



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 6LIO / pdb_00006lio
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

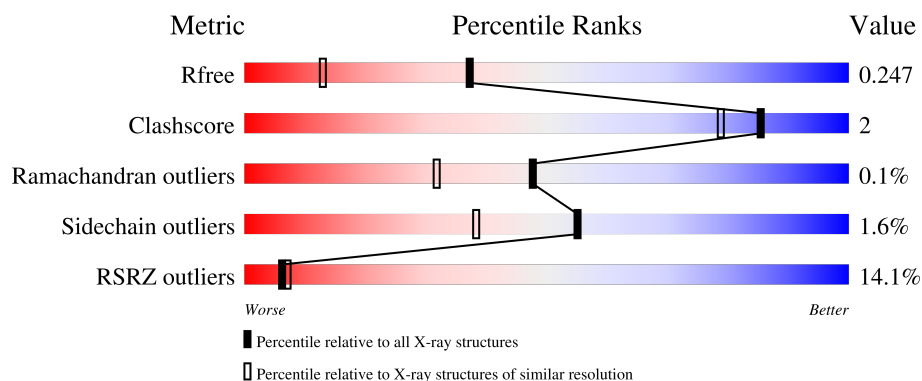
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 $\leq 5\%$. 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	411	16% 79% 7% 14%
1	B	411	9% 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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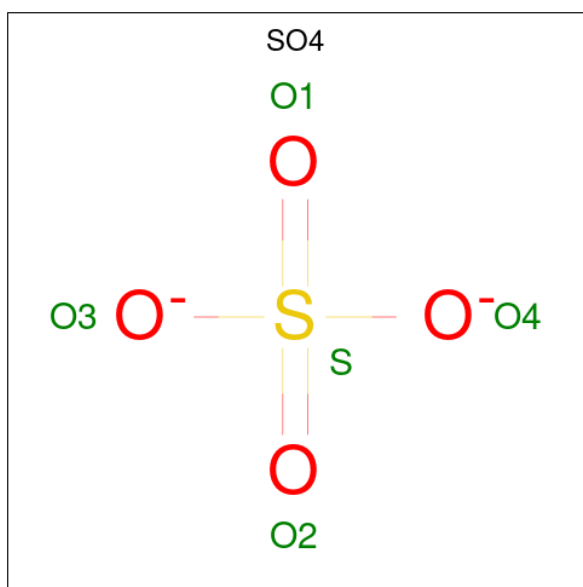
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q15119
A	1	ASP	-	expression tag	UNP Q15119
A	2	ASP	-	expression tag	UNP Q15119
A	3	ASP	-	expression tag	UNP Q15119
A	4	ASP	-	expression tag	UNP Q15119
A	5	LYS	-	expression tag	UNP Q15119
B	-24	MET	-	expression tag	UNP Q15119
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



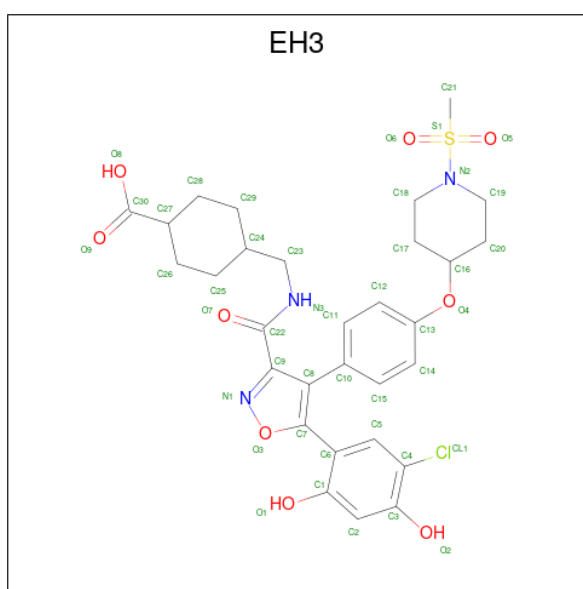
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 4-[[[5-[5-chloranyl-2,4-bis(oxidanyl)phenyl]-4-[4-(1-methylsulfonylpiperidin-4-yl)oxyphenyl]-1,2-oxazol-3-yl]carbonylamino]methyl]cyclohexane-1-carboxylic acid (CCD ID: EH3) (formula: C₃₀H₃₄ClN₃O₉S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	
			44	30	1	3	9	1	0
4	B	1	Total	C	Cl	N	O	S	
			44	30	1	3	9	1	0

