



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 8, 2025 – 10:06 AM EDT

PDB ID : 9DHN / pdb_00009dhn
Title : Crystal structure of PIsnA complexed with an imine intermediate
Authors : Kim, W.; Zhang, Y.J.; Guo, M.
Deposited on : 2024-09-04
Resolution : 2.94 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

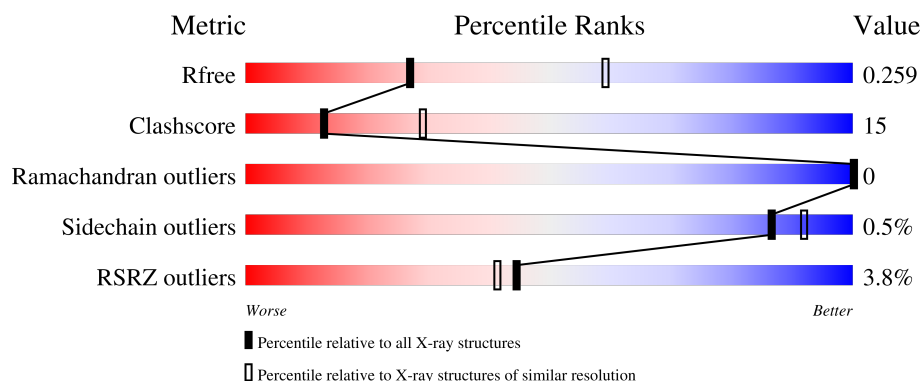
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div>4%</div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	B	315	<div> <div>4%</div> <div>66%</div> <div>34%</div> </div>

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
5	EDO	B	401	-	-	-	X

2 Entry composition [i](#)

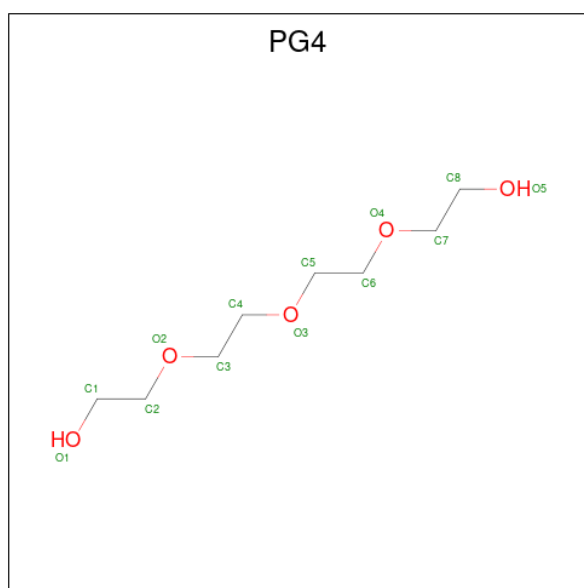
There are 7 unique types of molecules in this entry. The entry contains 5129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-tyrosine/L-tryptophan isonitrile synthase family protein.

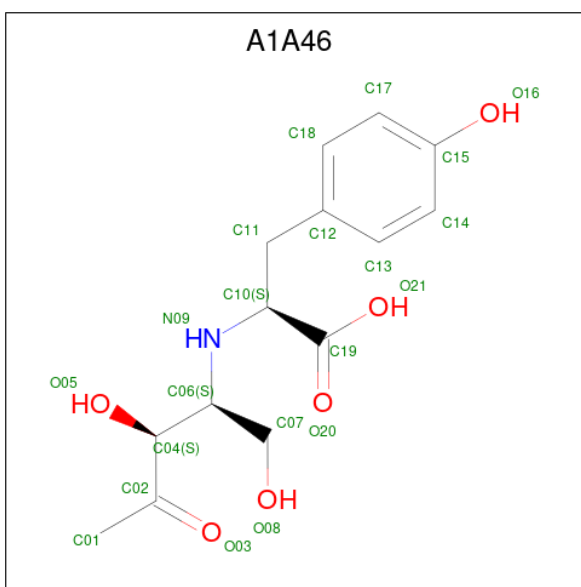
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2500	1593	443	453	11			
1	B	315	Total	C	N	O	S	0	0	0
			2542	1621	449	461	11			

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



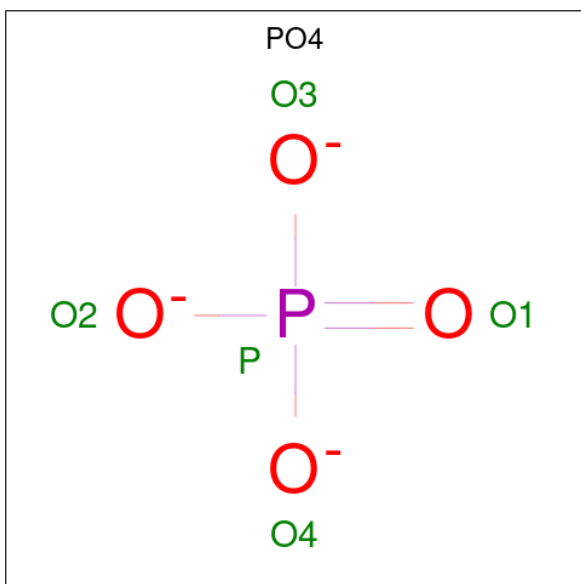
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is (2S)-2-[[[(2S,3S)-1,3-dihydroxy-4-oxopentan-2-yl]amino}-3-(4-hydroxyphenyl)propanoic acid (CCD ID: A1A46) (formula: C₁₄H₁₉NO₆) (labeled as "Ligand of Interest" by depositor).



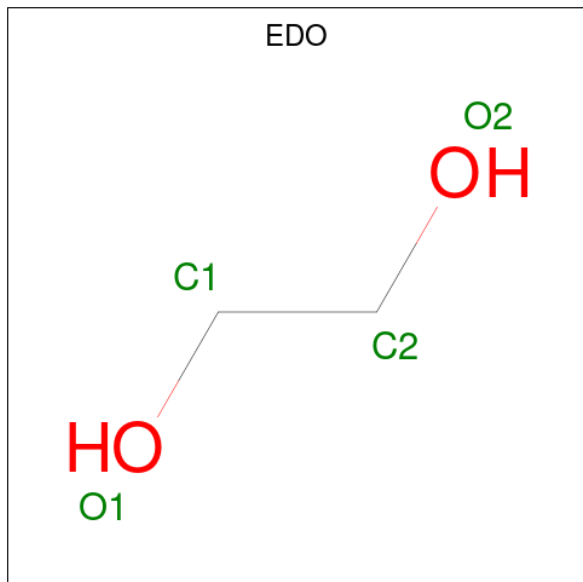
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	14	1	6		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



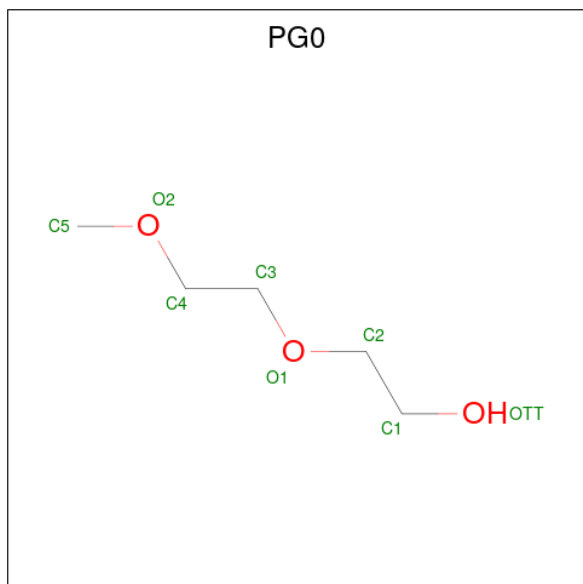
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



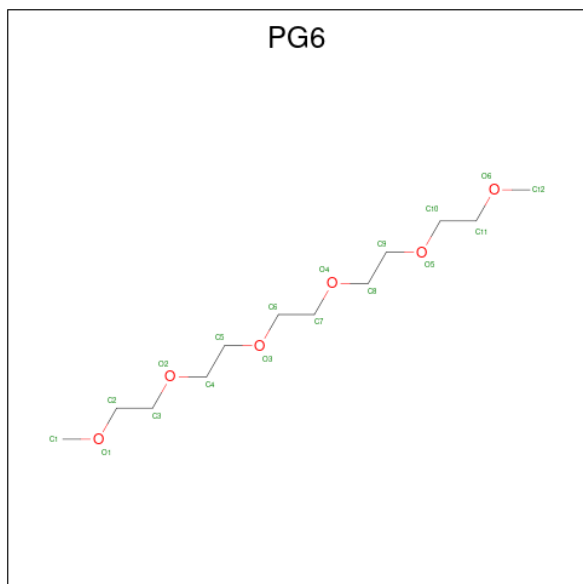
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: $C_{12}H_{26}O_6$) (labeled as "Ligand of Interest" by depositor).

