Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 06:15 AM JST

PDB ID	:	6LIO
Title	:	Crystal structure of human PDK2 complexed with GM67520
Authors	:	Kang, J.; Kim, J.
Deposited on	:	2019-12-12
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:

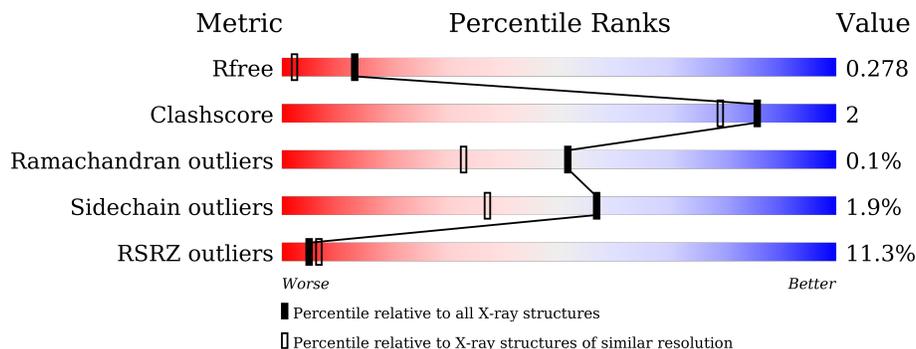|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.76 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 | Percentile Ranks | Value

Rfree — 0.278
Clashscore — 2
Ramachandran outliers — 0.1%
Sidechain outliers — 1.9%
RSRZ outliers — 11.3%

Worse — *Better*

▌Percentile relative to all X-ray structures
▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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% 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	411	13% / 79% 7% 14%
1	B	411	7% / 85% 5% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6397 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 [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	4	0
			2851	1825	477	531	18			
1	B	371	Total	C	N	O	S	0	2	0
			2969	1903	495	553	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP Q15119
A	-23	ALA	-	expression tag	UNP Q15119
A	-22	GLY	-	expression tag	UNP Q15119
A	-21	SER	-	expression tag	UNP Q15119
A	-20	HIS	-	expression tag	UNP Q15119
A	-19	HIS	-	expression tag	UNP Q15119
A	-18	HIS	-	expression tag	UNP Q15119
A	-17	HIS	-	expression tag	UNP Q15119
A	-16	HIS	-	expression tag	UNP Q15119
A	-15	HIS	-	expression tag	UNP Q15119
A	-14	GLY	-	expression tag	UNP Q15119
A	-13	MET	-	expression tag	UNP Q15119
A	-12	ALA	-	expression tag	UNP Q15119
A	-11	SER	-	expression tag	UNP Q15119
A	-10	MET	-	expression tag	UNP Q15119
A	-9	THR	-	expression tag	UNP Q15119
A	-8	GLY	-	expression tag	UNP Q15119
A	-7	GLY	-	expression tag	UNP Q15119
A	-6	GLN	-	expression tag	UNP Q15119
A	-5	GLN	-	expression tag	UNP Q15119
A	-4	MET	-	expression tag	UNP Q15119
A	-3	GLY	-	expression tag	UNP Q15119
A	-2	ARG	-	expression tag	UNP Q15119
A	-1	SER	-	expression tag	UNP Q15119

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q15119
A	1	ASP	-	expression tag	UNP Q15119
A	2	ASP	-	expression tag	UNP Q15119
A	3	ASP	-	expression tag	UNP Q15119
A	4	ASP	-	expression tag	UNP Q15119
A	5	LYS	-	expression tag	UNP Q15119
B	-24	MET	-	expression tag	UNP Q15119
B	-23	ALA	-	expression tag	UNP Q15119
B	-22	GLY	-	expression tag	UNP Q15119
B	-21	SER	-	expression tag	UNP Q15119
B	-20	HIS	-	expression tag	UNP Q15119
B	-19	HIS	-	expression tag	UNP Q15119
B	-18	HIS	-	expression tag	UNP Q15119
B	-17	HIS	-	expression tag	UNP Q15119
B	-16	HIS	-	expression tag	UNP Q15119
B	-15	HIS	-	expression tag	UNP Q15119
B	-14	GLY	-	expression tag	UNP Q15119
B	-13	MET	-	expression tag	UNP Q15119
B	-12	ALA	-	expression tag	UNP Q15119
B	-11	SER	-	expression tag	UNP Q15119
B	-10	MET	-	expression tag	UNP Q15119
B	-9	THR	-	expression tag	UNP Q15119
B	-8	GLY	-	expression tag	UNP Q15119
B	-7	GLY	-	expression tag	UNP Q15119
B	-6	GLN	-	expression tag	UNP Q15119
B	-5	GLN	-	expression tag	UNP Q15119
B	-4	MET	-	expression tag	UNP Q15119
B	-3	GLY	-	expression tag	UNP Q15119
B	-2	ARG	-	expression tag	UNP Q15119
B	-1	SER	-	expression tag	UNP Q15119
B	0	GLY	-	expression tag	UNP Q15119
B	1	ASP	-	expression tag	UNP Q15119
B	2	ASP	-	expression tag	UNP Q15119
B	3	ASP	-	expression tag	UNP Q15119
B	4	ASP	-	expression tag	UNP Q15119
B	5	LYS	-	expression tag	UNP Q15119

