wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 10:18 AM UTC

PDB ID	:	7ZID / pdb_00007zid
Title	:	Crystal Structure of truncated aspartate transcarbamoylase from Plasmodium falciparum in complex with BDA-14
Authors	:	Wang, C.; Zhang, B.
Deposited on	:	2022-04-07
Resolution	:	2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

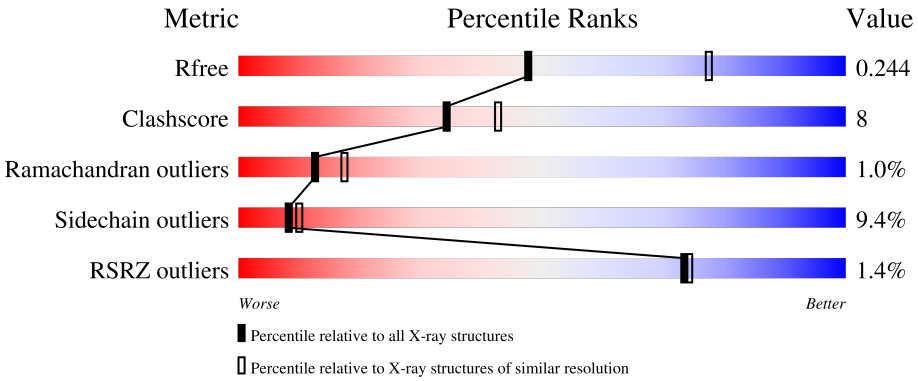
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	349	% 69% 19% • 8%
1	B	349	% 71% 17% 6% 5%
1	C	349	2% 72% 15% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15800 atoms, of which 7903 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	H	N	O	S	80	0	0
			5189	1649	2604	429	499	8			
1	B	331	Total	C	H	N	O	S	82	0	0
			5356	1704	2681	440	523	8			
1	C	319	Total	C	H	N	O	S	82	0	0
			5144	1634	2580	423	499	8			

There are 30 discrepancies between the modelled and reference sequences:

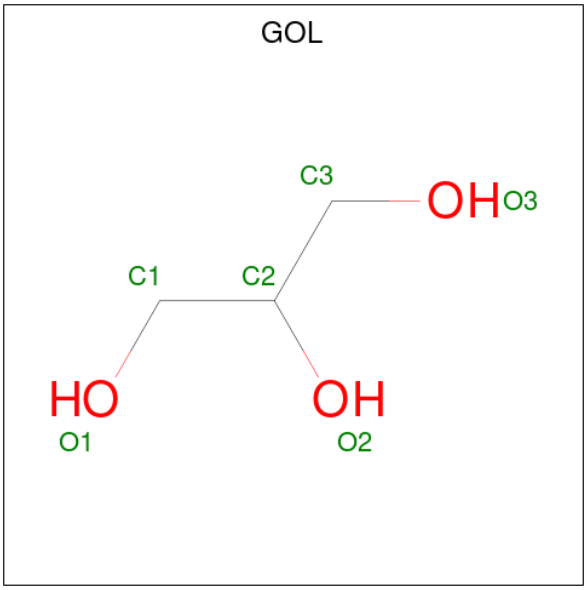
Chain	Residue	Modelled	Actual	Comment	Reference
A	376	SER	-	expression tag	UNP A0A5K1K910
A	377	ALA	-	expression tag	UNP A0A5K1K910
A	378	TRP	-	expression tag	UNP A0A5K1K910
A	379	SER	-	expression tag	UNP A0A5K1K910
A	380	HIS	-	expression tag	UNP A0A5K1K910
A	381	PRO	-	expression tag	UNP A0A5K1K910
A	382	GLN	-	expression tag	UNP A0A5K1K910
A	383	PHE	-	expression tag	UNP A0A5K1K910
A	384	GLU	-	expression tag	UNP A0A5K1K910
A	385	LYS	-	expression tag	UNP A0A5K1K910
B	376	SER	-	expression tag	UNP A0A5K1K910
B	377	ALA	-	expression tag	UNP A0A5K1K910
B	378	TRP	-	expression tag	UNP A0A5K1K910
B	379	SER	-	expression tag	UNP A0A5K1K910
B	380	HIS	-	expression tag	UNP A0A5K1K910
B	381	PRO	-	expression tag	UNP A0A5K1K910
B	382	GLN	-	expression tag	UNP A0A5K1K910
B	383	PHE	-	expression tag	UNP A0A5K1K910
B	384	GLU	-	expression tag	UNP A0A5K1K910
B	385	LYS	-	expression tag	UNP A0A5K1K910
C	376	SER	-	expression tag	UNP A0A5K1K910
C	377	ALA	-	expression tag	UNP A0A5K1K910
C	378	TRP	-	expression tag	UNP A0A5K1K910