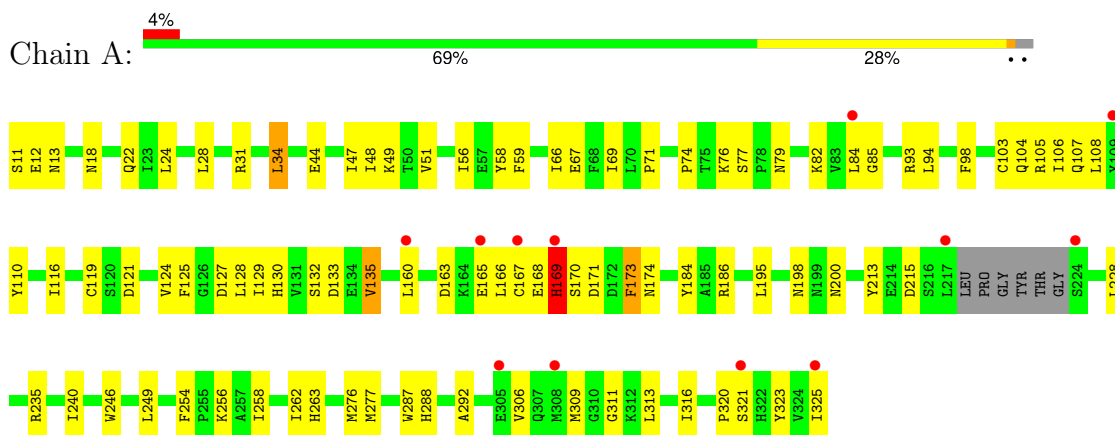


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			18	12	6		

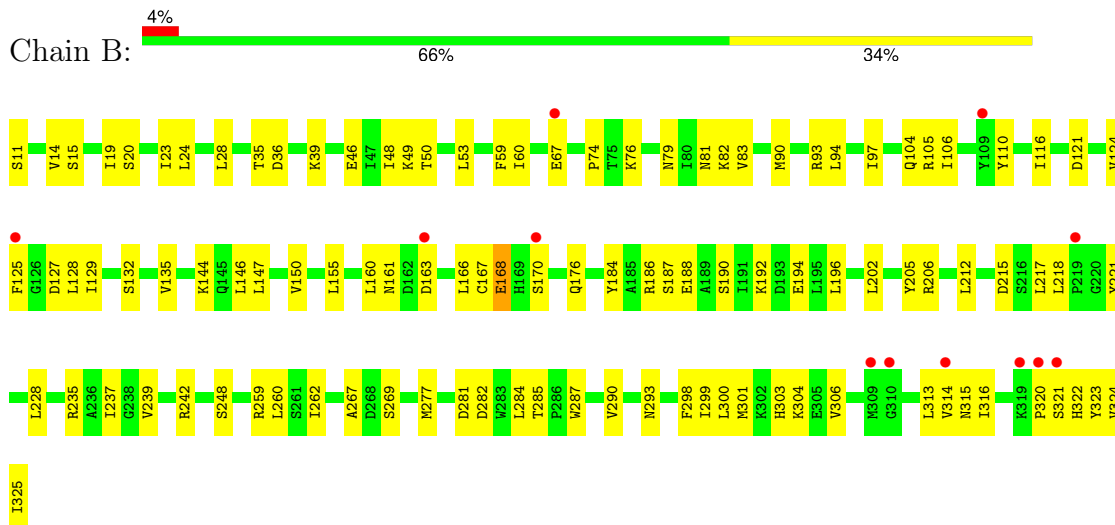
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: L-tyrosine/L-tryptophan isonitrile synthase family protein



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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.73Å 133.73Å 109.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.81 – 2.94 59.81 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.81-2.94) 99.9 (59.81-2.94)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.238 , 0.259 0.238 , 0.259	Depositor DCC
R_{free} test set	19625 reflections (9.25%)	wwPDB-VP
Wilson B-factor (Å ²)	103.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5129	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: PG4, PO4, A1A46, PG6, PG0, EDO

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	0/2556	1.06	12/3457 (0.3%)
1	B	0.57	0/2601	0.92	9/3521 (0.3%)
All	All	0.60	0/5157	0.99	21/6978 (0.3%)

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 (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	169	HIS	N-CA-C	10.52	125.48	110.23
1	A	106	ILE	N-CA-C	-9.49	100.94	110.62
1	A	130	HIS	N-CA-C	-9.40	99.92	110.91
1	B	269	SER	N-CA-C	8.86	122.23	110.53
1	A	133	ASP	N-CA-C	-8.36	102.25	111.36
1	A	167	CYS	N-CA-C	7.80	121.24	110.24
1	B	168	GLU	N-CA-C	-6.36	104.35	111.28
1	B	163	ASP	N-CA-C	-6.13	101.20	110.28
1	A	34	LEU	N-CA-C	-5.99	101.18	110.10
1	A	173	PHE	N-CA-C	-5.91	104.84	111.28
1	A	13	ASN	N-CA-C	5.88	119.56	112.38
1	B	267	ALA	N-CA-C	-5.79	105.31	112.38
1	A	74	PRO	CB-CA-C	-5.70	103.99	113.06
1	A	170	SER	N-CA-C	-5.53	105.25	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	VAL	N-CA-C	5.37	116.10	110.62
1	A	34	LEU	CB-CA-C	5.37	118.27	109.90
1	B	160	LEU	N-CA-C	-5.36	105.43	111.28
1	B	314	VAL	CA-C-N	-5.22	115.63	122.99
1	B	314	VAL	C-N-CA	-5.22	115.63	122.99
1	B	170	SER	N-CA-C	-5.13	105.68	111.28
1	B	74	PRO	CB-CA-C	-5.04	105.04	113.06

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Sidechain

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	2500	0	2508	75	0
1	B	2542	0	2549	75	0
2	A	26	0	36	4	0
3	A	21	0	0	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	B	4	0	6	2	0
6	B	8	0	12	4	0
7	B	18	0	26	1	0
All	All	5129	0	5137	152	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 15.

