Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 04:31 pm GMT

PDB ID	:	4BA5
Title	:	Crystal structure of omega-transaminase from Chromobacterium violaceum
Authors	:	Sayer, C.; Isupov, M.N.; Littlechild, J.A.
Deposited on	:	2012-09-11
Resolution	:	1.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

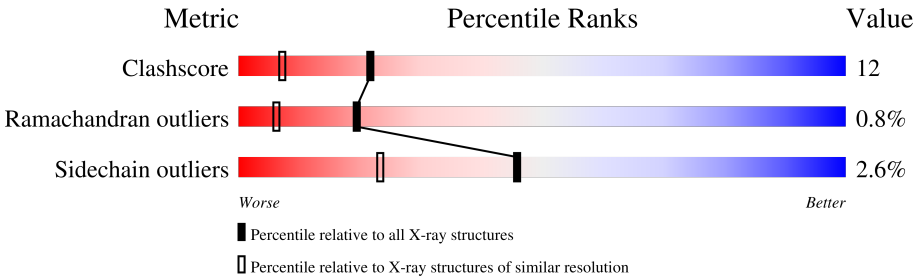
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.76 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))
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	459	78% 14% • 7%
1	B	459	76% 15% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PXG	A	470	-	-	X	-

2 Entry composition

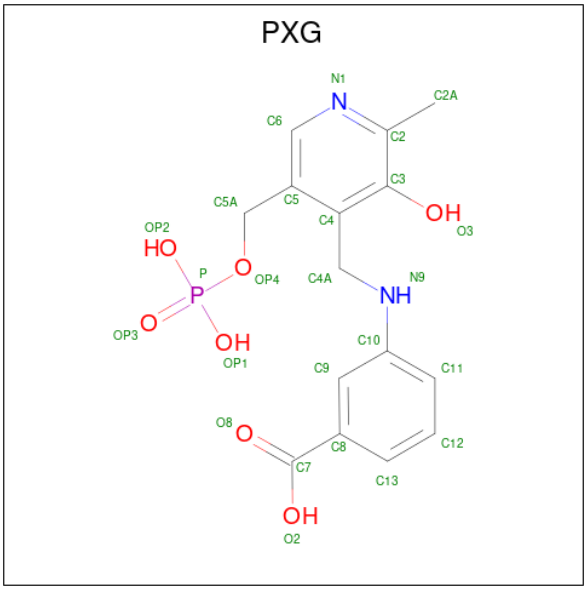
There are 4 unique types of molecules in this entry. The entry contains 7714 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AMINOTRANSFERASE.

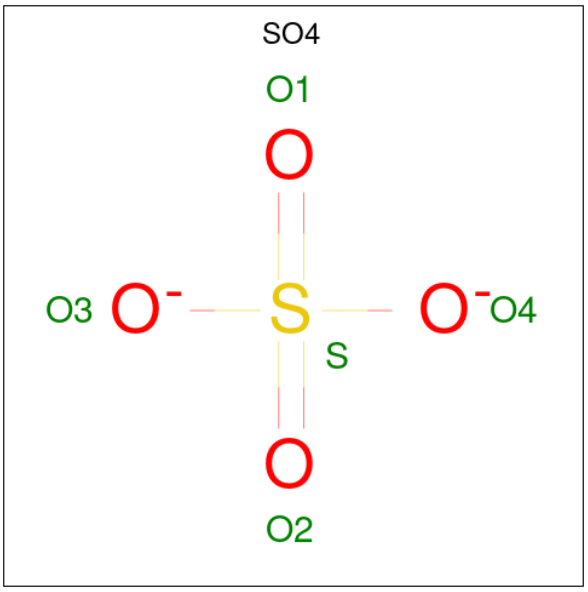
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	32	0
			3560	2282	623	632	23			
1	B	427	Total	C	N	O	S	0	26	0
			3517	2254	612	628	23			

- Molecule 2 is 3-[O-PHOSPHONOPYRIDOXYL]--AMINO-BENZOIC ACID (three-letter code: PXG) (formula: $C_{15}H_{17}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	15	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			25	15	2	7	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	307	Total O 307 307	0	0
4	B	275	Total O 275 275	0	0

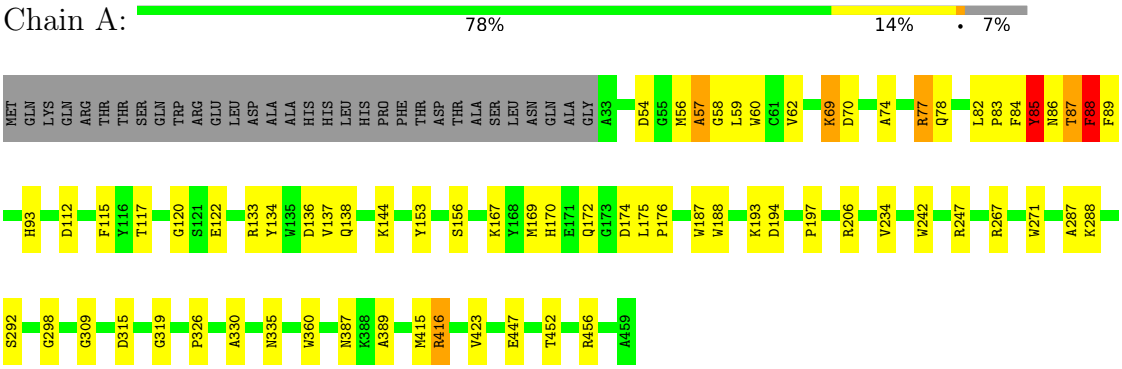
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

