C	481	Total 481	O 481	0	0
10	D	442	Total 442	O 442	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
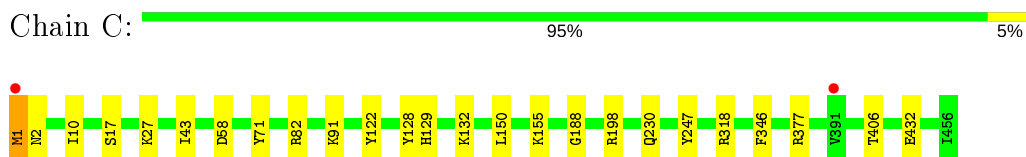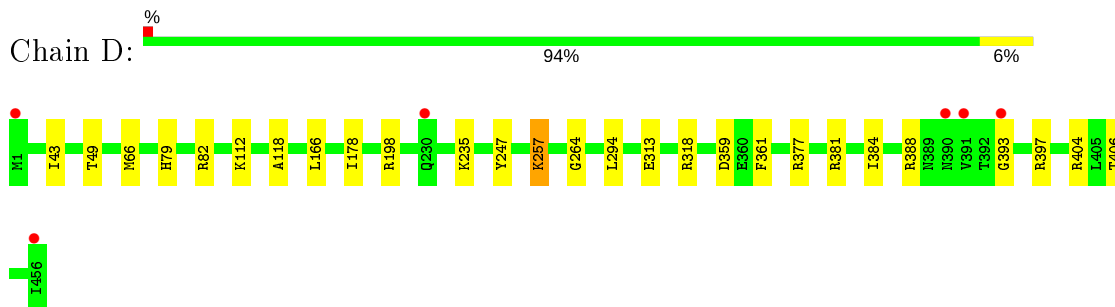
- Molecule 1: TYROSINE PHENOL-LYASE
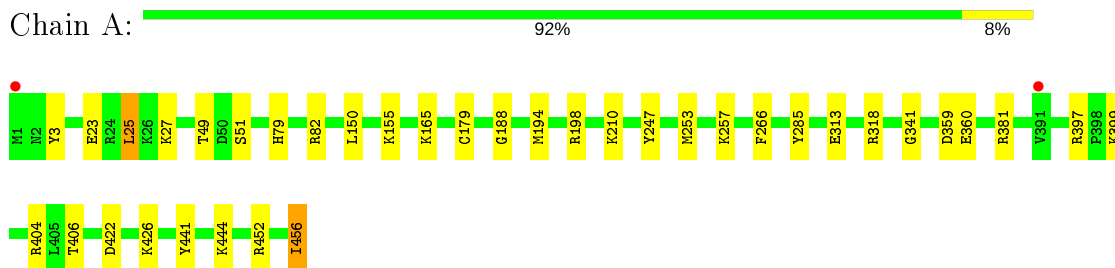
- Molecule 1: TYROSINE PHENOL-LYASE
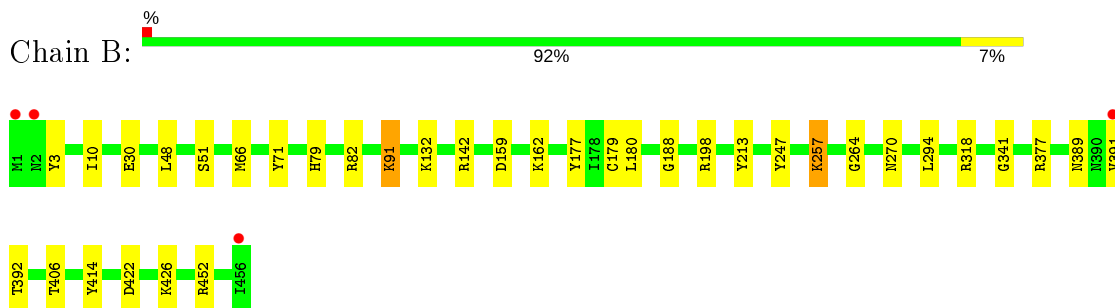
- Molecule 1: TYROSINE PHENOL-LYASE

- Molecule 1: TYROSINE PHENOL-LYASE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.42Å 143.76Å 118.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.00) 98.7 (29.83-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.141 , 0.175 0.157 , 0.184	Depositor DCC
R_{free} test set	1547 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.0	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16890	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7863e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: P61, PGE, K, EDO, 1PE, PG4, P33, 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	0.63	0/3758	0.64	1/5060 (0.0%)
1	B	0.60	0/3743	0.63	0/5041
1	C	0.62	0/3772	0.65	1/5078 (0.0%)
1	D	0.61	0/3745	0.64	0/5043
All	All	0.62	0/15018	0.64	2/20222 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	LEU	CA-CB-CG	5.52	127.99	115.30
1	C	58	ASP	CB-CG-OD1	5.28	123.05	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3661	0	3628	23	0
1	B	3652	0	3610	31	0
1	C	3672	0	3642	17	0
1	D	3651	0	3618	18	0
2	A	29	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	14	0	0
2	C	29	0	14	0	0
2	D	29	0	14	0	0
3	A	40	0	56	4	0
3	B	20	0	28	3	0
3	C	40	0	56	1	0
3	D	30	0	42	2	0
4	A	26	0	36	3	0
4	B	26	0	36	1	0
4	D	13	0	18	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	B	4	0	6	0	0
7	B	16	0	22	0	0
8	C	22	0	30	3	0
8	D	22	0	30	1	0
9	C	7	0	10	0	0
9	D	7	0	10	1	0
10	A	484	0	0	2	0
10	B	454	0	0	5	0
10	C	481	0	0	7	0
10	D	442	0	0	4	0
All	All	16890	0	14933	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 91 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LYS:HE3	9:D:1462:PEG:H12	1.49	0.93
1:A:179[A]:CYS:SG	10:A:2079:HOH:O	2.31	0.89
1:A:165:LYS:HD3	3:A:1457:PGE:H22	1.63	0.78
1:A:285:TYR:OH	1:B:132:LYS:HE3	1.85	0.76
1:D:79[B]:HIS:HD2	1:D:82:ARG:HH22	1.33	0.75