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
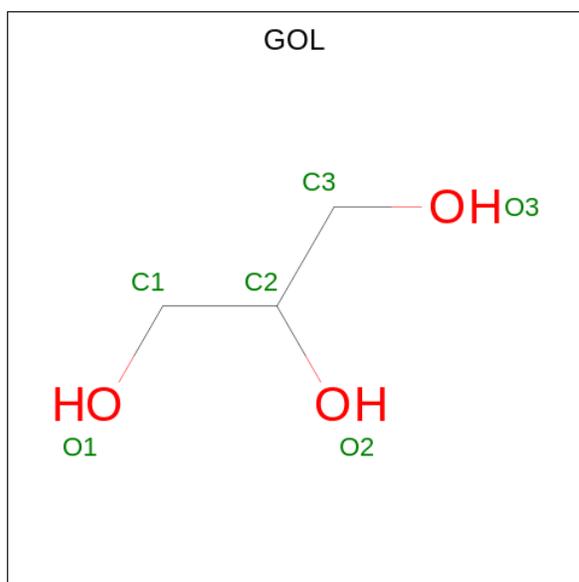
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

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

SO4

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

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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

- Molecule 4 is 4-[[[5-[5-chloranyl-2,4-bis(oxidanyl)phenyl]-4-[4-(1-methylsulfonylpiper idin-4-yl)oxyphenyl]-1,2-oxazol-3-yl]carbonylamino]methyl]cyclohexane-1-carboxylic acid (three-letter code: EH3) (formula: $C_{30}H_{34}ClN_3O_9S$) (labeled as "Ligand of Interest" by depositor).
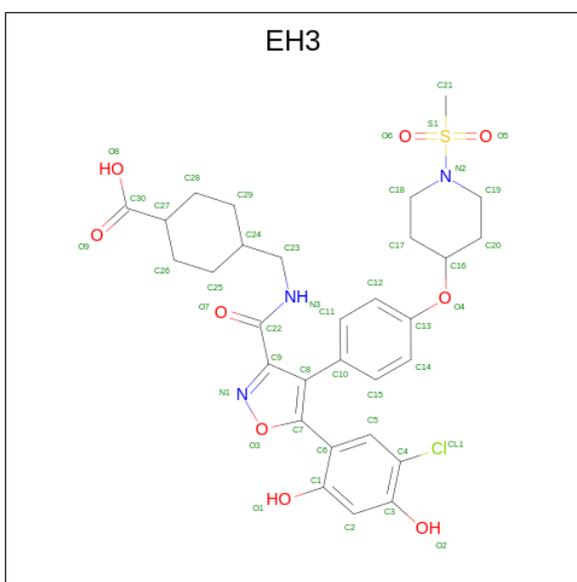
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 44	C 30	Cl 1	N 3	O 9	S 1	0	0
4	B	1	Total 44	C 30	Cl 1	N 3	O 9	S 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total 193	O 193	0	0
5	B	258	Total 258	O 258	0	0

