



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:30 PM UTC

PDB ID : 7T1I / pdb_00007t1i
Title : Crystal structure of CAB1 Pantothenate Kinase from *Saccharomyces cerevisiae* in complex with compound YU385597
Authors : Gihaz, S.; Ben Mamoun, C.
Deposited on : 2021-12-02
Resolution : 2.40 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

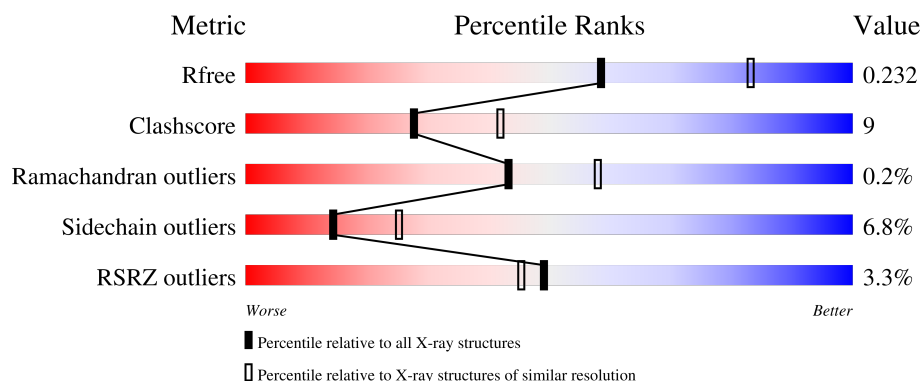
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	375	3% 66% 18% • 14%
1	B	375	2% 63% 19% • 16%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	405	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5335 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.

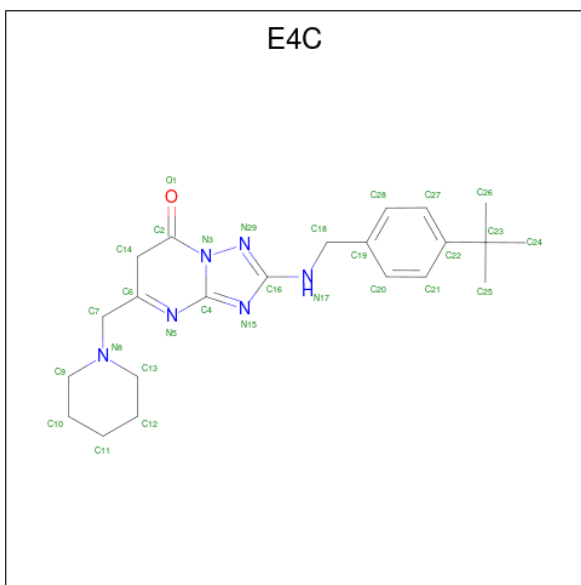
- Molecule 1 is a protein called Pantothenate kinase CAB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	3	0
			2537	1630	411	484	12			
1	B	314	Total	C	N	O	S	0	3	0
			2471	1595	399	466	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q04430
A	-6	ALA	-	expression tag	UNP Q04430
A	-5	HIS	-	expression tag	UNP Q04430
A	-4	HIS	-	expression tag	UNP Q04430
A	-3	HIS	-	expression tag	UNP Q04430
A	-2	HIS	-	expression tag	UNP Q04430
A	-1	HIS	-	expression tag	UNP Q04430
A	0	HIS	-	expression tag	UNP Q04430
B	-7	MET	-	initiating methionine	UNP Q04430
B	-6	ALA	-	expression tag	UNP Q04430
B	-5	HIS	-	expression tag	UNP Q04430
B	-4	HIS	-	expression tag	UNP Q04430
B	-3	HIS	-	expression tag	UNP Q04430
B	-2	HIS	-	expression tag	UNP Q04430
B	-1	HIS	-	expression tag	UNP Q04430
B	0	HIS	-	expression tag	UNP Q04430