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	462/456 (101%)	451 (98%)	11 (2%)	0	100	100
1	B	461/456 (101%)	450 (98%)	11 (2%)	0	100	100
1	C	464/456 (102%)	453 (98%)	11 (2%)	0	100	100
1	D	461/456 (101%)	452 (98%)	9 (2%)	0	100	100
All	All	1848/1824 (101%)	1806 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	386/379 (102%)	381 (99%)	5 (1%)	69	74
1	B	385/379 (102%)	381 (99%)	4 (1%)	76	81
1	C	388/379 (102%)	384 (99%)	4 (1%)	76	81
1	D	385/379 (102%)	382 (99%)	3 (1%)	81	86
All	All	1544/1516 (102%)	1528 (99%)	16 (1%)	73	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	ARG
1	B	406	THR
1	C	406	THR

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Mol	Chain	Res	Type
1	B	257	LYS
1	D	257	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	P61	B	600	-	26,30,30	1.79	2 (7%)	31,43,43	1.93	7 (22%)
8	P33	D	1457	-	21,21,21	0.46	0	20,20,20	0.32	0
3	PGE	D	1461	-	9,9,9	0.56	0	8,8,8	0.23	0
4	PG4	A	1464	-	12,12,12	0.57	0	11,11,11	0.41	0
3	PGE	A	1458	-	9,9,9	0.52	0	8,8,8	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	P61	C	600	-	26,30,30	1.95	2 (7%)	31,43,43	1.83	8 (25%)
3	PGE	B	1458	-	9,9,9	0.48	0	8,8,8	0.32	0
9	PEG	D	1462	-	6,6,6	0.48	0	5,5,5	0.38	0
3	PGE	A	1457	-	9,9,9	0.51	0	8,8,8	0.33	0
3	PGE	A	1459	-	9,9,9	0.42	0	8,8,8	0.38	0
6	EDO	B	1460	-	3,3,3	0.56	0	2,2,2	0.41	0
3	PGE	C	1460	-	9,9,9	0.60	0	8,8,8	0.31	0
4	PG4	B	1459	-	12,12,12	0.52	0	11,11,11	0.30	0
3	PGE	C	1458	-	9,9,9	0.52	0	8,8,8	0.47	0
4	PG4	D	1460	-	12,12,12	0.52	0	11,11,11	0.23	0
2	P61	A	600	-	26,30,30	1.77	2 (7%)	31,43,43	1.85	8 (25%)
8	P33	C	1457	-	21,21,21	0.49	0	20,20,20	0.33	0
4	PG4	B	1457	-	12,12,12	0.52	0	11,11,11	0.35	0
3	PGE	D	1458	-	9,9,9	0.47	0	8,8,8	0.32	0
7	1PE	B	1462	-	15,15,15	0.49	0	14,14,14	0.31	0
3	PGE	A	1461	-	9,9,9	0.48	0	8,8,8	0.30	0
2	P61	D	600	-	26,30,30	1.75	3 (11%)	31,43,43	1.95	7 (22%)
4	PG4	A	1460	-	12,12,12	0.53	0	11,11,11	0.27	0
3	PGE	B	1461	-	9,9,9	0.54	0	8,8,8	0.40	0
3	PGE	C	1459	-	9,9,9	0.48	0	8,8,8	0.33	0
9	PEG	C	1462	-	6,6,6	0.46	0	5,5,5	0.20	0
3	PGE	C	1461	-	9,9,9	0.48	0	8,8,8	0.32	0
3	PGE	D	1459	-	9,9,9	0.53	0	8,8,8	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P61	B	600	-	-	0/11/19/19	0/2/2/2
8	P33	D	1457	-	-	14/19/19/19	-
3	PGE	D	1461	-	-	3/7/7/7	-
4	PG4	A	1464	-	-	5/10/10/10	-
3	PGE	A	1458	-	-	2/7/7/7	-
2	P61	C	600	-	-	0/11/19/19	0/2/2/2
3	PGE	B	1458	-	-	5/7/7/7	-
9	PEG	D	1462	-	-	1/4/4/4	-
3	PGE	A	1457	-	-	3/7/7/7	-
3	PGE	A	1459	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	1460	-	-	1/1/1/1	-
3	PGE	C	1460	-	-	3/7/7/7	-
4	PG4	B	1459	-	-	4/10/10/10	-
3	PGE	C	1458	-	-	3/7/7/7	-
4	PG4	D	1460	-	-	2/10/10/10	-
2	P61	A	600	-	-	0/11/19/19	0/2/2/2
8	P33	C	1457	-	-	9/19/19/19	-
4	PG4	B	1457	-	-	3/10/10/10	-
3	PGE	D	1458	-	-	5/7/7/7	-
7	1PE	B	1462	-	-	6/13/13/13	-
3	PGE	A	1461	-	-	5/7/7/7	-
2	P61	D	600	-	-	0/11/19/19	0/2/2/2
4	PG4	A	1460	-	-	4/10/10/10	-
3	PGE	B	1461	-	-	5/7/7/7	-
3	PGE	C	1459	-	-	4/7/7/7	-
9	PEG	C	1462	-	-	3/4/4/4	-
3	PGE	C	1461	-	-	2/7/7/7	-
3	PGE	D	1459	-	-	5/7/7/7	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	P61	C3-C2	7.83	1.48	1.40
2	A	600	P61	C3-C2	6.94	1.47	1.40
2	B	600	P61	C3-C2	6.56	1.47	1.40
2	D	600	P61	C3-C2	6.47	1.47	1.40
2	B	600	P61	C-CA	-5.01	1.44	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	P61	C4-C3-C2	-6.93	115.90	120.19
2	A	600	P61	C4-C3-C2	-5.78	116.61	120.19
2	D	600	P61	C4-C3-C2	-5.20	116.97	120.19
2	D	600	P61	CG-CB-CA	-4.71	102.89	114.34
2	C	600	P61	C4-C3-C2	-4.50	117.40	120.19