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: [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial
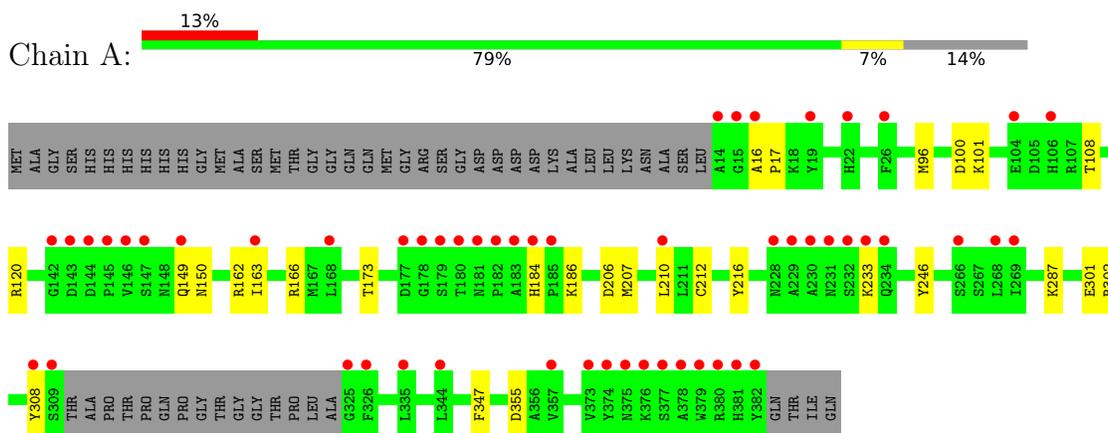
• Molecule 1: [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial
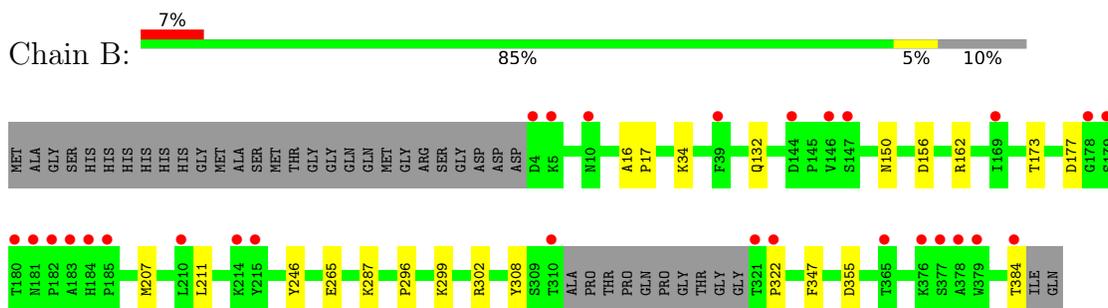
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.95Å 95.12Å 162.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.53 – 1.76 36.50 – 1.76	Depositor EDS
% Data completeness (in resolution range)	91.3 (36.53-1.76) 91.3 (36.50-1.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.234 , 0.269 0.246 , 0.278	Depositor DCC
R_{free} test set	4055 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.0	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6397	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EH3, GOL, SO4

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	0.72	0/2921	0.81	0/3959
1	B	0.72	0/3039	0.80	0/4118
All	All	0.72	0/5960	0.80	0/8077

There are no bond length outliers.

There are no bond angle outliers.

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	2851	0	2769	17	0
1	B	2969	0	2930	12	0
2	A	6	0	8	0	0
2	B	12	0	16	1	0
3	A	15	0	0	2	0
3	B	5	0	0	0	0
4	A	44	0	0	0	0
4	B	44	0	0	1	0
5	A	193	0	0	0	0
5	B	258	0	0	4	0
All	All	6397	0	5723	26	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 (26) 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:206:ASP:O	1:A:210:LEU:HD23	1.85	0.74
1:A:96:MET:HA	1:A:96:MET:HE2	1.84	0.58
1:B:173:THR:O	1:B:177:ASP:HB2	2.03	0.58
1:B:302:ARG:HG3	5:B:583:HOH:O	2.05	0.56
1:A:96:MET:HA	1:A:96:MET:CE	2.36	0.55
1:A:355:ASP:OD2	1:B:287:LYS:NZ	2.44	0.51
1:A:287:LYS:NZ	1:B:355:ASP:OD2	2.44	0.50
1:A:16:ALA:HB3	1:A:17:PRO:HD3	1.97	0.47
1:A:101:LYS:HE2	1:A:108:THR:HA	1.97	0.46
1:B:132:GLN:HG2	5:B:661:HOH:O	2.15	0.46
2:B:402:GOL:H32	5:B:602:HOH:O	2.15	0.46
1:A:347:PHE:CE2	1:B:347:PHE:HB3	2.51	0.46
1:A:207:MET:HG3	1:A:246:TYR:OH	2.16	0.44
1:A:347:PHE:CZ	1:B:347:PHE:HB3	2.52	0.44
1:B:265:GLU:HG3	5:B:716:HOH:O	2.17	0.44
1:A:301:GLU:HG3	1:A:302:ARG:N	2.33	0.43
1:A:162[B]:ARG:HG3	1:A:163:ILE:N	2.31	0.43
1:A:233:LYS:HB2	3:A:403:SO4:O1	2.19	0.42
1:B:207:MET:HG3	1:B:246:TYR:OH	2.19	0.42
1:A:96:MET:CE	1:A:96:MET:CA	2.97	0.42
1:A:166:ARG:NH2	3:A:404:SO4:O2	2.53	0.42
1:A:212[B]:CYS:SG	1:A:216:TYR:HD2	2.43	0.42
1:B:296:PRO:HG2	1:B:299:LYS:HD2	2.02	0.41
1:B:308:TYR:OH	4:B:404:EH3:O9	2.29	0.41
1:A:120:ARG:NH1	1:A:173:THR:OG1	2.53	0.41
1:B:16:ALA:HB3	1:B:17:PRO:HD3	2.03	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	354/411 (86%)	346 (98%)	8 (2%)	0	100	100
1	B	369/411 (90%)	358 (97%)	10 (3%)	1 (0%)	41	22
All	All	723/822 (88%)	704 (97%)	18 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	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	313/361 (87%)	307 (98%)	6 (2%)	57	37
1	B	329/361 (91%)	322 (98%)	7 (2%)	53	31
All	All	642/722 (89%)	629 (98%)	13 (2%)	57	34