All (152) 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:161:ASN:HA	1:B:166:LEU:HD13	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ASN:HA	1:B:320:PRO:HA	1.41	1.00
1:A:165:GLU:CD	1:A:166:LEU:HD12	1.93	0.94
1:A:165:GLU:OE2	1:A:166:LEU:HD12	1.66	0.93
1:A:124:VAL:HG12	1:A:160:LEU:HD21	1.54	0.90
1:A:124:VAL:CG1	1:A:160:LEU:HD11	2.05	0.85
1:A:124:VAL:HG13	1:A:160:LEU:HD11	1.59	0.85
1:B:290:VAL:HG22	1:B:301:MET:O	1.76	0.84
2:A:402:PG4:H21	7:B:403:PG6:H21	1.65	0.77
1:B:93:ARG:HG3	1:B:146:LEU:HD11	1.69	0.75
1:B:313:LEU:HD11	1:B:320:PRO:HB2	1.68	0.75
1:A:311:GLY:HA3	1:A:325:ILE:HG13	1.68	0.75
1:A:121:ASP:O	1:A:124:VAL:HG22	1.88	0.74
1:B:90:MET:HB2	1:B:321:SER:HB2	1.72	0.71
1:A:69:ILE:HD11	1:A:254:PHE:HB2	1.73	0.70
1:A:163:ASP:OD2	1:A:166:LEU:HD13	1.95	0.67
1:B:167:CYS:HB2	1:B:176:GLN:HG3	1.77	0.67
1:B:35:THR:HG23	1:B:282:ASP:OD2	1.95	0.67
1:B:127:ASP:OD1	1:B:128:LEU:HG	1.94	0.66
2:A:401:PG4:H82	1:B:104:GLN:NE2	2.11	0.66
1:B:105:ARG:HD3	5:B:401:EDO:H22	1.78	0.66
1:B:144:LYS:HA	1:B:147:LEU:HD12	1.79	0.65
1:B:79:ASN:HB3	1:B:82:LYS:HG3	1.81	0.63
1:A:94:LEU:HD12	1:A:277:MET:HE3	1.79	0.63
1:A:165:GLU:OE2	1:A:166:LEU:CD1	2.44	0.62
1:B:277:MET:HE2	1:B:300:LEU:HB2	1.80	0.62
1:B:186:ARG:NH2	1:B:194:GLU:OE1	2.33	0.61
1:A:165:GLU:CD	1:A:166:LEU:CD1	2.71	0.61
1:A:105:ARG:HD2	5:B:401:EDO:H21	1.82	0.60
1:A:18:ASN:O	1:A:22:GLN:HG3	2.01	0.59
1:A:31:ARG:NH2	1:A:44:GLU:OE1	2.36	0.59
1:A:313:LEU:HD21	1:A:320:PRO:HB3	1.85	0.59
1:A:127:ASP:OD1	1:A:128:LEU:N	2.36	0.59
1:B:262:ILE:HD13	1:B:287:TRP:HZ2	1.68	0.59
1:A:79:ASN:HB2	1:A:215:ASP:HA	1.84	0.58
2:A:402:PG4:H82	1:B:94:LEU:HD22	1.84	0.58
1:A:24:LEU:HD21	1:A:49:LYS:HA	1.85	0.58
1:B:121:ASP:O	1:B:124:VAL:HG22	2.02	0.58
1:B:20:SER:HB2	1:B:53:LEU:HD22	1.85	0.57
1:B:313:LEU:HD13	1:B:323:TYR:CE1	2.40	0.57
1:B:15:SER:O	1:B:19:ILE:HG13	2.05	0.57
1:B:281:ASP:HB3	1:B:284:LEU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD11	1:A:240:ILE:HD13	1.88	0.56
1:A:59:PHE:HB2	1:A:66:ILE:HD13	1.86	0.56
1:B:97:ILE:HG12	1:B:150:VAL:HG11	1.86	0.56
1:B:161:ASN:HA	1:B:166:LEU:CD1	2.27	0.56
1:A:69:ILE:HD11	1:A:254:PHE:CD1	2.41	0.55
1:B:202:LEU:O	1:B:206:ARG:HG3	2.06	0.55
1:B:259:ARG:NH1	1:B:260:LEU:O	2.38	0.54
1:A:213:TYR:HE1	1:A:228:LEU:HB3	1.73	0.53
1:A:124:VAL:HG13	1:A:160:LEU:CD1	2.35	0.53
1:A:44:GLU:O	1:A:48:ILE:HG13	2.09	0.53
1:B:49:LYS:HE3	1:B:53:LEU:HD12	1.92	0.51
1:A:263:HIS:NE2	3:A:403:A1A46:O05	2.43	0.51
1:A:105:ARG:HG3	1:A:108:LEU:HD12	1.93	0.51
1:B:46:GLU:O	1:B:50:THR:HG23	2.11	0.50
1:B:116:ILE:HB	1:B:155:LEU:HD22	1.94	0.50
1:A:59:PHE:CE1	1:A:67:GLU:HG2	2.46	0.50
1:B:221:TYR:CZ	1:B:228:LEU:HD21	2.46	0.50
1:A:76:LYS:HG2	1:A:85:GLY:O	2.12	0.49
1:A:103:CYS:SG	1:A:116:ILE:HD12	2.51	0.49
1:A:124:VAL:CG1	1:A:160:LEU:HD21	2.35	0.49
1:A:107:GLN:HA	1:A:110:TYR:O	2.13	0.49
1:A:169:HIS:CE1	1:A:171:ASP:HB2	2.47	0.49
1:A:93:ARG:HH22	1:A:316:ILE:HD11	1.78	0.49
1:A:168:GLU:HG3	1:A:169:HIS:N	2.28	0.49
1:A:98:PHE:HD1	6:B:402:PG0:H42	1.77	0.48
1:A:58:TYR:CZ	1:A:256:LYS:HD3	2.49	0.48
1:B:192:LYS:O	1:B:196:LEU:HG	2.13	0.48
1:A:47:ILE:O	1:A:51:VAL:HG23	2.13	0.47
1:A:56:ILE:HG13	1:A:258:ILE:CD1	2.45	0.47
1:A:84:LEU:HD21	1:A:323:TYR:HE1	1.79	0.47
1:B:11:SER:O	1:B:14:VAL:HG12	2.14	0.47
1:B:124:VAL:O	1:B:242:ARG:HG2	2.13	0.47
1:A:125:PHE:CD1	1:A:129:ILE:HD11	2.49	0.47
1:A:128:LEU:O	1:A:235:ARG:HD2	2.14	0.47
1:B:60:ILE:HG23	1:B:110:TYR:CE1	2.50	0.47
1:A:198:ASN:HB3	1:A:200:ASN:H	1.78	0.47
1:B:59:PHE:CE1	1:B:67:GLU:HG2	2.50	0.47
1:B:221:TYR:CE2	1:B:228:LEU:HD21	2.49	0.47
1:A:316:ILE:HG13	1:A:321:SER:HB2	1.97	0.47
1:A:132:SER:HB2	1:A:135:VAL:HG23	1.96	0.47
1:B:205:TYR:CE2	1:B:237:ILE:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.64	0.46
1:A:262:ILE:HG12	1:A:287:TRP:CH2	2.50	0.46
1:B:127:ASP:OD1	1:B:128:LEU:N	2.49	0.46
1:B:235:ARG:O	1:B:239:VAL:HG23	2.14	0.46
1:A:292:ALA:HA	1:A:323:TYR:O	2.15	0.46
1:A:288:HIS:HE1	3:A:403:A1A46:C14	2.29	0.46
1:B:24:LEU:O	1:B:28:LEU:HG	2.16	0.46
1:B:76:LYS:HE3	1:B:83:VAL:HG13	1.96	0.46
1:B:298:PHE:C	1:B:299:ILE:HD13	2.41	0.46
1:B:188:GLU:OE1	1:B:188:GLU:N	2.35	0.45
1:A:262:ILE:HG12	1:A:287:TRP:HH2	1.81	0.45
1:A:160:LEU:HD12	1:A:246:TRP:CH2	2.51	0.45
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.79	0.45
1:B:76:LYS:HG3	1:B:83:VAL:HG11	1.98	0.45
1:B:293:ASN:HB3	1:B:324:VAL:HG22	1.99	0.45
1:B:104:GLN:HB3	6:B:402:PG0:H22	1.99	0.45
1:B:97:ILE:CG1	1:B:150:VAL:HG11	2.46	0.45
1:B:125:PHE:CD1	1:B:129:ILE:HG13	2.52	0.45
1:B:132:SER:OG	1:B:135:VAL:HG23	2.17	0.45
1:B:20:SER:HB2	1:B:53:LEU:CD2	2.47	0.44
1:A:215:ASP:N	1:A:215:ASP:OD1	2.50	0.44
1:A:71:PRO:HA	1:A:119:CYS:O	2.17	0.44
1:B:36:ASP:HB3	1:B:39:LYS:HG3	1.99	0.44
1:B:298:PHE:O	1:B:299:ILE:HD13	2.18	0.44
1:A:165:GLU:OE1	1:A:166:LEU:CD1	2.65	0.44
1:B:23:ILE:HG12	1:B:106:ILE:HD12	1.99	0.44
1:B:59:PHE:CZ	1:B:67:GLU:HG2	2.52	0.44
1:B:262:ILE:HD13	1:B:287:TRP:CZ2	2.50	0.44
1:A:69:ILE:HD11	1:A:254:PHE:CB	2.46	0.44
1:A:306:VAL:HG13	1:A:325:ILE:HD11	1.99	0.44
1:B:284:LEU:HD12	1:B:285:THR:H	1.83	0.43
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.77	0.43
1:B:146:LEU:O	1:B:150:VAL:HG23	2.19	0.43
1:A:66:ILE:H	1:A:66:ILE:HG12	1.70	0.43
1:A:121:ASP:OD1	1:A:121:ASP:N	2.47	0.43
1:A:93:ARG:NH2	1:A:316:ILE:HD11	2.34	0.42
1:B:166:LEU:HD12	1:B:167:CYS:H	1.83	0.42
1:B:167:CYS:CB	1:B:176:GLN:HG3	2.46	0.42
1:A:104:GLN:O	1:A:107:GLN:HB2	2.19	0.42
1:B:82:LYS:HD2	1:B:215:ASP:OD1	2.18	0.42
1:A:121:ASP:HB3	1:A:246:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:SER:OG	1:A:12:GLU:N	2.53	0.42
1:A:69:ILE:CD1	1:A:254:PHE:HB2	2.46	0.42
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.84	0.42
1:B:81:ASN:HB3	1:B:304:LYS:HD3	2.01	0.42
1:B:303:HIS:O	1:B:306:VAL:HG12	2.19	0.42
1:A:69:ILE:HG21	1:A:69:ILE:HD13	1.72	0.42
1:A:311:GLY:CA	1:A:325:ILE:HG13	2.46	0.42
1:A:276:MET:HE3	1:A:276:MET:HB2	1.87	0.41
1:A:309:MET:HE3	1:A:309:MET:HB3	1.89	0.41
1:B:104:GLN:HE22	6:B:402:PG0:H52	1.84	0.41
1:B:316:ILE:HD13	1:B:316:ILE:HA	1.97	0.41
1:A:160:LEU:HD12	1:A:246:TRP:CZ3	2.55	0.41
1:A:184:TYR:CE1	1:A:249:LEU:HD12	2.55	0.41
1:B:104:GLN:NE2	6:B:402:PG0:H52	2.36	0.41
1:B:167:CYS:SG	1:B:168:GLU:N	2.93	0.41
1:B:313:LEU:HD12	1:B:322:HIS:O	2.20	0.41
1:B:212:LEU:HD12	1:B:235:ARG:NH2	2.36	0.41
1:A:173:PHE:O	1:A:174:ASN:C	2.62	0.41
2:A:401:PG4:H62	2:A:401:PG4:H42	1.60	0.41
1:A:168:GLU:HG3	1:A:169:HIS:H	1.86	0.41
1:B:187:SER:HB2	1:B:190:SER:H	1.86	0.41
1:B:93:ARG:O	1:B:97:ILE:HG13	2.21	0.41
1:A:69:ILE:HD11	1:A:254:PHE:CG	2.55	0.41
1:A:77:SER:OG	1:A:82:LYS:NZ	2.50	0.41
1:B:184:TYR:HB3	1:B:248:SER:HB3	2.03	0.41
1:B:217:LEU:C	1:B:218:LEU:HG	2.45	0.40
1:B:228:LEU:HD13	1:B:228:LEU:HA	1.91	0.40
1:B:262:ILE:HG21	1:B:287:TRP:HH2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/315 (97%)	300 (98%)	5 (2%)	0	100	100
1	B	313/315 (99%)	307 (98%)	6 (2%)	0	100	100
All	All	618/630 (98%)	607 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	278/282 (99%)	277 (100%)	1 (0%)	89	94
1	B	282/282 (100%)	280 (99%)	2 (1%)	81	89
All	All	560/564 (99%)	557 (100%)	3 (0%)	86	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	B	48	ILE
1	B	325	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	174	ASN
1	A	253	HIS
1	B	100	ASN
1	B	104	GLN
1	B	154	ASN
1	B	169	HIS
1	B	176	GLN
1	B	199	ASN
1	B	241	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
7	PG6	B	403	-	17,17,17	0.36	0	16,16,16	0.45	0
4	PO4	A	404	-	4,4,4	0.78	0	6,6,6	0.75	0
4	PO4	B	404	-	4,4,4	1.01	0	6,6,6	0.38	0
6	PG0	B	402	-	7,7,7	0.32	0	6,6,6	0.30	0
5	EDO	B	401	-	3,3,3	0.61	0	2,2,2	0.18	0
2	PG4	A	402	-	12,12,12	0.34	0	11,11,11	0.45	0
2	PG4	A	401	-	12,12,12	0.31	0	11,11,11	0.36	0
3	A1A46	A	403	-	21,21,21	1.13	2 (9%)	24,28,28	1.75	7 (29%)