Continued on next page...

Continued from previous page...

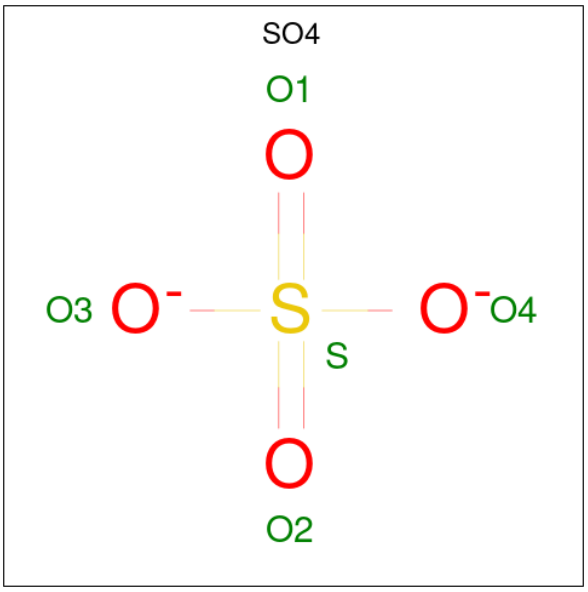
Chain	Residue	Modelled	Actual	Comment	Reference
C	379	SER	-	expression tag	UNP A0A5K1K910
C	380	HIS	-	expression tag	UNP A0A5K1K910
C	381	PRO	-	expression tag	UNP A0A5K1K910
C	382	GLN	-	expression tag	UNP A0A5K1K910
C	383	PHE	-	expression tag	UNP A0A5K1K910
C	384	GLU	-	expression tag	UNP A0A5K1K910
C	385	LYS	-	expression tag	UNP A0A5K1K910

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



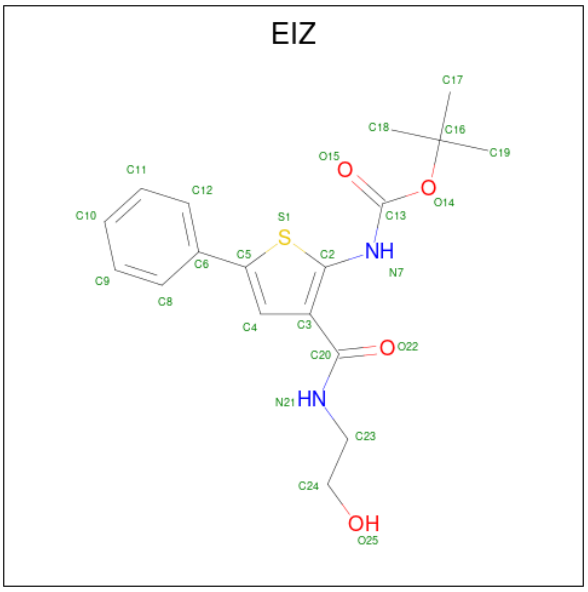
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			14	3	8	3		
2	A	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is tert-butyl N-[3-(2-hydroxyethylcarbamoyl)-5-phenyl-thiophen-2-yl]carbamate (CCD ID: EIZ) (formula: $C_{18}H_{22}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H N O S 47 18 22 2 4 1	1	0

- Molecule 5 is water.

