



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:03 PM UTC

PDB ID : 8T7D / pdb_00008t7d
Title : Crystal structure of wild type IDH1 bound to compound 1
Authors : Lu, J.; Abeywickrema, P.; Heo, M.R.; Parthasarathy, G.; McCoy, M.; Soisson, S.M.
Deposited on : 2023-06-20
Resolution : 3.44 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

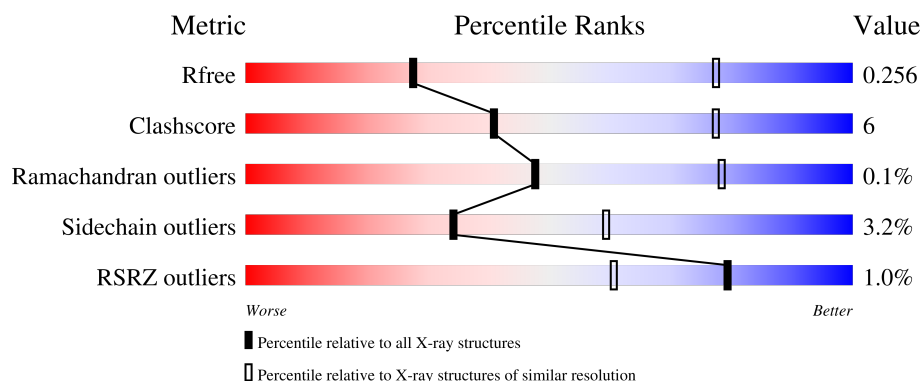
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	424	% 78% 14% 7%
1	B	424	77% 14% 8%
1	C	424	% 79% 12% 8%
1	D	424	% 77% 14% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11650 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2926	1861	491	556	18			
1	B	390	Total	C	N	O	S	0	0	0
			2913	1857	485	553	18			
1	C	390	Total	C	N	O	S	0	0	0
			2895	1844	483	550	18			
1	D	387	Total	C	N	O	S	0	0	0
			2796	1783	466	530	17			

There are 40 discrepancies between the modelled and reference sequences:

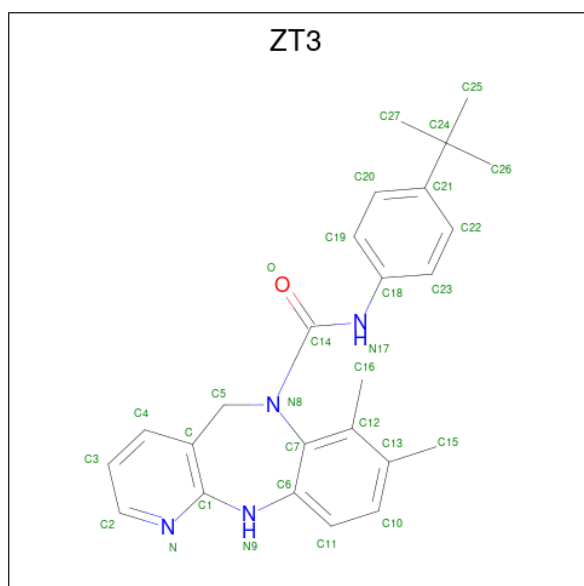
Chain	Residue	Modelled	Actual	Comment	Reference
A	415	LEU	-	expression tag	UNP O75874
A	416	GLU	-	expression tag	UNP O75874
A	417	HIS	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
B	415	LEU	-	expression tag	UNP O75874
B	416	GLU	-	expression tag	UNP O75874
B	417	HIS	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874
C	415	LEU	-	expression tag	UNP O75874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	416	GLU	-	expression tag	UNP O75874
C	417	HIS	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
D	415	LEU	-	expression tag	UNP O75874
D	416	GLU	-	expression tag	UNP O75874
D	417	HIS	-	expression tag	UNP O75874
D	418	HIS	-	expression tag	UNP O75874
D	419	HIS	-	expression tag	UNP O75874
D	420	HIS	-	expression tag	UNP O75874
D	421	HIS	-	expression tag	UNP O75874
D	422	HIS	-	expression tag	UNP O75874
D	423	HIS	-	expression tag	UNP O75874
D	424	HIS	-	expression tag	UNP O75874