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
7	PG6	B	403	-	-	6/15/15/15	-
6	PG0	B	402	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	401	-	-	0/1/1/1	-
2	PG4	A	402	-	-	5/10/10/10	-
2	PG4	A	401	-	-	6/10/10/10	-
3	A1A46	A	403	-	-	9/22/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	A1A46	C04-C02	2.27	1.54	1.52
3	A	403	A1A46	C01-C02	2.14	1.55	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	A1A46	C01-C02-C04	5.16	123.57	118.13
3	A	403	A1A46	C04-C06-N09	3.02	115.36	110.02
3	A	403	A1A46	O21-C19-C10	2.69	122.60	113.51
3	A	403	A1A46	O21-C19-O20	-2.33	118.79	124.08
3	A	403	A1A46	C11-C10-N09	2.26	114.63	109.35
3	A	403	A1A46	C19-C10-N09	2.14	116.30	109.40
3	A	403	A1A46	O05-C04-C06	2.08	114.30	108.43

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	A1A46	C19-C10-C11-C12
2	A	401	PG4	C6-C5-O3-C4
2	A	401	PG4	C4-C3-O2-C2
3	A	403	A1A46	N09-C10-C11-C12
7	B	403	PG6	O5-C10-C11-O6
6	B	402	PG0	O1-C3-C4-O2
2	A	402	PG4	O1-C1-C2-O2
2	A	402	PG4	O4-C7-C8-O5
2	A	401	PG4	O1-C1-C2-O2
7	B	403	PG6	O3-C6-C7-O4
3	A	403	A1A46	O05-C04-C06-C07
6	B	402	PG0	C3-C4-O2-C5
7	B	403	PG6	C8-C9-O5-C10
7	B	403	PG6	C11-C10-O5-C9

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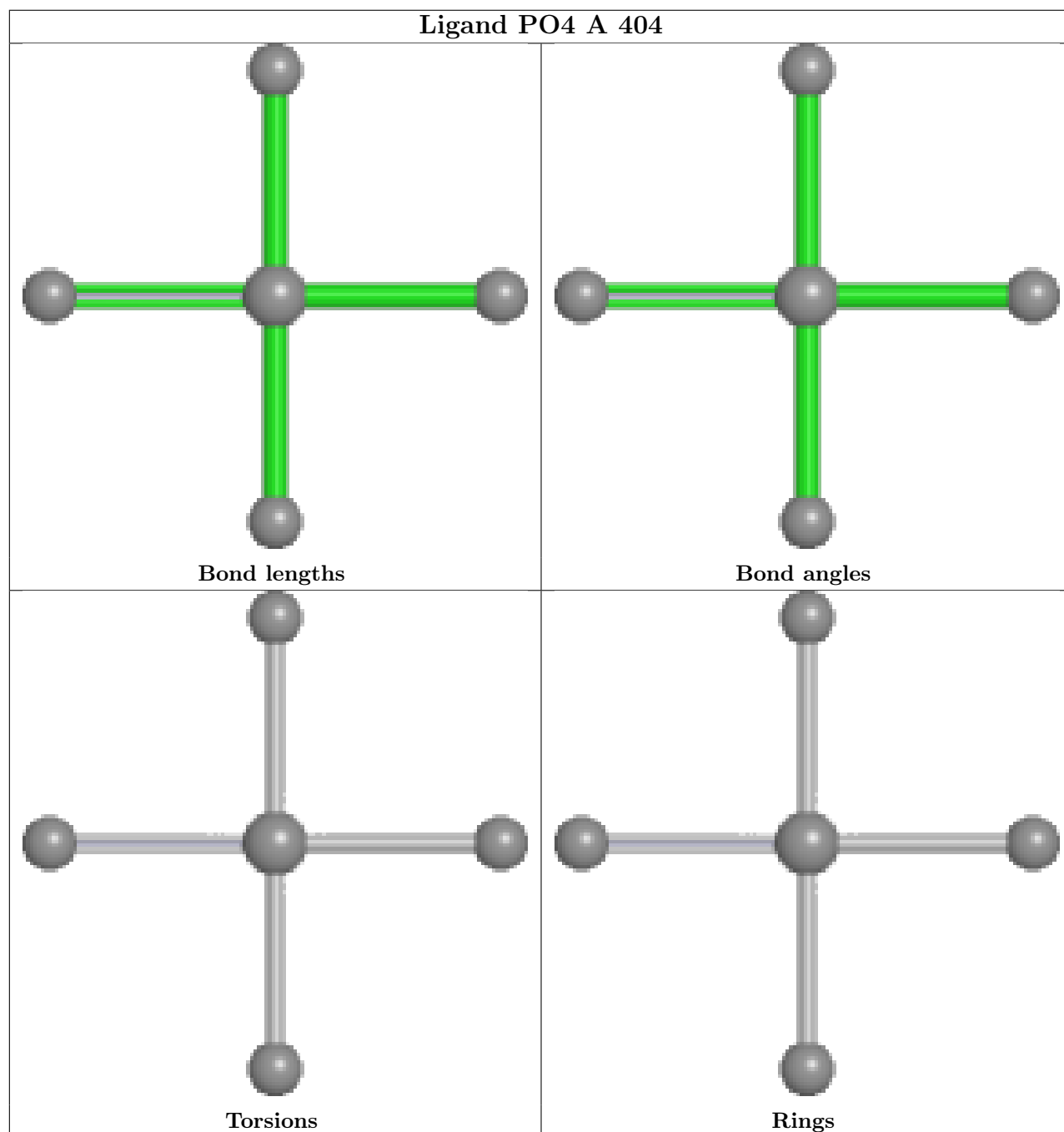
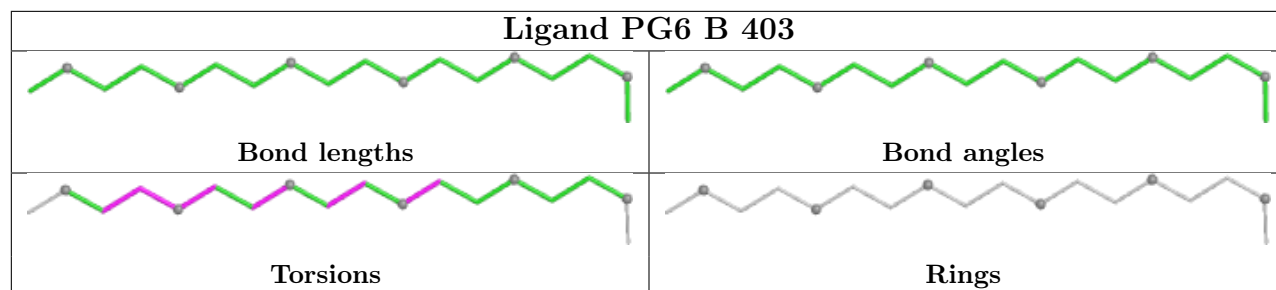
Mol	Chain	Res	Type	Atoms
3	A	403	A1A46	C11-C10-C19-O21
2	A	402	PG4	C6-C5-O3-C4
6	B	402	PG0	C1-C2-O1-C3
7	B	403	PG6	C4-C5-O3-C6
2	A	402	PG4	C3-C4-O3-C5
3	A	403	A1A46	C02-C04-C06-C07
3	A	403	A1A46	C04-C06-N09-C10
3	A	403	A1A46	C04-C06-C07-O08
2	A	401	PG4	O3-C5-C6-O4
3	A	403	A1A46	C11-C10-C19-O20
3	A	403	A1A46	C11-C10-N09-C06
7	B	403	PG6	C9-C8-O4-C7
2	A	401	PG4	O2-C3-C4-O3
2	A	401	PG4	O4-C7-C8-O5
2	A	402	PG4	C1-C2-O2-C3

