



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:53 am BST

PDB ID : 5G09
Title : The crystal structure of a S-selective transaminase from *Bacillus megaterium* bound with R-alpha-methylbenzylamine
Authors : van Oosterwijk, N.; Willies, S.; Hekelaar, J.; Terwisscha van Scheltinga, A.C.; Turner, N.J.; Dijkstra, B.W.
Deposited on : 2016-03-17
Resolution : 1.90 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 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

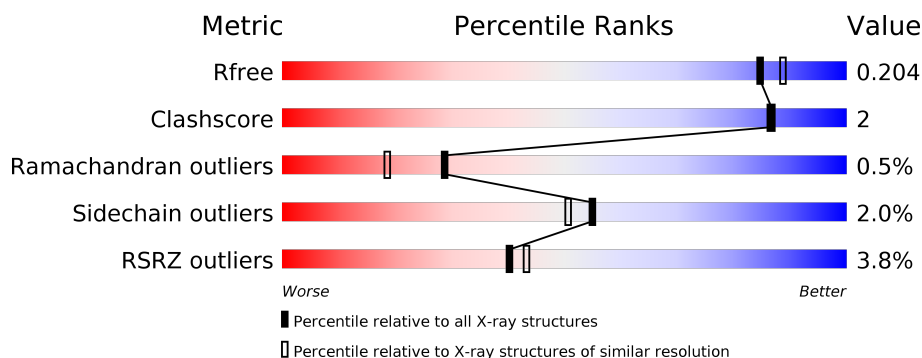
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	483	<div> <div>%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div>• •</div> </div>
1	B	483	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div></div> </div> <div>8%</div> <div>•</div> </div>
1	C	483	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div>5%</div> <div>•</div> </div>
1	D	483	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div></div> </div> <div>10%</div> <div>•</div> </div>

2 Entry composition [i](#)

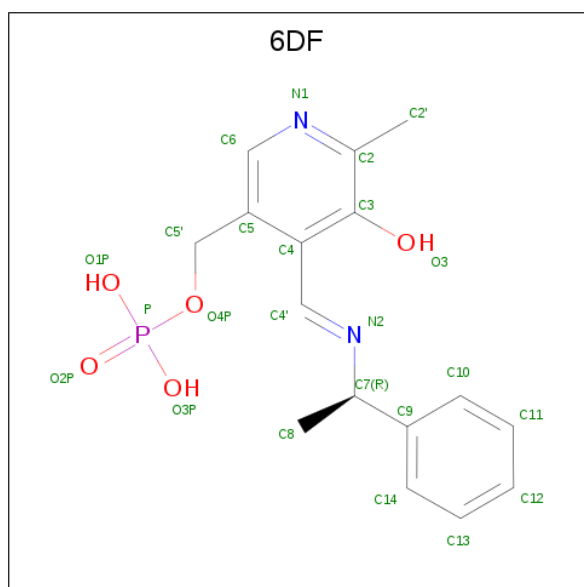
There are 7 unique types of molecules in this entry. The entry contains 15968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	1	1
			3696	2344	625	707	20			
1	B	471	Total	C	N	O	S	0	0	0
			3709	2354	626	710	19			
1	C	469	Total	C	N	O	S	0	0	1
			3688	2339	624	706	19			
1	D	473	Total	C	N	O	S	0	1	0
			3732	2367	630	715	20			

- Molecule 2 is [6-methyl-5-oxidanyl-4-[({E})-(1 {R})-1-phenylethyl]iminomethyl]pyridin-3-yl]methyl dihydrogen phosphate (three-letter code: 6DF) (formula: C₁₆H₁₉N₂O₅P).



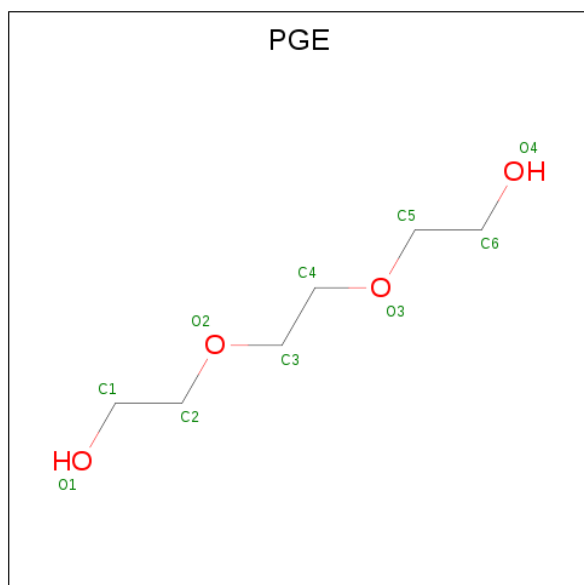
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	16	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			24	16	2	5	1		

Continued on next page...

Continued from previous page...

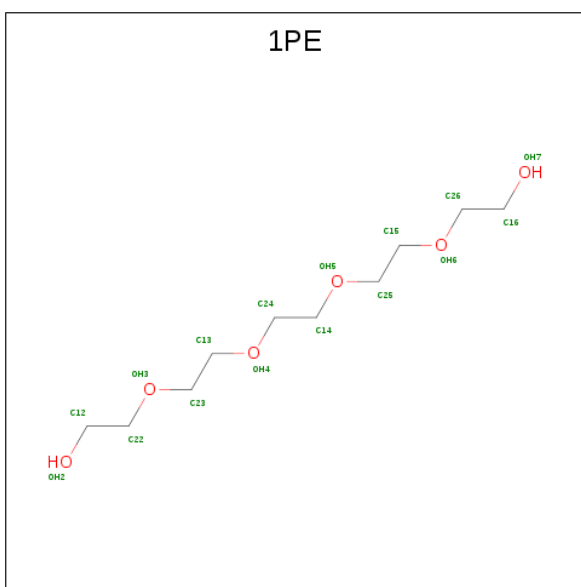
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			24	16	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			24	16	2	5	1		

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



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	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		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	8	5		
5	D	1	Total	C	O	0	0
			13	8	5		

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



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

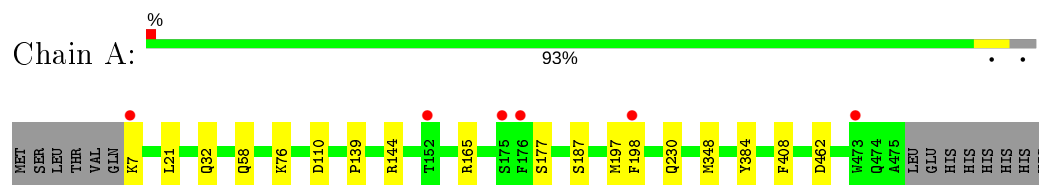
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	294	Total	O	0	0
			294	294		
7	B	210	Total	O	0	0
			210	210		
7	C	238	Total	O	0	0
			238	238		
7	D	176	Total	O	0	0
			176	176		