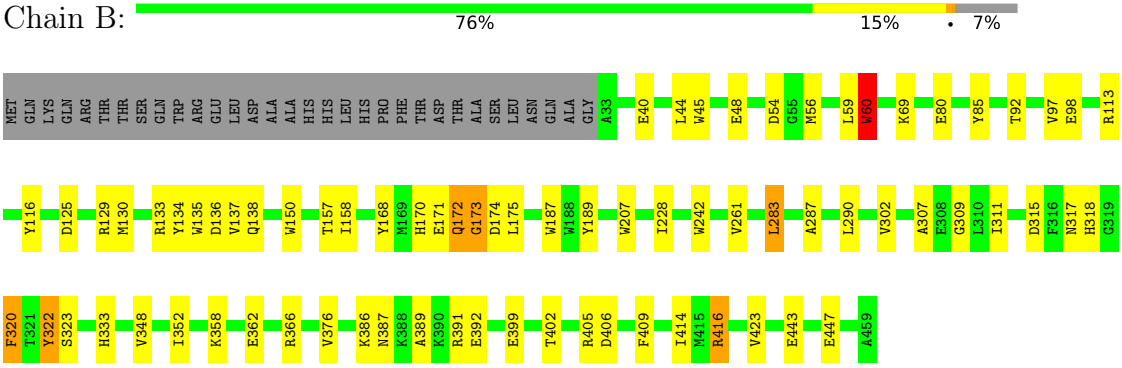
• Molecule 1: AMINOTRANSFERASE

Chain A:



• Molecule 1: AMINOTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.45Å 60.54Å 61.30Å 68.40° 76.18° 84.28°	Depositor
Resolution (Å)	56.75 – 1.76	Depositor
% Data completeness (in resolution range)	88.8 (56.75-1.76)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.233	Depositor
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.220	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7714	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PXG