- Molecule 2 is (8S)-2-{[(4-tert-butylphenyl)methyl]amino}-5-[(piperidin-1-yl)methyl][1,2,4]triazolo[1,5-a]pyrimidin-7(6H)-one (CCD ID: E4C) (formula: C₂₂H₃₀N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	22	6	1		
2	B	1	Total	C	N	O	0	0
			29	22	6	1		

- 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		
3	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	109	Total	O	0	0
			109	109		
6	B	114	Total	O	0	0
			114	114		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.97Å 92.11Å 99.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.87 – 2.40 65.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.87-2.40) 100.0 (65.87-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.233 0.181 , 0.232	Depositor DCC
R_{free} test set	1566 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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, E4C, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/2602	1.10	0/3516
1	B	0.59	0/2536	1.14	10/3427 (0.3%)
All	All	0.59	0/5138	1.12	10/6943 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	PHE	CA-CB-CG	7.64	121.44	113.80
1	B	102	ARG	CB-CG-CD	-6.16	97.12	111.30
1	B	242	PHE	CB-CA-C	5.84	120.57	110.94
1	B	14	TYR	CA-C-N	5.68	126.28	119.98
1	B	14	TYR	C-N-CA	5.68	126.28	119.98
1	B	278	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	170	ASN	CB-CA-C	5.14	118.54	111.23
1	B	168	PRO	CA-C-N	-5.08	114.66	123.25
1	B	168	PRO	C-N-CA	-5.08	114.66	123.25
1	B	167	GLU	CB-CA-C	-5.02	103.50	110.37

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	2537	0	2449	47	0
1	B	2471	0	2406	53	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	4	0	6	0	0
4	B	8	0	12	2	0
5	A	7	0	10	4	0
5	B	7	0	10	1	0
6	A	109	0	0	4	0
6	B	114	0	0	4	0
All	All	5335	0	4893	90	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 9.