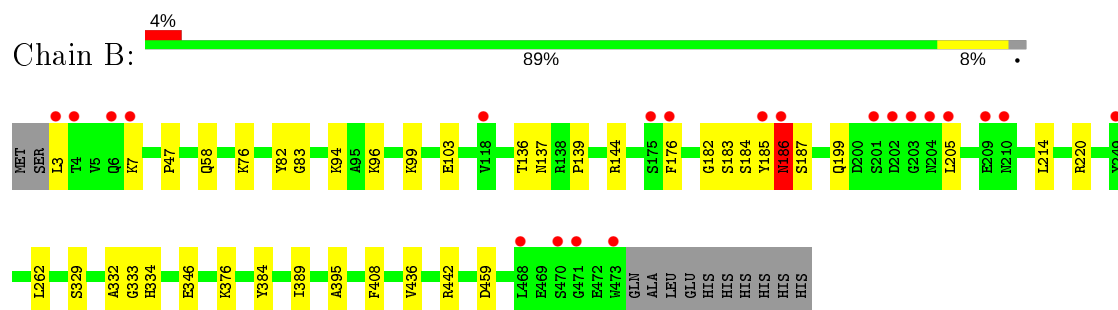
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

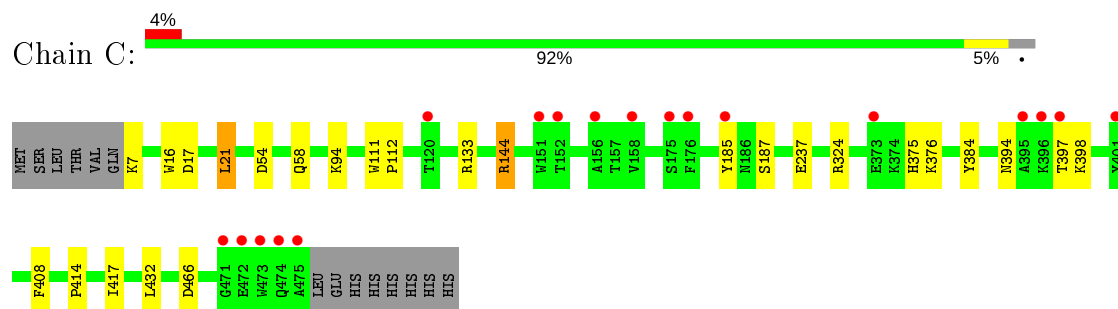
• Molecule 1: TRANSAMINASE



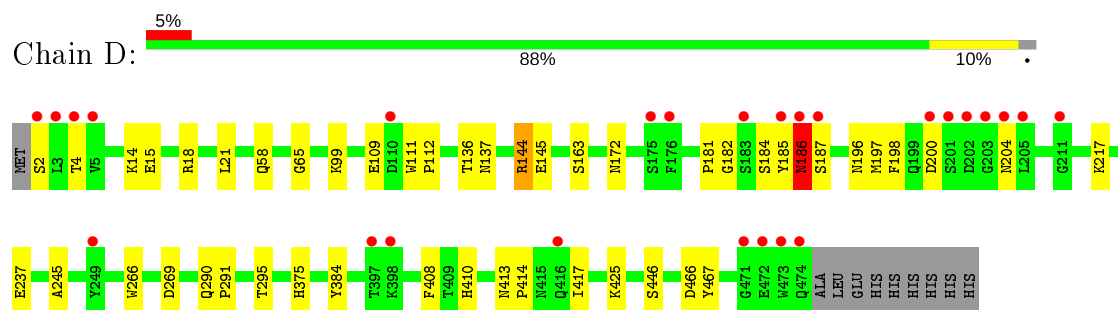
• Molecule 1: TRANSAMINASE



• Molecule 1: TRANSAMINASE



• Molecule 1: TRANSAMINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.32Å 124.59Å 126.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.46 – 1.90 44.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.46-1.90) 99.7 (44.46-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.166 , 0.203 0.167 , 0.204	Depositor DCC
R_{free} test set	7379 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15968	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PG4, PGE, 6DF, 1PE

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	0/3777	0.70	3/5116 (0.1%)
1	B	0.61	0/3790	0.70	0/5135
1	C	0.60	0/3769	0.67	1/5106 (0.0%)
1	D	0.59	0/3813	0.68	0/5165
All	All	0.61	0/15149	0.69	4/20522 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	324	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	462	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	348	MET	CG-SD-CE	-5.06	92.11	100.20

There are no chirality outliers.

There are no planarity outliers.

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	3696	0	3632	4	0
1	B	3709	0	3651	21	0
1	C	3688	0	3624	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3732	0	3672	30	0
2	A	24	0	0	0	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	0	0
3	A	30	0	42	1	0
3	B	20	0	28	3	0
3	C	30	0	42	1	0
4	A	16	0	22	0	0
5	D	26	0	36	2	0
6	D	7	0	10	1	0
7	A	294	0	0	1	0
7	B	210	0	0	3	0
7	C	238	0	0	1	0
7	D	176	0	0	1	0
All	All	15968	0	14759	62	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 2.