- Molecule 2 is N-(4-tert-butylphenyl)-7,8-dimethyl-5,11-dihydro-6H-pyrido[2,3-b][1,5]benzodiazepine-6-carboxamide (CCD ID: ZT3) (formula: C₂₅H₂₈N₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	25	4	1		

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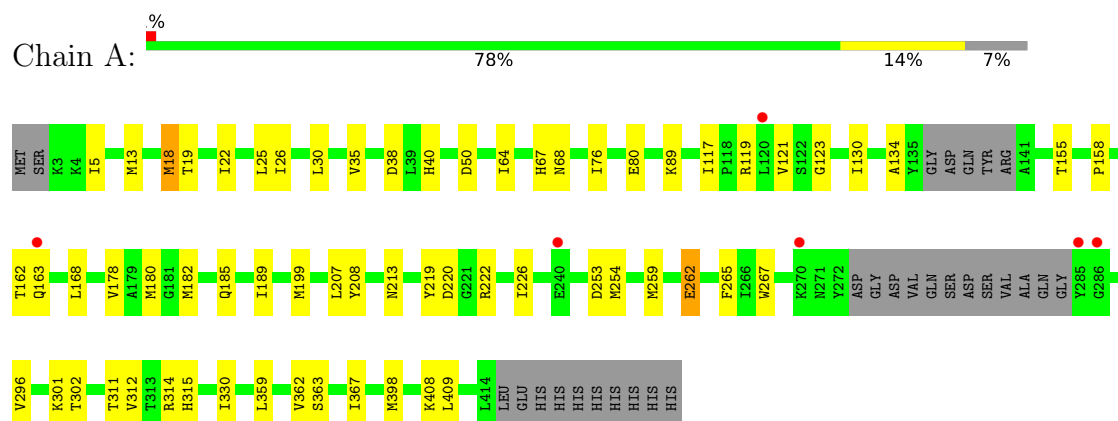
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			30	25	4	1		
2	C	1	Total	C	N	O	0	0
			30	25	4	1		
2	D	1	Total	C	N	O	0	0
			30	25	4	1		

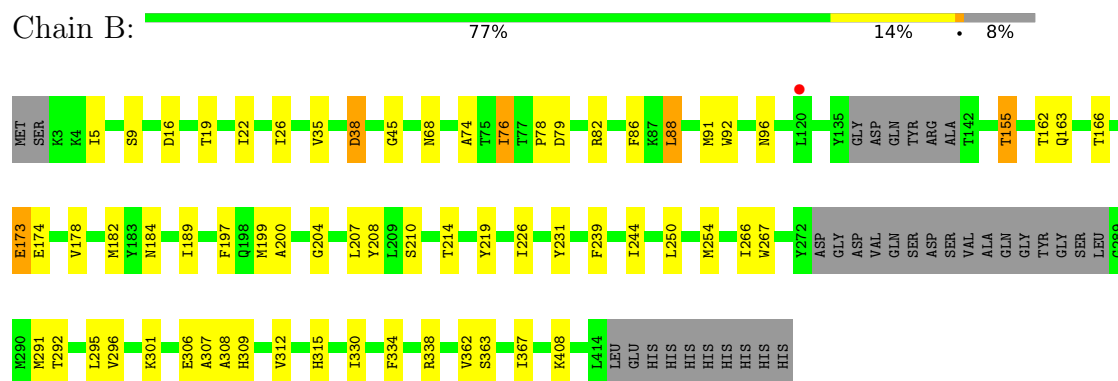
3 Residue-property plots

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.

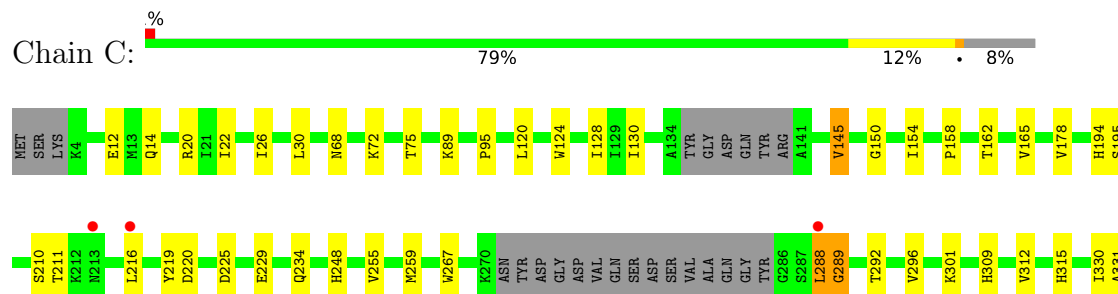
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

