



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:05 AM UTC

PDB ID : 6LIN / pdb_00006lin
Title : Crystal structure of human PDK2 complexed with GM10030
Authors : Kang, J.; Kim, J.
Deposited on : 2019-12-12
Resolution : 2.67 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

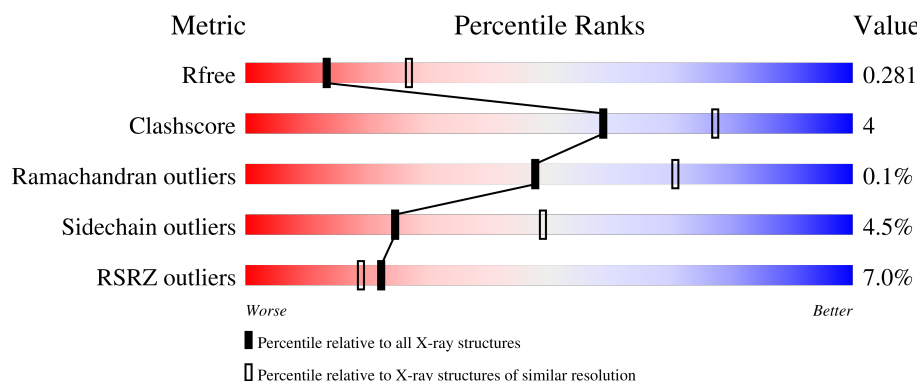
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	7% 76% 12% • 11%
1	B	411	6% 75% 12% • 12%
1	C	411	7% 80% 10% 11%
1	D	411	5% 75% 11% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11636 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	365	Total	C	N	O	S	0	0	0
			2822	1806	476	524	16			
1	B	362	Total	C	N	O	S	0	0	0
			2862	1836	477	532	17			
1	C	367	Total	C	N	O	S	0	0	0
			2831	1815	475	525	16			
1	D	354	Total	C	N	O	S	0	1	0
			2780	1784	461	518	17			

There are 120 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
C	-24	MET	-	expression tag	UNP Q15119
C	-23	ALA	-	expression tag	UNP Q15119

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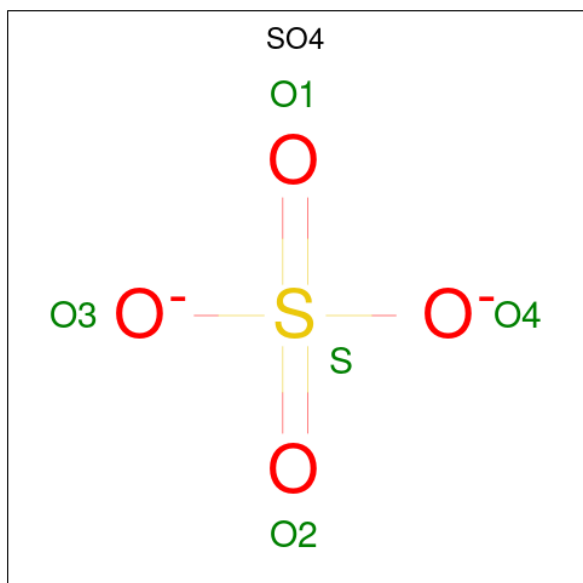
Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	GLY	-	expression tag	UNP Q15119
C	-21	SER	-	expression tag	UNP Q15119
C	-20	HIS	-	expression tag	UNP Q15119
C	-19	HIS	-	expression tag	UNP Q15119
C	-18	HIS	-	expression tag	UNP Q15119
C	-17	HIS	-	expression tag	UNP Q15119
C	-16	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	MET	-	expression tag	UNP Q15119
D	-9	THR	-	expression tag	UNP Q15119
D	-8	GLY	-	expression tag	UNP Q15119
D	-7	GLY	-	expression tag	UNP Q15119
D	-6	GLN	-	expression tag	UNP Q15119
D	-5	GLN	-	expression tag	UNP Q15119
D	-4	MET	-	expression tag	UNP Q15119
D	-3	GLY	-	expression tag	UNP Q15119
D	-2	ARG	-	expression tag	UNP Q15119
D	-1	SER	-	expression tag	UNP Q15119
D	0	GLY	-	expression tag	UNP Q15119
D	1	ASP	-	expression tag	UNP Q15119
D	2	ASP	-	expression tag	UNP Q15119
D	3	ASP	-	expression tag	UNP Q15119
D	4	ASP	-	expression tag	UNP Q15119
D	5	LYS	-	expression tag	UNP Q15119

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



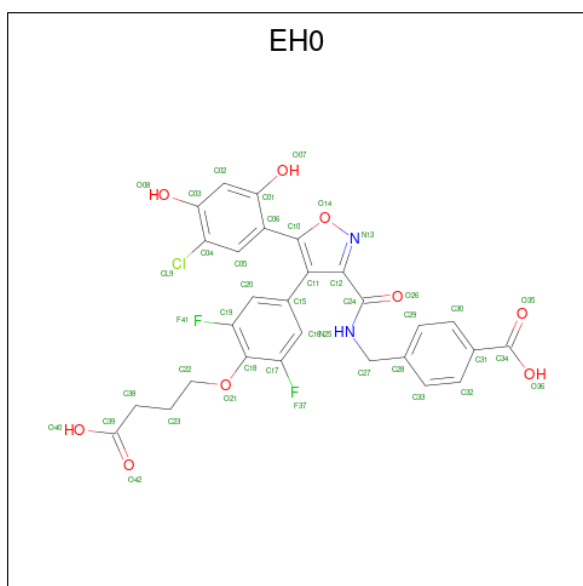
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 4-[[[4-[3,5-bis(fluoranyl)-4-(4-oxidanyl-4-oxidanylidene-butoxy)phenyl]-5-[5-chloranyl-2,4-bis(oxidanyl)phenyl]-1,2-oxazol-3-yl]carbonylamino]methyl]benzoic acid (CCD ID: EH0) (formula: C₂₈H₂₁ClF₂N₂O₉) (labeled as "Ligand of Interest" by depositor).



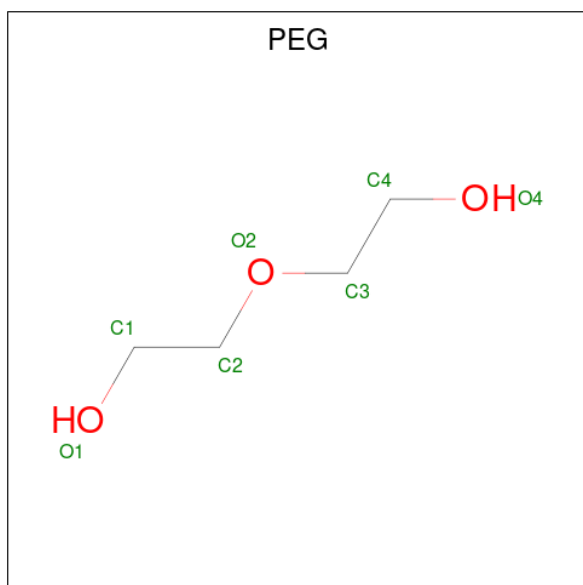
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			42	28	1	2	2	9		
4	B	1	Total	C	Cl	F	N	O	0	0
			42	28	1	2	2	9		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	Cl	F	N	O	0	0
			42	28	1	2	2	9		
4	D	1	Total	C	Cl	F	N	O	0	0
			42	28	1	2	2	9		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