All (62) 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:B:185:TYR:O	1:B:186:ASN:HB2	1.52	1.09
3:A:1479:PGE:H3	7:A:2037:HOH:O	1.68	0.92
3:C:1476:PGE:H22	7:C:2104:HOH:O	1.92	0.70
1:D:185:TYR:O	1:D:186:ASN:CB	2.40	0.68
1:D:185:TYR:O	1:D:186:ASN:HB2	1.96	0.64
1:D:14:LYS:HE2	1:D:18:ARG:HH22	1.66	0.61
1:B:183:SER:HB2	7:B:2123:HOH:O	2.00	0.60
1:A:76:LYS:HG2	1:B:76:LYS:HG2	1.86	0.58
1:D:182:GLY:HA2	1:D:185:TYR:CD1	2.39	0.57
1:A:21:LEU:HD13	1:B:94:LYS:HE3	1.88	0.55
1:C:94:LYS:HE3	1:D:21:LEU:HD13	1.88	0.54
1:D:137:ASN:OD1	5:D:1480:PG4:H21	2.07	0.54
1:B:99:LYS:HE2	1:B:103:GLU:OE1	2.08	0.54
1:B:136:THR:HG22	3:B:1475:PGE:H3	1.89	0.54
1:B:220:ARG:HG3	1:B:262:LEU:HD11	1.88	0.53
1:D:2:SER:HB2	1:D:4:THR:HG22	1.89	0.53
1:A:187:SER:OG	1:D:187:SER:O	2.26	0.52
1:B:96:LYS:CE	1:B:346:GLU:OE2	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:MET:O	1:D:198:PHE:HB2	2.10	0.52
1:D:172:ASN:OD1	1:D:413:ASN:HA	2.10	0.52
1:D:414:PRO:HA	1:D:417:ILE:HD12	1.93	0.51
1:C:414:PRO:HA	1:C:417:ILE:HD12	1.92	0.51
1:B:187:SER:O	1:C:187:SER:OG	2.27	0.51
1:C:17:ASP:HA	1:C:21:LEU:HD22	1.93	0.50
1:B:47:PRO:HD2	7:B:2034:HOH:O	2.12	0.49
1:C:375:HIS:HE1	1:C:466:ASP:OD1	1.94	0.49
1:B:182:GLY:HA2	1:B:185:TYR:CD1	2.48	0.48
3:B:1475:PGE:H52	7:B:2090:HOH:O	2.14	0.48
1:B:436:VAL:CG1	3:B:1476:PGE:H12	2.45	0.47
1:A:198:PHE:CE1	1:D:217:LYS:HD3	2.49	0.47
1:D:136:THR:HG22	6:D:1477:PEG:H21	1.97	0.47
1:B:389:ILE:HG23	1:B:442:ARG:NH1	2.30	0.47
1:D:425:LYS:HE2	1:D:467:TYR:CG	2.50	0.47
1:D:65:GLY:HA2	1:D:446:SER:OG	2.16	0.46
1:D:269:ASP:HA	1:D:295:THR:OG1	2.16	0.46
1:D:111:TRP:CD1	1:D:112:PRO:HD3	2.51	0.46
1:B:376:LYS:HB2	1:B:395:ALA:HB1	1.99	0.45
1:C:111:TRP:CD1	1:C:112:PRO:HD3	2.52	0.45
1:C:133:ARG:HB3	1:D:181:PRO:HD2	2.00	0.44
1:D:144:ARG:NH2	1:D:237:GLU:H	2.16	0.43
1:B:182:GLY:HA2	1:B:185:TYR:CE1	2.54	0.43
1:C:16:TRP:CE2	1:D:99:LYS:HG3	2.53	0.43
1:C:54:ASP:HA	1:C:432:LEU:HB2	2.00	0.43
1:C:144:ARG:NH2	1:C:237:GLU:H	2.18	0.42
1:B:199:GLN:HB3	1:B:205:LEU:HD13	2.02	0.42
1:D:111:TRP:CD1	1:D:290:GLN:HB3	2.55	0.42
1:C:394:ASN:HB3	1:C:397:THR:OG1	2.20	0.41
1:D:425:LYS:HE2	1:D:467:TYR:CD1	2.55	0.41
1:B:137:ASN:OD1	5:D:1480:PG4:H62	2.20	0.41
1:D:375:HIS:HE1	1:D:466:ASP:OD1	2.03	0.41
1:D:266:TRP:CE3	1:D:291:PRO:HA	2.56	0.41
1:D:145:GLU:OE1	7:D:2069:HOH:O	2.22	0.41
1:D:196:ASN:HD22	1:D:245:ALA:HB1	1.86	0.41
1:B:329:SER:HB3	1:B:332:ALA:HB2	2.02	0.40
1:B:82:TYR:HA	1:B:83:GLY:HA3	1.85	0.40
1:B:185:TYR:O	1:B:186:ASN:CB	2.38	0.40
1:B:333:GLY:O	1:B:334:HIS:C	2.60	0.40
1:D:197:MET:O	1:D:198:PHE:CB	2.68	0.40
1:D:109:GLU:HG2	1:D:290:GLN:NE2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:SER:HB2	1:D:410:HIS:CE1	2.57	0.40
1:C:111:TRP:N	1:C:112:PRO:CD	2.85	0.40
1:C:185:TYR:O	1:D:186:ASN:OD1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/483 (97%)	452 (97%)	12 (3%)	4 (1%)	17	7
1	B	469/483 (97%)	446 (95%)	20 (4%)	3 (1%)	25	15
1	C	467/483 (97%)	447 (96%)	19 (4%)	1 (0%)	47	38
1	D	472/483 (98%)	447 (95%)	23 (5%)	2 (0%)	34	24
All	All	1876/1932 (97%)	1792 (96%)	74 (4%)	10 (0%)	29	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	MET
1	D	186	ASN
1	B	58	GLN
1	A	58	GLN
1	B	186	ASN
1	C	58	GLN
1	D	58	GLN
1	A	177	SER
1	A	139	PRO
1	B	139	PRO

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	395/408 (97%)	388 (98%)	7 (2%)	59	55
1	B	397/408 (97%)	387 (98%)	10 (2%)	47	41
1	C	394/408 (97%)	387 (98%)	7 (2%)	59	55
1	D	400/408 (98%)	392 (98%)	8 (2%)	55	51
All	All	1586/1632 (97%)	1554 (98%)	32 (2%)	55	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	32	GLN
1	A	110	ASP
1	A	144	ARG
1	A	230	GLN
1	A	384	TYR
1	A	408	PHE
1	B	3	LEU
1	B	7	LYS
1	B	144	ARG
1	B	176	PHE
1	B	184	SER
1	B	186	ASN
1	B	214	LEU
1	B	384	TYR
1	B	408	PHE
1	B	459	ASP
1	C	7	LYS
1	C	21	LEU
1	C	144	ARG
1	C	376	LYS
1	C	384	TYR
1	C	398	LYS
1	C	408	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	15	GLU
1	D	144	ARG
1	D	184	SER
1	D	186	ASN
1	D	200	ASP
1	D	204	ASN
1	D	384	TYR
1	D	408	PHE