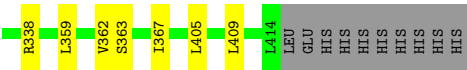


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

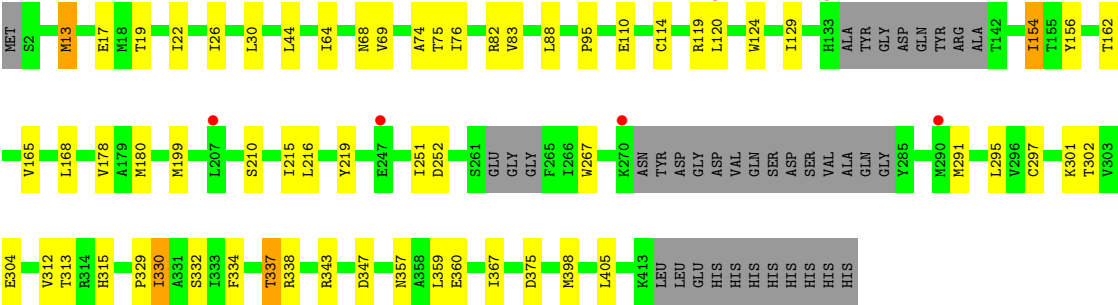
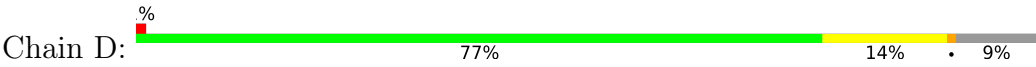


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic





● Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.59Å 120.99Å 139.27Å 90.00° 119.39° 90.00°	Depositor
Resolution (Å)	91.52 – 3.44 91.52 – 3.44	Depositor EDS
% Data completeness (in resolution range)	98.9 (91.52-3.44) 98.9 (91.52-3.44)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.240 , 0.267 0.223 , 0.256	Depositor DCC
R_{free} test set	1536 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11650	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: ZT3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	3/2989 (0.1%)	1.06	3/4072 (0.1%)
1	B	0.68	0/2977	1.04	2/4058 (0.0%)
1	C	0.67	0/2957	1.04	1/4029 (0.0%)
1	D	0.72	2/2856 (0.1%)	1.08	1/3904 (0.0%)
All	All	0.70	5/11779 (0.0%)	1.05	7/16063 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	MET	SD-CE	-7.33	1.61	1.79
1	A	134	ALA	CA-C	6.69	1.61	1.52
1	D	13	MET	SD-CE	-5.72	1.65	1.79
1	A	254	MET	SD-CE	-5.51	1.65	1.79
1	D	398	MET	SD-CE	-5.04	1.67	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASP	N-CA-C	-6.24	100.91	109.71
1	A	265	PHE	CA-CB-CG	5.74	119.54	113.80
1	B	79	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	253	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	252	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	38	ASP	N-CA-C	-5.28	99.38	108.56
1	C	145	VAL	N-CA-C	5.00	115.77	110.72

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	2926	0	2680	40	0
1	B	2913	0	2678	40	0
1	C	2895	0	2675	37	0
1	D	2796	0	2503	38	0
2	A	30	0	0	1	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
All	All	11650	0	10536	144	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 6.