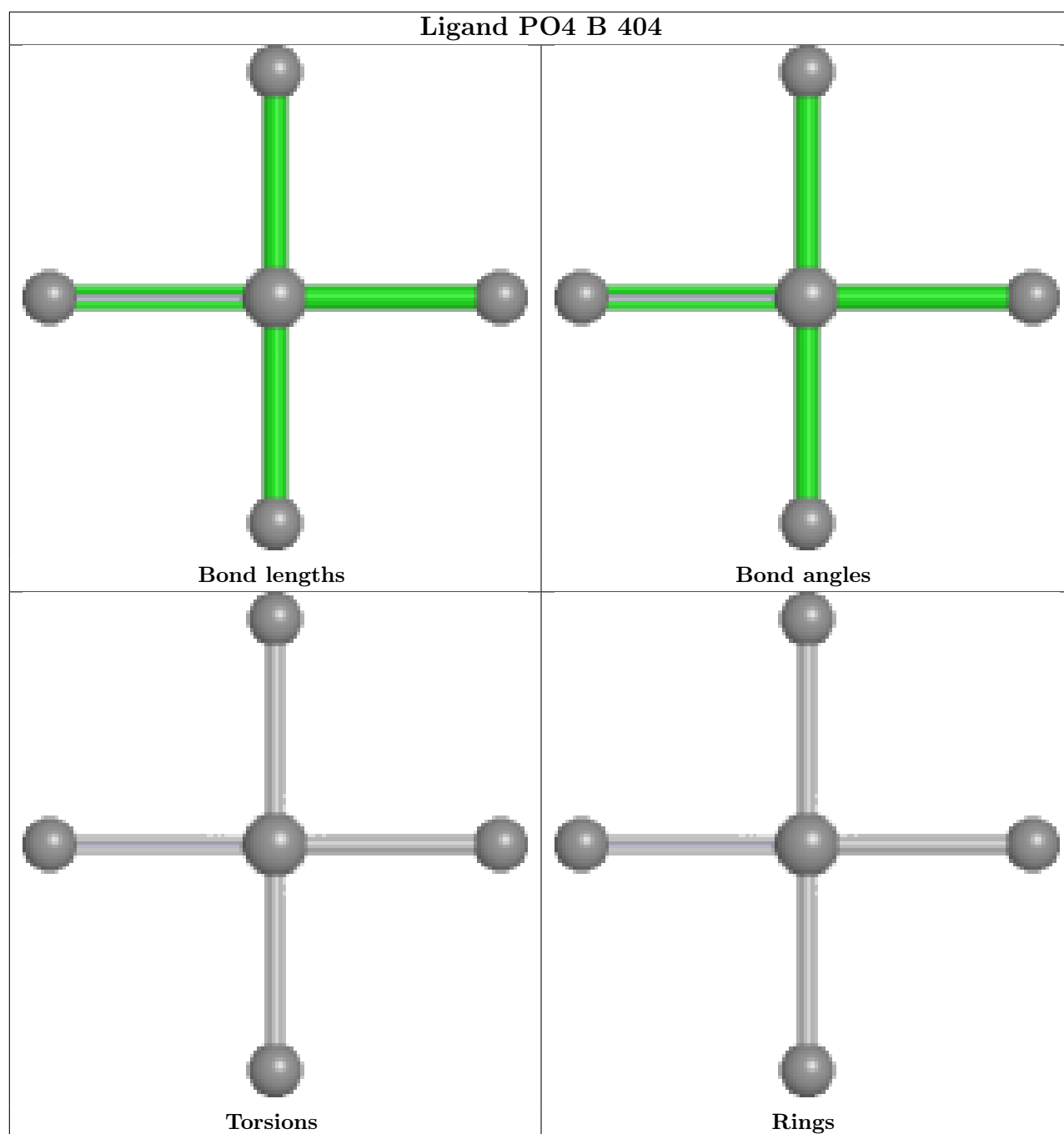
There are no ring outliers.

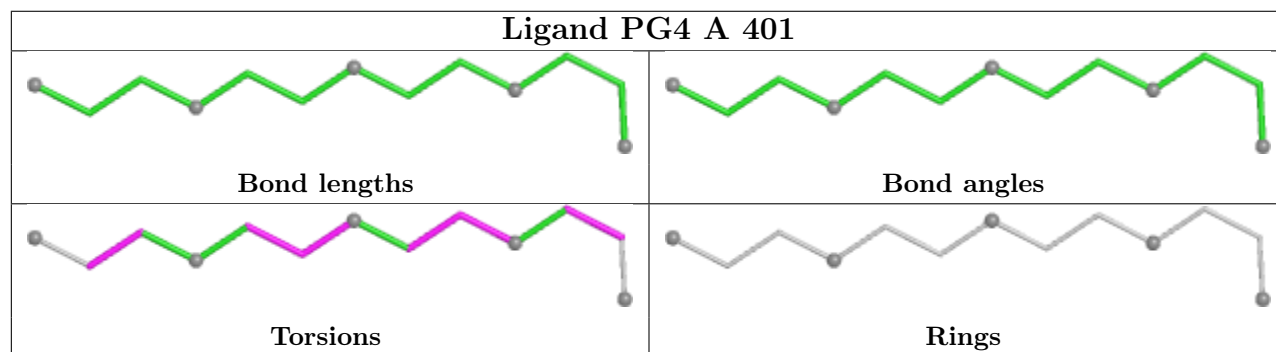
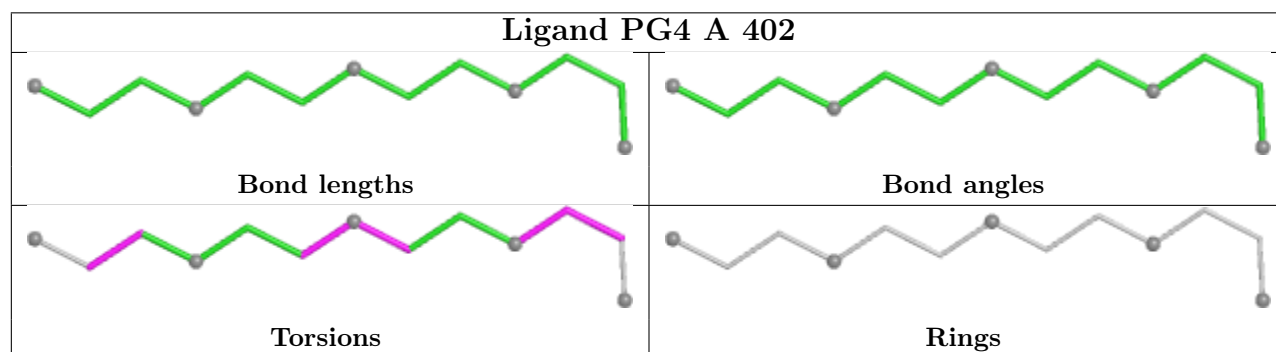
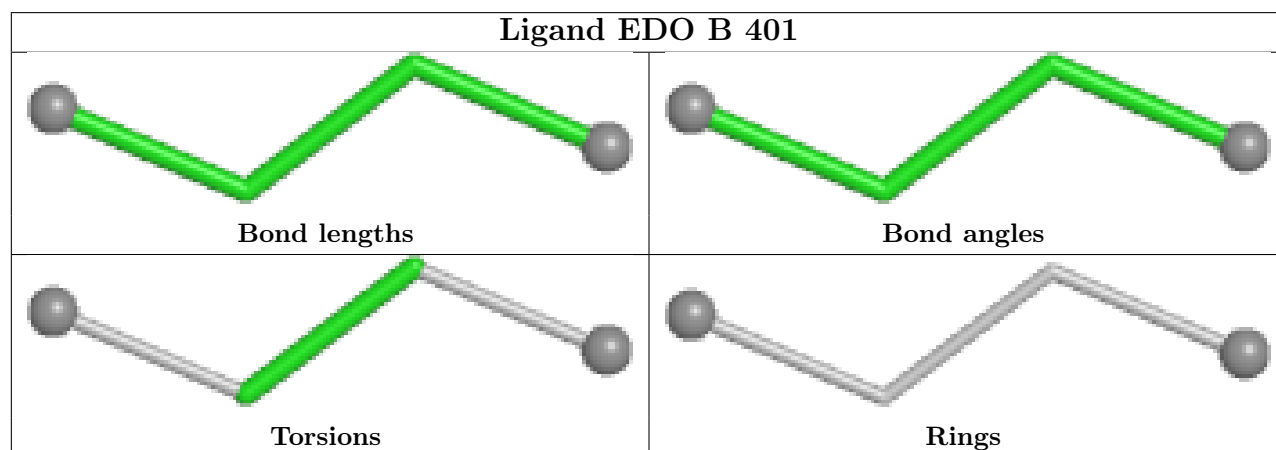
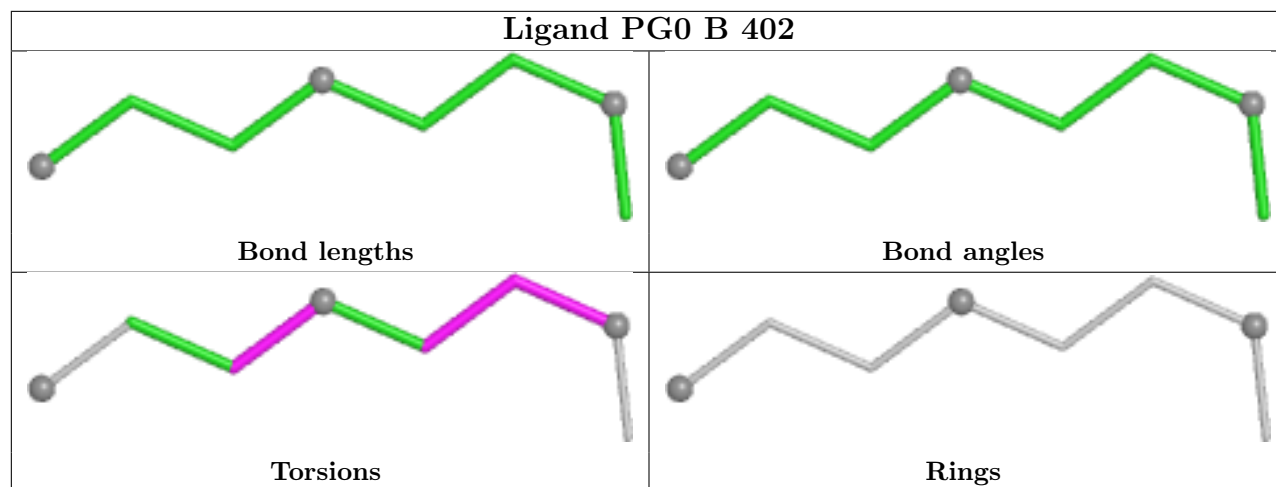
6 monomers are involved in 12 short contacts:

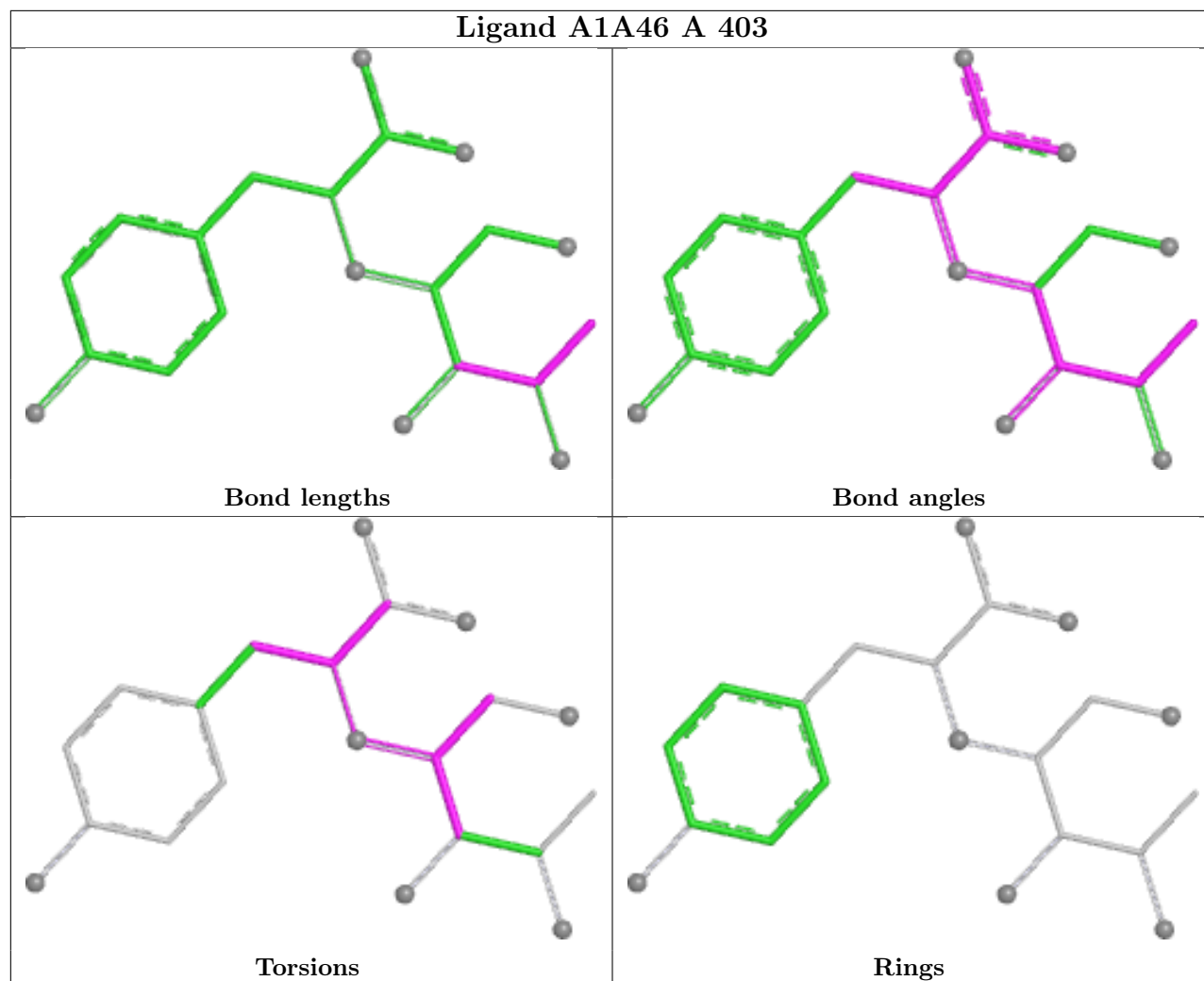
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	403	PG6	1	0
6	B	402	PG0	4	0
5	B	401	EDO	2	0
2	A	402	PG4	2	0
2	A	401	PG4	2	0
3	A	403	A1A46	2	0

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	309/315 (98%)	0.27	12 (3%)	44	41	65, 87, 120, 150	0
1	B	315/315 (100%)	0.25	12 (3%)	44	41	69, 93, 123, 165	0
All	All	624/630 (99%)	0.26	24 (3%)	44	41	65, 90, 123, 165	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	165	GLU	4.1
1	B	309	MET	3.6
1	B	320	PRO	3.2
1	A	84	LEU	3.1
1	A	160	LEU	2.9
1	B	163	ASP	2.8
1	B	310	GLY	2.8
1	B	321	SER	2.6
1	A	224	SER	2.5
1	B	125	PHE	2.4
1	A	305	GLU	2.4
1	A	308	MET	2.3
1	A	109	TYR	2.3
1	A	167	CYS	2.3
1	B	109	TYR	2.3
1	B	219	PRO	2.3
1	A	169	HIS	2.2
1	A	325	ILE	2.2
1	B	319	LYS	2.1
1	B	67	GLU	2.1
1	A	321	SER	2.1
1	B	314	VAL	2.1
1	A	217	LEU	2.0
1	B	170	SER	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

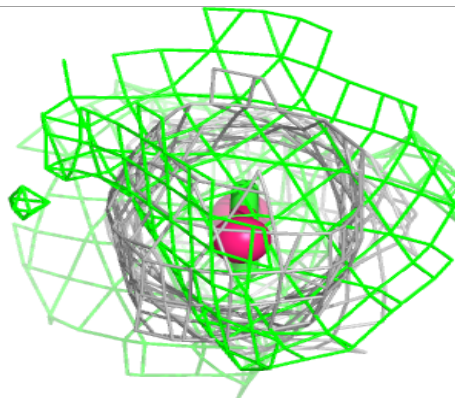
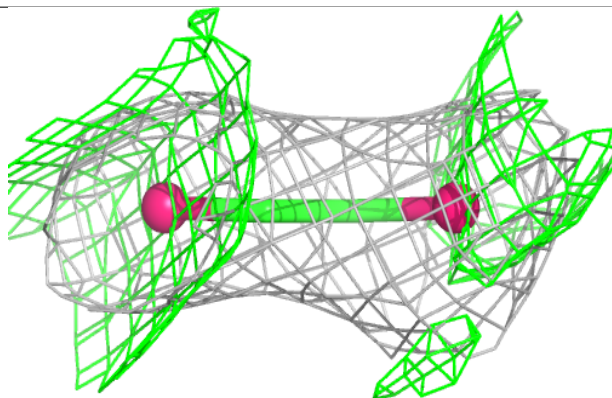
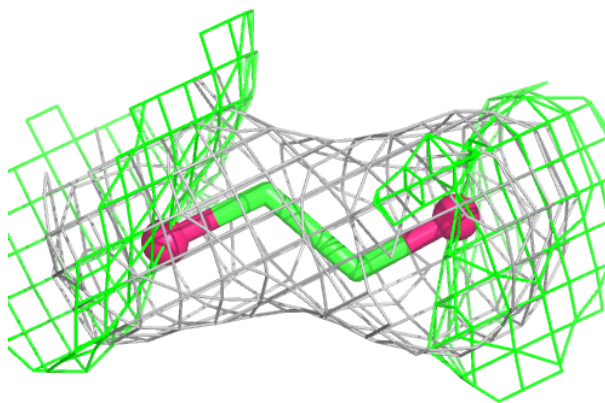
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	401	4/4	0.54	0.50	88,92,92,98	0
3	A1A46	A	403	21/21	0.74	0.26	77,99,107,111	0
2	PG4	A	402	13/13	0.84	0.22	90,95,104,109	0
6	PG0	B	402	8/8	0.85	0.19	78,92,94,100	0
7	PG6	B	403	18/18	0.86	0.19	82,101,119,119	0
2	PG4	A	401	13/13	0.91	0.15	82,91,108,109	0
4	PO4	B	404	5/5	0.95	0.06	75,78,87,89	0
4	PO4	A	404	5/5	0.97	0.06	74,78,82,87	0