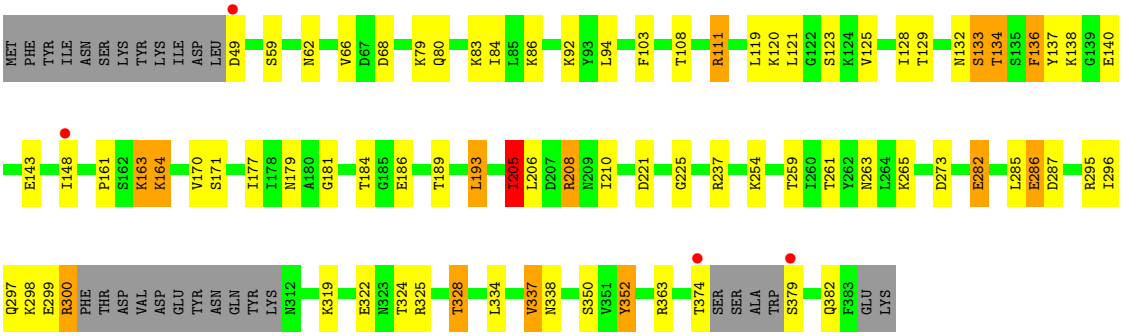
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	14	Total O 14 14	0	0
5	C	4	Total O 4 4	0	0

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.

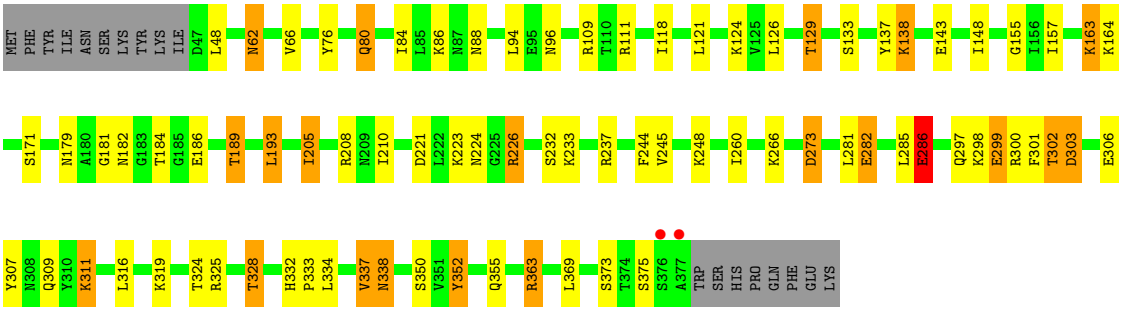
• Molecule 1: Aspartate carbamoyltransferase

Chain A:



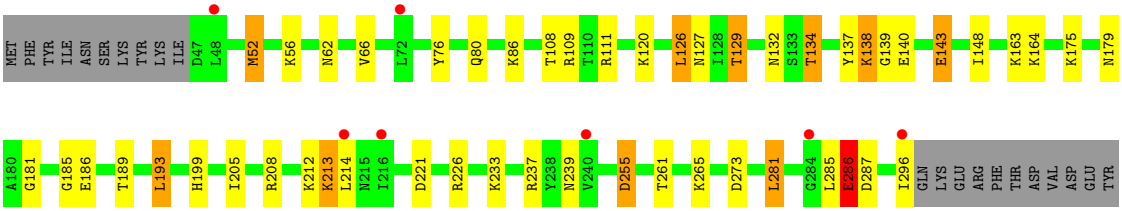
• Molecule 1: Aspartate carbamoyltransferase

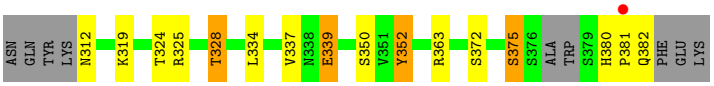
Chain B:



• Molecule 1: Aspartate carbamoyltransferase

Chain C:




ASN
GLN
TYR
LYS
N312
K319
T324
R325
T328
L334
V337
N338
E339
S350
V351
Y352
R363
S372
S375
S376
ALA
TRP
S379
H380
P381
Q382
PHE
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.26Å 90.02Å 136.94Å 90.00° 108.87° 90.00°	Depositor
Resolution (Å)	45.60 – 2.55 45.60 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.60-2.55) 95.7 (45.60-2.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.244 0.202 , 0.244	Depositor DCC
R_{free} test set	2205 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	67.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15800	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.14	4/2631 (0.2%)	1.51	6/3551 (0.2%)
1	B	1.18	5/2723 (0.2%)	1.57	10/3679 (0.3%)
1	C	1.11	1/2609 (0.0%)	1.49	5/3524 (0.1%)
All	All	1.15	10/7963 (0.1%)	1.53	21/10754 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	VAL	C-O	-7.36	1.16	1.23
1	B	244	PHE	C-O	7.26	1.32	1.24
1	B	245	VAL	C-O	-7.09	1.16	1.24
1	A	59	SER	C-O	-6.66	1.16	1.24
1	B	303	ASP	C-O	6.38	1.30	1.23

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	363	ARG	NE-CZ-NH1	-7.83	113.67	121.50
1	B	363	ARG	NE-CZ-NH2	7.03	125.52	119.20
1	B	205	ILE	N-CA-CB	6.69	119.64	110.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	PHE	CA-C-O	-6.55	113.94	121.47
1	A	205	ILE	N-CA-CB	6.07	118.79	110.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ILE	Peptide
1	C	139	GLY	Peptide

5.2 Too-close contacts (i)

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	2585	2604	2595	47	0
1	B	2675	2681	2675	46	0
1	C	2564	2580	2571	37	0
2	A	12	16	16	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	B	25	22	0	0	0
5	A	8	0	0	0	0
5	B	14	0	0	0	0
5	C	4	0	0	0	0
All	All	7897	7903	7857	120	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 8.

The worst 5 of 120 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:299:GLU:OE2	1:A:299:GLU:N	2.06	0.89
1:A:382:GLN:HA	1:A:382:GLN:OE1	1.77	0.84
1:B:307:TYR:CE2	1:B:311:LYS:HD2	2.20	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:O	1:A:300:ARG:HB3	1.85	0.77
1:A:285:LEU:O	1:A:286:GLU:O	2.04	0.76

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	314/349 (90%)	295 (94%)	16 (5%)	3 (1%)	12	17
1	B	329/349 (94%)	312 (95%)	14 (4%)	3 (1%)	14	20
1	C	313/349 (90%)	287 (92%)	22 (7%)	4 (1%)	9	12
All	All	956/1047 (91%)	894 (94%)	52 (5%)	10 (1%)	12	17

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	286	GLU
1	B	286	GLU
1	C	138	LYS
1	C	286	GLU

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	300/328 (92%)	272 (91%)	28 (9%)	8 10
1	B	310/328 (94%)	276 (89%)	34 (11%)	6 6
1	C	299/328 (91%)	276 (92%)	23 (8%)	12 17
All	All	909/984 (92%)	824 (91%)	85 (9%)	8 10

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	319	LYS
1	C	143	GLU
1	B	352	TYR
1	C	108	THR
1	C	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	ASN
1	B	338	ASN
1	C	280	ASN
1	B	312	ASN
1	B	355	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)