All (144) 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:C:211:THR:HG23	1:C:220:ASP:HB3	1.37	1.00
1:D:13:MET:HE1	1:D:64:ILE:HD11	1.44	0.99
1:C:211:THR:HB	1:C:248:HIS:HE1	1.28	0.95
1:C:211:THR:HB	1:C:248:HIS:CE1	2.10	0.87
1:A:180:MET:HE2	1:A:182:MET:HE1	1.56	0.86
1:A:13:MET:HE1	1:A:64:ILE:HD11	1.59	0.83
1:D:13:MET:CE	1:D:64:ILE:HD11	2.13	0.79
1:B:239:PHE:CD2	1:B:244:ILE:HG22	2.19	0.78
1:B:362:VAL:HG22	1:B:408:LYS:HD3	1.69	0.75
1:A:362:VAL:HG22	1:A:408:LYS:HD2	1.68	0.74
1:A:362:VAL:CG2	1:A:408:LYS:HD2	2.16	0.74
1:B:16:ASP:OD1	1:B:45:GLY:HA2	1.86	0.73
1:C:211:THR:CG2	1:C:220:ASP:HB3	2.18	0.72
1:D:69:VAL:HG21	1:D:343:ARG:HD2	1.75	0.69
1:A:178:VAL:HG21	1:B:219:TYR:HA	1.76	0.68
1:A:219:TYR:HA	1:B:178:VAL:HG21	1.76	0.67
1:A:130:ILE:HG22	1:A:267:TRP:HB3	1.75	0.67
1:A:13:MET:CE	1:A:64:ILE:HD11	2.24	0.67
1:A:76:ILE:HG23	1:A:311:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:SER:OG	1:C:267:TRP:NE1	2.29	0.66
1:B:76:ILE:HG21	1:B:82:ARG:HE	1.62	0.64
1:C:225:ASP:O	1:C:229:GLU:HG3	1.97	0.64
1:A:199:MET:HE2	1:A:296:VAL:HG21	1.79	0.64
1:B:199:MET:HE2	1:B:296:VAL:HG21	1.80	0.63
1:C:219:TYR:HA	1:D:178:VAL:HG21	1.81	0.62
1:C:330:ILE:HG13	1:C:367:ILE:HD11	1.80	0.62
1:A:30:LEU:HD23	1:A:359:LEU:HD11	1.83	0.60
1:C:75:THR:OG1	1:C:95:PRO:HG2	2.01	0.60
1:A:312:VAL:HG12	1:A:315:HIS:HB2	1.83	0.60
1:C:120:LEU:HD13	1:D:120:LEU:HD21	1.83	0.59
1:B:330:ILE:HG13	1:B:367:ILE:HD11	1.83	0.59
1:C:154:ILE:HB	1:D:154:ILE:HD12	1.84	0.59
1:A:330:ILE:HG13	1:A:367:ILE:HD11	1.84	0.58
1:C:72:LYS:NZ	1:C:75:THR:HG23	2.18	0.58
1:D:334:PHE:HA	1:D:337:THR:HG22	1.87	0.57
1:D:13:MET:HB3	1:D:44:LEU:HD12	1.86	0.56
1:B:204:GLY:HA2	1:B:244:ILE:HD11	1.88	0.56
1:C:130:ILE:HG22	1:C:267:TRP:HB3	1.88	0.56
1:A:180:MET:CE	1:A:182:MET:HE1	2.30	0.55
1:B:362:VAL:CG2	1:B:408:LYS:HD3	2.37	0.55
1:C:210:SER:CB	1:C:267:TRP:HE1	2.19	0.55
1:D:17:GLU:OE1	1:D:313:THR:HG22	2.07	0.55
1:D:295:LEU:HB3	1:D:304:GLU:HB3	1.88	0.55
1:C:359:LEU:HA	1:C:362:VAL:HG12	1.89	0.54
1:B:22:ILE:O	1:B:26:ILE:HG13	2.07	0.54
1:B:291:MET:HB3	1:B:308:ALA:HB3	1.89	0.54
1:D:68:ASN:HB3	1:D:301:LYS:O	2.08	0.54
1:B:312:VAL:HG12	1:B:315:HIS:HB2	1.89	0.54
1:C:292:THR:OG1	1:C:338:ARG:NH1	2.40	0.54
1:D:75:THR:OG1	1:D:95:PRO:HG2	2.07	0.53
1:B:292:THR:OG1	1:B:338:ARG:NH1	2.42	0.53
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.44	0.53