All (90) 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:185:TRP:HB3	1:B:242:PHE:HD2	1.13	1.12
1:A:185:TRP:HB3	1:B:242:PHE:CD2	1.85	1.12
1:A:77:ILE:HD11	1:A:103:PHE:HB2	1.40	1.01
1:A:185:TRP:CB	1:B:242:PHE:HD2	1.93	0.78
1:B:224:TYR:HA	5:B:401:PEG:H21	1.70	0.72
6:A:570:HOH:O	1:B:85:LYS:HE3	1.90	0.71
1:B:188:LEU:O	1:B:192:THR:OG1	2.07	0.71
1:B:25:ILE:HB	1:B:82:GLY:HA3	1.74	0.70
1:A:224:TYR:CE1	5:A:405:PEG:H32	2.29	0.67
1:B:316:GLY:HA2	1:B:321:MET:CE	2.29	0.63
1:A:77:ILE:CD1	1:A:103:PHE:HB2	2.23	0.63
1:B:316:GLY:HA2	1:B:321:MET:HE1	1.81	0.61
1:A:179:LEU:HD21	1:B:286:ALA:HB1	1.83	0.61
1:A:77:ILE:HD11	1:A:103:PHE:CB	2.24	0.61
1:B:72:ARG:O	1:B:98:LYS:HB2	2.01	0.61
1:A:185:TRP:HB3	1:B:242:PHE:CE2	2.36	0.60
1:A:244:ASN:HD21	1:A:273:MET:HE2	1.67	0.59
1:B:315:ARG:HA	6:B:591:HOH:O	2.02	0.58
1:B:64:LYS:HD2	6:B:575:HOH:O	2.04	0.58
1:B:8:ILE:HG21	1:B:120:ILE:HD12	1.87	0.57
1:A:300:LYS:HD3	1:B:301:ILE:HD13	1.86	0.55
1:A:115:PHE:CG	1:A:354:LEU:HD11	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:HE2	1:A:315:ARG:HD3	1.72	0.55
5:A:405:PEG:H41	1:B:84:PHE:HE2	1.72	0.55
1:A:244:ASN:ND2	1:A:273:MET:HE2	2.22	0.54
1:B:36:PRO:HG3	1:B:66:HIS:HB3	1.90	0.54
1:B:98:LYS:HD3	6:B:509:HOH:O	2.07	0.53
1:B:356:ALA:O	1:B:357:SER:C	2.52	0.53
1:A:329:ASN:ND2	1:A:334:GLY:HA2	2.24	0.53
1:B:75:HIS:HD2	6:B:533:HOH:O	1.91	0.53
1:A:6:GLN:CD	1:A:6:GLN:N	2.68	0.52
1:A:274:PHE:HB2	1:A:279:ILE:HD11	1.92	0.51
1:A:286:ALA:HB1	1:B:179:LEU:HD21	1.92	0.51
1:B:116:PHE:CZ	1:B:350:MET:HE3	2.45	0.51
1:B:192:THR:HB	1:B:203:TRP:HZ3	1.74	0.51
5:A:405:PEG:H41	1:B:84:PHE:CE2	2.46	0.51
1:A:117:ILE:O	1:A:138:THR:HG23	2.11	0.50
1:A:65:GLU:HB2	6:A:600:HOH:O	2.11	0.50
1:B:112:GLY:HA3	1:B:347:LEU:O	2.12	0.50
1:B:22:ALA:HB3	1:B:33[B]:VAL:HG22	1.94	0.49
1:A:127:TYR:CZ	1:A:318:LEU:HG	2.48	0.48
1:A:356:ALA:O	1:A:357:SER:C	2.56	0.48
1:A:23:ILE:HD12	1:A:25:ILE:HD11	1.95	0.48
1:B:37:ILE:HG22	1:B:38:HIS:CD2	2.49	0.48
1:B:184:LEU:HD21	1:B:284:LEU:HD12	1.95	0.48
1:A:156:ILE:HG23	1:A:160:VAL:HG22	1.95	0.48
1:B:113:LEU:HD22	1:B:153[B]:LEU:HG	1.95	0.48
5:A:405:PEG:H21	6:A:597:HOH:O	2.14	0.48
1:A:37:ILE:HG22	1:A:38:HIS:CD2	2.48	0.48
1:A:190:LEU:HG	1:A:268:LYS:HE2	1.96	0.48
1:B:192:THR:HB	1:B:203:TRP:CZ3	2.50	0.47
1:B:133:GLU:OE2	1:B:135:ILE:HD11	2.14	0.47
1:A:116:PHE:HB3	1:A:123:GLU:HG2	1.96	0.47
1:A:220:TYR:CE2	1:B:81:GLY:HA2	2.50	0.47
1:A:113:LEU:HD22	1:A:153:LEU:HD13	1.97	0.47
1:B:29:LEU:HD12	4:B:406:EDO:H12	1.96	0.47
1:A:293:GLN:NE2	6:A:507:HOH:O	2.49	0.47
1:A:83:ALA:O	1:A:87:TYR:HB2	2.15	0.46
1:A:267:GLU:HG3	1:A:268:LYS:HD2	1.97	0.46
1:B:44:PHE:CE2	1:B:350:MET:CE	2.98	0.46
1:A:60:HIS:HD2	1:A:71:TYR:OH	1.99	0.46
1:A:220:TYR:CD2	1:B:81:GLY:HA2	2.51	0.46
1:B:33[B]:VAL:CG2	1:B:353:PHE:HB2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:NE1	1:A:197:TYR:CE1	2.84	0.45
1:A:276:ASN:N	1:A:277:PRO:CD	2.79	0.45
1:B:167:GLU:HB3	1:B:168:PRO:HD2	1.98	0.45
1:B:276:ASN:HB2	1:B:277:PRO:HD3	1.98	0.45
1:A:36:PRO:HG3	1:A:66:HIS:HB3	1.99	0.45
1:B:29:LEU:HB2	4:B:406:EDO:H12	1.99	0.44
1:B:122:ASP:HA	1:B:135:ILE:CG2	2.48	0.44
1:B:56:MET:HG3	1:B:93:ASN:ND2	2.32	0.44
1:A:25:ILE:HB	1:A:82:GLY:HA3	2.00	0.44
1:B:315:ARG:HB3	1:B:317:HIS:CD2	2.53	0.43
1:B:164:LYS:HD3	1:B:174:VAL:CG1	2.49	0.43
1:A:16:ASP:OD1	1:A:16:ASP:C	2.62	0.43
1:A:268:LYS:HE3	1:B:191:ILE:HG23	2.00	0.43
1:A:110:ILE:HD12	1:A:110:ILE:HA	1.91	0.43
1:A:81:GLY:HA3	1:B:219:ILE:HG22	2.00	0.42
1:B:164:LYS:HD3	1:B:174:VAL:HG11	2.01	0.42
1:B:51:LYS:HB3	1:B:54:LYS:HG2	2.02	0.42
1:A:34:PHE:CE2	1:A:62:ILE:HD13	2.55	0.42
1:A:127:TYR:CD2	1:A:127:TYR:C	2.98	0.42
1:B:44:PHE:CZ	1:B:350:MET:HE1	2.54	0.42
1:A:44:PHE:HB3	1:A:346:TYR:CZ	2.54	0.42
1:B:114:ASP:O	1:B:118:HIS:HD2	2.04	0.41
1:B:11:ASN:HA	1:B:40:ASN:OD1	2.21	0.41
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.97	0.40
1:B:316:GLY:HA2	1:B:321:MET:HE2	2.02	0.40
1:A:146:LYS:C	1:A:148:ILE:H	2.30	0.40
1:B:33[B]:VAL:HG23	1:B:353:PHE:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/375 (86%)	310 (97%)	10 (3%)	1 (0%)	36	50
1	B	311/375 (83%)	303 (97%)	8 (3%)	0	100	100
All	All	632/750 (84%)	613 (97%)	18 (3%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	GLU