There are no chirality outliers.
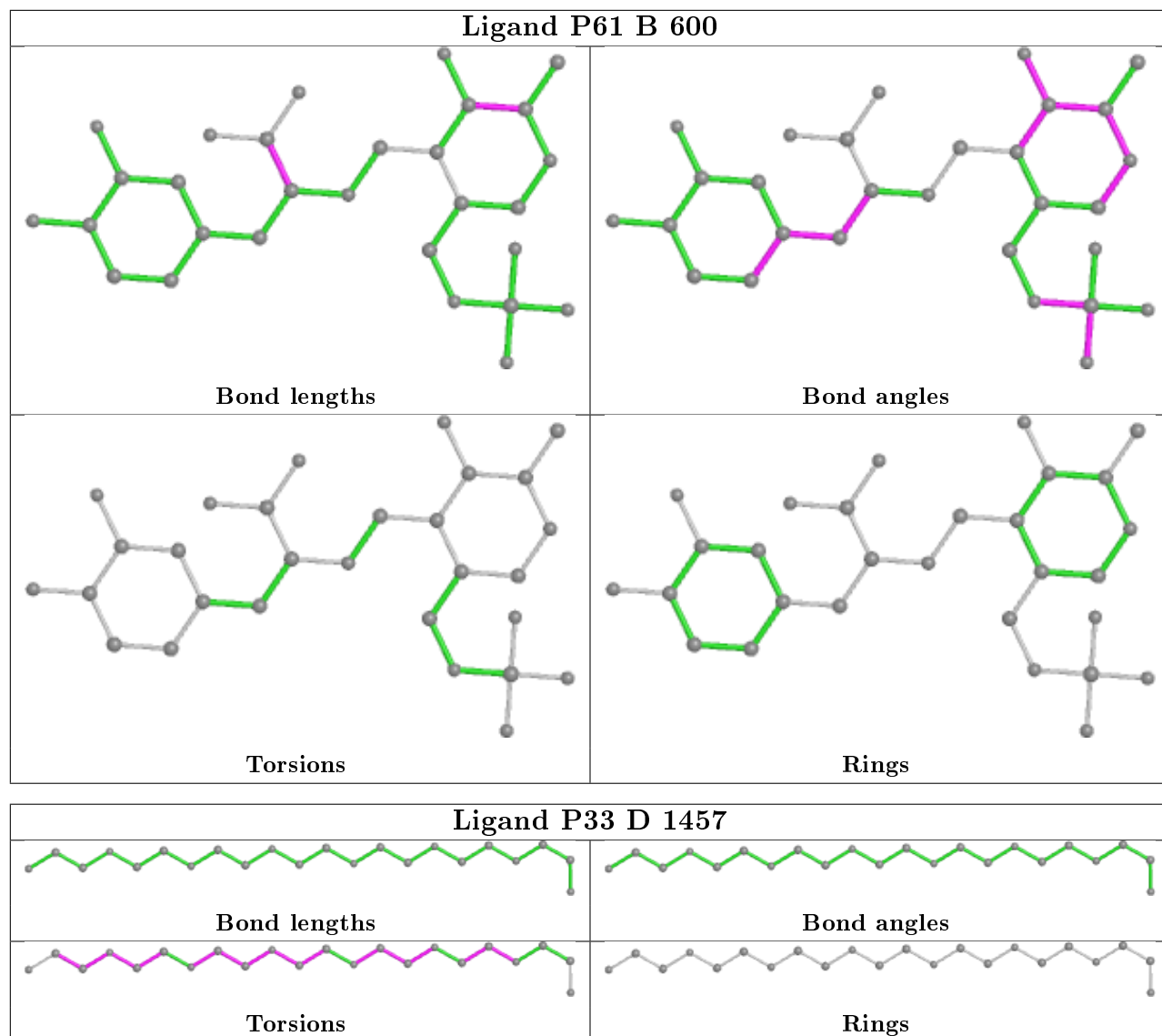
5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	1457	P33	O10-C11-C12-O13
7	B	1462	1PE	OH6-C15-C25-OH5
8	D	1457	P33	O16-C17-C18-O19
3	D	1459	PGE	O2-C3-C4-O3
8	C	1457	P33	O4-C5-C6-O7

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1457	P33	1	0
4	A	1464	PG4	1	0
9	D	1462	PEG	1	0
3	A	1457	PGE	1	0
3	A	1459	PGE	2	0
3	C	1458	PGE	1	0
8	C	1457	P33	3	0
4	B	1457	PG4	1	0
3	D	1458	PGE	1	0
3	A	1461	PGE	1	0
4	A	1460	PG4	2	0
3	B	1461	PGE	3	0
3	D	1459	PGE	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 P61 B 600

Bond lengths

Bond angles

Torsions

Rings

Ligand P33 D 1457

Bond lengths

Bond angles

Torsions

Rings

Ligand P61 C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand P61 A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand P33 C 1457