1:D:26:ILE:HG23	1:D:30:LEU:HD12	1.91	0.52
1:C:288:LEU:HD12	1:C:289:GLY:H	1.73	0.52
1:A:68:ASN:HB3	1:A:301:LYS:O	2.10	0.52
1:B:189:ILE:HG21	1:B:226:ILE:HD13	1.92	0.52
1:B:208:TYR:HB3	1:B:254:MET:HE3	1.92	0.52
1:D:119:ARG:NH1	1:D:124:TRP:O	2.43	0.51
1:D:215:ILE:HG22	1:D:216:LEU:HD12	1.93	0.51
1:B:214:THR:HG23	1:B:250:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HA	1:A:30:LEU:HD13	1.93	0.51
1:C:362:VAL:HG11	1:C:405:LEU:HD13	1.92	0.51
1:C:26:ILE:HG23	1:C:30:LEU:HD12	1.93	0.50
1:A:158:PRO:HG2	1:A:162:THR:HB	1.93	0.50
1:C:312:VAL:HG12	1:C:315:HIS:HB2	1.92	0.49
1:B:155:THR:HG22	1:B:166:THR:HG23	1.94	0.49
1:D:337:THR:HG21	1:D:360:GLU:HG2	1.95	0.49
1:C:195:SER:HB3	1:C:296:VAL:HG23	1.94	0.49
1:D:210:SER:HB3	1:D:267:TRP:HE1	1.78	0.49
1:A:262:GLU:H	1:A:262:GLU:CD	2.20	0.48
1:D:297:CYS:HB2	1:D:302:THR:OG1	2.14	0.48
1:C:178:VAL:HG21	1:D:219:TYR:HA	1.95	0.48
1:A:162:THR:HG22	1:A:163:GLN:H	1.79	0.48
1:A:22:ILE:O	1:A:26:ILE:HG13	2.14	0.47
1:A:362:VAL:HG23	1:A:408:LYS:HD2	1.95	0.47
1:B:76:ILE:CG2	1:B:82:ARG:HE	2.28	0.47
1:B:78:PRO:HG2	1:B:92:TRP:O	2.15	0.47
1:D:22:ILE:O	1:D:26:ILE:HG13	2.15	0.46
1:D:82:ARG:HH22	1:D:313:THR:HG21	1.80	0.46
1:B:162:THR:HG22	1:B:163:GLN:H	1.80	0.46
1:C:12:GLU:OE2	1:C:14:GLN:NE2	2.42	0.46
1:C:194:HIS:HE1	1:C:234:GLN:OE1	1.99	0.46
1:C:216:LEU:HD12	1:C:219:TYR:CB	2.45	0.46
1:D:343:ARG:NH1	1:D:347:ASP:OD2	2.49	0.46
1:D:110:GLU:HB2	1:D:129:ILE:HG12	1.96	0.46
1:D:330:ILE:HG13	1:D:367:ILE:HD11	1.98	0.46
1:B:208:TYR:HB3	1:B:254:MET:CE	2.46	0.46
1:C:22:ILE:O	1:C:26:ILE:HG13	2.15	0.45
1:A:180:MET:HB2	1:B:219:TYR:CE2	2.52	0.45
1:C:124:TRP:CE2	1:C:128:ILE:HD11	2.51	0.45
1:C:150:GLY:HA3	1:D:156:TYR:CE1	2.52	0.45
1:C:158:PRO:HG2	1:C:162:THR:HB	1.98	0.45
1:A:121:VAL:HG12	1:A:123:GLY:H	1.80	0.45
1:B:68:ASN:HB3	1:B:301:LYS:O	2.17	0.45
1:A:207:LEU:HD23	1:A:208:TYR:N	2.32	0.45
1:B:307:ALA:HB1	1:B:309:HIS:CD2	2.52	0.45
1:B:9:SER:HA	1:B:38:ASP:HB3	1.99	0.45
1:B:96:ASN:ND2	1:B:306:GLU:OE1	2.49	0.45
1:C:72:LYS:HZ3	1:C:75:THR:HG23	1.81	0.45
1:D:312:VAL:HG12	1:D:315:HIS:HB2	1.99	0.44
1:D:334:PHE:O	1:D:337:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.99	0.44
1:A:25:LEU:HB3	1:A:398:MET:HE2	2.00	0.44
1:B:182:MET:HE2	1:B:182:MET:HB3	1.89	0.44
1:D:359:LEU:HD13	1:D:405:LEU:HD22	1.99	0.44