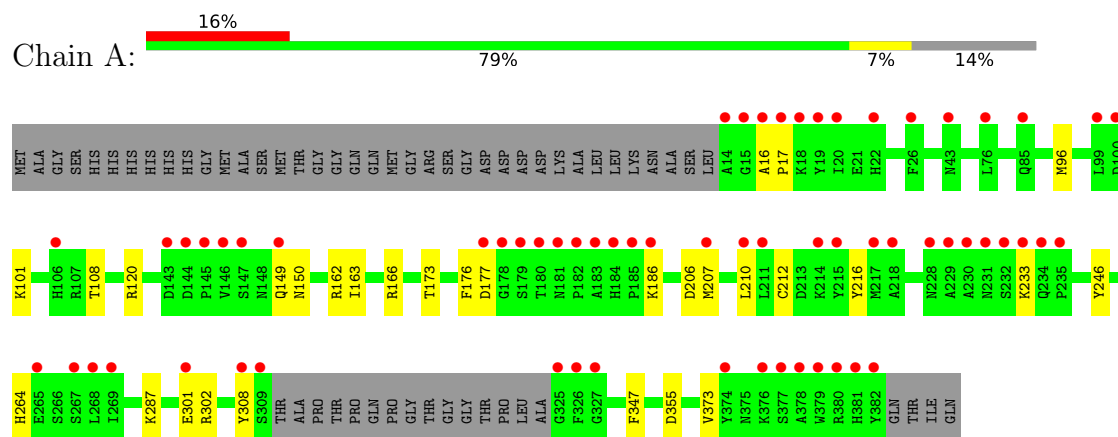
- Molecule 5 is water.

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

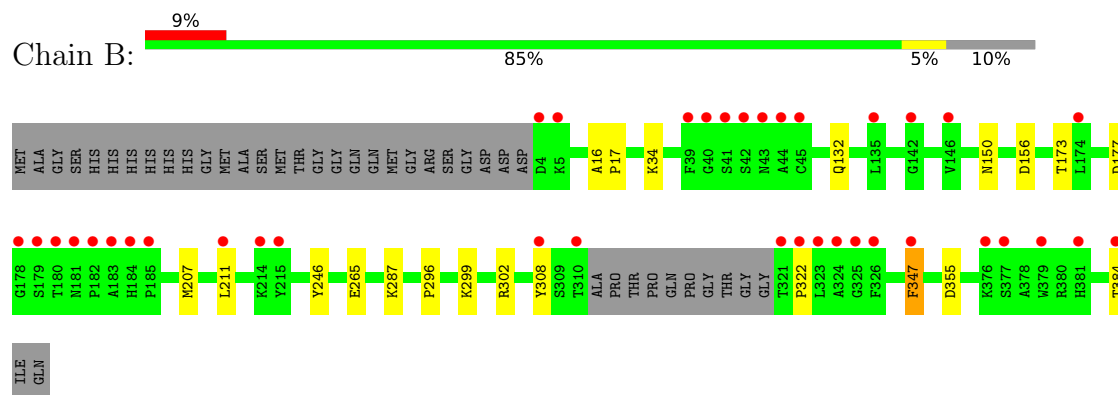
3 Residue-property plots

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 36.53 – 1.76	Depositor EDS
% Data completeness (in resolution range)	91.3 (36.53-1.76) 91.3 (36.53-1.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.234 , 0.269 (Not available) , 0.247	Depositor DCC
R_{free} test set	4055 reflections (4.59%)	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 , 38.3	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	0.93	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.*