Bond lengths

Bond angles

Torsions

Rings

Ligand P61 D 600

Bond lengths

Bond angles

Torsions

Rings
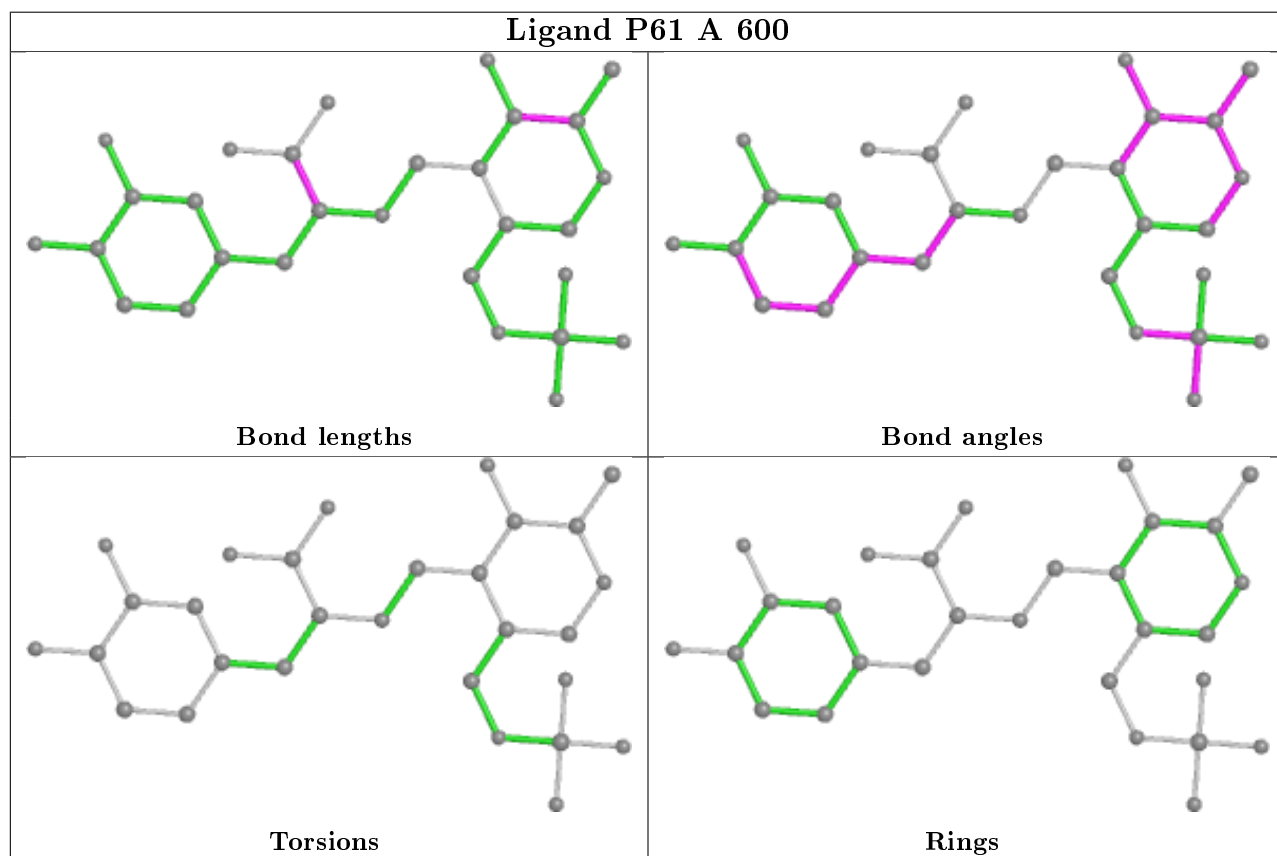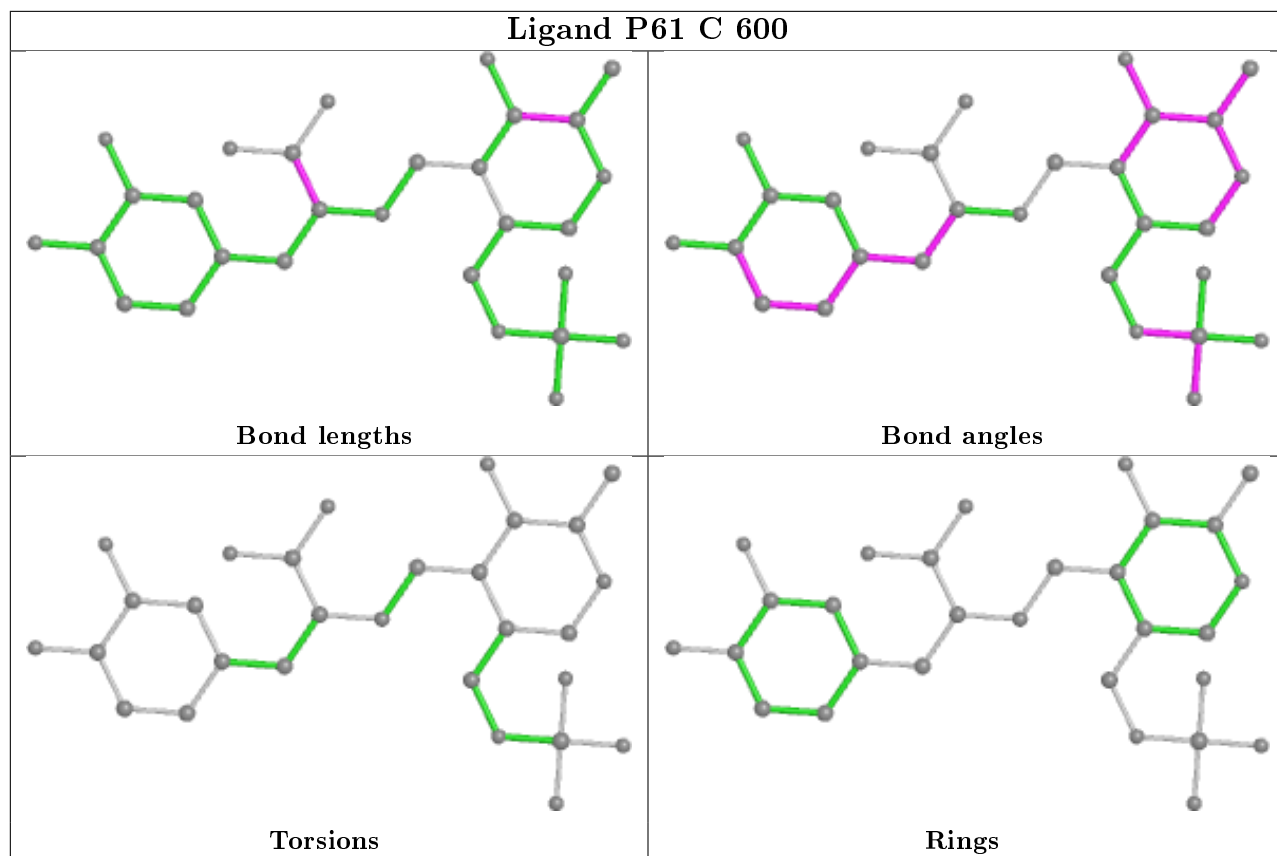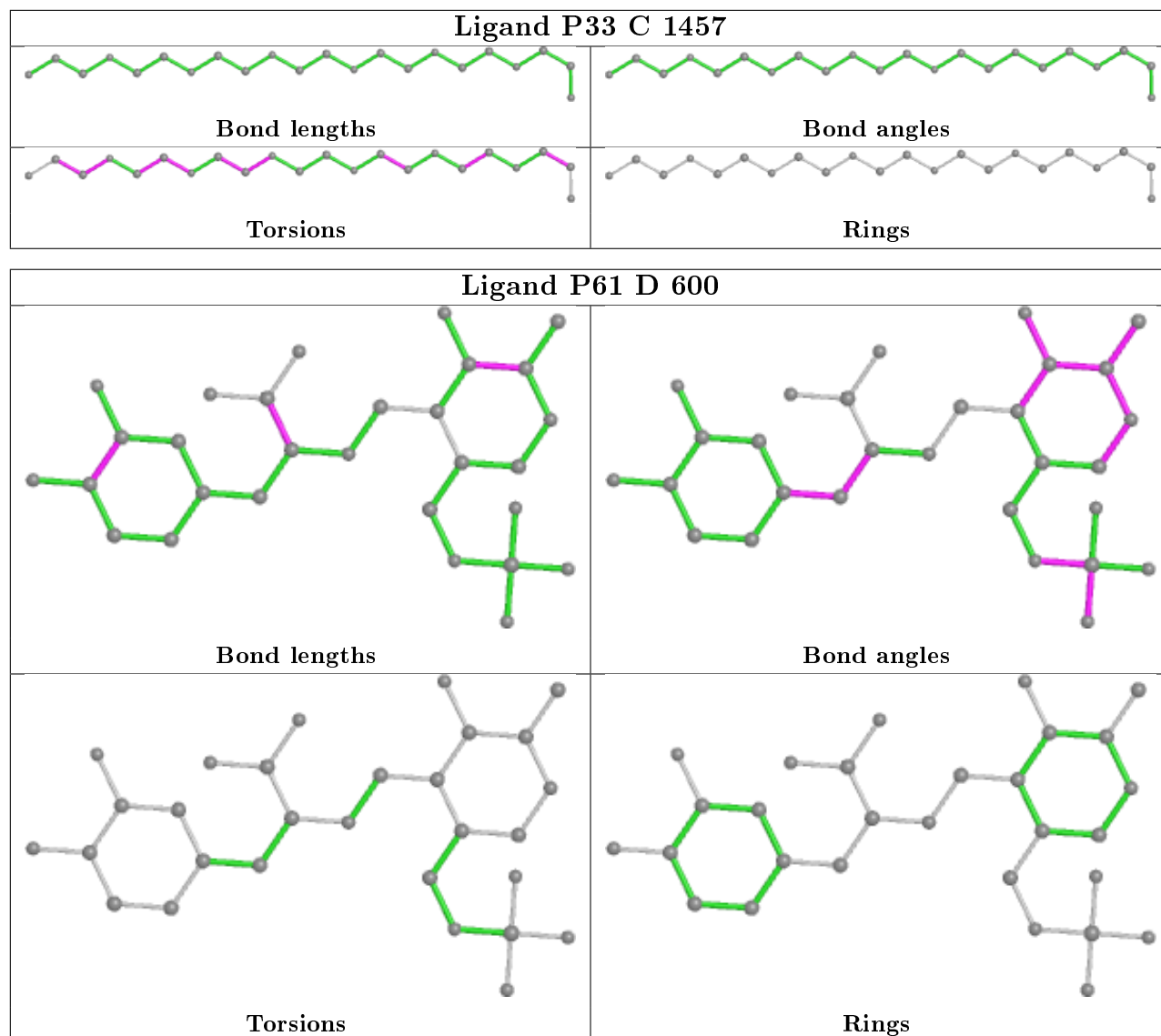
5.7 Other polymers (i)