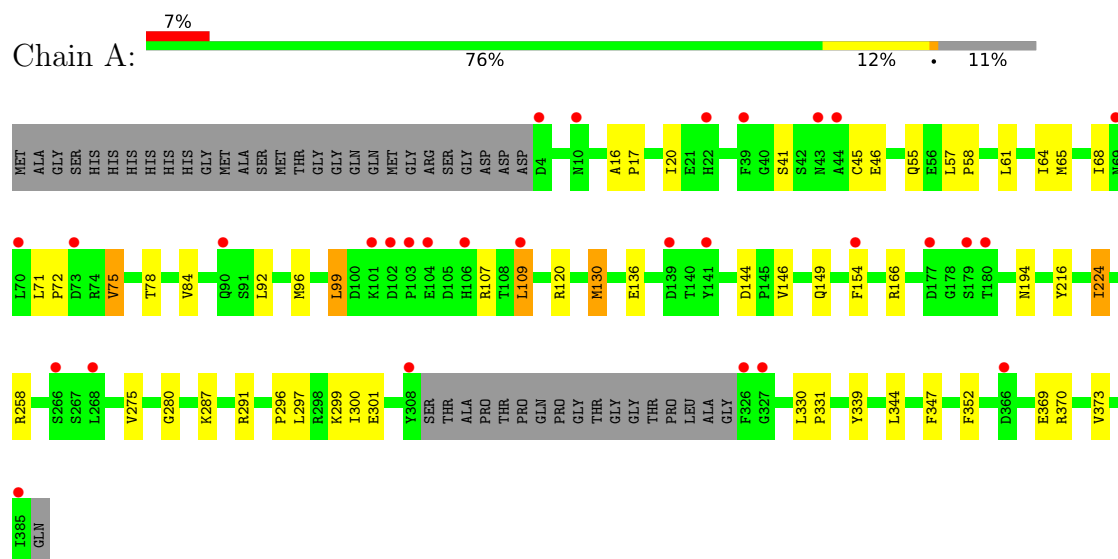
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	44	Total	O	0	0
			44	44		
6	C	34	Total	O	0	0
			34	34		
6	D	43	Total	O	0	0
			43	43		

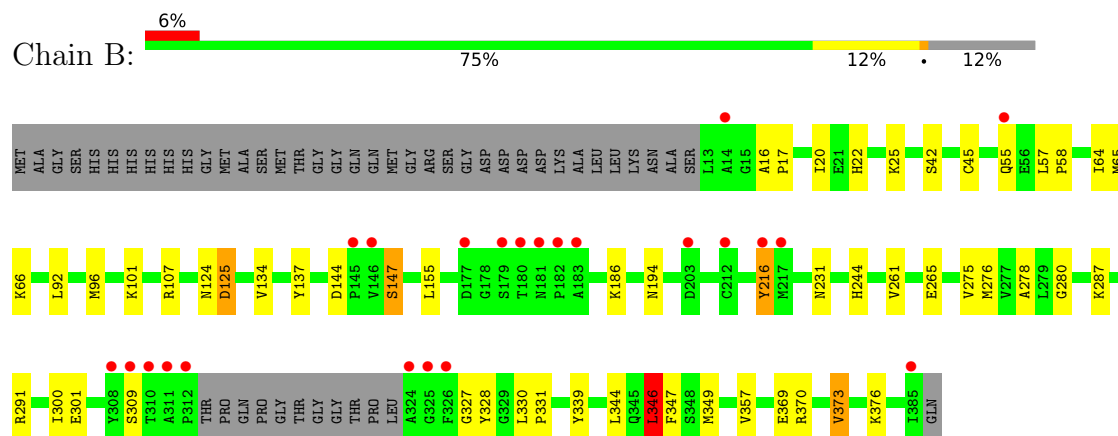
3 Residue-property plots [i](#)

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 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.

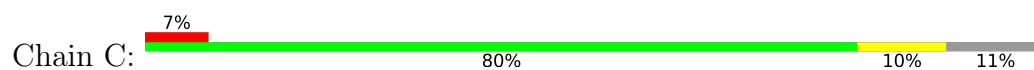
- Molecule 1: [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial

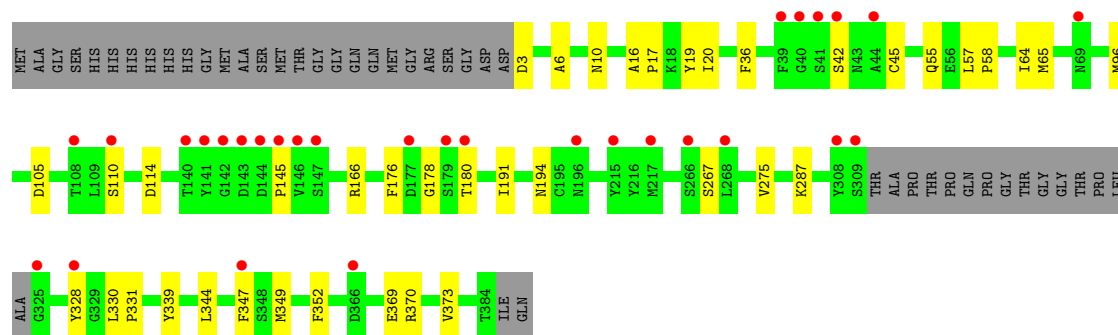


- Molecule 1: [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial

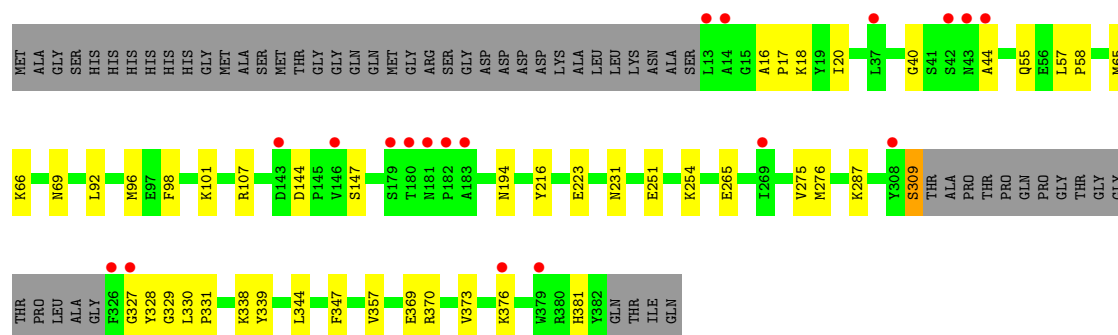
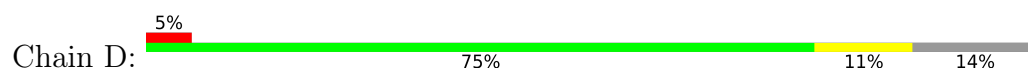


- Molecule 1: [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial





- Molecule 1: [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.42Å 156.19Å 102.01Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	39.08 – 2.67 39.08 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.08-2.67) 99.7 (39.08-2.67)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.223 , 0.280 0.229 , 0.281	Depositor DCC
R_{free} test set	2442 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11636	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, GOL, EH0

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	0/2888	1.46	1/3926 (0.0%)
1	B	1.03	1/2931 (0.0%)	1.49	10/3976 (0.3%)
1	C	1.03	0/2898	1.46	3/3941 (0.1%)
1	D	1.04	0/2846	1.45	3/3862 (0.1%)
All	All	1.03	1/11563 (0.0%)	1.47	17/15705 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	HIS	CE1-NE2	5.47	1.38	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	45	CYS	CA-C-O	-6.10	114.42	120.70
1	B	346	LEU	CB-CA-C	6.04	120.64	109.70
1	D	216	TYR	CA-C-O	-5.97	114.48	121.46
1	D	328	TYR	CA-C-N	5.84	126.59	119.99
1	D	328	TYR	C-N-CA	5.84	126.59	119.99
1	B	216	TYR	CA-C-O	-5.50	115.03	121.46
1	B	124	ASN	CA-C-N	5.49	132.26	122.06
1	B	124	ASN	C-N-CA	5.49	132.26	122.06
1	B	328	TYR	CA-C-N	5.24	125.91	119.99
1	B	328	TYR	C-N-CA	5.24	125.91	119.99
1	C	328	TYR	CA-C-N	5.17	125.83	119.99
1	C	328	TYR	C-N-CA	5.17	125.83	119.99
1	A	280	GLY	CA-C-O	-5.16	116.60	122.33
1	C	105	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	280	GLY	CA-C-O	-5.11	116.66	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	SER	CA-C-O	-5.02	116.34	121.87

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	2822	0	2713	35	0
1	B	2862	0	2801	32	0
1	C	2831	0	2704	23	0
1	D	2780	0	2695	19	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	6	0	8	0	0
4	A	42	0	0	0	0
4	B	42	0	0	0	0
4	C	42	0	0	0	0
4	D	42	0	0	0	0
5	C	7	0	10	3	0
6	A	29	0	0	0	0
6	B	44	0	0	1	0
6	C	34	0	0	0	0
6	D	43	0	0	0	0
All	All	11636	0	10931	99	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 4.