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: EH3, SO4, GOL

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	1.04	0/2921	1.27	4/3959 (0.1%)
1	B	1.04	0/3039	1.24	1/4118 (0.0%)
All	All	1.04	0/5960	1.25	5/8077 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ASP	CB-CA-C	-5.30	101.66	110.68
1	A	176	PHE	CA-C-N	5.08	127.34	120.38
1	A	176	PHE	C-N-CA	5.08	127.34	120.38
1	B	347	PHE	CB-CA-C	5.05	117.92	110.14
1	A	264	HIS	CB-CA-C	5.02	118.42	110.19

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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:96:MET:HA	1:A:96:MET:HE2	1.57	0.87
1:A:206:ASP:O	1:A:210:LEU:HD23	1.85	0.74
1:A:96:MET:HE2	1:A:96:MET:CA	2.26	0.65
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: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:96:MET:HA	1:A:96:MET:CE	2.36	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: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 [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	354/411 (86%)	346 (98%)	8 (2%)	0	100	100
1	B	369/411 (90%)	358 (97%)	10 (3%)	1 (0%)	36	21
All	All	723/822 (88%)	704 (97%)	18 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	PRO

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	313/361 (87%)	308 (98%)	5 (2%)	55	38
1	B	329/361 (91%)	324 (98%)	5 (2%)	57	41
All	All	642/722 (89%)	632 (98%)	10 (2%)	55	38

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	150	ASN

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Mol	Chain	Res	Type
1	A	186	LYS
1	A	308	TYR
1	A	373	VAL
1	B	34	LYS
1	B	150	ASN
1	B	156	ASP
1	B	211	LEU
1	B	384	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	150	ASN
1	A	231	ASN
1	B	90	GLN
1	B	187	HIS
1	B	345	GLN
1	B	383	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	404	-	4,4,4	0.32	0	6,6,6	0.11	0
2	GOL	B	401	-	5,5,5	0.22	0	5,5,5	0.47	0
3	SO4	A	403	-	4,4,4	0.33	0	6,6,6	0.17	0
2	GOL	A	401	-	5,5,5	0.10	0	5,5,5	0.26	0
3	SO4	B	403	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO4	A	402	-	4,4,4	0.33	0	6,6,6	0.19	0