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	0.65	5/3725 (0.1%)	0.68	0/5028
1	B	0.64	7/3670 (0.2%)	0.67	2/4954 (0.0%)
All	All	0.65	12/7395 (0.2%)	0.67	2/9982 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	TRP	CD2-CE2	5.88	1.48	1.41
1	A	360	TRP	CD2-CE2	5.79	1.48	1.41
1	A	271	TRP	CD2-CE2	5.68	1.48	1.41
1	A	188	TRP	CD2-CE2	5.54	1.48	1.41
1	B	242	TRP	CD2-CE2	5.41	1.47	1.41
1	B	135	TRP	CD2-CE2	5.25	1.47	1.41
1	A	187	TRP	CD2-CE2	5.22	1.47	1.41
1	B	207	TRP	CD2-CE2	5.21	1.47	1.41
1	B	45	TRP	CD2-CE2	5.14	1.47	1.41
1	B	60	TRP	CD2-CE2	5.10	1.47	1.41
1	B	187	TRP	CD2-CE2	5.08	1.47	1.41
1	B	150	TRP	CD2-CE2	5.07	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	LEU	CA-CB-CG	6.03	129.17	115.30
1	B	290	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	THR	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	3560	0	3544	104	0
1	B	3517	0	3484	67	0
2	A	25	0	14	29	0
2	B	25	0	14	8	0
3	B	5	0	0	0	0
4	A	307	0	0	20	0
4	B	275	0	0	8	0
All	All	7714	0	7056	169	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 12.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59[B]:LEU:CD2	2:A:470:PXG:H13	1.38	1.52
1:A:59[B]:LEU:HD22	2:A:470:PXG:C13	1.46	1.43
1:A:59[B]:LEU:HB3	2:A:470:PXG:C12	1.52	1.38
1:A:69[A]:LYS:HE3	4:A:2037:HOH:O	1.19	1.30
1:A:167[B]:LYS:CE	4:A:2138:HOH:O	1.73	1.29
1:A:59[B]:LEU:CB	2:A:470:PXG:H12	1.65	1.25
1:A:69[A]:LYS:CE	4:A:2037:HOH:O	1.73	1.23
1:A:59[B]:LEU:HD13	2:A:470:PXG:C12	1.71	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:HG22	1:A:88:PHE:CA	1.73	1.19
1:A:167[B]:LYS:CD	4:A:2138:HOH:O	1.83	1.15
2:A:470:PXG:H13	4:A:2025:HOH:O	1.05	1.15
1:A:87:THR:HG22	1:A:88:PHE:HA	1.13	1.13
1:B:406:ASP:OD1	4:B:2252:HOH:O	1.66	1.11
1:A:167[B]:LYS:HE2	4:A:2138:HOH:O	1.35	1.09
2:B:470:PXG:H9	4:B:2273:HOH:O	0.88	1.06
1:A:59[B]:LEU:CD1	2:A:470:PXG:H12	1.86	1.05
1:A:174[B]:ASP:OD2	4:A:2148:HOH:O	1.74	1.04
1:A:59[B]:LEU:HB3	2:A:470:PXG:H12	1.18	1.02
1:A:60[B]:TRP:HE1	2:A:470:PXG:C7	1.72	1.02
1:A:60[B]:TRP:CH2	1:A:423[B]:VAL:HG11	1.96	1.00
1:A:59[B]:LEU:CB	2:A:470:PXG:C12	2.30	1.00
1:A:87:THR:CG2	1:A:88:PHE:HA	1.91	0.99
1:A:59[B]:LEU:CD1	2:A:470:PXG:C12	2.41	0.98
1:A:69[A]:LYS:CD	4:A:2037:HOH:O	2.00	0.96
1:A:167[B]:LYS:HD3	4:A:2138:HOH:O	1.54	0.94
1:B:172[B]:GLN:O	1:B:174[B]:ASP:N	2.01	0.93
1:A:87:THR:HG22	1:A:88:PHE:N	1.83	0.93
1:A:85:TYR:CE1	1:A:93:HIS:HB2	2.05	0.92
1:A:59[B]:LEU:CG	2:A:470:PXG:H12	2.01	0.90
1:A:59[B]:LEU:HD13	2:A:470:PXG:H12	1.48	0.89
1:A:69[A]:LYS:HG3	4:A:2037:HOH:O	1.70	0.89
1:A:133[A]:ARG:HG2	1:A:315[A]:ASP:OD2	1.73	0.89
1:B:170[A]:HIS:O	1:B:171[A]:GLU:OE1	1.90	0.89
1:B:170[A]:HIS:C	1:B:171[A]:GLU:OE1	2.12	0.89
1:A:59[B]:LEU:HD13	2:A:470:PXG:C13	2.07	0.85
1:B:60:TRP:HE1	2:B:470:PXG:C7	1.89	0.84
2:A:470:PXG:H11	4:A:2235:HOH:O	1.79	0.81
1:A:59[B]:LEU:CG	2:A:470:PXG:H13	2.10	0.81
1:A:59[B]:LEU:CG	2:A:470:PXG:C12	2.59	0.80
1:A:85:TYR:HE1	1:A:93:HIS:HB2	1.49	0.78
1:A:60[B]:TRP:HH2	1:A:423[B]:VAL:HG11	1.49	0.77
1:A:84:PHE:O	1:A:85:TYR:HB2	1.85	0.76
1:A:59[B]:LEU:CD2	2:A:470:PXG:C13	2.28	0.76
1:B:44:LEU:CD1	1:B:54:ASP:HB2	2.15	0.76
1:B:171[B]:GLU:O	1:B:172[B]:GLN:C	2.24	0.75
1:A:136[B]:ASP:OD1	4:A:2108:HOH:O	2.06	0.74
1:A:59[B]:LEU:CG	2:A:470:PXG:C13	2.64	0.73
2:B:470:PXG:C9	4:B:2273:HOH:O	1.68	0.72
1:B:113:ARG:HD3	1:B:307:ALA:HB1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69[B]:LYS:CD	1:B:69[B]:LYS:H	2.04	0.71
2:B:470:PXG:O3	4:B:2273:HOH:O	2.09	0.70
1:B:59:LEU:HB3	2:B:470:PXG:C12	2.22	0.70
1:B:69[B]:LYS:NZ	4:B:2024:HOH:O	2.23	0.70
1:A:74:ALA:O	1:A:77[A]:ARG:HD3	1.92	0.69
1:B:172[B]:GLN:C	1:B:174[B]:ASP:H	1.94	0.69
1:A:115:PHE:CE2	1:A:319:GLY:HA3	2.28	0.68
1:A:59[B]:LEU:CD1	2:A:470:PXG:C13	2.70	0.68
1:B:56[B]:MET:SD	1:B:414:ILE:HG22	2.34	0.67
1:A:89:PHE:HB2	4:A:2058:HOH:O	1.94	0.67
1:A:78[A]:GLN:NE2	1:A:82:LEU:HB2	2.10	0.66
1:B:171[B]:GLU:O	1:B:173[B]:GLY:N	2.28	0.66
1:A:78[B]:GLN:HG3	1:A:330:ALA:CB	2.26	0.66
1:B:170[B]:HIS:O	1:B:172[B]:GLN:HG3	1.96	0.66
1:A:88:PHE:HB2	1:B:409[B]:PHE:CE2	2.31	0.66
1:A:58[B]:GLY:O	1:B:85:TYR:CE1	2.50	0.65
1:B:56[B]:MET:SD	1:B:414:ILE:CG2	2.87	0.63
1:A:58[B]:GLY:O	1:B:85:TYR:HE1	1.81	0.62
2:A:470:PXG:C13	4:A:2025:HOH:O	1.75	0.62
1:B:69[B]:LYS:H	1:B:69[B]:LYS:HD2	1.63	0.62
1:A:59[B]:LEU:HB3	2:A:470:PXG:C13	2.23	0.60
1:B:44:LEU:HD11	1:B:54:ASP:HB2	1.82	0.60
1:B:320:PHE:H	1:B:320:PHE:HD1	1.48	0.60
1:B:170[A]:HIS:O	1:B:171[A]:GLU:HB3	2.02	0.59
1:A:167[A]:LYS:HG2	4:A:2138:HOH:O	2.03	0.59