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	271/322 (84%)	247 (91%)	24 (9%)	9	15
1	B	265/322 (82%)	250 (94%)	15 (6%)	18	33
All	All	536/644 (83%)	497 (93%)	39 (7%)	14	22

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	28[A]	THR
1	A	28[B]	THR
1	A	31	LYS
1	A	32[A]	VAL
1	A	32[B]	VAL
1	A	45	TYR
1	A	48	GLU
1	A	50	GLU
1	A	77	ILE
1	A	96	GLN
1	A	110	ILE
1	A	158	SER
1	A	167	GLU
1	A	196	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	LEU
1	A	205	GLN
1	A	211	SER
1	A	238	PHE
1	A	241	VAL
1	A	243	GLN
1	A	281	LYS
1	A	318	LEU
1	A	357	SER
1	B	6	GLN
1	B	9	SER
1	B	28[A]	THR
1	B	28[B]	THR
1	B	31	LYS
1	B	47	ILE
1	B	54	LYS
1	B	56	MET
1	B	98	LYS
1	B	130	GLN
1	B	199	GLN
1	B	201	LEU
1	B	226	LYS
1	B	243	GLN
1	B	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	38	HIS
1	A	60	HIS
1	A	75	HIS
1	A	96	GLN
1	A	155	ASN
1	A	205	GLN
1	A	225	ASN
1	A	244	ASN
1	A	293	GLN
1	A	302	ASN
1	A	306	ASN
1	A	317	HIS
1	B	38	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	75	HIS
1	B	93	ASN
1	B	118	HIS
1	B	293	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](#)