1:D:83:VAL:HG12	1:D:88:LEU:HD12	2.00	0.44
1:A:68:ASN:HA	1:A:302:THR:HG23	2.00	0.44
1:A:189:ILE:HG21	1:A:226:ILE:HD13	1.99	0.44
1:C:216:LEU:HD12	1:C:219:TYR:HB2	1.99	0.44
1:A:40:HIS:HE1	1:A:67:HIS:CE1	2.36	0.43
1:D:337:THR:CG2	1:D:360:GLU:OE2	2.67	0.43
1:A:50:ASP:OD1	1:A:89:LYS:HG3	2.18	0.43
1:B:5:ILE:HB	1:B:35:VAL:HG22	2.01	0.43
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.99	0.43
1:D:329:PRO:HD2	1:D:330:ILE:HD13	2.01	0.43
1:D:334:PHE:O	1:D:338:ARG:HG2	2.18	0.43
1:A:130:ILE:HD11	2:A:501:ZT3:C15	2.48	0.43
1:C:150:GLY:HA3	1:D:156:TYR:HE1	1.83	0.43
1:A:5:ILE:HB	1:A:35:VAL:HG22	2.01	0.42
1:A:222:ARG:HG3	1:A:226:ILE:HD11	2.01	0.42
1:A:180:MET:HB2	1:B:219:TYR:CD2	2.54	0.42
1:A:182:MET:HE3	1:A:182:MET:HB3	1.96	0.42
1:B:19:THR:HG21	1:B:74:ALA:HB3	2.00	0.42
1:B:334:PHE:O	1:B:338:ARG:HG2	2.20	0.42
1:C:216:LEU:HD11	1:D:180:MET:SD	2.59	0.42
1:D:210:SER:OG	1:D:251:ILE:HD12	2.18	0.42
1:A:259:MET:HE2	1:A:259:MET:HB3	1.96	0.42
1:B:200:ALA:HA	1:B:266:ILE:HG13	2.02	0.42
1:B:207:LEU:HD12	1:B:266:ILE:HB	2.01	0.42
1:A:330:ILE:HD12	1:A:363:SER:HB3	2.01	0.42
1:A:158:PRO:CG	1:A:162:THR:HB	2.50	0.42
1:C:309:HIS:CE1	1:C:331:ALA:HB3	2.55	0.42
1:D:199:MET:O	1:D:199:MET:HE3	2.19	0.42
1:A:40:HIS:CE1	1:A:67:HIS:CE1	3.08	0.41
1:B:86:PHE:HB2	1:B:88:LEU:HD12	2.01	0.41
1:C:255:VAL:O	1:C:259:MET:HG2	2.20	0.41
1:B:210:SER:OG	1:B:267:TRP:NE1	2.30	0.41
1:B:91:MET:O	1:B:91:MET:HG3	2.21	0.41
1:A:19:THR:HA	1:A:22:ILE:HG12	2.02	0.41
1:A:213:ASN:HA	1:A:220:ASP:HB2	2.03	0.40
1:B:207:LEU:HD12	1:B:266:ILE:CG2	2.51	0.40
1:D:19:THR:HG21	1:D:74:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:HB3	1:C:301:LYS:O	2.22	0.40
1:D:337:THR:HG23	1:D:360:GLU:OE2	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	389/424 (92%)	374 (96%)	15 (4%)	0	100	100
1	B	384/424 (91%)	373 (97%)	10 (3%)	1 (0%)	36	66
1	C	384/424 (91%)	365 (95%)	18 (5%)	1 (0%)	36	66
1	D	379/424 (89%)	361 (95%)	18 (5%)	0	100	100
All	All	1536/1696 (91%)	1473 (96%)	61 (4%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	289	GLY
1	B	173	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	282/360 (78%)	272 (96%)	10 (4%)	32	57
1	B	284/360 (79%)	277 (98%)	7 (2%)	42	63
1	C	283/360 (79%)	277 (98%)	6 (2%)	47	66
1	D	261/360 (72%)	249 (95%)	12 (5%)	24	51
All	All	1110/1440 (77%)	1075 (97%)	35 (3%)	34	59