All (99) 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:300:ILE:HD12	1:B:346:LEU:HD11	1.48	0.93
1:A:352:PHE:CG	1:B:276:MET:HE1	2.20	0.77
1:B:300:ILE:HD12	1:B:346:LEU:CD1	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ALA:HB3	1:D:17:PRO:HD3	1.75	0.68
1:C:19:TYR:CG	1:C:96:MET:HE1	2.29	0.67
1:C:19:TYR:CD2	1:C:96:MET:HE1	2.29	0.67
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.78	0.66
1:C:16:ALA:HB3	1:C:17:PRO:HD3	1.78	0.65
1:C:352:PHE:CZ	1:D:276:MET:HE1	2.31	0.65
1:B:346:LEU:C	1:B:346:LEU:HD12	2.22	0.63
1:A:16:ALA:HB3	1:A:17:PRO:HD3	1.80	0.63
1:A:352:PHE:CD2	1:B:276:MET:HE1	2.35	0.61
1:A:224:ILE:C	1:A:224:ILE:HD13	2.26	0.61
1:B:22:HIS:O	1:B:25:LYS:HG2	2.02	0.60
1:A:216:TYR:OH	1:A:258:ARG:HG3	2.02	0.59
1:C:166:ARG:HH11	5:C:401:PEG:H42	1.68	0.59
1:A:57:LEU:O	1:A:61:LEU:HD13	2.02	0.59
1:A:291:ARG:HD2	1:A:352:PHE:CE1	2.39	0.57
1:A:46:GLU:HG2	1:A:109:LEU:HG	1.85	0.57
1:C:352:PHE:CE1	1:D:276:MET:HE1	2.40	0.57
1:C:166:ARG:NH1	5:C:401:PEG:H42	2.20	0.56
1:B:373:VAL:HG12	6:B:522:HOH:O	2.06	0.55
1:B:22:HIS:O	1:B:25:LYS:CG	2.54	0.55
1:A:299:LYS:NZ	2:A:401:SO4:O4	2.40	0.54
1:D:20:ILE:HD11	1:D:65:MET:HE2	1.89	0.54
1:B:96:MET:HA	1:B:96:MET:HE2	1.91	0.53
1:A:71:LEU:HD13	1:A:75:VAL:CG2	2.38	0.52
1:D:98:PHE:HA	1:D:101:LYS:HG3	1.91	0.52
1:C:347:PHE:HB3	1:D:347:PHE:CZ	2.45	0.52
1:A:347:PHE:CZ	1:B:347:PHE:HB3	2.45	0.52
1:A:96:MET:HA	1:A:99:LEU:HD13	1.92	0.51
1:D:57:LEU:HB2	1:D:58:PRO:HD3	1.92	0.51
1:B:57:LEU:HB2	1:B:58:PRO:HD3	1.92	0.51
1:A:20:ILE:HD11	1:A:65:MET:HE2	1.92	0.51
1:C:344:LEU:C	1:C:344:LEU:HD23	2.36	0.51
1:A:297:LEU:HA	1:A:300:ILE:HD13	1.93	0.51
1:D:96:MET:HE2	1:D:96:MET:HA	1.92	0.50
1:C:330:LEU:HB3	1:C:331:PRO:HD3	1.92	0.50
1:A:96:MET:HA	1:A:96:MET:HE2	1.94	0.49
1:A:330:LEU:HB3	1:A:331:PRO:HD3	1.92	0.49
1:C:3:ASP:HA	1:C:6:ALA:HB2	1.94	0.49
1:C:57:LEU:HB2	1:C:58:PRO:HD3	1.94	0.49
1:A:78:THR:HB	1:A:136:GLU:OE2	2.13	0.48
1:A:57:LEU:HB2	1:A:58:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:O	1:B:96:MET:HG2	2.13	0.48
1:A:344:LEU:C	1:A:344:LEU:HD23	2.39	0.48
1:D:330:LEU:HB3	1:D:331:PRO:HD3	1.95	0.47
1:B:20:ILE:HD11	1:B:65:MET:HE2	1.95	0.47
1:D:92:LEU:O	1:D:96:MET:HG2	2.14	0.47
1:B:330:LEU:HB3	1:B:331:PRO:HD3	1.96	0.47
1:A:146:VAL:HA	1:A:149:GLN:HE21	1.79	0.47
1:B:276:MET:HE3	1:B:278:ALA:HB2	1.96	0.47
1:A:92:LEU:O	1:A:96:MET:HG2	2.14	0.47
1:A:347:PHE:CD2	1:B:347:PHE:CD1	3.02	0.47
1:B:344:LEU:C	1:B:344:LEU:HD23	2.41	0.46
1:B:134:VAL:HG21	1:B:155:LEU:HD11	1.98	0.46
1:A:72:PRO:O	1:A:75:VAL:HG13	2.16	0.46
1:A:296:PRO:HG2	1:A:299:LYS:HD2	1.97	0.46
1:B:346:LEU:CD1	1:B:346:LEU:C	2.88	0.46
1:D:344:LEU:C	1:D:344:LEU:HD23	2.41	0.45
1:C:20:ILE:HD11	1:C:65:MET:HE2	1.96	0.45
1:A:71:LEU:HD13	1:A:75:VAL:HG21	1.98	0.45
1:B:216:TYR:CG	1:B:261:VAL:HG11	2.51	0.45
1:C:42:SER:CB	1:C:45:CYS:SG	3.05	0.45
1:D:309:SER:HB3	1:D:327:GLY:HA3	1.99	0.44
1:D:251:GLU:HG2	1:D:329:GLY:CA	2.46	0.44
1:B:339:TYR:CZ	1:B:369:GLU:HG2	2.53	0.44
1:A:64:ILE:HD12	1:A:64:ILE:HA	1.90	0.43
1:A:352:PHE:CB	1:B:276:MET:HE1	2.48	0.43
1:A:84:VAL:HG21	1:A:130:MET:CE	2.48	0.43
1:C:176:PHE:C	1:C:178:GLY:H	2.26	0.43
1:C:64:ILE:HD12	1:C:64:ILE:HA	1.91	0.43
1:B:275:VAL:HA	1:B:287:LYS:O	2.19	0.43
1:A:120:ARG:HD2	1:A:166:ARG:NH2	2.33	0.43
1:D:55:GLN:C	1:D:58:PRO:HD2	2.44	0.43
1:C:36:PHE:HB3	1:C:191:ILE:CD1	2.48	0.42
1:A:120:ARG:HD2	1:A:166:ARG:HH22	1.84	0.42
1:B:55:GLN:C	1:B:58:PRO:HD2	2.44	0.42
1:B:309:SER:CB	1:B:327:GLY:O	2.67	0.42
1:D:339:TYR:CZ	1:D:369:GLU:HG2	2.54	0.42
1:C:55:GLN:C	1:C:58:PRO:HD2	2.44	0.42
1:A:68:ILE:HG12	1:A:154:PHE:HZ	1.83	0.42
1:B:346:LEU:HD12	1:B:346:LEU:O	2.18	0.42
1:A:287:LYS:HE2	1:B:349:MET:SD	2.59	0.42
1:D:40:GLY:C	1:D:44:ALA:HB2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:VAL:HA	1:D:287:LYS:O	2.20	0.42
1:A:55:GLN:C	1:A:58:PRO:HD2	2.45	0.42
1:B:137:TYR:OH	1:B:147:SER:HB3	2.20	0.42
1:C:55:GLN:O	1:C:58:PRO:HD2	2.20	0.42
1:B:216:TYR:CD2	1:B:261:VAL:HG11	2.55	0.41
1:C:339:TYR:CZ	1:C:369:GLU:HG2	2.54	0.41
1:C:275:VAL:HA	1:C:287:LYS:O	2.20	0.41
1:C:166:ARG:NH1	5:C:401:PEG:C4	2.83	0.41
1:A:339:TYR:CZ	1:A:369:GLU:HG2	2.55	0.41
1:B:344:LEU:HA	1:B:357:VAL:O	2.21	0.41
1:C:349:MET:SD	1:D:287:LYS:HB2	2.61	0.41
1:B:64:ILE:HD12	1:B:64:ILE:HA	1.98	0.40
1:A:275:VAL:HA	1:A:287:LYS:O	2.20	0.40
1:D:344:LEU:HA	1:D:357:VAL:O	2.22	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	361/411 (88%)	349 (97%)	12 (3%)	0	100	100
1	B	358/411 (87%)	345 (96%)	13 (4%)	0	100	100
1	C	363/411 (88%)	342 (94%)	20 (6%)	1 (0%)	36	57
1	D	351/411 (85%)	335 (95%)	16 (5%)	0	100	100
All	All	1433/1644 (87%)	1371 (96%)	61 (4%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	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	299/361 (83%)	286 (96%)	13 (4%)	26	51
1	B	313/361 (87%)	297 (95%)	16 (5%)	21	44
1	C	297/361 (82%)	289 (97%)	8 (3%)	39	67
1	D	300/361 (83%)	283 (94%)	17 (6%)	18	40
All	All	1209/1444 (84%)	1155 (96%)	54 (4%)	24	49