11 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	E4C	B	403	-	28,32,32	1.06	1 (3%)	33,46,46	2.39	11 (33%)
4	EDO	B	406	-	3,3,3	0.27	0	2,2,2	0.67	0
5	PEG	A	405	-	6,6,6	0.60	0	5,5,5	0.52	0
3	SO4	B	404	-	4,4,4	0.38	0	6,6,6	0.15	0
4	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.62	0
3	SO4	B	405	-	4,4,4	0.33	0	6,6,6	0.10	0
2	E4C	A	401	-	28,32,32	1.12	1 (3%)	33,46,46	2.04	9 (27%)
5	PEG	B	401	-	6,6,6	0.24	0	5,5,5	0.15	0
3	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	402	-	3,3,3	0.22	0	2,2,2	0.58	0
3	SO4	A	403	-	4,4,4	0.28	0	6,6,6	0.14	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	E4C	B	403	-	-	0/13/35/35	0/4/4/4
4	EDO	B	406	-	-	1/1/1/1	-
5	PEG	A	405	-	-	3/4/4/4	-
4	EDO	A	404	-	-	1/1/1/1	-
5	PEG	B	401	-	-	2/4/4/4	-
2	E4C	A	401	-	-	1/13/35/35	0/4/4/4
4	EDO	B	402	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	E4C	C14-C6	-3.72	1.34	1.49
2	A	401	E4C	C14-C6	-3.66	1.35	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	E4C	N3-C4-N5	-7.64	115.97	122.61
2	B	403	E4C	N5-C4-N15	5.55	136.53	127.73
2	A	401	E4C	N3-C4-N5	-4.73	118.50	122.61
2	A	401	E4C	N5-C4-N15	4.50	134.87	127.73
2	B	403	E4C	C11-C10-C9	4.33	119.20	111.19
2	A	401	E4C	C4-N3-N29	4.09	113.46	110.41
2	A	401	E4C	N3-C4-N15	-3.85	106.63	109.14
2	B	403	E4C	O1-C2-C14	3.48	128.54	118.60
2	A	401	E4C	C12-C11-C10	-3.41	101.06	111.19
2	A	401	E4C	O1-C2-C14	3.40	128.31	118.60
2	B	403	E4C	N3-C4-N15	-2.52	107.50	109.14
2	B	403	E4C	C6-N5-C4	2.47	119.86	117.06
2	B	403	E4C	C18-C19-C28	-2.40	116.04	120.94
2	B	403	E4C	N29-C16-N15	-2.40	113.48	116.67
2	A	401	E4C	C11-C10-C9	2.31	115.47	111.19
2	A	401	E4C	C11-C12-C13	2.31	115.47	111.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	E4C	C18-C19-C20	2.25	125.52	120.94
2	B	403	E4C	C25-C23-C24	-2.17	101.91	108.36
2	A	401	E4C	C12-C13-N8	-2.08	108.07	111.30
2	B	403	E4C	C7-N8-C13	-2.02	108.00	111.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