1:A:416[A]:ARG:HB3	1:A:423[A]:VAL:HG22	1.84	0.59
1:A:78[A]:GLN:HE22	1:A:82:LEU:HD12	1.66	0.58
1:B:130[B]:MET:HE1	1:B:302:VAL:HG22	1.85	0.58
1:A:60[B]:TRP:NE1	2:A:470:PXG:C7	2.55	0.57
1:A:59[B]:LEU:CB	2:A:470:PXG:C13	2.83	0.57
1:A:172:GLN:HG2	1:B:133[B]:ARG:HD2	1.87	0.57
1:A:56[B]:MET:HG2	1:A:415:MET:HA	1.86	0.57
1:B:133[B]:ARG:HE	1:B:133[B]:ARG:HA	1.69	0.57
1:A:133[A]:ARG:CG	1:A:315[A]:ASP:OD2	2.51	0.56
1:B:168:TYR:HD1	4:B:2109:HOH:O	1.88	0.56
1:A:416[A]:ARG:HB3	1:A:423[A]:VAL:CG2	2.35	0.55
1:A:172:GLN:HG2	1:B:133[A]:ARG:HD3	1.88	0.55
1:B:133[A]:ARG:HE	1:B:315:ASP:CG	2.09	0.55
1:B:387:ASN:OD1	1:B:389:ALA:HB3	2.07	0.55
1:B:158:ILE:HG23	1:B:175:LEU:HD21	1.88	0.54
1:B:386:LYS:HD3	1:B:392:GLU:OE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ALA:HA	1:A:298:GLY:HA2	1.89	0.54
1:A:78[B]:GLN:HG3	1:A:330:ALA:HB2	1.89	0.53
1:B:443:GLU:O	1:B:447[A]:GLU:HG2	2.09	0.53
1:A:59[B]:LEU:HD22	2:A:470:PXG:H13	0.59	0.53
1:B:171[B]:GLU:C	1:B:173[B]:GLY:N	2.60	0.53
1:B:56[A]:MET:SD	1:B:416:ARG:HB2	2.50	0.52
1:A:60[B]:TRP:NE1	2:A:470:PXG:O8	2.33	0.52
1:A:56[B]:MET:SD	1:A:416[B]:ARG:HB2	2.51	0.51
1:A:82:LEU:HD23	1:A:83:PRO:HD2	1.92	0.51
1:A:87:THR:CG2	1:A:88:PHE:CA	2.60	0.51
1:A:69[A]:LYS:NZ	4:A:2039:HOH:O	2.24	0.51
1:A:153:TYR:HE1	1:A:169:MET:SD	2.34	0.51
1:B:416:ARG:HB3	1:B:423:VAL:CG2	2.41	0.51
1:B:92:THR:HB	1:B:97:VAL:HG22	1.92	0.50
1:A:175:LEU:HB3	1:A:176:PRO:HA	1.94	0.49
1:B:98:GLU:HG2	1:B:333:HIS:CD2	2.47	0.49
1:A:156:SER:O	1:B:129[B]:ARG:NH1	2.45	0.49
1:A:60[B]:TRP:HE1	2:A:470:PXG:C8	2.22	0.49
1:A:78[A]:GLN:HE22	1:A:82:LEU:CD1	2.26	0.49
1:A:69[B]:LYS:HG2	1:B:80:GLU:HG2	1.95	0.48
1:B:59:LEU:HD13	2:B:470:PXG:H12	1.95	0.48
1:B:44:LEU:HD12	1:B:54:ASP:HB2	1.94	0.48
1:B:358:LYS:NZ	1:B:362:GLU:OE2	2.47	0.48
1:A:120:GLY:CA	1:A:287:ALA:HB2	2.44	0.48
1:A:85:TYR:HE1	1:A:93:HIS:CB	2.25	0.48
1:A:234:VAL:O	1:A:234:VAL:HG12	2.14	0.47
1:A:54:ASP:OD2	1:A:57[A]:ALA:HB2	2.14	0.47
1:B:116:TYR:O	1:B:323[A]:SER:HB3	2.14	0.47
1:A:87:THR:CG2	1:A:88:PHE:N	2.50	0.47
1:B:320:PHE:C	1:B:322:TYR:H	2.18	0.46
1:A:60[A]:TRP:HE1	1:B:322:TYR:HH	1.63	0.46
1:A:292:SER:OG	1:A:335:ASN:ND2	2.47	0.46
1:B:189:TYR:CE1	1:B:391[A]:ARG:HG2	2.51	0.46
1:A:60[B]:TRP:NE1	2:A:470:PXG:C8	2.78	0.46
1:A:56[B]:MET:HG3	1:A:416[B]:ARG:HB2	1.98	0.45
1:B:116:TYR:O	1:B:323[B]:SER:HB2	2.15	0.45
1:B:261:VAL:HG13	1:B:287:ALA:HB3	1.97	0.45
1:A:387:ASN:OD1	1:A:389:ALA:HB3	2.16	0.45
1:A:170:HIS:HA	1:A:175:LEU:HB2	1.98	0.45
1:A:117:THR:HB	1:A:122[B]:GLU:HB3	1.98	0.45
1:A:59[B]:LEU:C	1:A:60[B]:TRP:CD1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:HB3	4:A:2029:HOH:O	2.18	0.44
1:A:58[A]:GLY:HA3	1:A:267:ARG:NH2	2.32	0.44
1:B:134:TYR:O	1:B:138:GLN:HG2	2.17	0.44
1:A:69[A]:LYS:HD2	1:A:70:ASP:H	1.81	0.44
1:B:59:LEU:HB3	2:B:470:PXG:C13	2.47	0.44
1:B:125[B]:ASP:OD1	1:B:157:THR:OG1	2.35	0.43
1:A:452:THR:O	1:A:456:ARG:HG2	2.19	0.43
1:A:167[A]:LYS:HD3	4:A:2138:HOH:O	2.18	0.43
1:B:311:ILE:HA	1:B:317:ASN:HD21	1.84	0.42
4:A:2104:HOH:O	1:B:172[A]:GLN:NE2	2.36	0.42
1:B:92:THR:HB	1:B:97:VAL:CG2	2.49	0.42
2:B:470:PXG:N9	4:B:2273:HOH:O	2.37	0.42
1:B:137:VAL:HG11	1:B:309:GLY:O	2.19	0.42
1:B:402:THR:HG23	1:B:405:ARG:NH2	2.34	0.42
1:A:172:GLN:OE1	1:B:315:ASP:HB3	2.19	0.42
1:A:234:VAL:HG21	1:A:423[B]:VAL:HG13	2.02	0.42
1:A:85:TYR:CZ	1:A:93:HIS:HB2	2.52	0.42
1:B:348:VAL:HA	1:B:352:ILE:HG22	2.02	0.42
1:A:137:VAL:HG11	1:A:309:GLY:O	2.20	0.41
1:B:130[B]:MET:HE1	1:B:302:VAL:CG2	2.49	0.41
1:B:189:TYR:CZ	1:B:391[A]:ARG:HG2	2.55	0.41
1:B:130[B]:MET:HB3	1:B:130[B]:MET:HE2	1.87	0.41
1:A:60[B]:TRP:CH2	1:A:423[B]:VAL:CG1	2.86	0.41
1:A:167[A]:LYS:CD	4:A:2138:HOH:O	2.68	0.41
1:B:228:ILE:HD11	1:B:376[B]:VAL:CG1	2.51	0.41
1:A:59[B]:LEU:CD1	2:A:470:PXG:H13	2.43	0.41
1:A:93:HIS:CE1	1:A:326:PRO:HB3	2.55	0.41
1:A:206:ARG:HE	1:A:247:ARG:HH21	1.69	0.41
1:A:134:TYR:O	1:A:138:GLN:HG2	2.21	0.41
1:A:288:LYS:HB2	1:A:288:LYS:HE2	1.86	0.41
1:A:57[A]:ALA:HB1	1:A:62:VAL:HB	2.03	0.41
1:A:62:VAL:HA	1:A:292:SER:O	2.21	0.41
1:B:48:GLU:HG2	4:B:2007:HOH:O	2.20	0.41
1:A:193:LYS:HB3	1:A:194:ASP:H	1.64	0.40
1:B:416:ARG:HB3	1:B:423:VAL:HG22	2.02	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	457/459 (100%)	431 (94%)	21 (5%)	5 (1%)	14 3
1	B	451/459 (98%)	418 (93%)	28 (6%)	5 (1%)	14 3
All	All	908/918 (99%)	849 (94%)	49 (5%)	10 (1%)	19 3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	B	318	HIS
1	B	172[A]	GLN
1	B	172[B]	GLN
1	B	173[A]	GLY
1	B	173[B]	GLY
1	A	57[A]	ALA
1	A	57[B]	ALA
1	A	88	PHE
1	A	86	ASN