4	EH3	A	405	-	48,48,48	0.80	3 (6%)	67,70,70	1.89	17 (25%)
4	EH3	B	404	-	48,48,48	0.95	3 (6%)	67,70,70	1.74	13 (19%)
2	GOL	B	402	-	5,5,5	0.21	0	5,5,5	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	401	-	-	1/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
4	EH3	A	405	-	-	9/31/51/51	1/5/5/5
4	EH3	B	404	-	-	2/31/51/51	1/5/5/5
2	GOL	B	402	-	-	1/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	EH3	O8-C30	-2.91	1.21	1.30
4	B	404	EH3	O3-N1	2.70	1.47	1.42
4	A	405	EH3	C8-C9	-2.68	1.36	1.44
4	B	404	EH3	C19-N2	-2.63	1.45	1.47
4	A	405	EH3	O8-C30	-2.37	1.23	1.30
4	A	405	EH3	O3-N1	2.30	1.46	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	EH3	C19-N2-C18	6.57	119.67	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	EH3	C10-C8-C7	-5.39	119.21	127.60
4	A	405	EH3	C20-C19-N2	5.25	116.13	109.33
4	B	404	EH3	C18-C17-C16	4.89	115.61	110.32
4	A	405	EH3	C10-C8-C7	-4.81	120.12	127.60
4	B	404	EH3	C19-C20-C16	4.01	114.67	110.32
4	B	404	EH3	C8-C9-N1	-3.99	107.70	112.66
4	A	405	EH3	O5-S1-N2	3.77	110.16	107.02
4	B	404	EH3	C20-C16-C17	3.70	119.22	111.67
4	A	405	EH3	C8-C9-N1	-3.69	108.07	112.66
4	A	405	EH3	C19-C20-C16	3.65	114.27	110.32
4	B	404	EH3	C22-C9-N1	3.55	131.15	121.45
4	A	405	EH3	C22-C9-N1	3.46	130.90	121.45
4	B	404	EH3	O4-C16-C17	-3.12	101.03	108.31
4	B	404	EH3	O4-C13-C12	-2.75	106.44	119.90
4	A	405	EH3	C18-C17-C16	-2.74	107.36	110.32
4	B	404	EH3	O4-C13-C14	2.71	133.18	119.90
4	A	405	EH3	C7-O3-N1	-2.63	105.61	108.94
4	A	405	EH3	C21-S1-N2	-2.60	104.22	107.27
4	B	404	EH3	O3-C7-C6	2.47	120.62	115.50
4	B	404	EH3	C20-C19-N2	-2.38	106.25	109.33
4	A	405	EH3	O3-N1-C9	2.30	107.79	104.88
4	A	405	EH3	C2-C3-C4	2.29	119.57	118.44
4	A	405	EH3	C9-C22-N3	2.28	118.51	115.57
4	A	405	EH3	O4-C16-C20	-2.27	103.02	108.31
4	B	404	EH3	C7-O3-N1	-2.27	106.07	108.94
4	A	405	EH3	C17-C18-N2	2.20	112.19	109.33
4	A	405	EH3	O6-S1-N2	2.19	108.85	107.02
4	B	404	EH3	O3-N1-C9	2.14	107.58	104.88
4	A	405	EH3	O9-C30-C27	-2.04	117.45	122.86