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	149	GLN
1	A	150	ASN
1	A	184	HIS
1	A	186	LYS
1	A	308	TYR
1	B	34	LYS
1	B	150	ASN
1	B	156	ASP
1	B	162[A]	ARG
1	B	162[B]	ARG
1	B	211	LEU

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Mol	Chain	Res	Type
1	B	384	THR

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

Mol	Chain	Res	Type
1	A	149	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	A	403	-	4,4,4	0.36	0	6,6,6	0.13	0
3	SO4	A	402	-	4,4,4	0.38	0	6,6,6	0.18	0
2	GOL	B	402	-	5,5,5	0.20	0	5,5,5	0.61	0
3	SO4	A	404	-	4,4,4	0.33	0	6,6,6	0.07	0
4	EH3	A	405	-	44,48,48	0.90	2 (4%)	62,70,70	2.01	14 (22%)
2	GOL	A	401	-	5,5,5	0.10	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SO4	B	403	-	4,4,4	0.30	0	6,6,6	0.17	0
2	GOL	B	401	-	5,5,5	0.22	0	5,5,5	0.47	0
4	EH3	B	404	-	44,48,48	0.86	2 (4%)	62,70,70	1.79	10 (16%)

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	GOL	B	402	-	-	1/4/4/4	-
4	EH3	A	405	-	-	10/23/51/51	1/5/5/5
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	B	401	-	-	1/4/4/4	-
4	EH3	B	404	-	-	0/23/51/51	1/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	EH3	C8-C9	-4.30	1.36	1.41
4	B	404	EH3	O8-C30	-2.80	1.21	1.30
4	B	404	EH3	C19-N2	-2.59	1.45	1.47
4	A	405	EH3	O8-C30	-2.28	1.23	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	EH3	C19-N2-C18	6.78	119.67	112.17
4	A	405	EH3	C9-C8-C7	6.43	110.22	104.90
4	B	404	EH3	C9-C8-C7	6.21	110.03	104.90
4	A	405	EH3	C8-C9-C22	-5.11	121.00	130.97
4	B	404	EH3	C8-C9-C22	-5.04	121.13	130.97
4	A	405	EH3	C20-C19-N2	4.92	116.13	109.43
4	B	404	EH3	C18-C17-C16	4.81	115.61	110.32
4	B	404	EH3	C19-C20-C16	3.95	114.67	110.32
4	B	404	EH3	C20-C16-C17	3.87	119.22	111.74
4	A	405	EH3	O5-S1-N2	3.73	110.16	107.03
4	A	405	EH3	C21-S1-N2	-3.62	104.22	107.36
4	A	405	EH3	C19-C20-C16	3.59	114.27	110.32
4	B	404	EH3	O4-C16-C17	-3.29	101.03	108.31
4	A	405	EH3	C9-C22-N3	2.92	118.51	115.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	404	EH3	O4-C13-C12	-2.77	106.44	119.93
4	B	404	EH3	O4-C13-C14	2.72	133.18	119.93
4	A	405	EH3	C18-C17-C16	-2.69	107.36	110.32
4	A	405	EH3	O4-C16-C20	-2.39	103.02	108.31
4	B	404	EH3	C20-C19-N2	-2.33	106.25	109.43
4	A	405	EH3	C2-C3-C4	2.31	119.57	118.44
4	B	404	EH3	C18-N2-S1	2.25	119.07	116.30
4	A	405	EH3	O9-C30-C27	-2.24	117.45	122.93
4	A	405	EH3	O6-S1-N2	2.16	108.85	107.03
4	A	405	EH3	C17-C18-N2	2.02	112.19	109.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	EH3	C19-N2-S1-C21
4	A	405	EH3	C19-N2-S1-O5
4	A	405	EH3	C19-N2-S1-O6
2	A	401	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
4	A	405	EH3	C18-N2-S1-O5
4	A	405	EH3	C18-N2-S1-O6
2	B	401	GOL	C1-C2-C3-O3
4	A	405	EH3	C14-C13-O4-C16
4	A	405	EH3	C12-C13-O4-C16
4	A	405	EH3	C26-C27-C30-O8
4	A	405	EH3	C26-C27-C30-O9
4	A	405	EH3	C18-N2-S1-C21

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	EH3	C24-C25-C26-C27-C28-C29
4	B	404	EH3	C24-C25-C26-C27-C28-C29

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	SO4	1	0
2	B	402	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	SO4	1	0
4	B	404	EH3	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand EH3 A 405