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	45	CYS
1	A	75	VAL
1	A	99	LEU
1	A	107	ARG
1	A	109	LEU
1	A	130	MET
1	A	144	ASP
1	A	194	ASN
1	A	224	ILE
1	A	301	GLU
1	A	370	ARG
1	A	373	VAL
1	B	66	LYS
1	B	101	LYS
1	B	107	ARG
1	B	125	ASP
1	B	144	ASP
1	B	147	SER
1	B	186	LYS
1	B	194	ASN
1	B	231	ASN
1	B	265	GLU
1	B	291	ARG

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Mol	Chain	Res	Type
1	B	301	GLU
1	B	346	LEU
1	B	370	ARG
1	B	373	VAL
1	B	376	LYS
1	C	10	ASN
1	C	110	SER
1	C	114	ASP
1	C	180	THR
1	C	194	ASN
1	C	267	SER
1	C	370	ARG
1	C	373	VAL
1	D	18	LYS
1	D	66	LYS
1	D	69	ASN
1	D	107	ARG
1	D	144	ASP
1	D	147	SER
1	D	194	ASN
1	D	223	GLU
1	D	231	ASN
1	D	254	LYS
1	D	265	GLU
1	D	309	SER
1	D	338	LYS
1	D	370	ARG
1	D	373	VAL
1	D	376	LYS
1	D	381	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	149	GLN
1	A	170	ASN
1	A	194	ASN
1	A	237	HIS
1	A	345	GLN
1	A	381	HIS
1	B	43	ASN

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Mol	Chain	Res	Type
1	B	85	GLN
1	C	149	GLN
1	C	184	HIS
1	D	85	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](#)

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
2	SO4	A	401	-	4,4,4	0.32	0	6,6,6	0.15	0
5	PEG	C	401	-	6,6,6	0.41	0	5,5,5	0.25	0
4	EH0	A	403	-	45,45,45	1.78	10 (22%)	59,64,64	3.66	21 (35%)
2	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.11	0
4	EH0	C	402	-	45,45,45	1.61	7 (15%)	59,64,64	2.46	21 (35%)
4	EH0	B	402	-	45,45,45	1.73	8 (17%)	59,64,64	2.49	18 (30%)
4	EH0	D	401	-	45,45,45	1.50	5 (11%)	59,64,64	2.75	19 (32%)
3	GOL	A	402	-	5,5,5	0.10	0	5,5,5	0.25	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
5	PEG	C	401	-	-	3/4/4/4	-
4	EH0	A	403	-	-	10/28/28/28	0/4/4/4
4	EH0	C	402	-	-	2/28/28/28	0/4/4/4
4	EH0	B	402	-	-	5/28/28/28	0/4/4/4
4	EH0	D	401	-	-	6/28/28/28	0/4/4/4
3	GOL	A	402	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	EH0	C24-N25	6.19	1.44	1.33
4	B	402	EH0	C24-N25	6.06	1.43	1.33
4	C	402	EH0	C24-N25	5.76	1.43	1.33
4	D	401	EH0	C24-N25	5.21	1.42	1.33
4	A	403	EH0	C06-C10	3.87	1.53	1.47
4	B	402	EH0	C05-C06	-3.65	1.34	1.39
4	A	403	EH0	O26-C24	-3.41	1.17	1.23
4	D	401	EH0	O26-C24	-3.30	1.17	1.23
4	B	402	EH0	O26-C24	-3.17	1.17	1.23
4	A	403	EH0	C11-C10	3.05	1.40	1.36
4	B	402	EH0	C11-C12	-2.99	1.35	1.44
4	A	403	EH0	C31-C34	2.83	1.55	1.49
4	D	401	EH0	C12-C24	2.69	1.53	1.48
4	C	402	EH0	C38-C39	2.68	1.56	1.50
4	B	402	EH0	C31-C34	2.67	1.55	1.49
4	D	401	EH0	C11-C12	-2.65	1.36	1.44
4	D	401	EH0	C38-C39	2.49	1.56	1.50
4	A	403	EH0	O14-C10	-2.46	1.32	1.36
4	A	403	EH0	C11-C12	-2.38	1.37	1.44
4	B	402	EH0	O14-N13	-2.37	1.38	1.42
4	C	402	EH0	C11-C12	-2.35	1.37	1.44
4	A	403	EH0	O08-C03	2.35	1.41	1.36
4	A	403	EH0	C04-CL9	2.32	1.79	1.73
4	C	402	EH0	O08-C03	2.28	1.40	1.36
4	B	402	EH0	C06-C01	-2.22	1.37	1.40
4	C	402	EH0	C15-C11	2.16	1.53	1.49
4	A	403	EH0	C38-C39	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	EH0	O07-C01	2.13	1.40	1.36
4	C	402	EH0	O42-C39	2.07	1.28	1.22
4	C	402	EH0	O14-C10	-2.04	1.32	1.36