There are no chirality outliers.

All (15) 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
2	B	401	GOL	C1-C2-C3-O3
4	A	405	EH3	C14-C13-O4-C16

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Mol	Chain	Res	Type	Atoms
4	A	405	EH3	C12-C13-O4-C16
4	B	404	EH3	N3-C22-C9-C8
4	A	405	EH3	C18-N2-S1-O5
4	A	405	EH3	C18-N2-S1-O6
4	A	405	EH3	C26-C27-C30-O8
4	B	404	EH3	N3-C22-C9-N1
4	A	405	EH3	C26-C27-C30-O9

All (2) ring outliers are listed below:

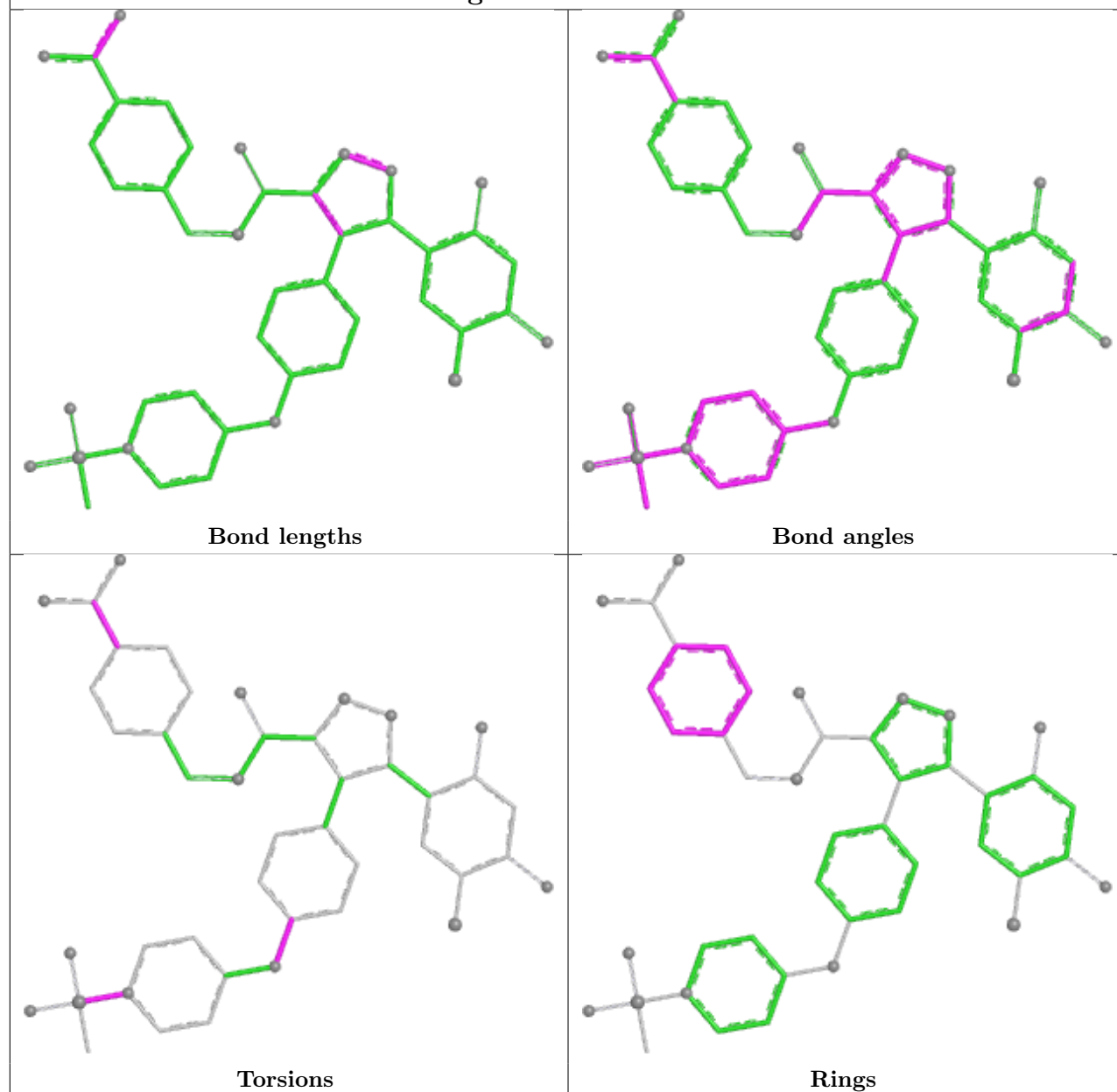
Mol	Chain	Res	Type	Atoms
4	A	405	EH3	C24-C25-C26-C27-C28-C29
4	B	404	EH3	C24-C25-C26-C27-C28-C29