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	456/456 (100%)	-0.40	2 (0%)	92	92	13, 20, 35, 58	0
1	B	456/456 (100%)	-0.38	4 (0%)	84	83	14, 22, 39, 59	1 (0%)
1	C	456/456 (100%)	-0.45	2 (0%)	92	92	13, 21, 36, 58	0
1	D	456/456 (100%)	-0.40	6 (1%)	77	76	14, 21, 39, 60	0
All	All	1824/1824 (100%)	-0.41	14 (0%)	86	85	13, 21, 37, 60	1 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	4.7
1	D	391	VAL	4.7
1	B	1	MET	4.4
1	A	1	MET	4.2
1	B	391	VAL	3.4

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

There are no non-standard protein/DNA/RNA residues in this entry.
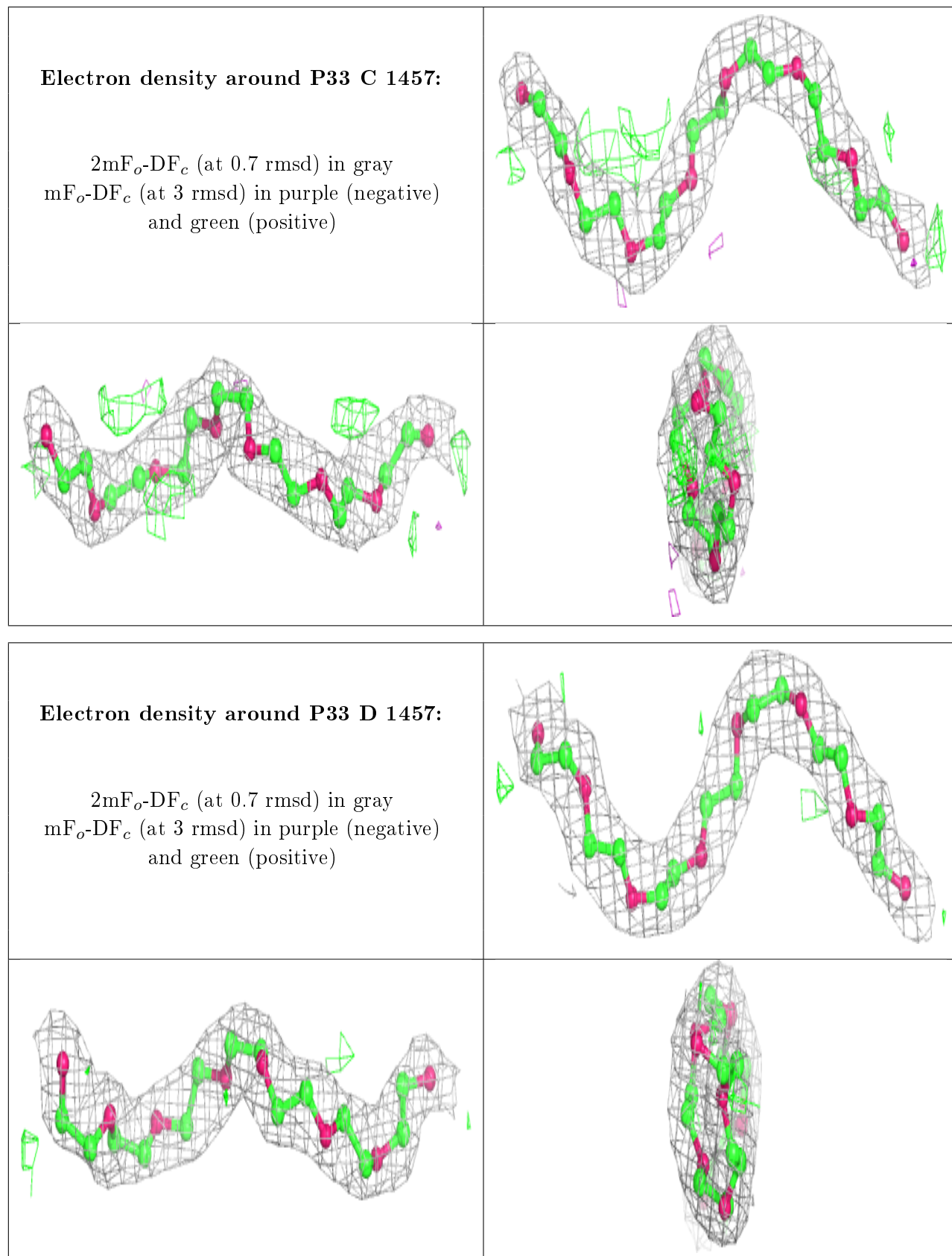
6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å²)	Q<0.9
3	PGE	A	1458	10/10	0.70	0.36	62,72,75,76	0
3	PGE	C	1459	10/10	0.72	0.18	53,65,67,69	0
3	PGE	C	1460	10/10	0.73	0.28	45,64,69,69	0
3	PGE	D	1459	10/10	0.74	0.28	55,62,66,67	0
3	PGE	B	1458	10/10	0.76	0.32	58,65,69,69	0
3	PGE	A	1457	10/10	0.78	0.25	59,64,67,68	0
3	PGE	D	1461	10/10	0.81	0.26	53,57,60,61	0
4	PG4	A	1460	13/13	0.82	0.35	49,55,65,66	0
3	PGE	D	1458	10/10	0.83	0.22	49,53,56,59	0
9	PEG	D	1462	7/7	0.83	0.19	52,54,58,61	0