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	EH0	C12-C24-N25	16.99	137.52	115.57
4	D	401	EH0	O36-C34-O35	7.67	139.84	123.35
4	C	402	EH0	O36-C34-O35	7.56	139.60	123.35
4	A	403	EH0	C27-N25-C24	7.38	132.62	122.07
4	D	401	EH0	C12-C24-N25	7.35	125.07	115.57
4	A	403	EH0	O26-C24-C12	-6.86	110.58	121.60
4	B	402	EH0	C12-C24-N25	6.85	124.41	115.57
4	B	402	EH0	O36-C34-O35	6.81	137.99	123.35
4	A	403	EH0	C11-C12-N13	-6.79	104.20	112.66
4	A	403	EH0	C02-C03-C04	6.58	121.67	118.44
4	A	403	EH0	O26-C24-N25	-6.35	111.89	123.35
4	D	401	EH0	O14-C10-C06	6.16	128.28	115.50
4	A	403	EH0	C28-C27-N25	-6.13	100.15	113.07
4	C	402	EH0	C27-N25-C24	-6.13	113.31	122.07
4	A	403	EH0	O36-C34-O35	6.07	136.39	123.35
4	D	401	EH0	C28-C27-N25	-6.03	100.36	113.07
4	A	403	EH0	O14-N13-C12	5.71	112.09	104.88
4	D	401	EH0	C11-C12-N13	-5.50	105.81	112.66
4	D	401	EH0	O26-C24-N25	-5.45	113.51	123.35
4	A	403	EH0	C15-C11-C10	-5.29	119.37	127.60
4	B	402	EH0	O35-C34-C31	-5.17	107.91	121.46
4	D	401	EH0	C05-C04-C03	5.11	123.91	120.92
4	C	402	EH0	C05-C04-C03	5.03	123.86	120.92
4	B	402	EH0	C03-C02-C01	-4.86	115.18	120.17
4	B	402	EH0	C02-C03-C04	4.79	120.79	118.44
4	C	402	EH0	O35-C34-C31	-4.66	109.25	121.46
4	A	403	EH0	C03-C02-C01	-4.54	115.50	120.17
4	B	402	EH0	C05-C04-CL9	-4.37	111.30	118.45
4	C	402	EH0	C05-C06-C01	4.35	122.82	118.72
4	C	402	EH0	C12-C24-N25	4.19	120.98	115.57
4	C	402	EH0	C11-C12-N13	-4.10	107.56	112.66
4	D	401	EH0	C05-C06-C01	4.08	122.56	118.72
4	C	402	EH0	O14-N13-C12	4.02	109.96	104.88
4	B	402	EH0	O26-C24-C12	-3.98	115.20	121.60
4	B	402	EH0	C16-C17-C18	-3.98	117.66	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	EH0	O07-C01-C06	-3.95	114.39	121.71
4	C	402	EH0	C15-C11-C10	-3.94	121.46	127.60
4	D	401	EH0	C06-C10-C11	-3.93	122.58	134.99
4	C	402	EH0	C38-C23-C22	3.92	120.19	112.33
4	A	403	EH0	O14-C10-C06	3.90	123.59	115.50
4	D	401	EH0	O14-N13-C12	3.88	109.79	104.88
4	B	402	EH0	C11-C12-N13	-3.69	108.07	112.66
4	D	401	EH0	O35-C34-C31	-3.68	111.82	121.46
4	A	403	EH0	O35-C34-C31	-3.60	112.01	121.46
4	B	402	EH0	O14-C10-C06	3.59	122.94	115.50
4	B	402	EH0	C03-C04-CL9	3.56	125.77	119.43
4	B	402	EH0	C05-C06-C01	3.49	122.01	118.72
4	B	402	EH0	C05-C04-C03	3.44	122.93	120.92
4	C	402	EH0	C01-C06-C10	-3.33	115.88	122.94
4	D	401	EH0	C24-C12-N13	3.32	130.51	121.45
4	B	402	EH0	O14-N13-C12	3.06	108.75	104.88
4	D	401	EH0	C02-C03-C04	2.89	119.86	118.44
4	C	402	EH0	C10-O14-N13	-2.89	105.28	108.94
4	C	402	EH0	C23-C38-C39	2.87	121.99	114.51
4	D	401	EH0	C27-C28-C33	-2.85	115.13	120.94
4	D	401	EH0	C03-C02-C01	-2.72	117.38	120.17
4	C	402	EH0	C06-C05-C04	-2.69	114.91	119.95
4	C	402	EH0	O14-C10-C06	2.68	121.06	115.50
4	D	401	EH0	C06-C05-C04	-2.67	114.94	119.95
4	C	402	EH0	C03-C02-C01	-2.59	117.50	120.17
4	A	403	EH0	O42-C39-C38	-2.58	114.90	123.09
4	C	402	EH0	C28-C27-N25	-2.57	107.65	113.07
4	D	401	EH0	C10-O14-N13	-2.57	105.68	108.94
4	A	403	EH0	C01-C06-C10	-2.54	117.55	122.94
4	D	401	EH0	O36-C34-C31	-2.53	108.34	114.84
4	A	403	EH0	F37-C17-C18	2.49	120.92	117.62
4	A	403	EH0	C10-O14-N13	-2.43	105.86	108.94
4	C	402	EH0	C06-C10-C11	-2.36	127.54	134.99
4	A	403	EH0	C05-C06-C01	2.35	120.94	118.72
4	A	403	EH0	C20-C19-C18	-2.34	119.96	123.24
4	B	402	EH0	C06-C10-C11	-2.32	127.66	134.99
4	B	402	EH0	C27-N25-C24	-2.24	118.87	122.07
4	A	403	EH0	C06-C10-C11	-2.19	128.06	134.99
4	B	402	EH0	C01-C06-C10	-2.19	118.30	122.94
4	D	401	EH0	C32-C31-C34	-2.19	116.04	120.37
4	C	402	EH0	C15-C11-C12	2.12	132.66	127.31
4	A	403	EH0	O07-C01-C06	-2.11	117.80	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	EH0	C02-C03-C04	2.10	119.47	118.44
4	C	402	EH0	O26-C24-N25	-2.03	119.68	123.35

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3
4	A	403	EH0	C11-C12-C24-N25
4	A	403	EH0	N13-C12-C24-N25
4	A	403	EH0	N13-C12-C24-O26
4	A	403	EH0	C12-C24-N25-C27
4	A	403	EH0	O26-C24-N25-C27
4	B	402	EH0	C28-C27-N25-C24
4	A	403	EH0	O21-C22-C23-C38
5	C	401	PEG	O1-C1-C2-O2
5	C	401	PEG	O2-C3-C4-O4
3	A	402	GOL	O1-C1-C2-O2
4	D	401	EH0	O21-C22-C23-C38
4	A	403	EH0	C22-C23-C38-C39
4	B	402	EH0	N13-C12-C24-O26
4	B	402	EH0	C23-C22-O21-C18
4	A	403	EH0	C11-C12-C24-O26
4	B	402	EH0	C11-C12-C24-O26
4	D	401	EH0	C22-C23-C38-C39
4	A	403	EH0	C23-C22-O21-C18
4	C	402	EH0	C23-C38-C39-O42
4	D	401	EH0	C23-C38-C39-O42
4	D	401	EH0	C23-C38-C39-O40
4	C	402	EH0	C23-C38-C39-O40
5	C	401	PEG	C1-C2-O2-C3
4	B	402	EH0	N13-C12-C24-N25
4	D	401	EH0	N13-C12-C24-N25
4	A	403	EH0	C23-C38-C39-O40
4	D	401	EH0	N13-C12-C24-O26

There are no ring outliers.