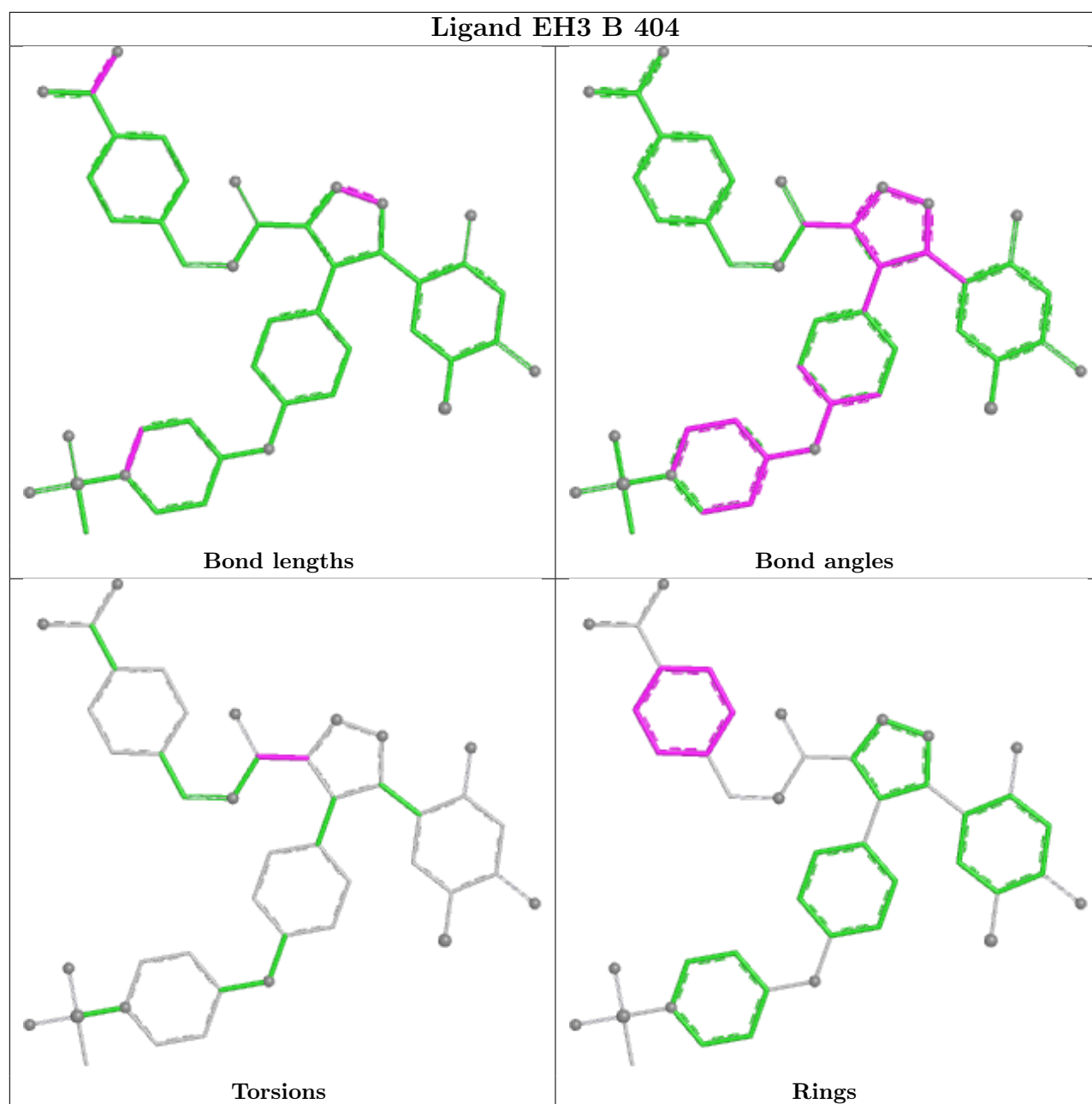
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	SO4	1	0
3	A	403	SO4	1	0
4	B	404	EH3	1	0
2	B	402	GOL	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.