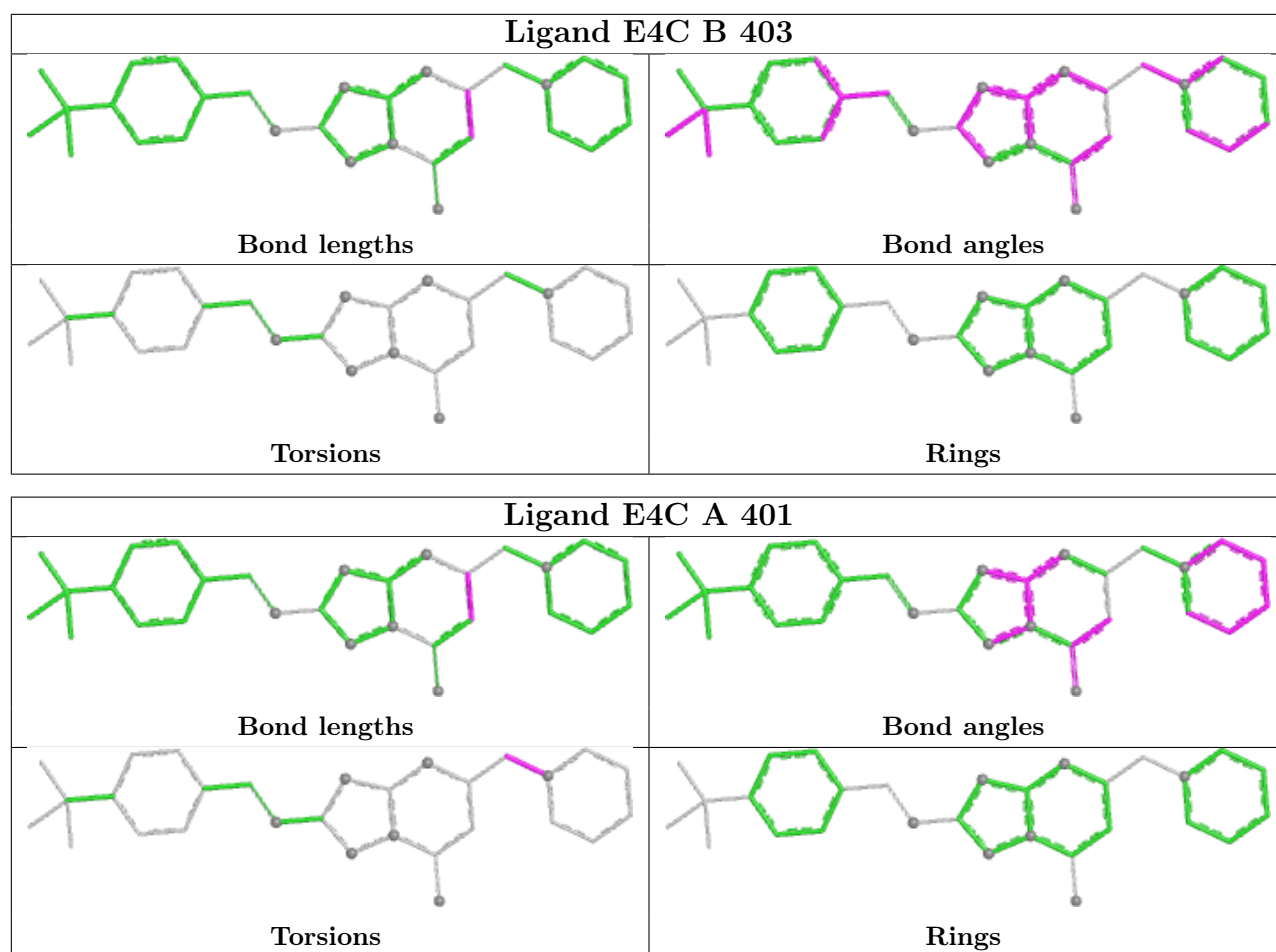
Mol	Chain	Res	Type	Atoms
5	A	405	PEG	O2-C3-C4-O4
5	A	405	PEG	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2
5	B	401	PEG	O2-C3-C4-O4
2	A	401	E4C	C6-C7-N8-C13
5	A	405	PEG	C4-C3-O2-C2
5	B	401	PEG	C1-C2-O2-C3
4	B	406	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	406	EDO	2	0
5	A	405	PEG	4	0
5	B	401	PEG	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.



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	324/375 (86%)	-0.34	13 (4%) 42 38	15, 29, 63, 126	3 (0%)
1	B	314/375 (83%)	-0.26	8 (2%) 58 54	12, 31, 64, 94	3 (0%)
All	All	638/750 (85%)	-0.30	21 (3%) 49 45	12, 30, 65, 126	6 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	GLN	4.8
1	A	266	ILE	4.7
1	A	271	GLY	4.3
1	A	185	TRP	4.2
1	A	270	ASN	3.7
1	A	267	GLU	3.5
1	B	146	LYS	3.4
1	A	138	THR	3.3
1	A	146	LYS	3.3
1	A	244	ASN	3.3
1	A	268	LYS	3.1
1	A	242	PHE	2.9
1	A	269	ASN	2.6
1	B	357	SER	2.5
1	A	357	SER	2.4
1	A	147	ALA	2.4
1	B	147	ALA	2.3
1	B	316	GLY	2.2
1	B	197	TYR	2.1
1	B	242	PHE	2.0
1	B	137	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