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

Mol	Chain	Res	Type
1	A	268	ASN
1	C	268	ASN
1	D	268	ASN
1	D	290	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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGE	B	1476	-	9,9,9	0.41	0	8,8,8	0.83	0
3	PGE	A	1477	-	9,9,9	0.46	0	8,8,8	0.46	0
3	PGE	B	1475	-	9,9,9	0.32	0	8,8,8	0.44	0
6	PEG	D	1477	-	6,6,6	0.45	0	5,5,5	0.26	0
3	PGE	C	1477	-	9,9,9	0.43	0	8,8,8	0.32	0
4	1PE	A	1478	-	15,15,15	0.54	0	14,14,14	0.36	0
2	6DF	D	1476	-	25,25,25	0.83	0	33,35,35	1.82	5 (15%)
3	PGE	C	1480	-	9,9,9	0.53	0	8,8,8	0.41	0
2	6DF	A	1475	-	25,25,25	1.04	2 (8%)	33,35,35	1.73	3 (9%)
3	PGE	A	1479	-	9,9,9	0.58	0	8,8,8	0.47	0
2	6DF	B	1474	-	25,25,25	1.08	1 (4%)	33,35,35	1.82	4 (12%)
5	PG4	D	1475	-	12,12,12	0.58	0	11,11,11	0.41	0
5	PG4	D	1480	-	12,12,12	0.50	0	11,11,11	0.58	0
3	PGE	A	1476	-	9,9,9	0.33	0	8,8,8	0.60	0
3	PGE	C	1476	-	9,9,9	0.41	0	8,8,8	0.41	0
2	6DF	C	1475	-	25,25,25	1.01	1 (4%)	33,35,35	1.84	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	B	1476	-	-	3/7/7/7	-
3	PGE	A	1477	-	-	4/7/7/7	-
3	PGE	B	1475	-	-	5/7/7/7	-
6	PEG	D	1477	-	-	2/4/4/4	-
3	PGE	C	1477	-	-	2/7/7/7	-
4	1PE	A	1478	-	-	4/13/13/13	-
2	6DF	D	1476	-	-	2/15/15/15	0/2/2/2
3	PGE	C	1480	-	-	1/7/7/7	-
2	6DF	A	1475	-	-	2/15/15/15	0/2/2/2
3	PGE	A	1479	-	-	4/7/7/7	-
2	6DF	B	1474	-	-	2/15/15/15	0/2/2/2
5	PG4	D	1475	-	-	3/10/10/10	-
5	PG4	D	1480	-	-	7/10/10/10	-
3	PGE	A	1476	-	-	1/7/7/7	-
3	PGE	C	1476	-	-	6/7/7/7	-
2	6DF	C	1475	-	-	3/15/15/15	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1475	6DF	C3-C2	-2.89	1.38	1.40
2	B	1474	6DF	C4-C5	-2.50	1.38	1.42
2	A	1475	6DF	C4-C4'	2.13	1.50	1.46
2	A	1475	6DF	C3-C2	-2.04	1.38	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1474	6DF	C7-N2-C4'	7.55	131.23	118.00
2	D	1476	6DF	C7-N2-C4'	7.02	130.30	118.00
2	A	1475	6DF	C7-N2-C4'	6.96	130.20	118.00
2	C	1475	6DF	C7-N2-C4'	6.90	130.10	118.00
2	C	1475	6DF	C8-C7-N2	4.32	116.77	108.54
2	A	1475	6DF	C8-C7-N2	4.03	116.22	108.54
2	B	1474	6DF	C8-C7-N2	3.95	116.06	108.54
2	C	1475	6DF	C5-C6-N1	-3.19	118.50	123.82
2	D	1476	6DF	C8-C7-N2	3.18	114.60	108.54
2	B	1474	6DF	C9-C7-N2	3.10	115.63	109.58
2	D	1476	6DF	C9-C7-N2	2.81	115.06	109.58
2	D	1476	6DF	C2'-C2-C3	2.73	124.26	120.89
2	A	1475	6DF	C9-C7-N2	2.57	114.60	109.58
2	C	1475	6DF	C6-N1-C2	2.53	123.86	119.17
2	B	1474	6DF	C4-C3-C2	2.48	121.72	120.19
2	C	1475	6DF	C9-C7-N2	2.37	114.21	109.58
2	D	1476	6DF	C4-C4'-N2	-2.28	117.94	123.01
2	C	1475	6DF	C14-C9-C10	2.03	120.82	118.29

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1476	6DF	C8-C7-N2-C4'
2	A	1475	6DF	C8-C7-N2-C4'
2	B	1474	6DF	C8-C7-N2-C4'
2	C	1475	6DF	C8-C7-N2-C4'
3	A	1479	PGE	O2-C3-C4-O3
5	D	1475	PG4	O1-C1-C2-O2
3	B	1475	PGE	O2-C3-C4-O3
3	C	1477	PGE	O2-C3-C4-O3
3	C	1476	PGE	O3-C5-C6-O4
3	C	1480	PGE	O3-C5-C6-O4

Continued on next page...

Continued from previous page...

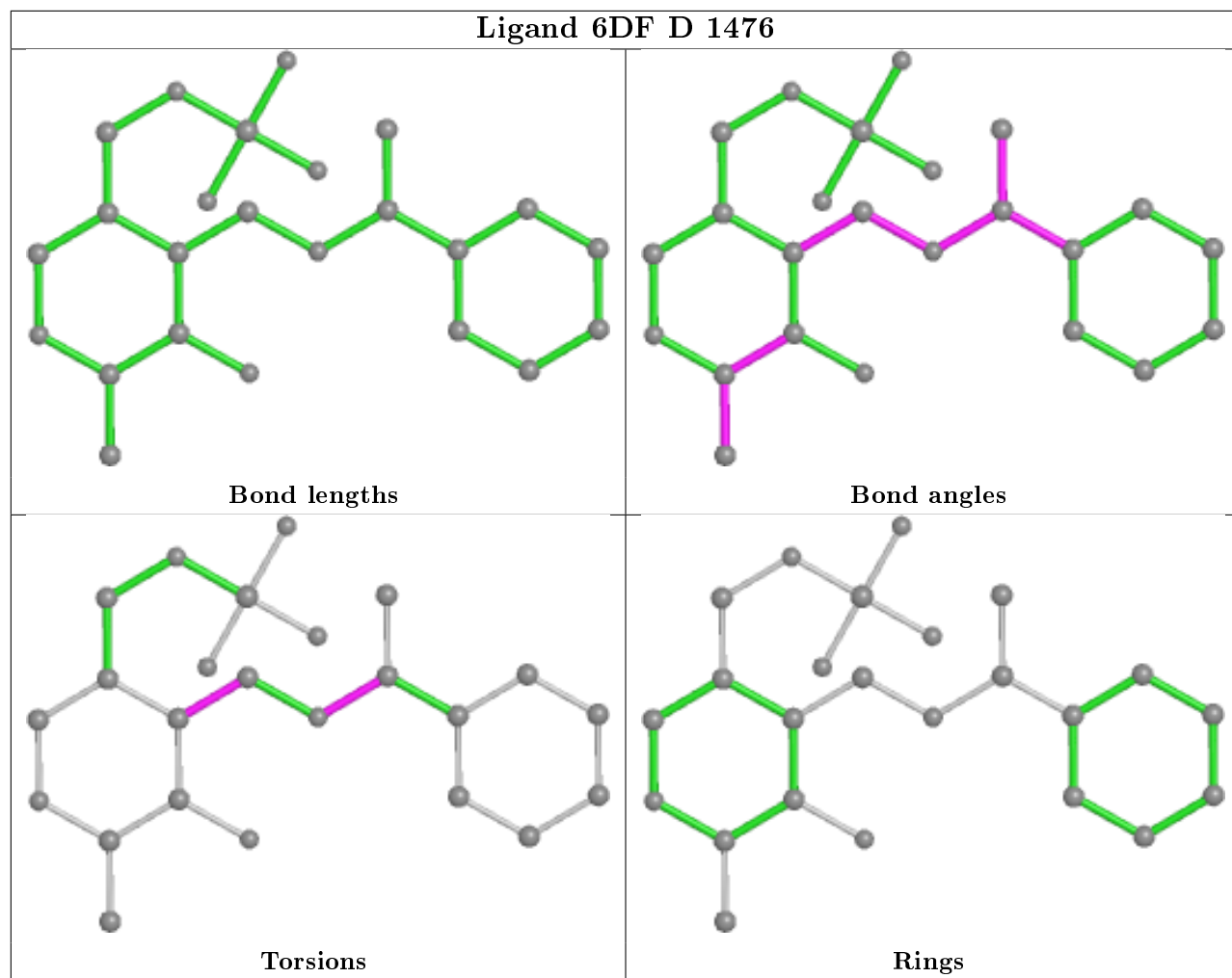
Mol	Chain	Res	Type	Atoms
5	D	1480	PG4	O3-C5-C6-O4
5	D	1480	PG4	O4-C7-C8-O5
3	C	1476	PGE	O2-C3-C4-O3
5	D	1475	PG4	O4-C7-C8-O5
3	C	1476	PGE	O1-C1-C2-O2
2	B	1474	6DF	C9-C7-N2-C4'
5	D	1480	PG4	O2-C3-C4-O3
3	B	1475	PGE	O3-C5-C6-O4
3	A	1479	PGE	C3-C4-O3-C5
4	A	1478	1PE	C13-C23-OH3-C22
3	B	1475	PGE	C3-C4-O3-C5
3	A	1477	PGE	C4-C3-O2-C2
4	A	1478	1PE	OH6-C15-C25-OH5
3	A	1476	PGE	C6-C5-O3-C4
3	A	1477	PGE	C3-C4-O3-C5
3	B	1475	PGE	C1-C2-O2-C3
3	C	1476	PGE	C6-C5-O3-C4
3	A	1477	PGE	C6-C5-O3-C4
3	A	1479	PGE	O1-C1-C2-O2
6	D	1477	PEG	O1-C1-C2-O2
2	A	1475	6DF	C9-C7-N2-C4'
2	C	1475	6DF	C9-C7-N2-C4'
4	A	1478	1PE	OH4-C13-C23-OH3
2	D	1476	6DF	C3-C4-C4'-N2
3	B	1475	PGE	O1-C1-C2-O2
5	D	1480	PG4	O1-C1-C2-O2
3	B	1476	PGE	C1-C2-O2-C3
3	C	1476	PGE	C3-C4-O3-C5
3	A	1479	PGE	O3-C5-C6-O4
3	C	1477	PGE	C6-C5-O3-C4
5	D	1480	PG4	C6-C5-O3-C4
4	A	1478	1PE	OH7-C16-C26-OH6
5	D	1480	PG4	C8-C7-O4-C6
3	B	1476	PGE	C4-C3-O2-C2
2	C	1475	6DF	C3-C4-C4'-N2
3	B	1476	PGE	O1-C1-C2-O2
3	C	1476	PGE	C4-C3-O2-C2
6	D	1477	PEG	O2-C3-C4-O4
5	D	1480	PG4	C1-C2-O2-C3
5	D	1475	PG4	C1-C2-O2-C3
3	A	1477	PGE	O2-C3-C4-O3