Ligand EH3 A 405





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	354/411 (86%)	1.04	64 (18%) 3 4	15, 33, 77, 121	4 (1%)
1	B	371/411 (90%)	0.75	38 (10%) 12 14	13, 31, 64, 113	2 (0%)
All	All	725/822 (88%)	0.90	102 (14%) 6 7	13, 32, 69, 121	6 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	VAL	7.5
1	A	326	PHE	7.2
1	A	145	PRO	6.5
1	A	14	ALA	6.5
1	A	229	ALA	5.5
1	A	309	SER	5.3
1	B	323	LEU	5.2
1	B	4	ASP	5.0
1	B	321	THR	5.0
1	B	322	PRO	4.9
1	A	308	TYR	4.9
1	A	181	ASN	4.8
1	A	147	SER	4.7
1	B	183	ALA	4.7
1	A	182	PRO	4.7
1	B	310	THR	4.6
1	B	180	THR	4.5
1	B	384	THR	4.5
1	B	181	ASN	4.5
1	A	106	HIS	4.3
1	A	179	SER	4.3
1	A	268	LEU	4.2
1	B	182	PRO	4.2
1	B	184	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	183	ALA	4.1
1	A	180	THR	4.1
1	B	39	PHE	4.0
1	A	230	ALA	4.0
1	B	179	SER	3.9
1	A	382	TYR	3.9
1	A	379	TRP	3.9
1	A	178	GLY	3.8
1	A	233	LYS	3.7
1	A	325	GLY	3.7
1	A	185	PRO	3.7
1	A	232	SER	3.6
1	B	215	TYR	3.6
1	B	379	TRP	3.6
1	B	326	PHE	3.6
1	A	378	ALA	3.5
1	A	235	PRO	3.5
1	A	15	GLY	3.4
1	A	16	ALA	3.4
1	A	376	LYS	3.4
1	A	269	ILE	3.3
1	B	325	GLY	3.2
1	A	177	ASP	3.2
1	A	381	HIS	3.1
1	B	5	LYS	3.0
1	A	377	SER	3.0
1	A	374	TYR	2.9
1	B	324	ALA	2.9
1	B	40	GLY	2.9
1	B	178	GLY	2.9
1	B	146	VAL	2.8
1	A	184	HIS	2.8
1	B	211	LEU	2.8
1	A	215	TYR	2.8
1	A	327	GLY	2.8
1	A	19	TYR	2.7
1	A	211	LEU	2.7
1	A	218	ALA	2.7
1	B	135	LEU	2.7
1	A	380	ARG	2.7
1	A	20	ILE	2.7
1	A	99	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	376	LYS	2.6
1	A	143	ASP	2.6
1	A	210	LEU	2.6
1	A	17	PRO	2.6
1	B	43	ASN	2.6
1	A	231	ASN	2.6
1	A	214	LYS	2.5
1	A	149	GLN	2.5
1	A	228	ASN	2.5
1	A	234	GLN	2.5
1	B	347	PHE	2.5
1	B	44	ALA	2.5
1	B	142	GLY	2.4
1	A	267	SER	2.4
1	A	18	LYS	2.4
1	A	217	MET	2.4
1	A	186	LYS	2.3
1	A	26	PHE	2.3
1	A	22	HIS	2.3
1	B	45	CYS	2.3
1	B	377	SER	2.3
1	B	214	LYS	2.3
1	A	76	LEU	2.3
1	B	308	TYR	2.3
1	B	41	SER	2.2
1	B	42	SER	2.2
1	A	43	ASN	2.2
1	B	381	HIS	2.1
1	A	207	MET	2.1
1	A	85	GLN	2.1
1	B	185	PRO	2.1
1	A	100	ASP	2.1
1	A	144	ASP	2.1
1	B	174	LEU	2.1
1	A	301	GLU	2.0
1	A	265	GLU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