Bond lengths

Bond angles

Torsions

Rings

Ligand EH3 B 404

Bond lengths

Bond angles

Torsions

Rings
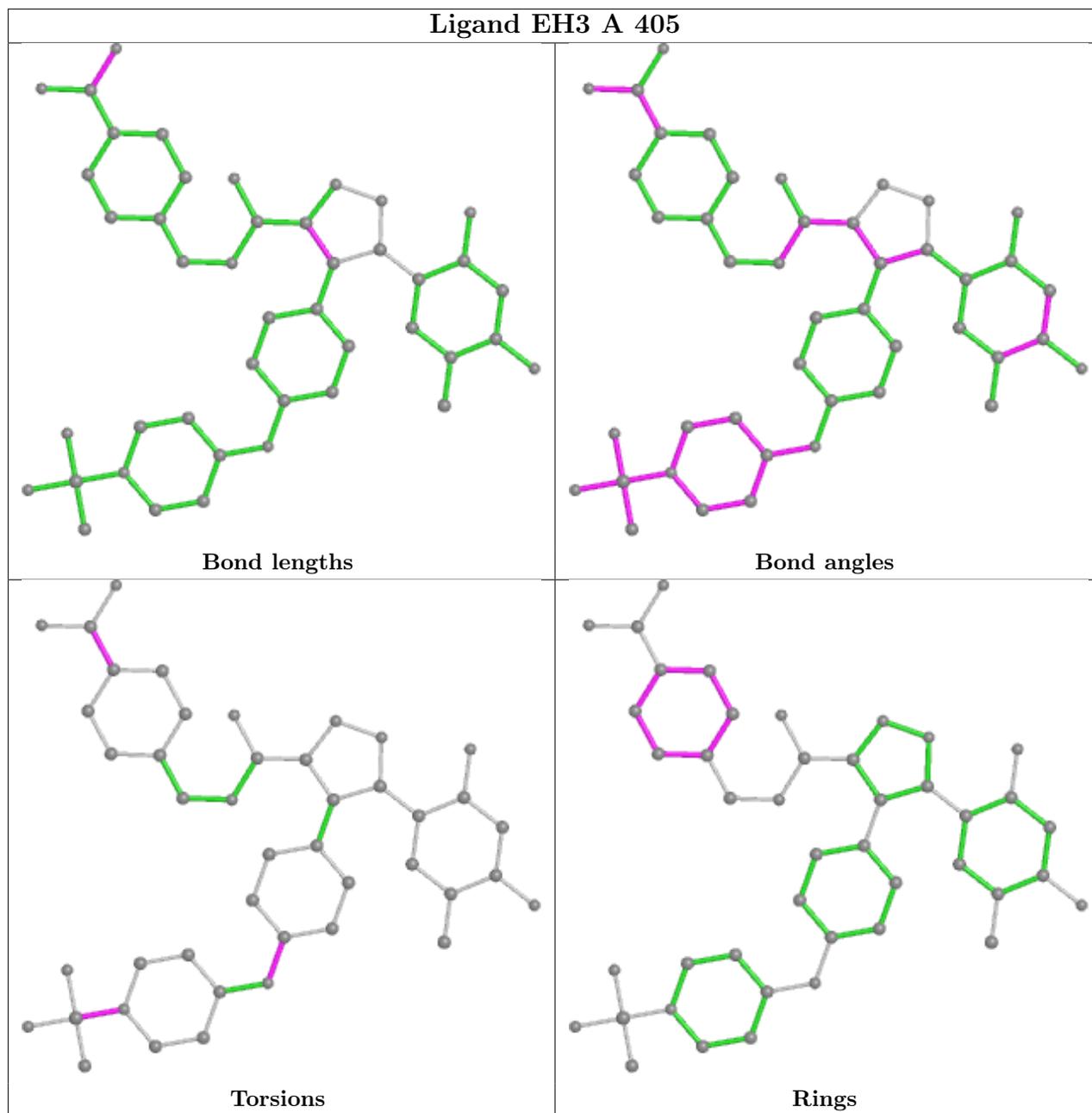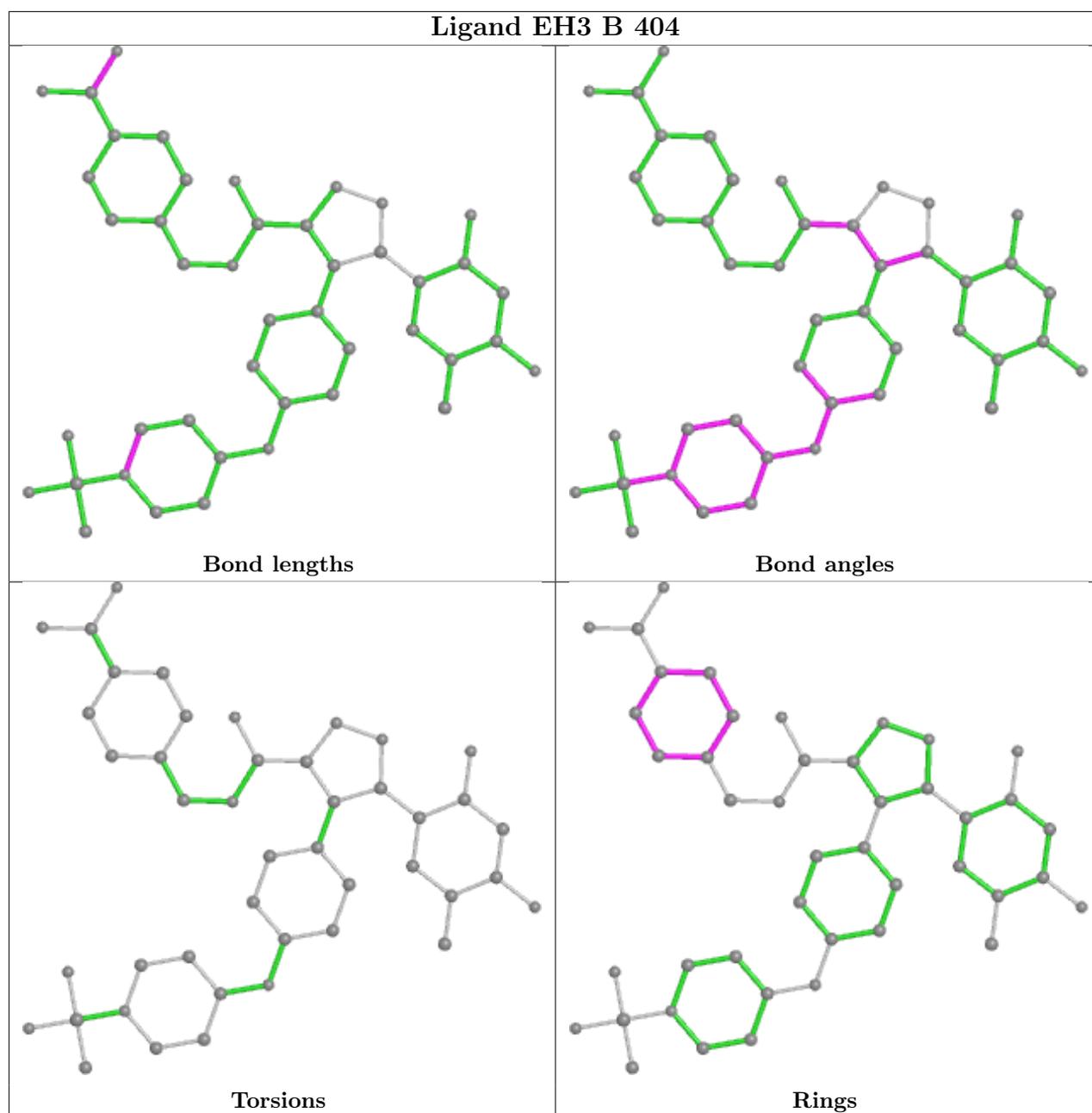
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	354/411 (86%)	0.81	54 (15%)	2	3	24, 33, 77, 121	0
1	B	371/411 (90%)	0.42	28 (7%)	14	19	22, 31, 64, 113	0
All	All	725/822 (88%)	0.61	82 (11%)	5	7	22, 32, 69, 121	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	ASN	11.6
1	A	180	THR	11.1
1	A	179	SER	9.6
1	B	384	THR	9.2
1	A	181	ASN	8.9
1	B	321	THR	8.4
1	A	147	SER	7.9
1	B	180	THR	7.9
1	A	183	ALA	7.3
1	B	179	SER	7.3
1	A	146	VAL	6.5
1	A	178	GLY	6.4
1	A	182	PRO	6.1
1	A	268	LEU	6.1
1	A	379	TRP	6.0
1	A	145	PRO	5.8
1	B	182	PRO	5.7
1	B	183	ALA	5.7
1	A	229	ALA	5.7
1	A	14	ALA	5.6
1	A	15	GLY	5.4
1	A	326	PHE	5.1
1	A	19	TYR	4.6
1	B	215	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	4	ASP	4.5