2 monomers are involved in 4 short contacts:

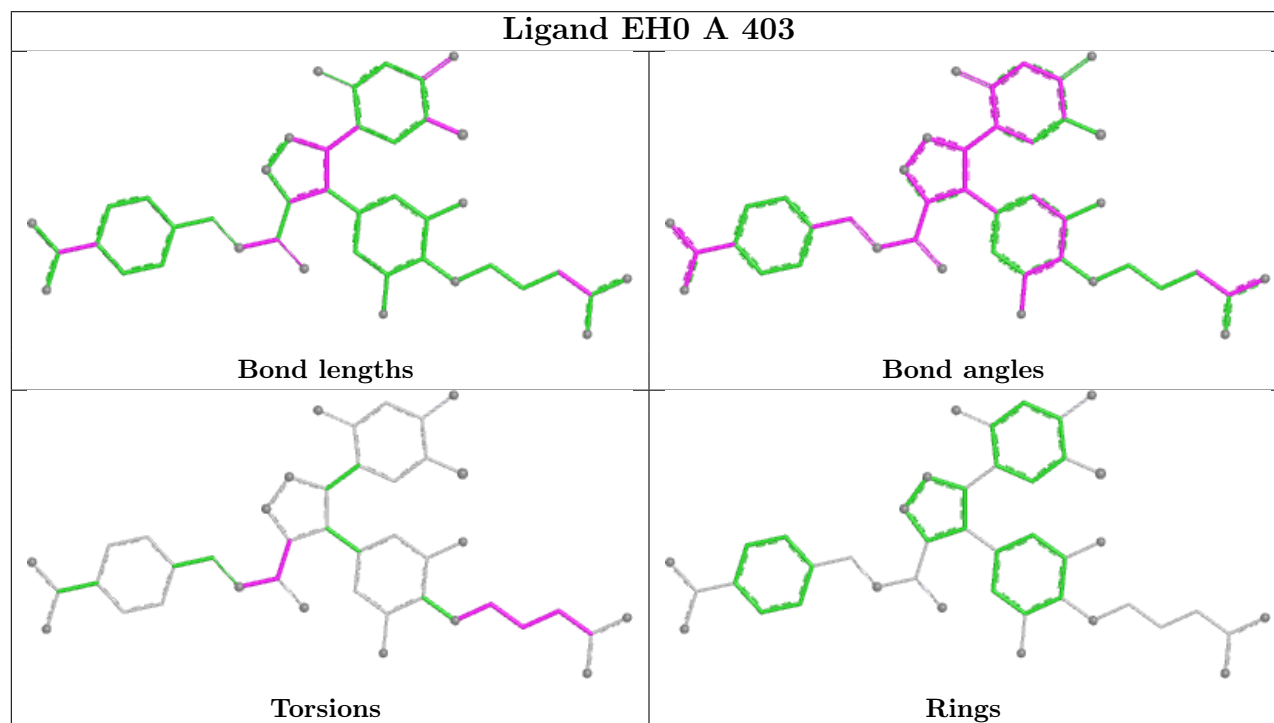
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0

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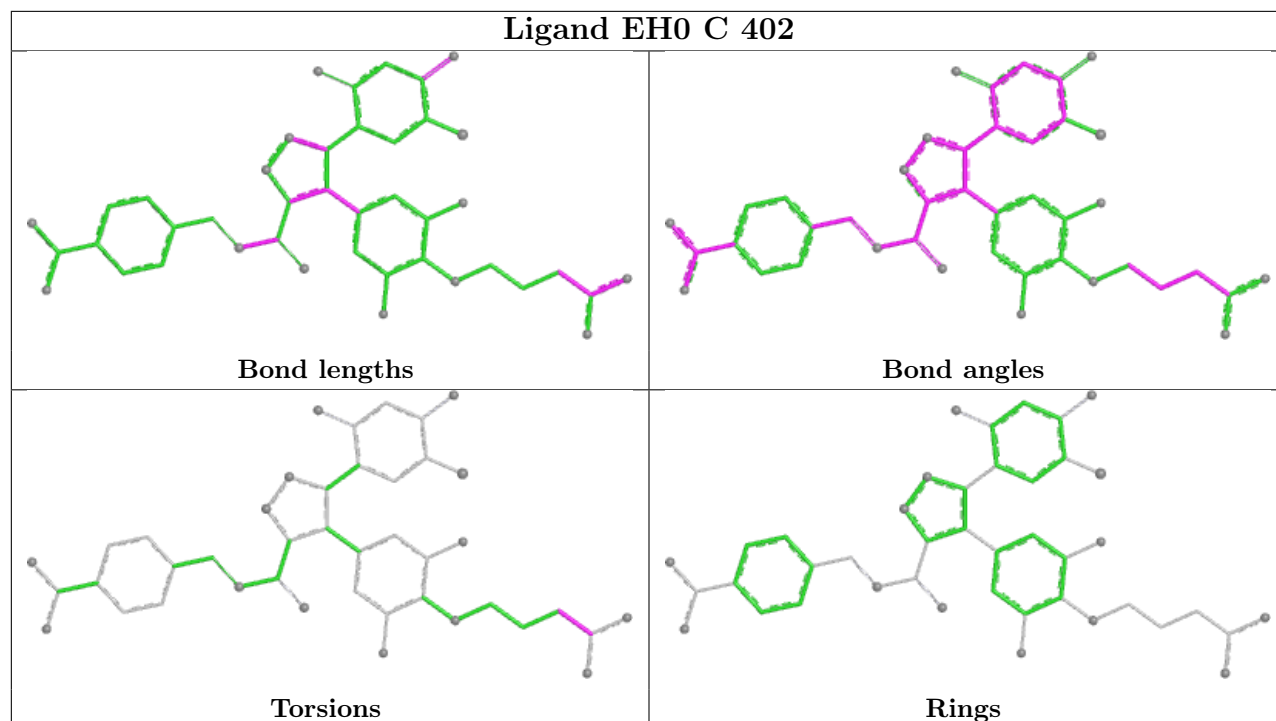
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	PEG	3	0

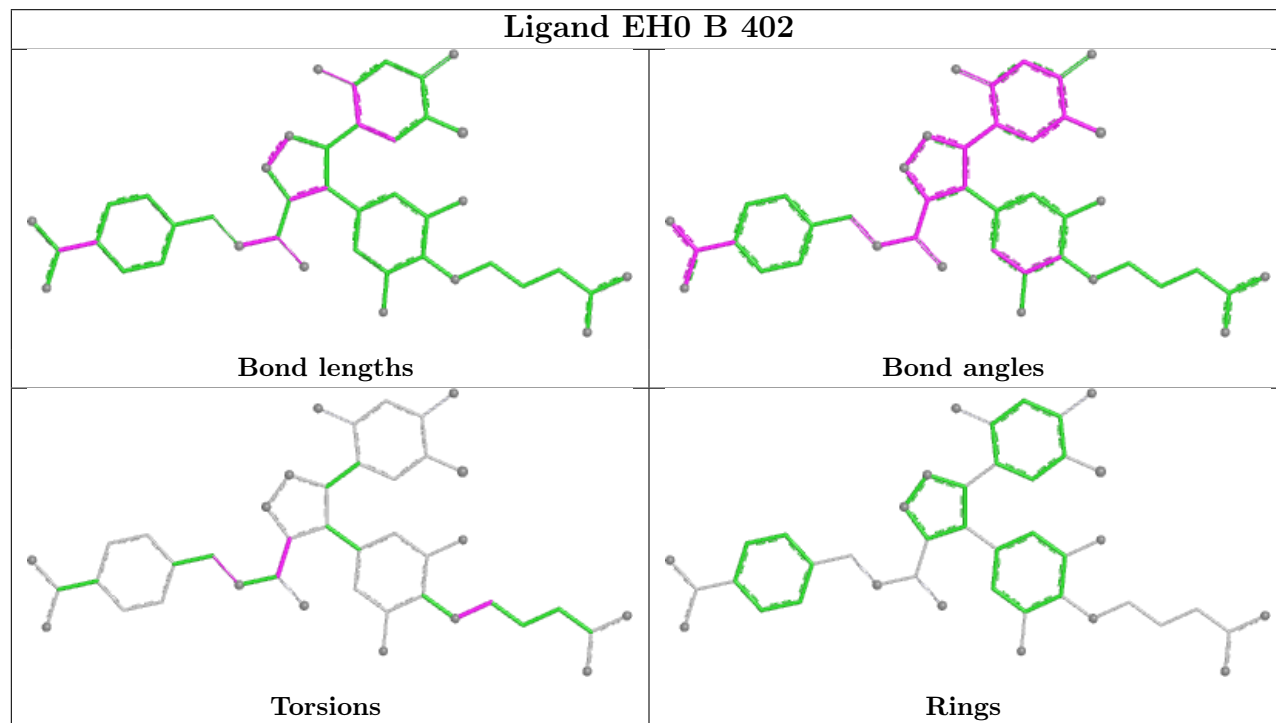
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