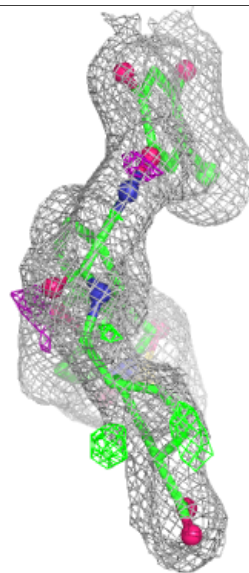
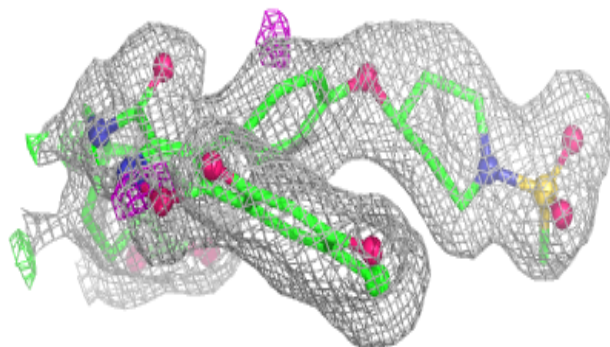
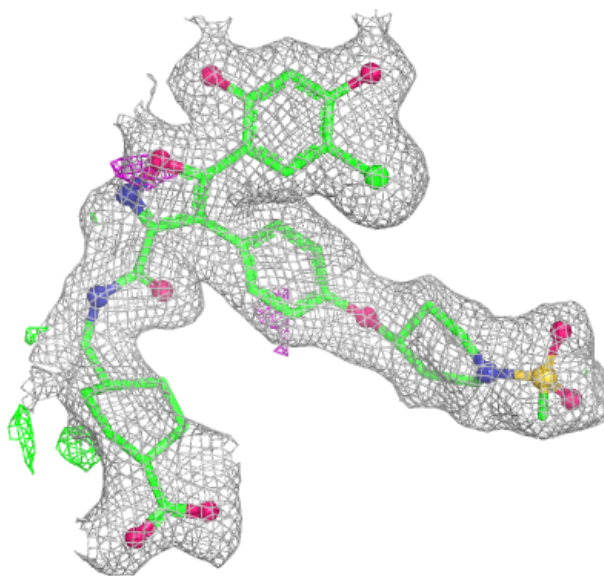
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	404	5/5	0.53	0.17	96,102,105,105	0
3	SO4	A	402	5/5	0.82	0.10	66,70,76,88	0
2	GOL	B	401	6/6	0.82	0.15	31,51,58,58	0
3	SO4	B	403	5/5	0.84	0.11	50,62,69,80	0
2	GOL	A	401	6/6	0.86	0.21	51,62,71,71	0
3	SO4	A	403	5/5	0.86	0.10	63,72,82,84	0
2	GOL	B	402	6/6	0.89	0.17	42,60,61,64	0
4	EH3	A	405	44/44	0.95	0.09	25,31,57,61	0
4	EH3	B	404	44/44	0.96	0.08	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.

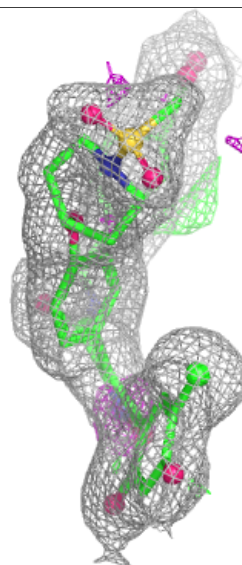
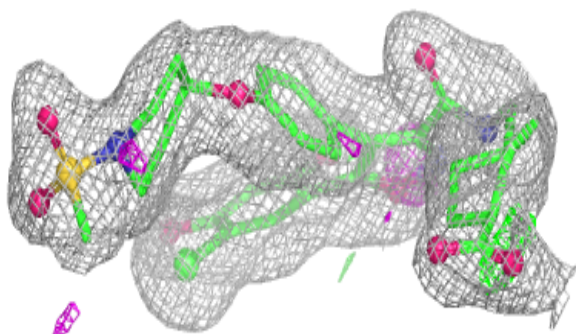
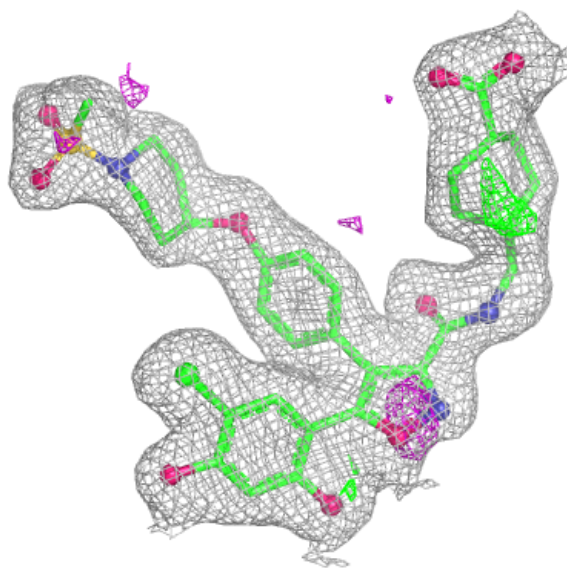
Electron density around EH3 A 405:

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



Electron density around EH3 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.