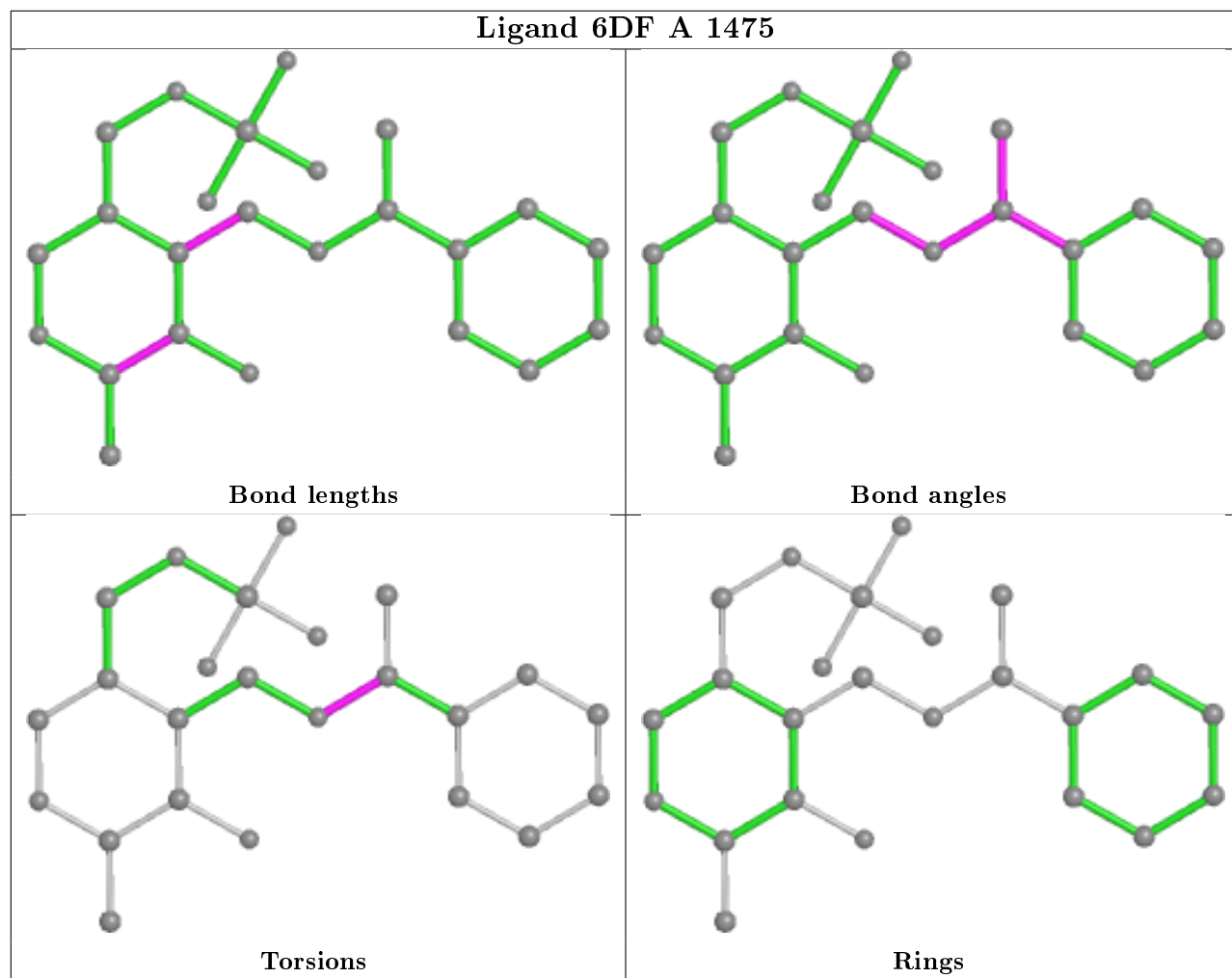
There are no ring outliers.