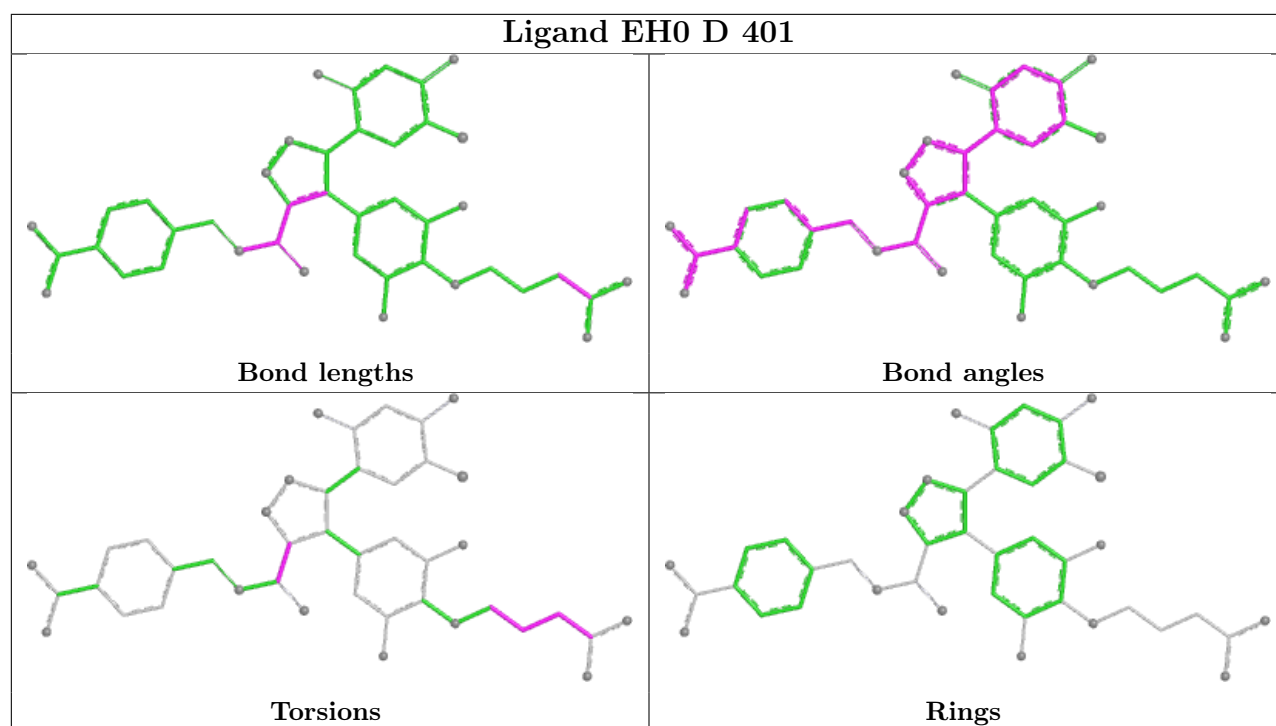


Ligand EH0 C 402



Ligand EH0 B 402





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	365/411 (88%)	0.67	29 (7%)	18	15	30, 55, 91, 130	0
1	B	362/411 (88%)	0.45	23 (6%)	25	22	29, 45, 94, 128	0
1	C	367/411 (89%)	0.60	30 (8%)	17	14	29, 52, 93, 116	0
1	D	354/411 (86%)	0.42	19 (5%)	31	27	19, 47, 91, 130	1 (0%)
All	All	1448/1644 (88%)	0.53	101 (6%)	22	19	19, 50, 93, 130	1 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	ALA	7.0
1	C	41	SER	6.9
1	B	326	PHE	4.8
1	D	326	PHE	4.7
1	D	43	ASN	4.7
1	A	43	ASN	4.6
1	C	42	SER	4.5
1	B	385	ILE	4.4
1	A	326	PHE	4.3
1	C	40	GLY	4.3
1	C	266	SER	4.2
1	A	179	SER	3.9
1	B	312	PRO	3.9
1	A	308	TYR	3.8
1	C	145	PRO	3.8
1	D	180	THR	3.8
1	C	308	TYR	3.8
1	A	109	LEU	3.7
1	B	310	THR	3.7
1	C	179	SER	3.7
1	C	39	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	102	ASP	3.6
1	B	179	SER	3.6
1	C	44	ALA	3.5
1	D	146	VAL	3.5
1	C	143	ASP	3.4
1	B	145	PRO	3.3
1	D	44	ALA	3.3
1	A	385	ILE	3.3
1	B	180	THR	3.2
1	B	183	ALA	3.2
1	D	327	GLY	3.2
1	D	179	SER	3.1
1	C	108	THR	3.1
1	B	14	ALA	3.1
1	A	104	GLU	3.1
1	B	308	TYR	3.0
1	B	181	ASN	3.0
1	C	141	TYR	3.0
1	B	182	PRO	2.9
1	C	180	THR	2.8
1	A	180	THR	2.8
1	B	309	SER	2.8
1	A	268	LEU	2.7
1	C	146	VAL	2.7
1	D	308	TYR	2.7
1	C	309	SER	2.7
1	B	177	ASP	2.6
1	D	14	ALA	2.6
1	B	203	ASP	2.5
1	C	366	ASP	2.5
1	C	268	LEU	2.5
1	C	215	TYR	2.5
1	C	325	GLY	2.5
1	B	55	GLN	2.5
1	A	4	ASP	2.5
1	A	139	ASP	2.5
1	D	143	ASP	2.5
1	A	141	TYR	2.5
1	D	182	PRO	2.5
1	A	106	HIS	2.4
1	C	147	SER	2.4
1	A	103	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	144	ASP	2.4
1	C	140	THR	2.3
1	A	10	ASN	2.3
1	C	110	SER	2.3
1	C	217	MET	2.3
1	D	379	TRP	2.3
1	D	37	LEU	2.3
1	A	22	HIS	2.3
1	C	142	GLY	2.3
1	D	269	ILE	2.3
1	D	376	LYS	2.3
1	D	181	ASN	2.3
1	A	73	ASP	2.3
1	A	266	SER	2.3
1	A	366	ASP	2.3
1	A	177	ASP	2.2
1	B	325	GLY	2.2
1	D	13	LEU	2.2
1	B	217	MET	2.2
1	C	347	PHE	2.2
1	A	327	GLY	2.2
1	B	146	VAL	2.2
1	A	44	ALA	2.1
1	B	311	ALA	2.1
1	A	69	ASN	2.1
1	B	216	TYR	2.1
1	A	70	LEU	2.1
1	D	42	SER	2.1
1	D	183	ALA	2.1
1	C	177	ASP	2.1
1	B	212	CYS	2.1
1	C	69	ASN	2.1
1	C	328	TYR	2.1
1	C	196	ASN	2.1
1	A	154	PHE	2.1
1	A	90	GLN	2.0
1	A	39	PHE	2.0
1	A	101	LYS	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](#)