4	PG4	B	1459	13/13	0.83	0.37	37,54,72,72	0
4	PG4	B	1457	13/13	0.83	0.26	58,60,63,63	0
6	EDO	B	1460	4/4	0.85	0.28	35,35,44,52	0
3	PGE	B	1461	10/10	0.85	0.24	40,48,56,56	0
4	PG4	A	1464	13/13	0.88	0.15	36,49,65,65	0
3	PGE	C	1458	10/10	0.88	0.16	45,50,56,61	0
9	PEG	C	1462	7/7	0.90	0.20	40,44,46,49	0
3	PGE	C	1461	10/10	0.90	0.31	48,50,58,58	0
4	PG4	D	1460	13/13	0.90	0.29	44,53,67,67	0
7	1PE	B	1462	16/16	0.91	0.20	27,46,57,58	0
3	PGE	A	1461	10/10	0.91	0.29	45,49,63,64	0
8	P33	C	1457	22/22	0.93	0.12	28,39,51,54	0
3	PGE	A	1459	10/10	0.94	0.12	31,38,47,49	0
8	P33	D	1457	22/22	0.95	0.10	31,38,47,52	0
2	P61	B	600	29/29	0.97	0.14	12,18,20,23	0
2	P61	A	600	29/29	0.98	0.11	13,17,21,22	0
2	P61	C	600	29/29	0.98	0.13	10,16,19,21	0
2	P61	D	600	29/29	0.98	0.12	12,15,18,19	0
5	K	A	1462	1/1	0.99	0.08	15,15,15,15	0
5	K	C	1464	1/1	1.00	0.07	16,16,16,16	0
5	K	A	1463	1/1	1.00	0.06	16,16,16,16	0
5	K	C	1463	1/1	1.00	0.06	17,17,17,17	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.
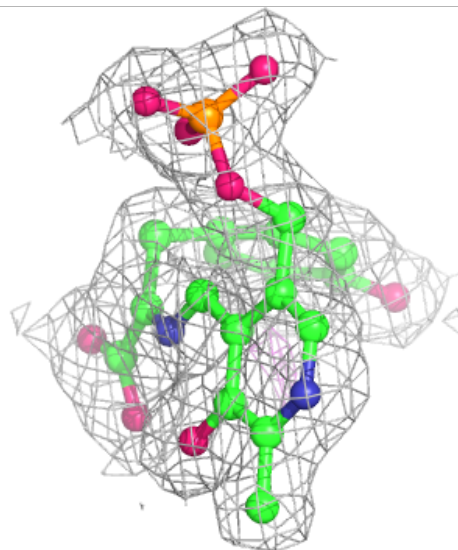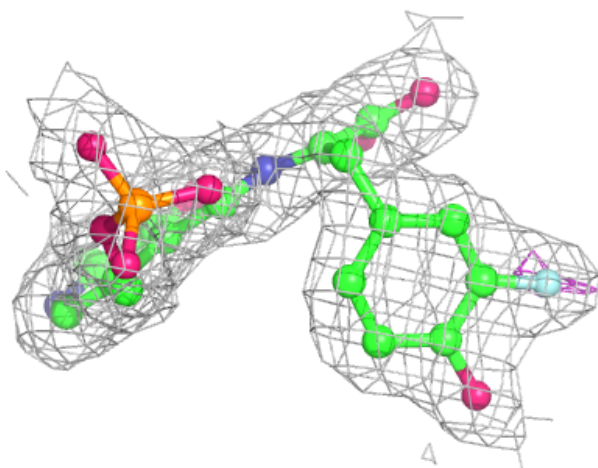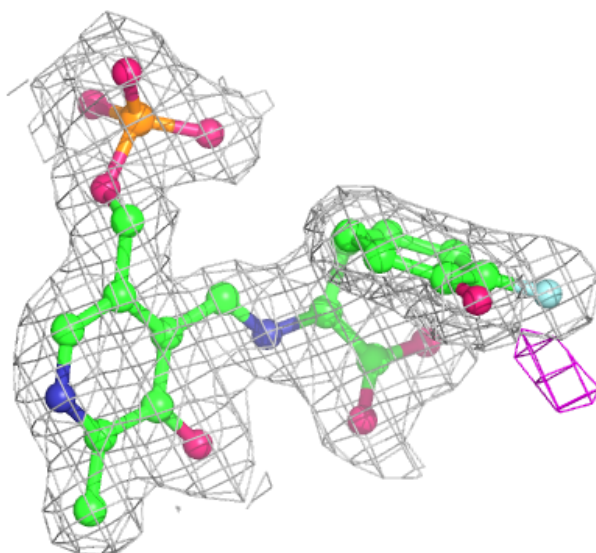
Electron density around P33 C 1457:

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 D 1457:

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 P61 B 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
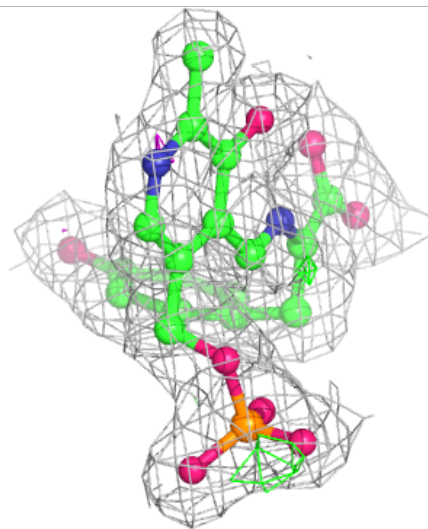mF_o-DF_c (at 3 rmsd) in purple (negative)
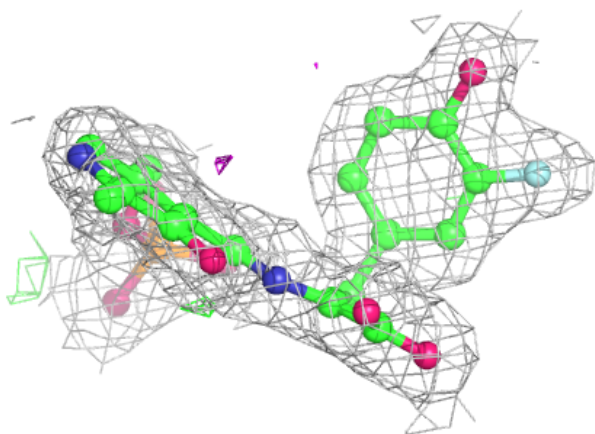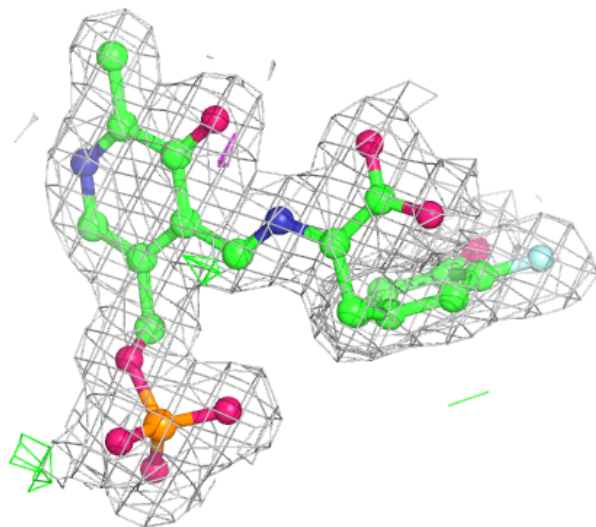and green (positive)
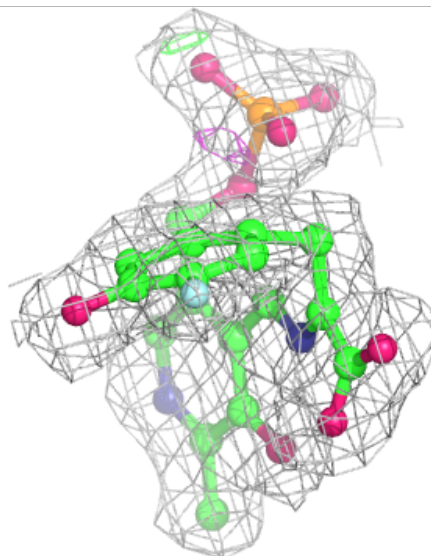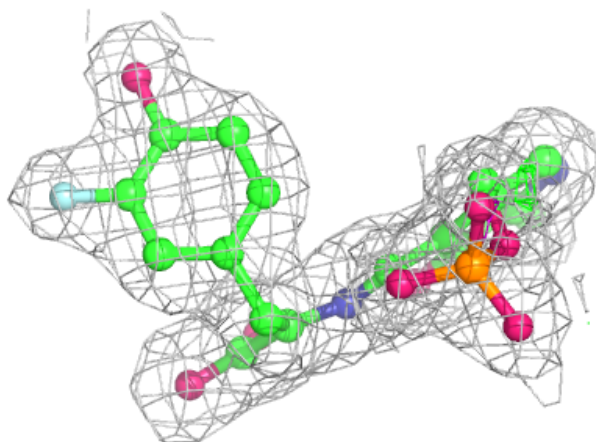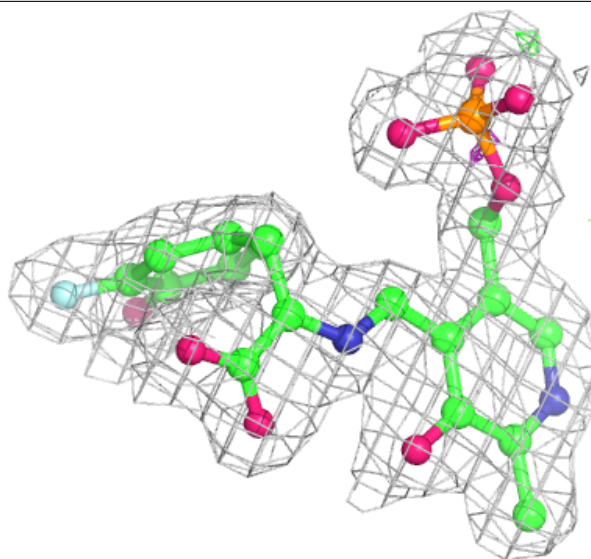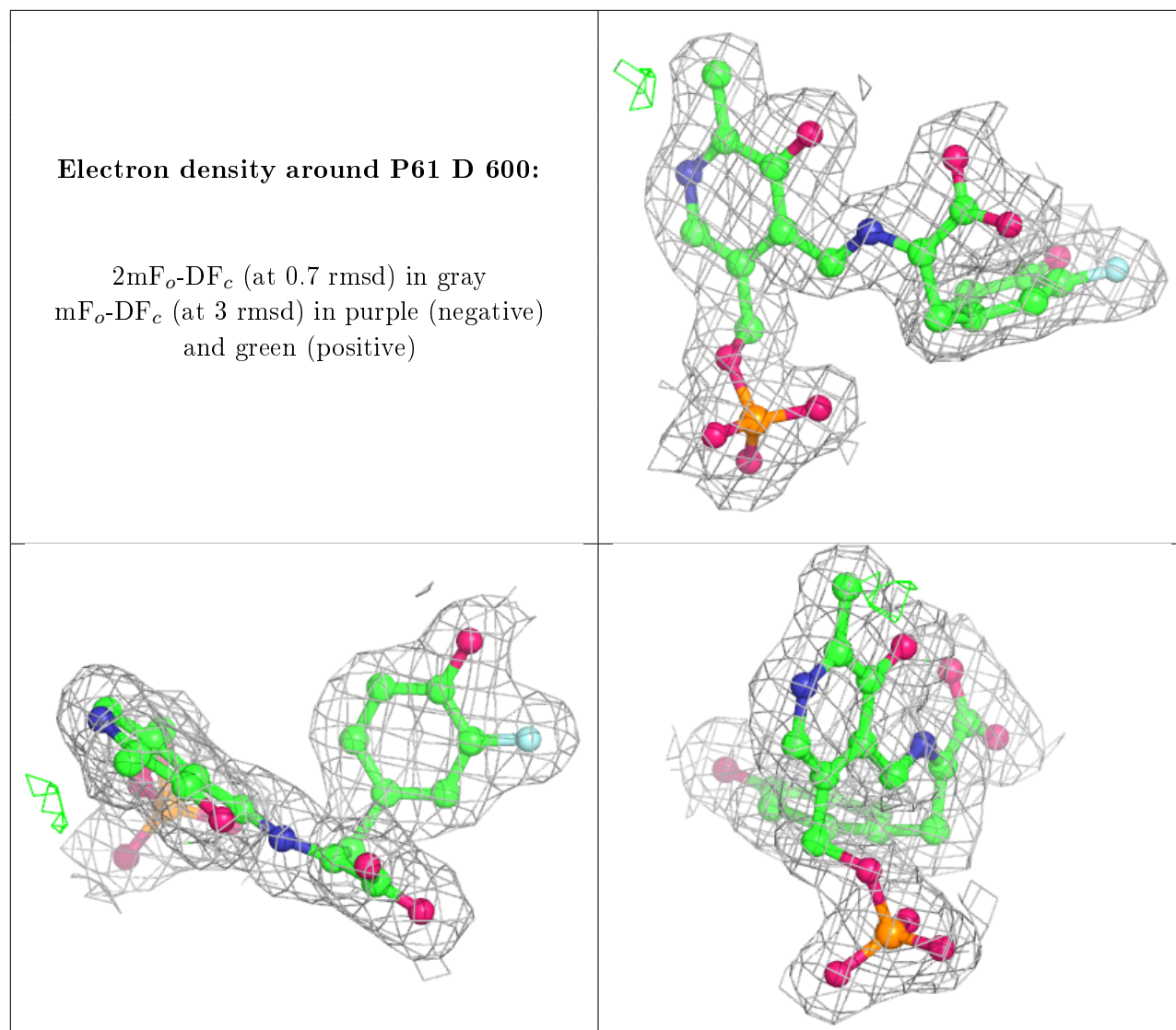
Electron density around P61 A 600:

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

Electron density around P61 C 600:

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

Electron density around P61 D 600:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.