5 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	$\#\|Z\| > 2$
4	EIZ	B	401	-	26,26,26	0.71	0	35,36,36	3.05	8 (22%)
3	SO4	B	402	-	4,4,4	0.62	0	6,6,6	0.45	0
2	GOL	A	402	-	5,5,5	0.33	0	5,5,5	0.43	0
3	SO4	A	403	-	4,4,4	0.34	0	6,6,6	0.16	0
2	GOL	A	401	-	5,5,5	0.17	0	5,5,5	0.28	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	A	402	-	-	4/4/4/4	-
4	EIZ	B	401	-	-	8/21/21/21	0/2/2/2
2	GOL	A	401	-	-	4/4/4/4	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	EIZ	C3-C2-S1	-14.38	106.61	111.64
4	B	401	EIZ	C4-C3-C2	-8.26	104.41	111.67
4	B	401	EIZ	C3-C2-N7	3.58	129.74	125.01
4	B	401	EIZ	O14-C16-C18	3.09	119.42	107.21
4	B	401	EIZ	C4-C3-C20	2.22	131.29	125.97

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3
2	A	402	GOL	O1-C1-C2-O2
2	A	402	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

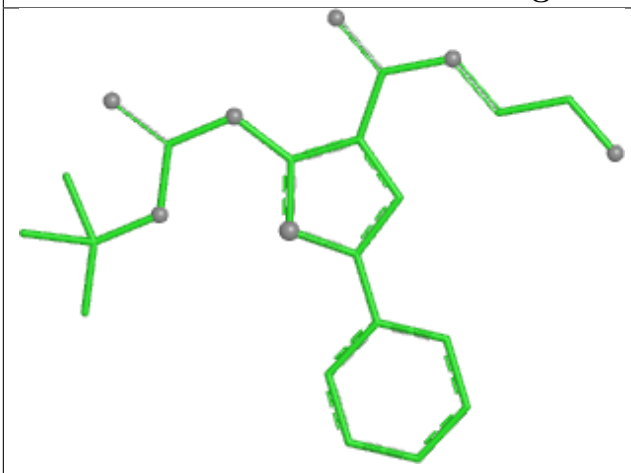
Mol	Chain	Res	Type	Atoms
2	A	402	GOL	O2-C2-C3-O3
4	B	401	EIZ	S1-C2-N7-C13

There are no ring outliers.

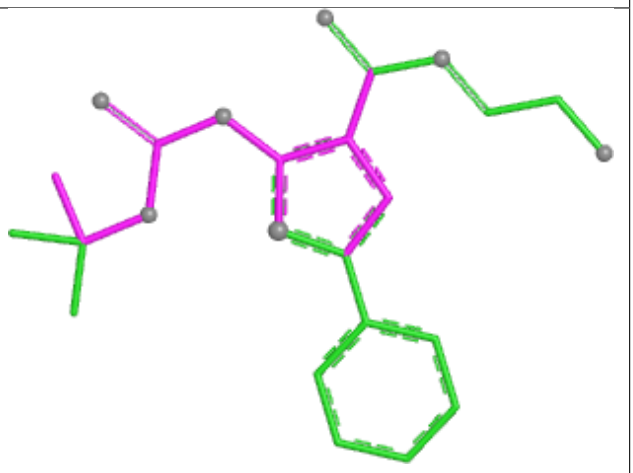
No monomer is involved in short contacts.