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	371/368 (101%)	356 (96%)	15 (4%)	31 10
1	B	366/368 (100%)	355 (97%)	11 (3%)	41 18
All	All	737/736 (100%)	711 (96%)	26 (4%)	46 13

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69[A]	LYS
1	A	69[B]	LYS
1	A	77[A]	ARG
1	A	77[B]	ARG
1	A	85	TYR
1	A	88	PHE
1	A	112[A]	ASP
1	A	112[B]	ASP
1	A	144[A]	LYS
1	A	144[B]	LYS
1	A	197	PRO
1	A	416[A]	ARG
1	A	416[B]	ARG
1	A	447[A]	GLU
1	A	447[B]	GLU
1	B	40[A]	GLU
1	B	40[B]	GLU
1	B	60	TRP
1	B	136	ASP
1	B	283	LEU
1	B	320	PHE
1	B	322	TYR
1	B	366[A]	ARG
1	B	366[B]	ARG
1	B	399	GLU
1	B	416	ARG

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	50	ASN
1	A	335	ASN
1	B	317	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

3 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	SO4	B	1460	-	4,4,4	0.23	0	6,6,6	0.19	0
2	PXG	A	470	-	26,26,26	0.95	1 (3%)	35,37,37	1.58	7 (20%)
2	PXG	B	470	-	26,26,26	0.76	0	35,37,37	1.17	3 (8%)

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	PXG	A	470	-	-	8/15/15/15	0/2/2/2
2	PXG	B	470	-	-	8/15/15/15	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	470	PXG	C9-C8	2.08	1.42	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	470	PXG	C9-C8-C7	4.35	127.86	119.98
2	A	470	PXG	C13-C8-C7	-4.19	112.15	120.39
2	A	470	PXG	O2-C7-C8	2.45	121.21	114.85
2	B	470	PXG	C5-C6-N1	-2.43	119.77	123.82
2	A	470	PXG	C5-C6-N1	-2.33	119.94	123.82
2	A	470	PXG	C11-C10-N9	-2.25	116.30	120.97
2	A	470	PXG	C6-N1-C2	2.14	123.14	119.17
2	B	470	PXG	C4A-N9-C10	-2.11	116.71	122.15
2	B	470	PXG	C6-C5-C4	2.06	119.58	118.12
2	A	470	PXG	C12-C11-C10	2.02	122.14	119.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	470	PXG	C5-C4-C4A-N9
2	B	470	PXG	O8-C7-C8-C9
2	B	470	PXG	O8-C7-C8-C13
2	A	470	PXG	O2-C7-C8-C13
2	B	470	PXG	O2-C7-C8-C9
2	A	470	PXG	C11-C10-N9-C4A
2	B	470	PXG	C9-C10-N9-C4A
2	B	470	PXG	O2-C7-C8-C13
2	A	470	PXG	C5-C4-C4A-N9
2	B	470	PXG	C11-C10-N9-C4A
2	A	470	PXG	C9-C10-N9-C4A
2	A	470	PXG	O2-C7-C8-C9
2	A	470	PXG	O8-C7-C8-C13
2	B	470	PXG	C3-C4-C4A-N9
2	A	470	PXG	O8-C7-C8-C9
2	A	470	PXG	C4-C4A-N9-C10

There are no ring outliers.