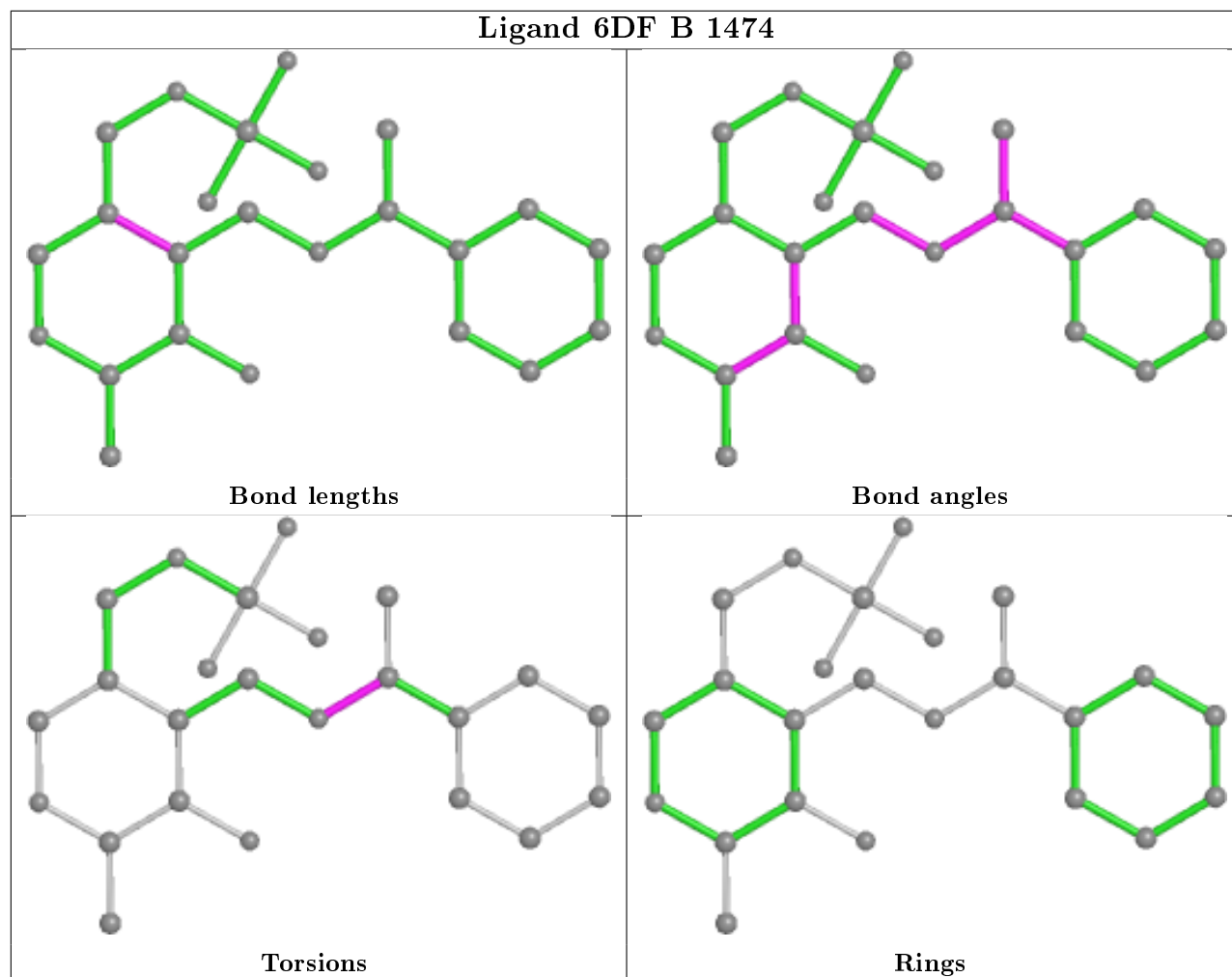
6 monomers are involved in 8 short contacts:

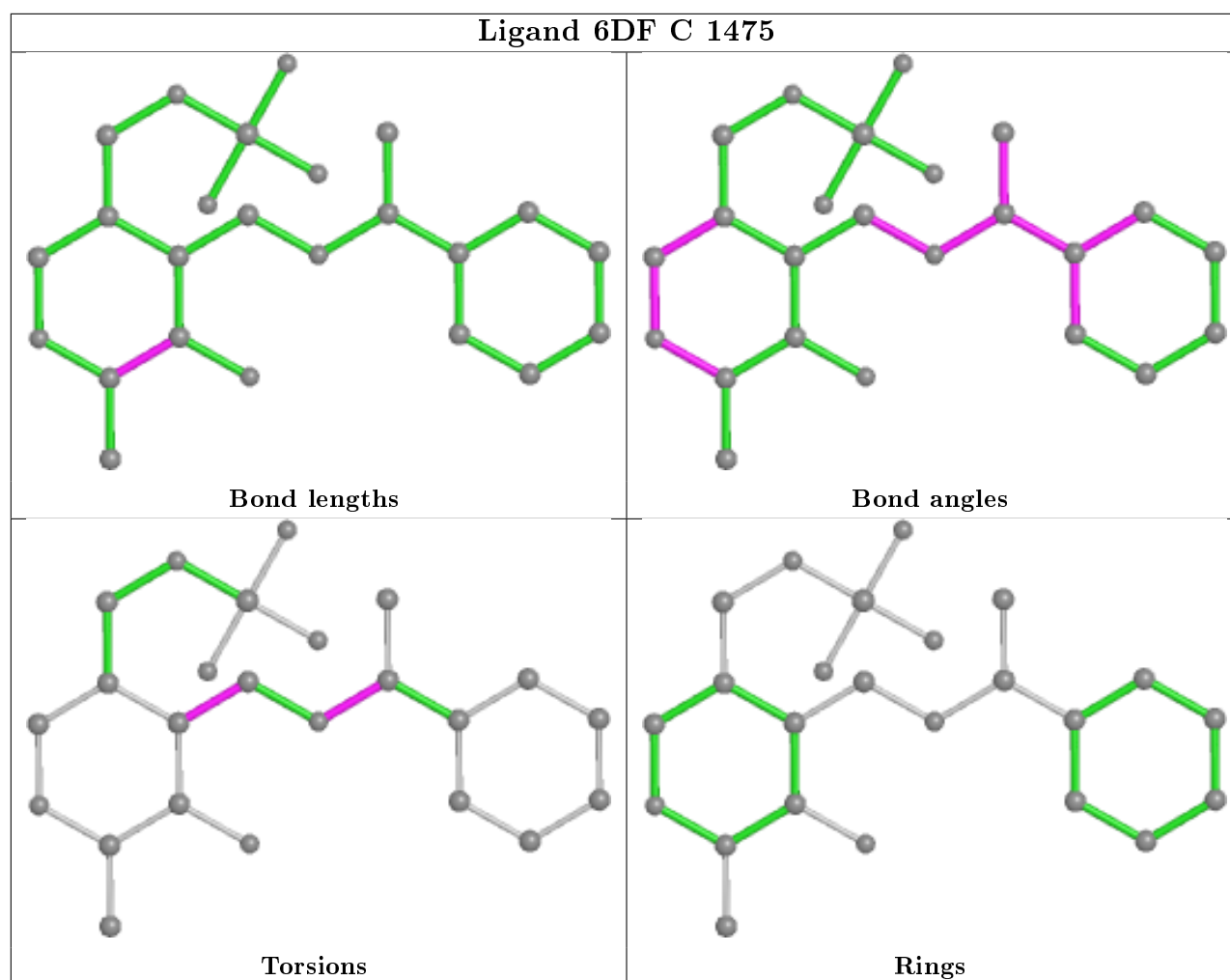
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1476	PGE	1	0
3	B	1475	PGE	2	0
6	D	1477	PEG	1	0
3	A	1479	PGE	1	0
5	D	1480	PG4	2	0
3	C	1476	PGE	1	0