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

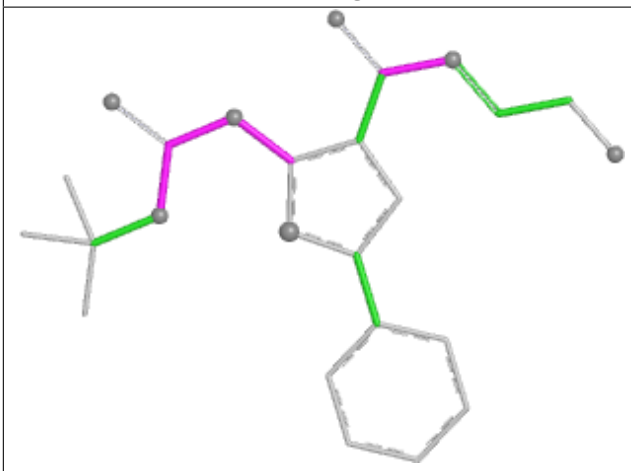
Ligand EIZ B 401



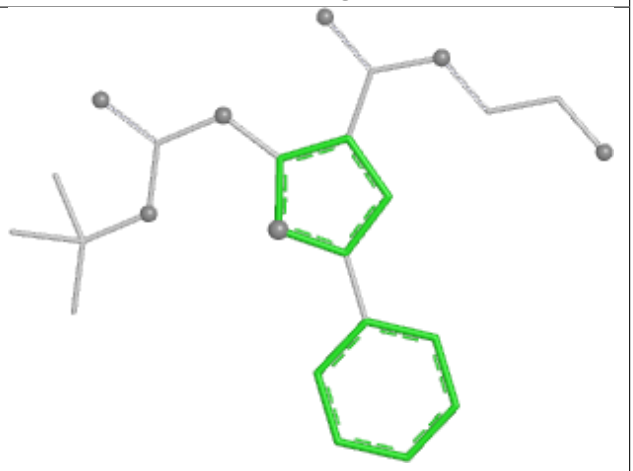
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	320/349 (91%)	-0.05	4 (1%)	75	75	46, 78, 111, 126	0
1	B	331/349 (94%)	-0.27	2 (0%)	85	88	44, 67, 103, 140	0
1	C	319/349 (91%)	0.33	8 (2%)	58	59	48, 93, 135, 159	0
All	All	970/1047 (92%)	0.00	14 (1%)	73	74	44, 77, 124, 159	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	ALA	6.5
1	C	381	PRO	4.2
1	A	374	THR	3.5
1	C	48	LEU	3.2
1	C	214	LEU	3.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

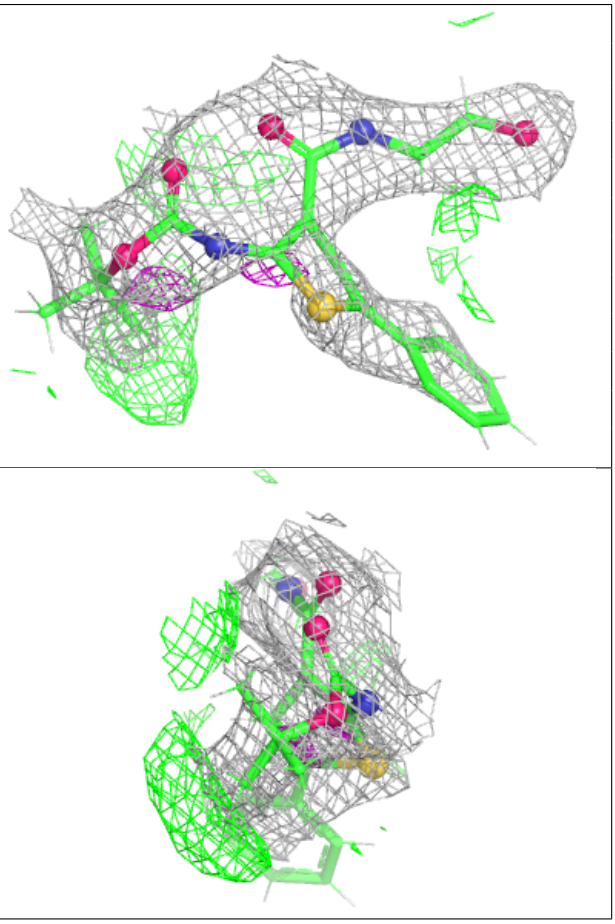
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EIZ	B	401	25/25	0.80	0.19	30,116,138,140	1
2	GOL	A	401	6/6	0.81	0.15	30,107,112,112	2
3	SO4	A	403	5/5	0.83	0.09	73,94,99,107	0
2	GOL	A	402	6/6	0.91	0.12	30,99,102,102	2
3	SO4	B	402	5/5	0.95	0.14	70,71,76,80	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 EIZ B 401:

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



6.5 Other polymers

There are no such residues in this entry.