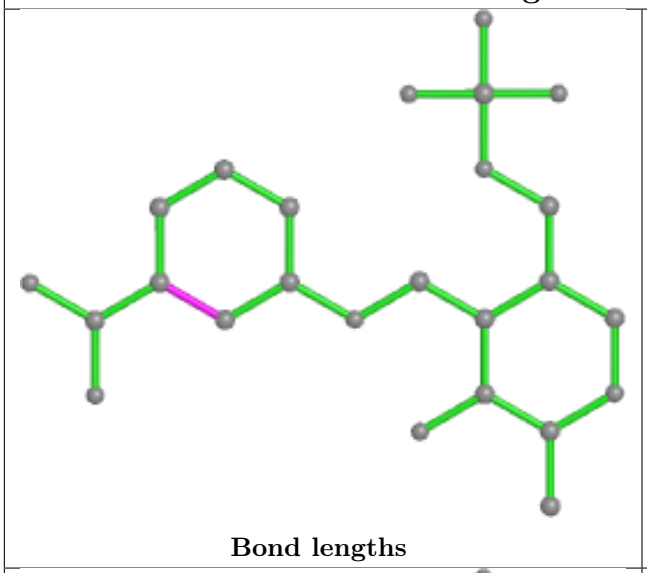
2 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	470	PXG	29	0
2	B	470	PXG	8	0

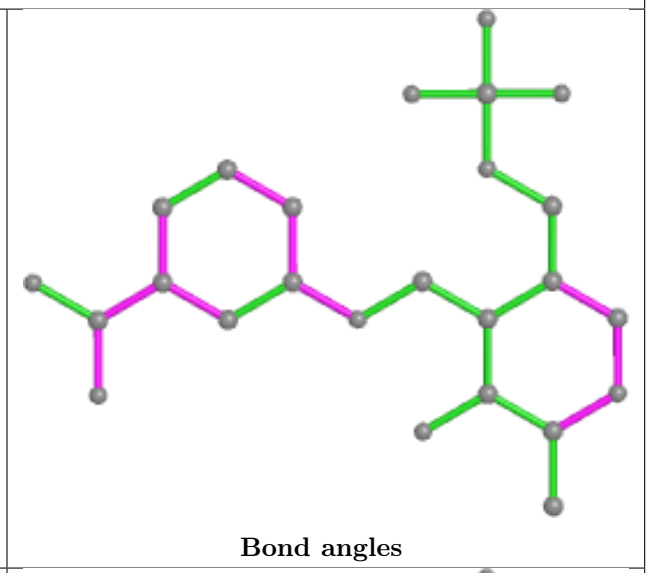
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