1	B	184	HIS	4.5
1	A	378	ALA	4.3
1	A	231	ASN	4.1
1	A	325	GLY	4.1
1	B	185	PRO	4.0
1	A	308	TYR	4.0
1	A	377	SER	4.0
1	A	382	TYR	3.9
1	A	16	ALA	3.8
1	A	185	PRO	3.8
1	A	230	ALA	3.7
1	A	380	ARG	3.6
1	A	381	HIS	3.6
1	A	106	HIS	3.5
1	B	178	GLY	3.4
1	A	335	LEU	3.4
1	A	374	TYR	3.4
1	B	376	LYS	3.3
1	B	310	THR	3.2
1	A	143	ASP	3.1
1	A	233	LYS	3.1
1	A	144	ASP	3.0
1	A	232	SER	2.9
1	A	149	GLN	2.9
1	A	269	ILE	2.8
1	A	266	SER	2.8
1	B	10	ASN	2.8
1	B	146	VAL	2.7
1	A	357	VAL	2.7
1	A	376	LYS	2.7
1	A	184	HIS	2.6
1	B	5	LYS	2.6
1	A	228	ASN	2.6
1	A	309	SER	2.6
1	B	39	PHE	2.6
1	B	214	LYS	2.5
1	B	322	PRO	2.5
1	A	177	ASP	2.4
1	A	163	ILE	2.4
1	A	344	LEU	2.4
1	A	26	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	22	HIS	2.4
1	B	379	TRP	2.3
1	A	210	LEU	2.3
1	B	210	LEU	2.3
1	B	377	SER	2.2
1	A	168	LEU	2.2
1	A	234	GLN	2.1
1	A	104	GLU	2.1
1	A	142	GLY	2.1