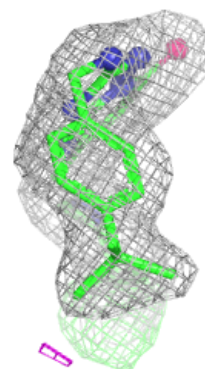
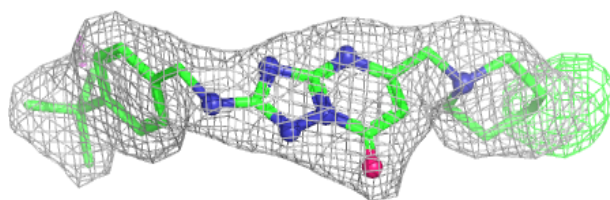
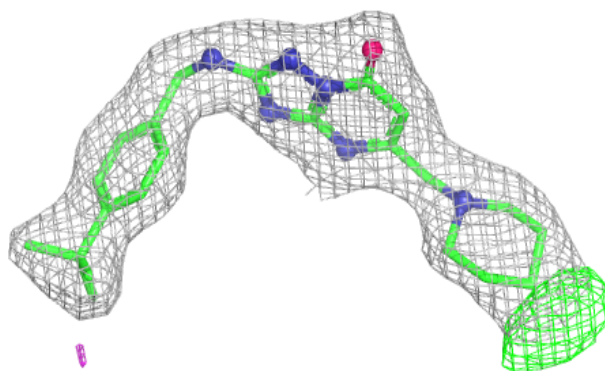
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EDO	B	402	4/4	0.82	0.21	58,62,64,67	0
3	SO4	A	403	5/5	0.86	0.12	59,63,75,81	0
4	EDO	A	404	4/4	0.88	0.15	44,46,49,54	0
5	PEG	A	405	7/7	0.90	0.15	29,41,44,48	0
3	SO4	B	405	5/5	0.93	0.11	59,60,69,70	0
2	E4C	A	401	29/29	0.93	0.07	19,24,35,39	0
5	PEG	B	401	7/7	0.93	0.12	39,48,51,52	0
2	E4C	B	403	29/29	0.95	0.07	20,23,28,31	0
3	SO4	A	402	5/5	0.96	0.07	46,47,51,52	0
4	EDO	B	406	4/4	0.96	0.10	36,40,43,48	0
3	SO4	B	404	5/5	0.98	0.06	39,40,44,46	0

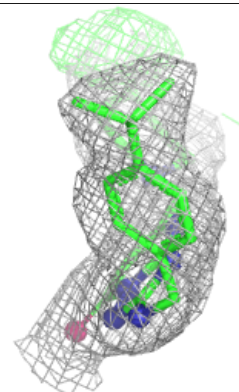
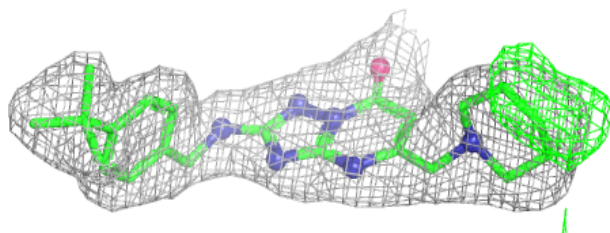
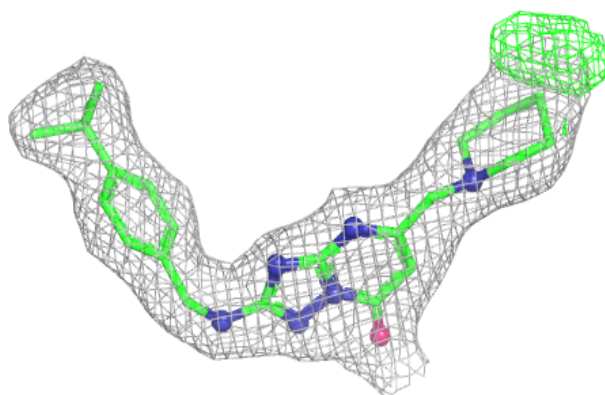
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around E4C A 401:

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

**Electron density around E4C B 403:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.