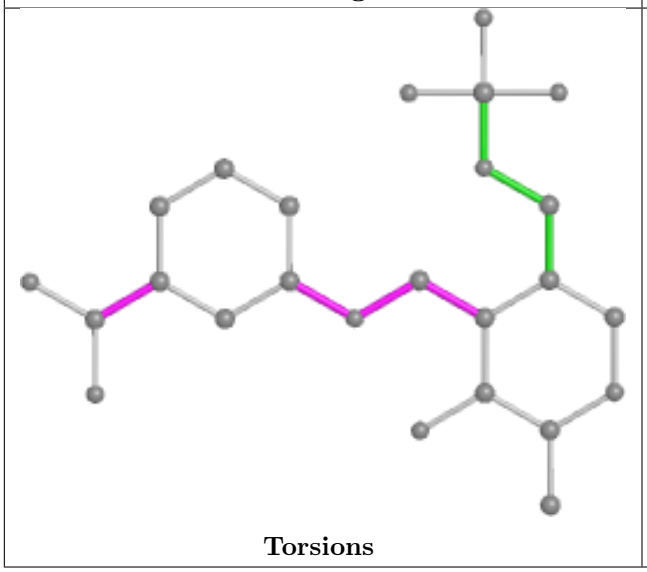
Ligand PXG A 470



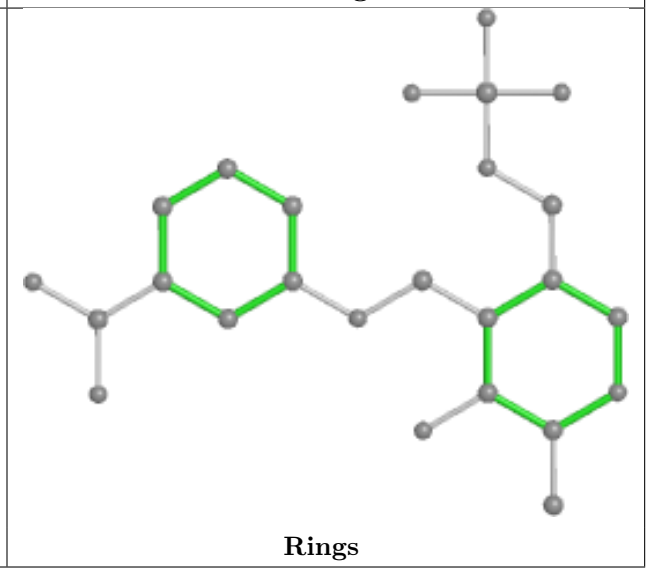
Bond lengths



Bond angles

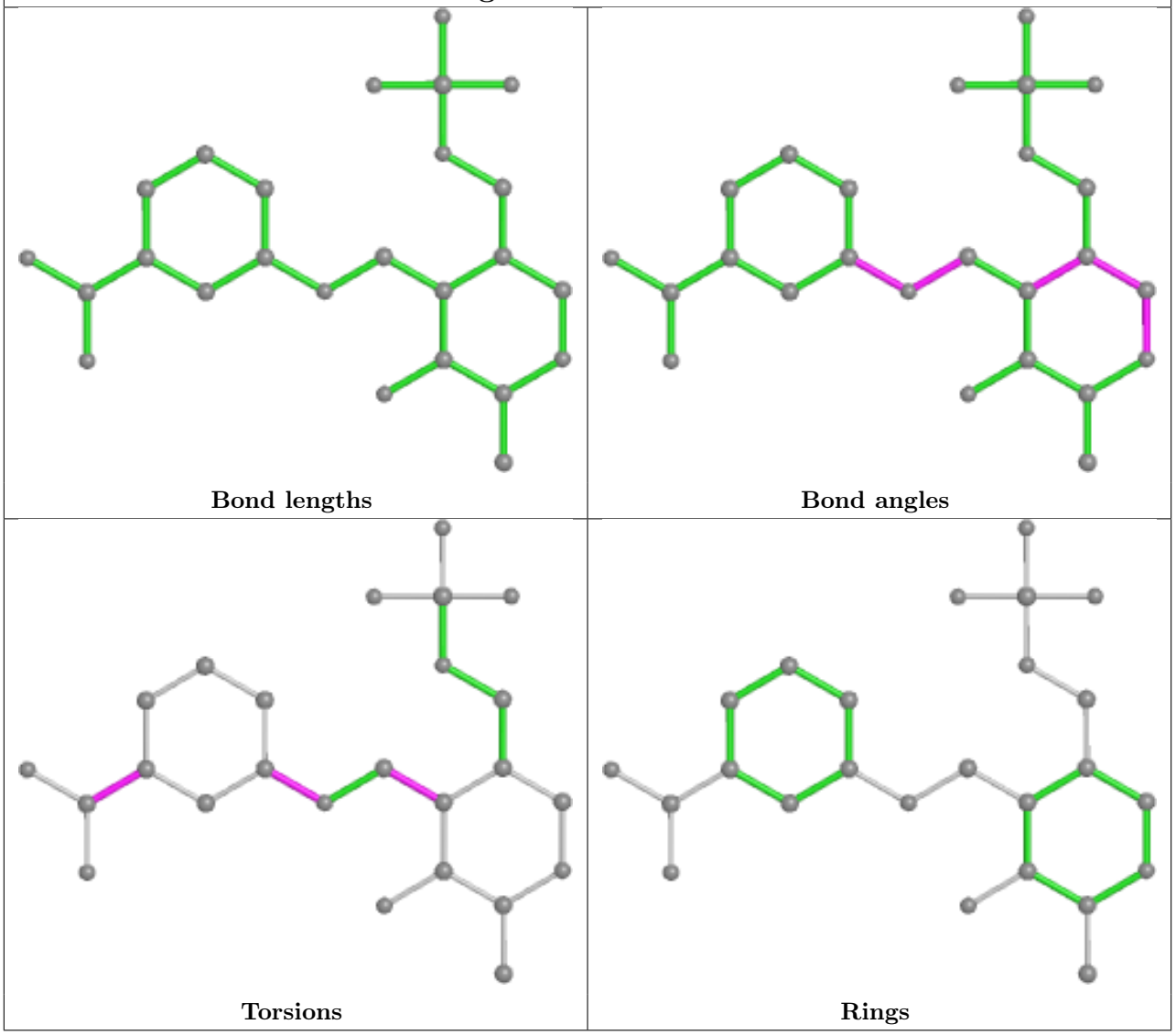


Torsions



Rings

Ligand PXG B 470



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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