1	A	375	ASN	2.1
1	A	373	VAL	2.1
1	B	365	THR	2.0
1	B	147	SER	2.0
1	B	169	ILE	2.0
1	B	144	ASP	2.0
1	B	378	ALA	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 monosaccharides 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.
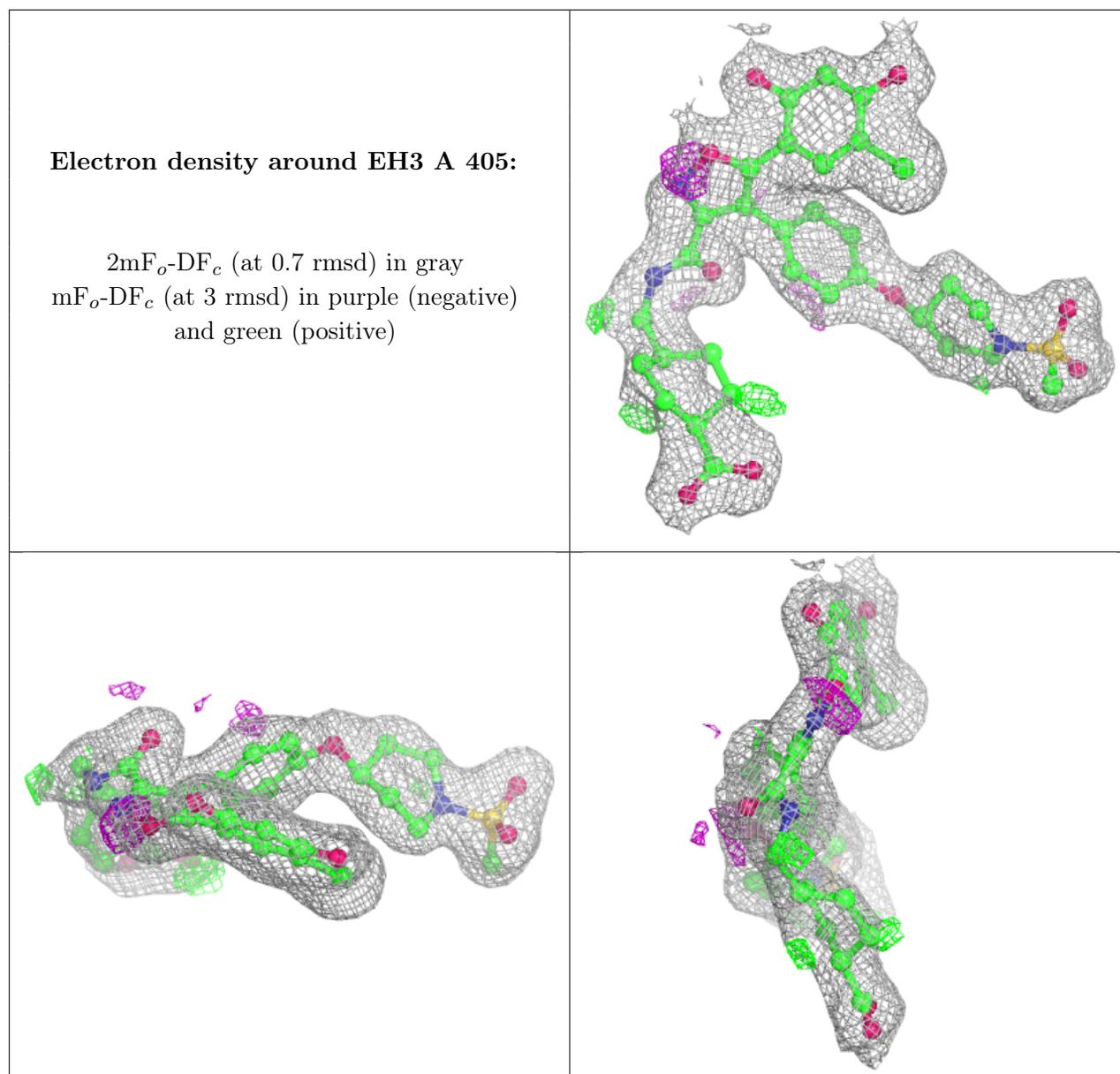
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	404	5/5	0.71	0.26	96,102,105,105	0
2	GOL	B	402	6/6	0.85	0.20	42,60,61,64	0
2	GOL	B	401	6/6	0.88	0.16	31,51,58,58	0
3	SO4	A	402	5/5	0.89	0.26	66,70,76,88	0
2	GOL	A	401	6/6	0.90	0.25	51,62,71,71	0
3	SO4	B	403	5/5	0.94	0.09	50,62,69,80	0
4	EH3	A	405	44/44	0.94	0.11	25,31,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	403	5/5	0.95	0.24	63,72,82,84	0
4	EH3	B	404	44/44	0.95	0.10	23,29,52,53	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 EH3 A 405:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around EH3 B 404:

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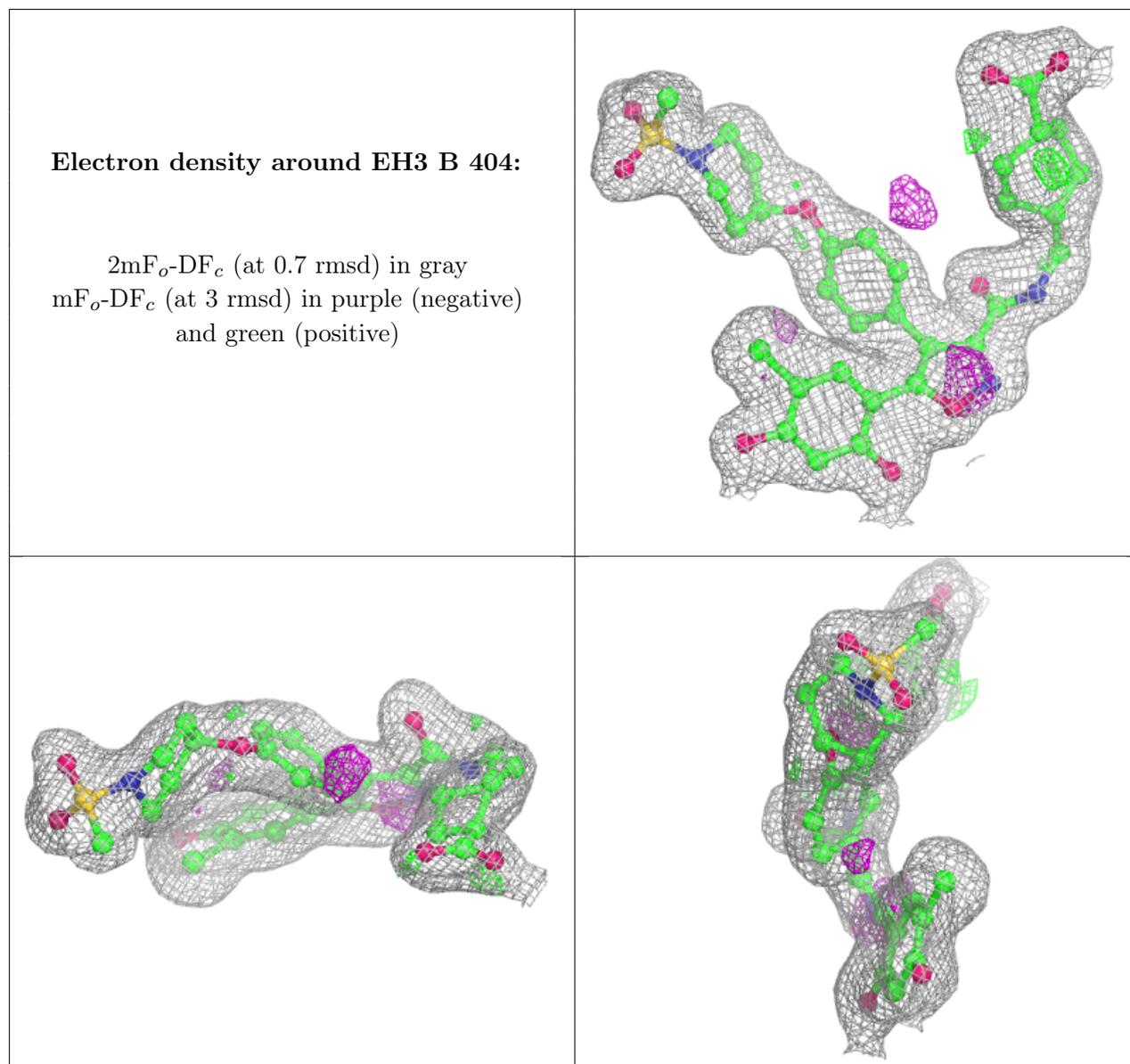
6.5 Other polymers (i)

There are no such residues in this entry.