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 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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	469/483 (97%)	-0.23	6 (1%) 77 79	11, 19, 36, 64	0
1	B	471/483 (97%)	0.00	21 (4%) 33 36	12, 21, 50, 88	0
1	C	469/483 (97%)	0.01	18 (3%) 40 43	13, 23, 45, 81	0
1	D	473/483 (97%)	0.06	26 (5%) 25 28	13, 23, 47, 86	0
All	All	1882/1932 (97%)	-0.04	71 (3%) 40 43	11, 22, 45, 88	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	LEU	8.0
1	D	201	SER	7.0
1	B	176	PHE	6.3
1	A	175	SER	5.7
1	D	2	SER	5.0
1	C	475	ALA	4.9
1	A	176	PHE	4.8
1	B	3	LEU	4.8
1	C	176	PHE	4.6
1	D	202	ASP	4.5
1	D	473	TRP	4.4
1	D	203	GLY	4.1
1	D	4	THR	4.1
1	C	471	GLY	4.1
1	C	473	TRP	3.9
1	D	176	PHE	3.7
1	B	202	ASP	3.6
1	B	210	ASN	3.5
1	D	204	ASN	3.5
1	B	203	GLY	3.4
1	C	474	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	175	SER	3.2
1	D	471	GLY	3.0
1	C	175	SER	3.0
1	B	471	GLY	3.0
1	B	201	SER	3.0
1	C	396	LYS	2.9
1	B	205	LEU	2.8
1	B	209	GLU	2.8
1	D	200	ASP	2.8
1	C	185	TYR	2.7
1	B	473	TRP	2.7
1	B	186	ASN	2.7
1	D	416	GLN	2.6
1	B	7	LYS	2.6
1	B	4	THR	2.6
1	D	249	TYR	2.5
1	C	151	TRP	2.5
1	A	198	PHE	2.5
1	B	470	SER	2.5
1	D	5	VAL	2.5
1	D	183	SER	2.4
1	D	186	ASN	2.4
1	C	397	THR	2.4
1	D	398	LYS	2.3
1	B	6	GLN	2.3
1	D	205	LEU	2.3
1	C	156	ALA	2.3
1	A	152	THR	2.3
1	C	373	GLU	2.3
1	C	120	THR	2.3
1	C	395	ALA	2.2
1	C	152	THR	2.2
1	C	401	TYR	2.2
1	B	468	LEU	2.2
1	B	204	ASN	2.2
1	A	7	LYS	2.1
1	D	110	ASP	2.1
1	D	211	GLY	2.1
1	D	185	TYR	2.1
1	D	175	SER	2.1
1	C	472	GLU	2.1
1	B	249	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	118	VAL	2.1
1	D	472	GLU	2.1
1	B	185	TYR	2.0
1	C	158	VAL	2.0
1	A	473	TRP	2.0
1	D	474	GLN	2.0
1	D	187	SER	2.0
1	D	397	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	PGE	A	1479	10/10	0.85	0.14	32,36,42,43	0
3	PGE	C	1476	10/10	0.87	0.19	36,39,43,46	0
3	PGE	B	1476	10/10	0.88	0.15	33,38,42,48	0
5	PG4	D	1475	13/13	0.88	0.14	37,40,46,46	0
3	PGE	B	1475	10/10	0.88	0.16	37,41,43,44	0
5	PG4	D	1480	13/13	0.89	0.16	38,44,48,48	0
3	PGE	A	1477	10/10	0.89	0.17	42,45,46,50	0
3	PGE	C	1480	10/10	0.89	0.20	46,48,50,50	0
4	1PE	A	1478	16/16	0.93	0.20	36,40,43,44	0
6	PEG	D	1477	7/7	0.93	0.15	35,36,40,41	0
3	PGE	A	1476	10/10	0.93	0.15	41,42,45,45	0
3	PGE	C	1477	10/10	0.96	0.10	30,34,35,38	0
2	6DF	B	1474	24/24	0.97	0.13	13,17,34,36	0
2	6DF	A	1475	24/24	0.98	0.14	12,16,28,30	0
2	6DF	D	1476	24/24	0.98	0.15	15,18,32,33	0

Continued on next page...

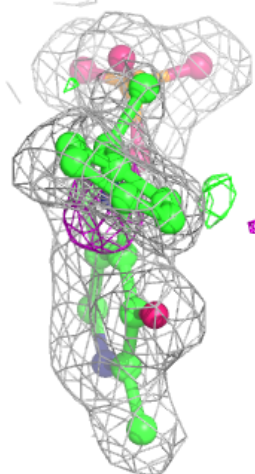
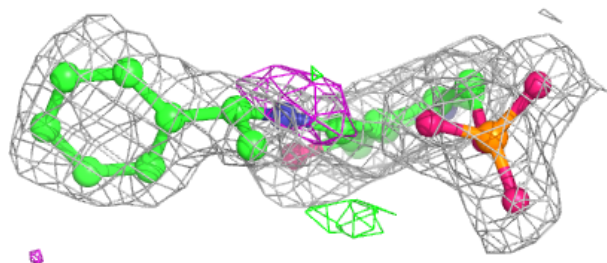
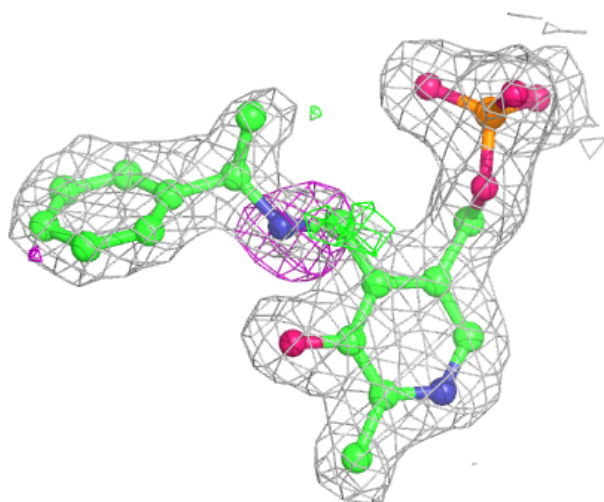
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	6DF	C	1475	24/24	0.98	0.16	15,17,32,33	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.

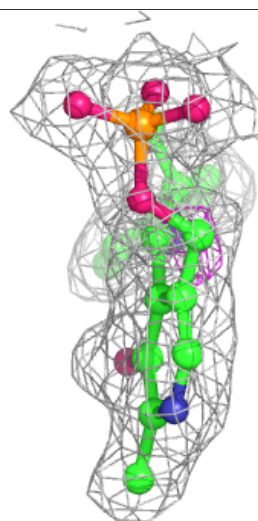
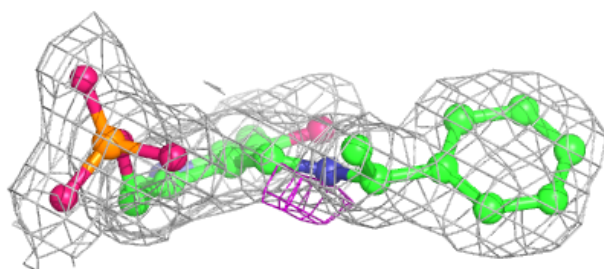
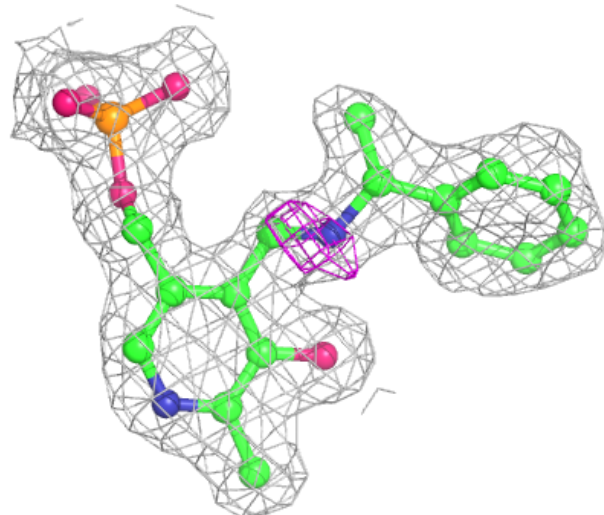
Electron density around 6DF B 1474:

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



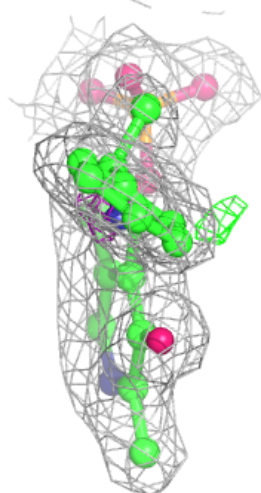
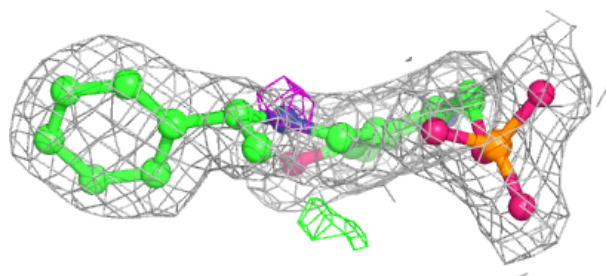
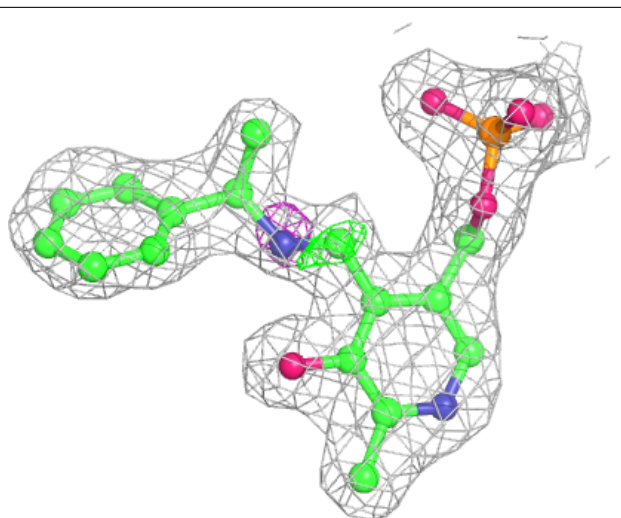
Electron density around 6DF A 1475:

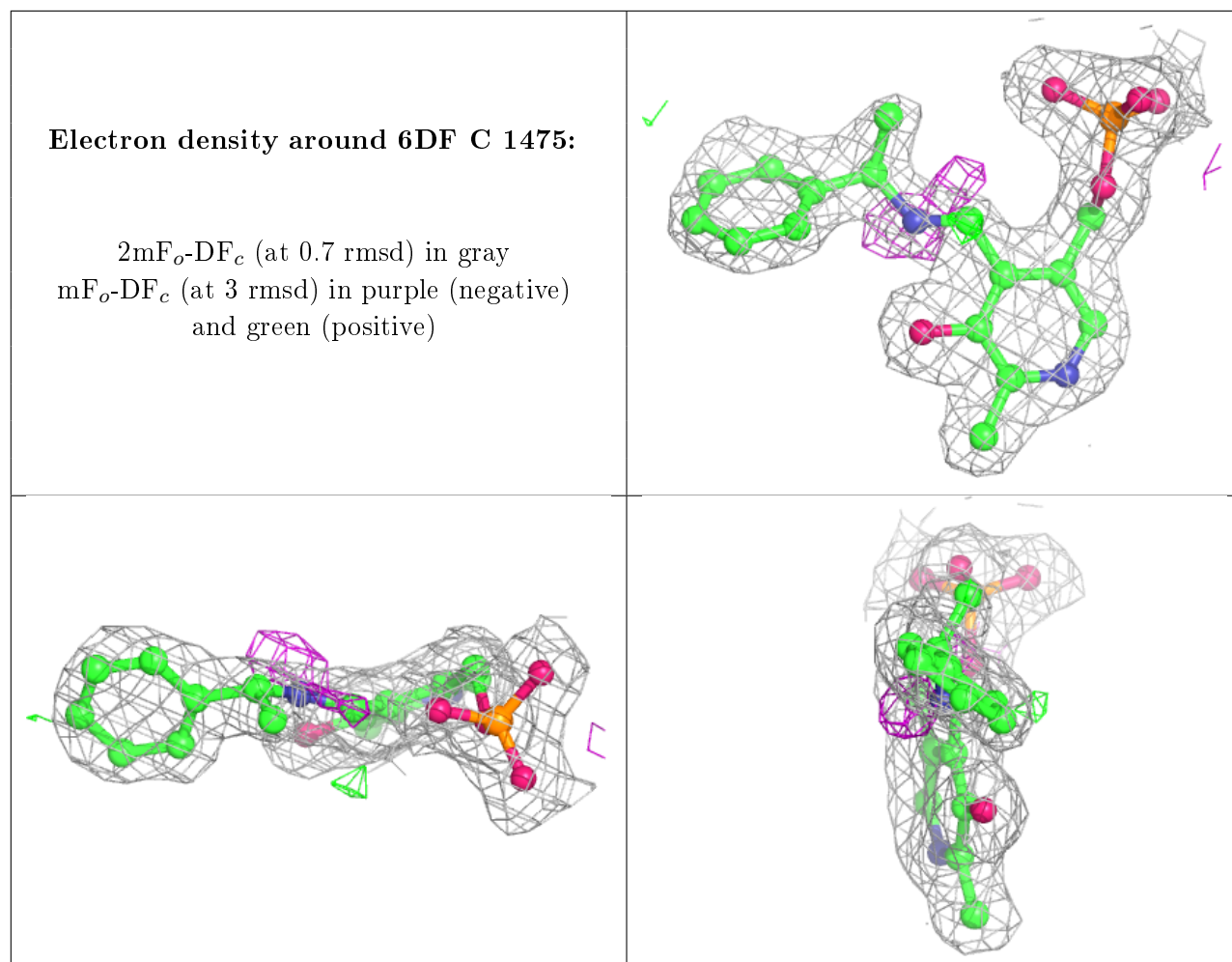
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6DF D 1476:

$2mF_o-DF_c$ (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.