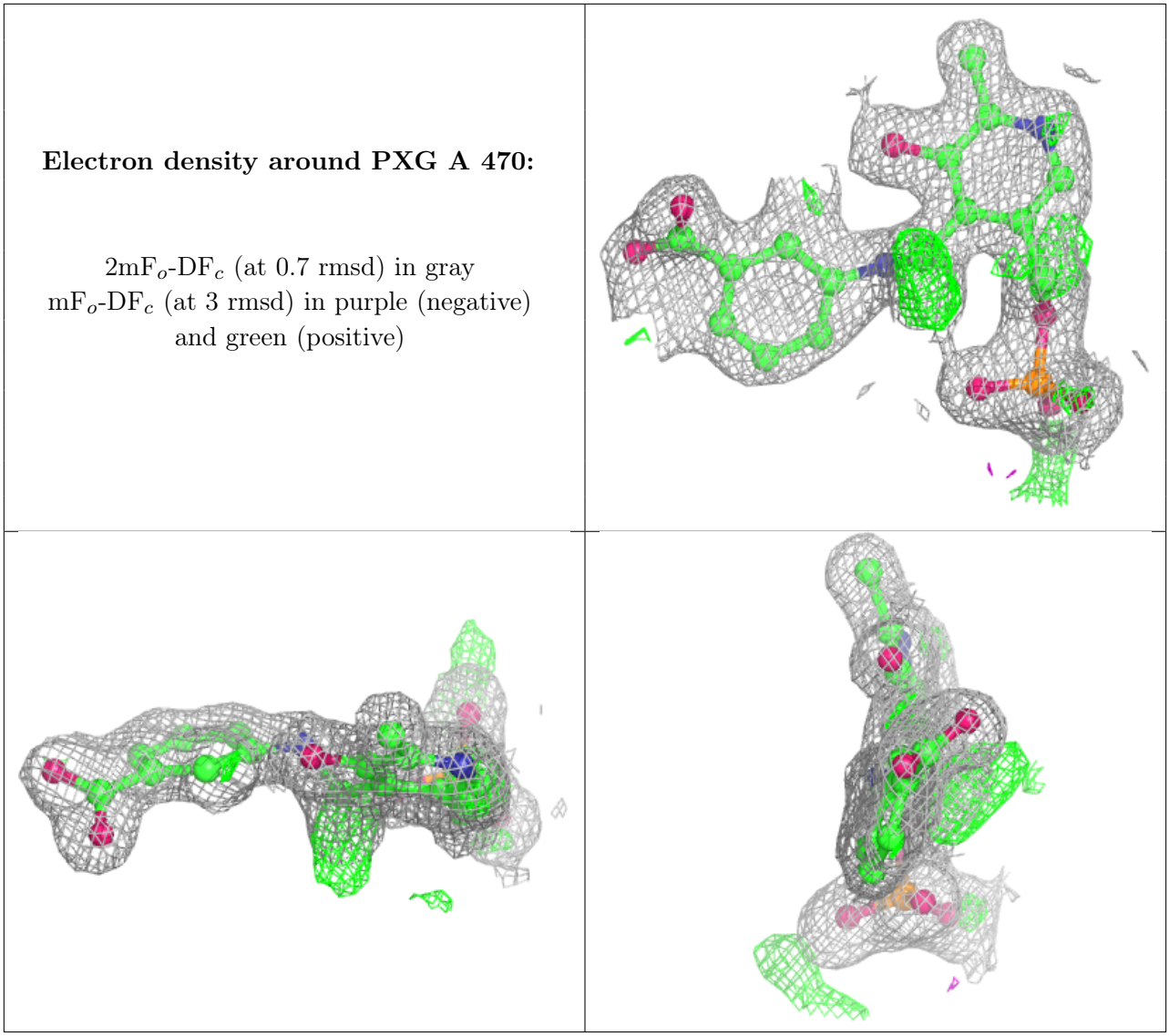
6.4 Ligands

EDS failed to run properly - this section is therefore empty.

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.

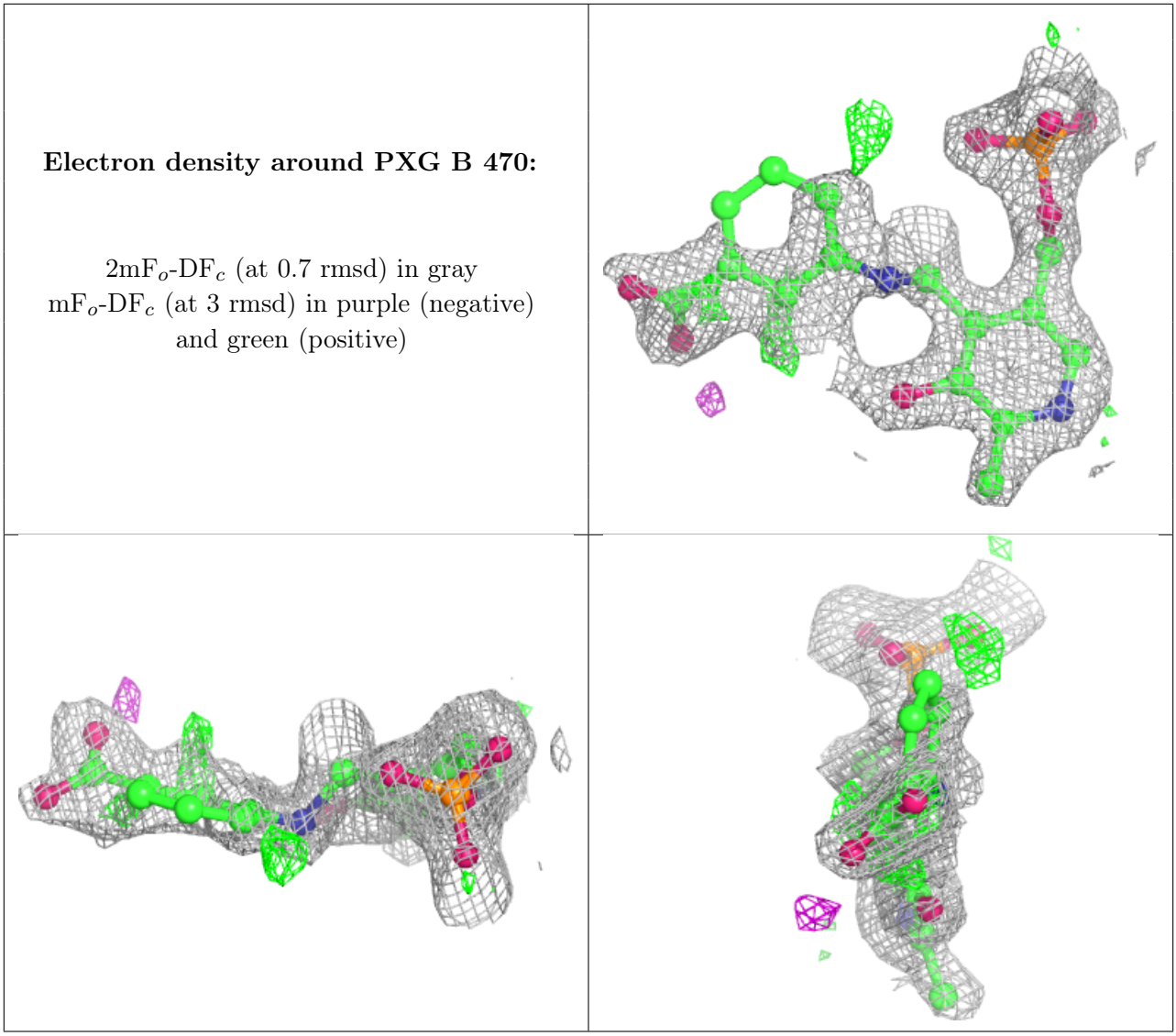
Electron density around PXG A 470:

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



Electron density around PXG B 470:

$2mF_o$-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)

EDS failed to run properly - this section is therefore empty.