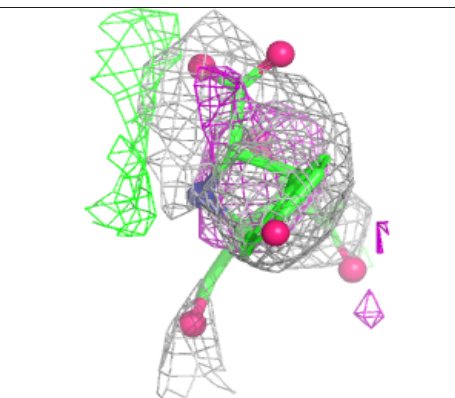
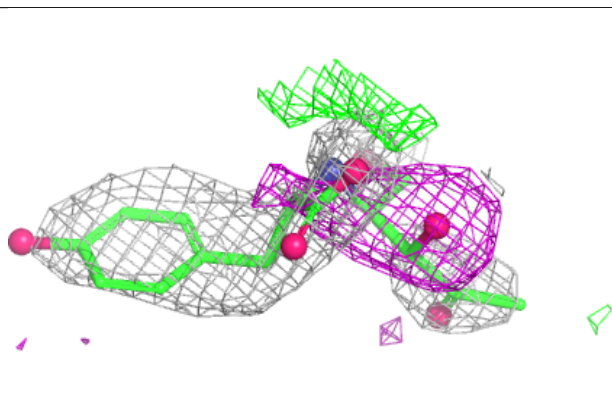
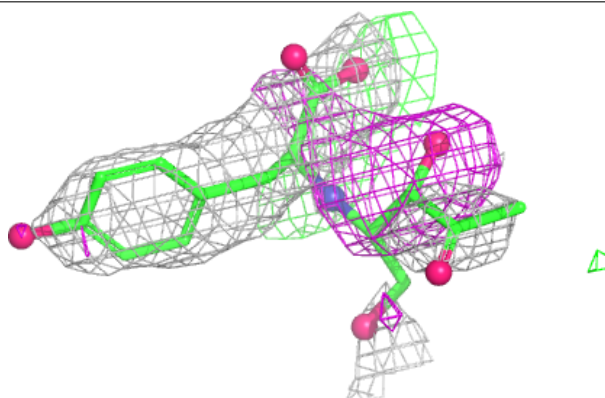
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO B 401:

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

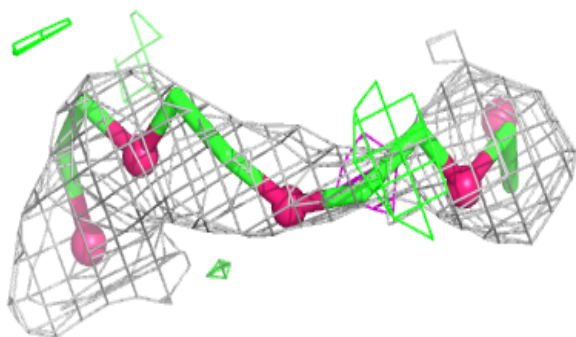
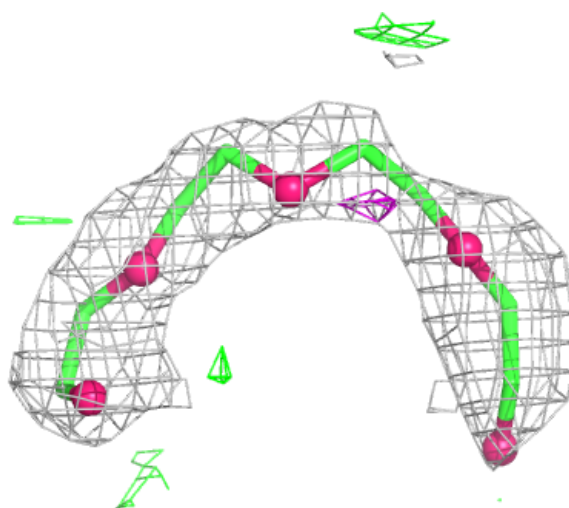
**Electron density around A1A46 A 403:**

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



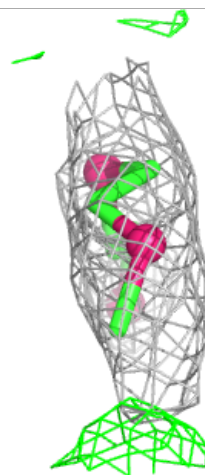
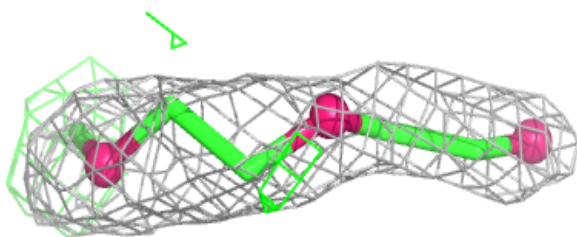
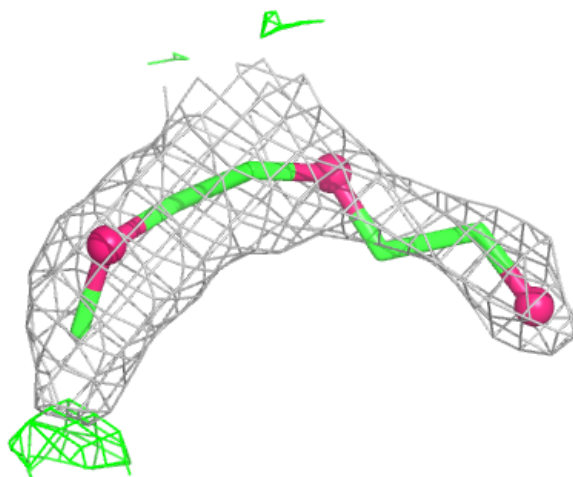
Electron density around PG4 A 402:

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



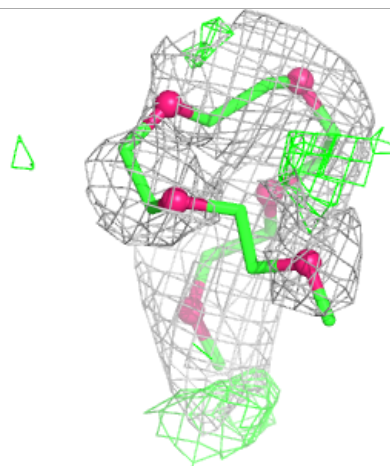
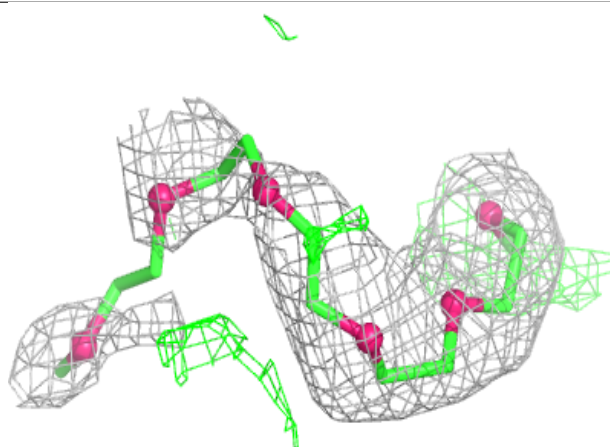
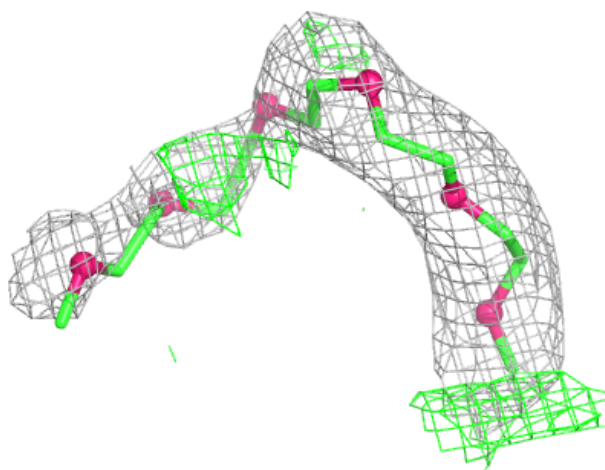
Electron density around PG0 B 402:

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



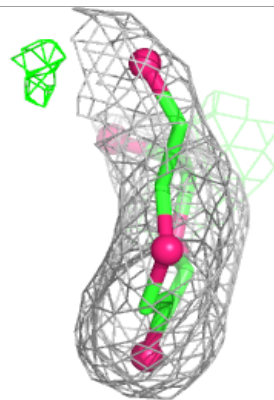
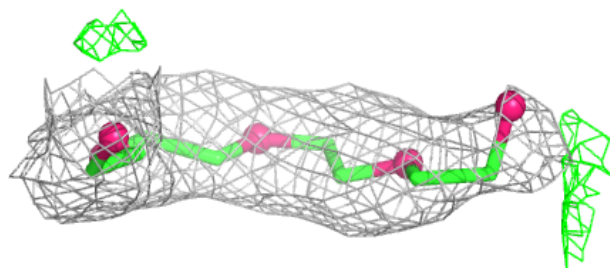
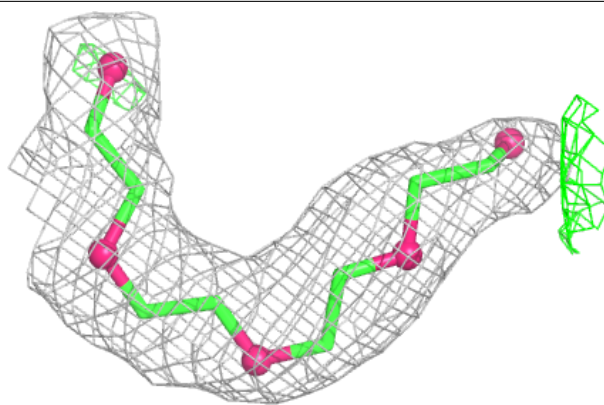
Electron density around PG6 B 403:

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



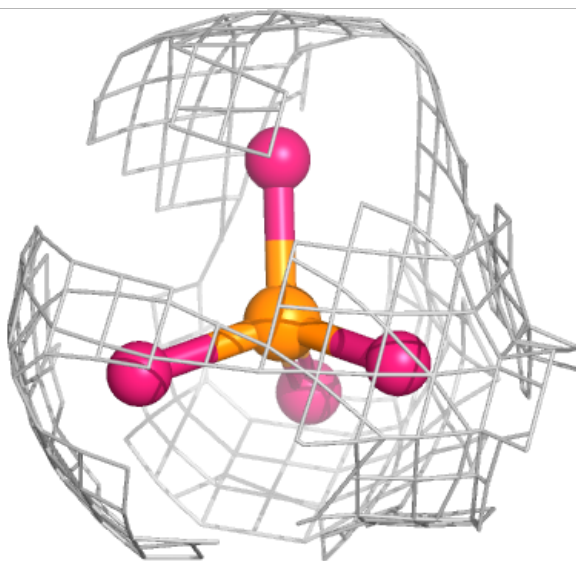
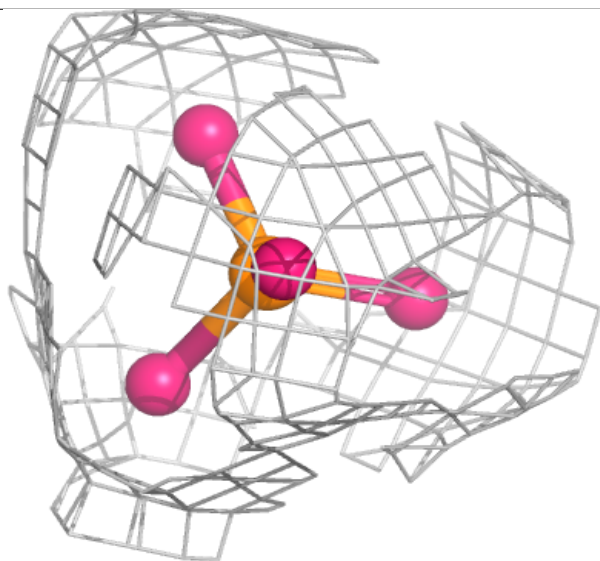
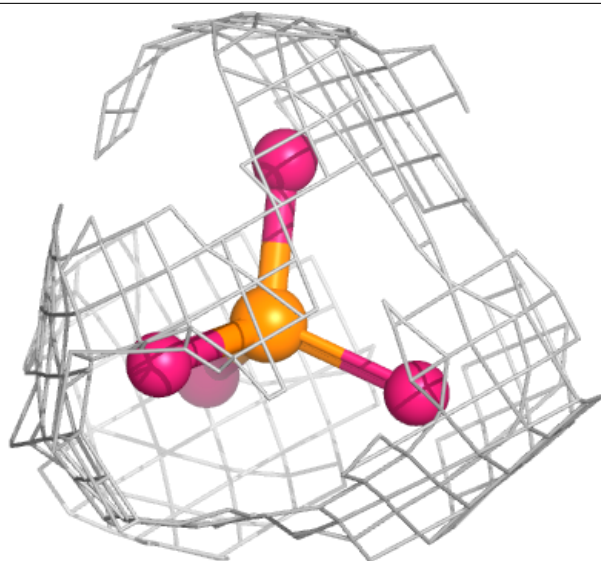
Electron density around PG4 A 401:

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



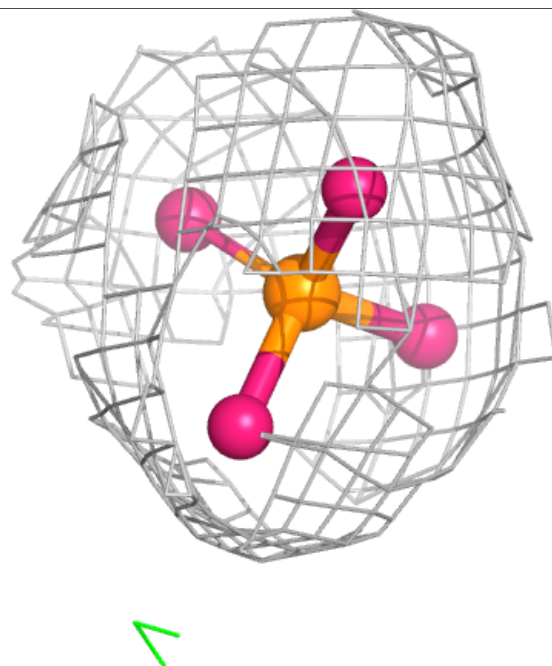
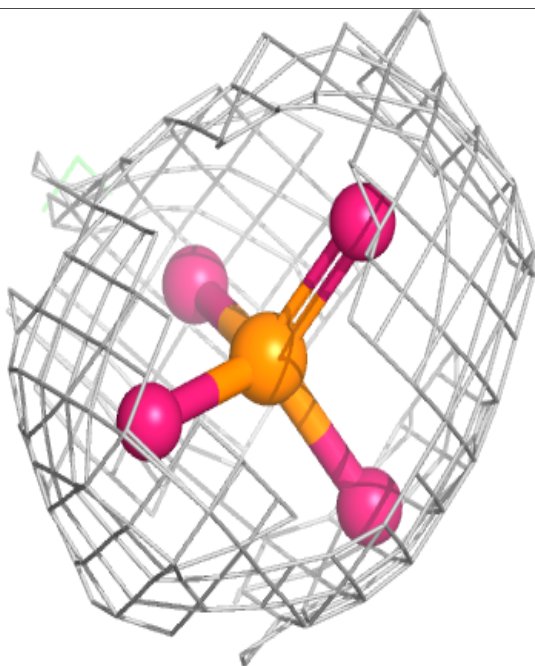
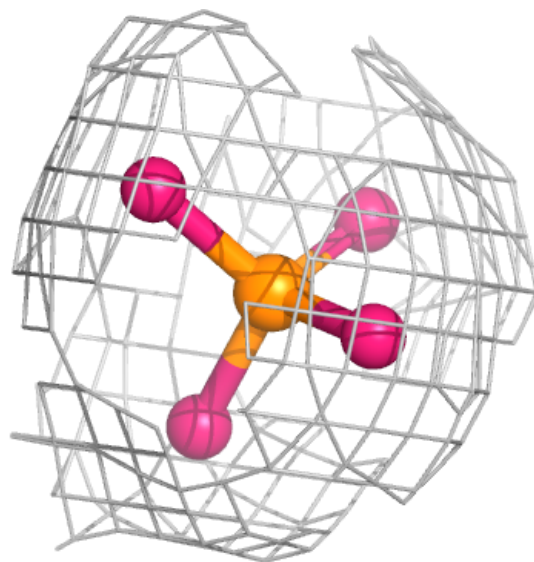
Electron density around PO4 B 404:

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



Electron density around PO4 A 404:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.