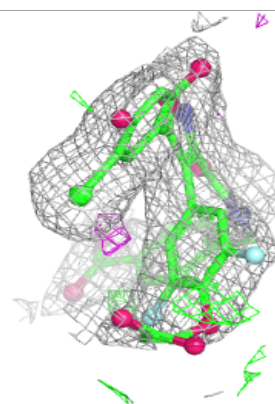
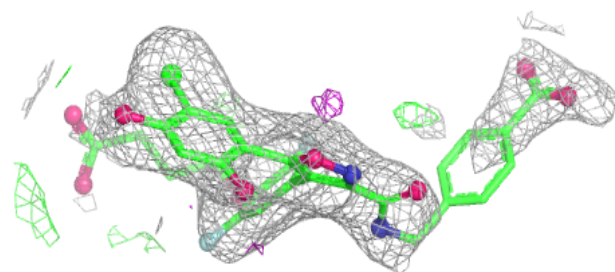
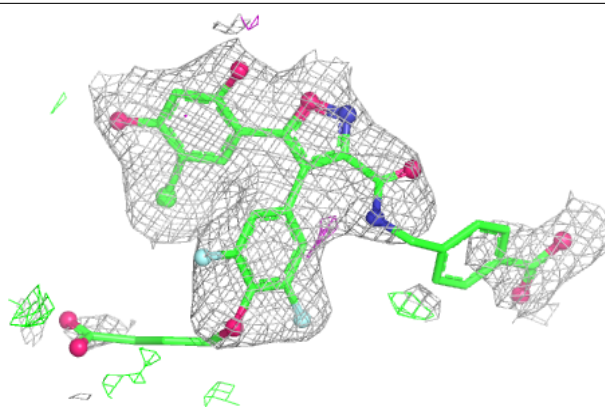
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	402	6/6	0.60	0.20	53,62,63,66	0
2	SO4	B	401	5/5	0.73	0.17	82,85,97,100	0
5	PEG	C	401	7/7	0.77	0.18	56,61,70,71	0
2	SO4	A	401	5/5	0.83	0.14	35,37,41,41	5
4	EH0	B	402	42/42	0.90	0.13	31,59,103,123	0
4	EH0	C	402	42/42	0.91	0.12	33,50,85,96	0
4	EH0	D	401	42/42	0.91	0.12	24,52,100,103	0
4	EH0	A	403	42/42	0.91	0.13	32,51,95,100	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.

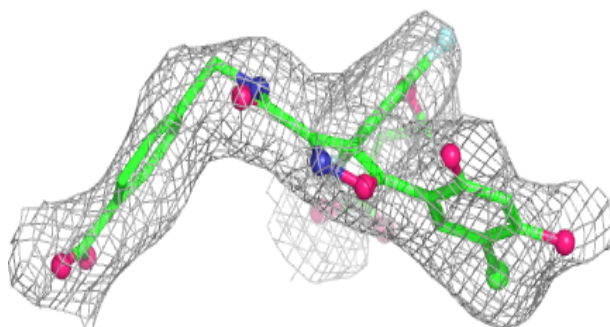
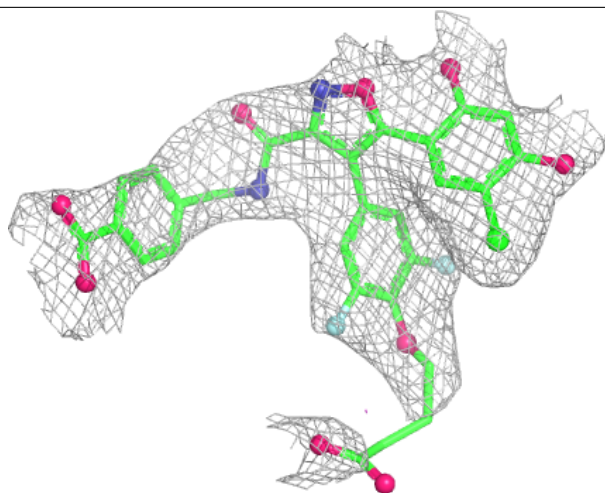
Electron density around EH0 B 402:

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



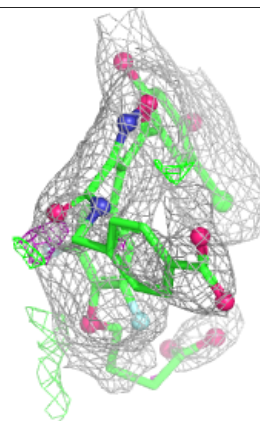
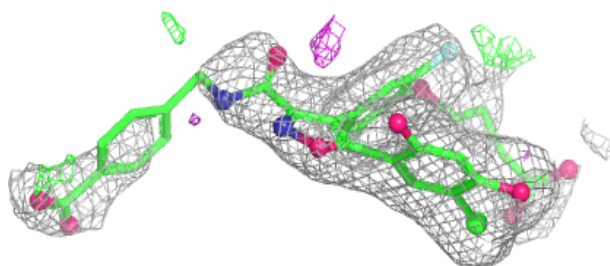
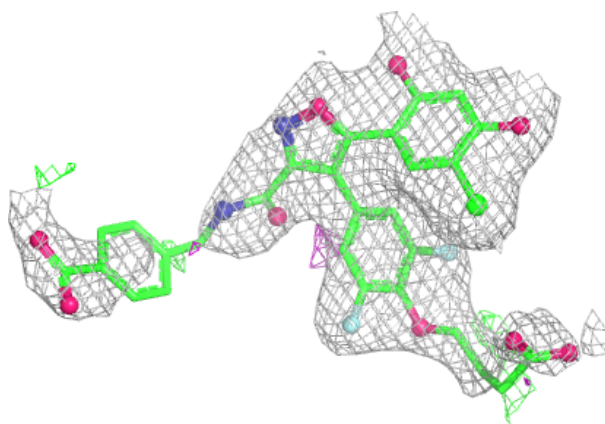
Electron density around EH0 C 402:

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



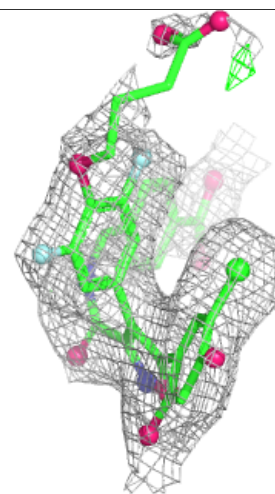
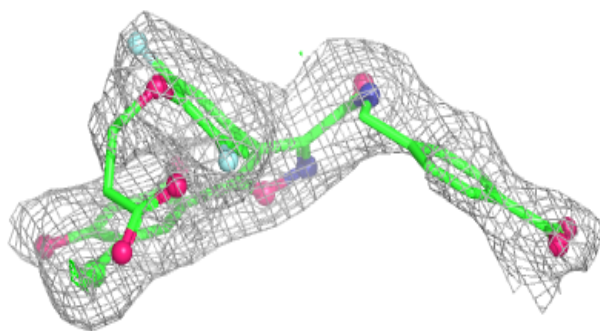
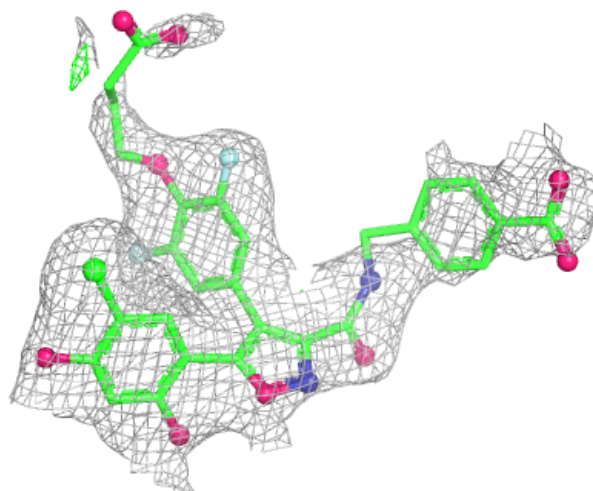
Electron density around EH0 D 401:

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



Electron density around EH0 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.