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	80	GLU
1	A	117	ILE
1	A	119	ARG
1	A	155	THR
1	A	168	LEU
1	A	185	GLN
1	A	262	GLU
1	A	314	ARG
1	A	409	LEU
1	B	76	ILE
1	B	88	LEU
1	B	155	THR
1	B	173	GLU
1	B	174	GLU
1	B	184	ASN
1	B	295	LEU
1	C	20	ARG
1	C	89	LYS
1	C	145	VAL
1	C	165	VAL
1	C	288	LEU
1	C	409	LEU
1	D	76	ILE
1	D	114	CYS
1	D	154	ILE
1	D	162	THR
1	D	165	VAL
1	D	168	LEU
1	D	291	MET
1	D	330	ILE
1	D	332	SER
1	D	337	THR

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Mol	Chain	Res	Type
1	D	357	ASN
1	D	375	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	184	ASN
1	B	67	HIS
1	B	198	GLN
1	B	348	ASN
1	C	90	GLN
1	C	171	ASN
1	C	198	GLN
1	C	248	HIS
1	C	348	ASN
1	D	68	ASN
1	D	90	GLN
1	D	320	GLN
1	D	385	ASN

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](#)

4 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	ZT3	D	501	-	33,33,33	1.48	3 (9%)	43,49,49	1.09	2 (4%)
2	ZT3	C	501	-	33,33,33	1.36	3 (9%)	43,49,49	1.47	6 (13%)
2	ZT3	B	501	-	33,33,33	1.44	3 (9%)	43,49,49	0.94	2 (4%)
2	ZT3	A	501	-	33,33,33	1.50	4 (12%)	43,49,49	1.39	2 (4%)

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	ZT3	D	501	-	-	5/13/26/26	0/3/4/4
2	ZT3	C	501	-	-	2/13/26/26	0/3/4/4
2	ZT3	B	501	-	-	6/13/26/26	0/3/4/4
2	ZT3	A	501	-	-	4/13/26/26	0/3/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ZT3	C7-N8	-5.27	1.39	1.43
2	D	501	ZT3	C7-N8	-4.77	1.39	1.43
2	B	501	ZT3	C7-N8	-4.45	1.39	1.43
2	C	501	ZT3	C5-N8	-3.96	1.43	1.47
2	D	501	ZT3	C5-N8	-3.89	1.43	1.47
2	B	501	ZT3	C5-N8	-3.58	1.43	1.47
2	A	501	ZT3	C5-N8	-3.40	1.43	1.47
2	C	501	ZT3	C7-N8	-3.33	1.40	1.43
2	B	501	ZT3	C-C1	-2.89	1.38	1.41
2	C	501	ZT3	C-C1	-2.62	1.38	1.41
2	D	501	ZT3	C-C1	-2.57	1.38	1.41
2	A	501	ZT3	C-C1	-2.39	1.38	1.41
2	A	501	ZT3	C5-C	-2.02	1.48	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ZT3	C18-N17-C14	-6.11	113.69	126.04
2	C	501	ZT3	C6-C7-N8	-3.81	117.15	121.62
2	C	501	ZT3	N17-C14-N8	-3.71	112.18	115.94
2	D	501	ZT3	C18-N17-C14	-3.42	119.14	126.04
2	C	501	ZT3	C16-C12-C13	-3.01	114.47	119.67
2	A	501	ZT3	C6-C7-N8	-2.76	118.39	121.62
2	B	501	ZT3	C6-C7-N8	-2.61	118.56	121.62
2	D	501	ZT3	C6-C7-N8	-2.49	118.70	121.62
2	C	501	ZT3	C16-C12-C7	2.24	125.57	121.20
2	C	501	ZT3	C7-C6-N9	2.11	126.13	122.41
2	B	501	ZT3	C6-N9-C1	2.10	133.23	120.58
2	C	501	ZT3	C27-C24-C21	-2.06	105.49	110.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	ZT3	N17-C14-N8-C5
2	A	501	ZT3	C19-C18-N17-C14
2	A	501	ZT3	C23-C18-N17-C14
2	C	501	ZT3	O-C14-N17-C18
2	C	501	ZT3	N8-C14-N17-C18
2	D	501	ZT3	C19-C18-N17-C14
2	A	501	ZT3	N8-C14-N17-C18
2	D	501	ZT3	C23-C18-N17-C14
2	A	501	ZT3	O-C14-N17-C18
2	D	501	ZT3	N8-C14-N17-C18
2	D	501	ZT3	O-C14-N17-C18
2	B	501	ZT3	C22-C21-C24-C26
2	B	501	ZT3	C20-C21-C24-C26
2	B	501	ZT3	C22-C21-C24-C27
2	B	501	ZT3	C20-C21-C24-C25
2	B	501	ZT3	C22-C21-C24-C25
2	B	501	ZT3	C20-C21-C24-C27

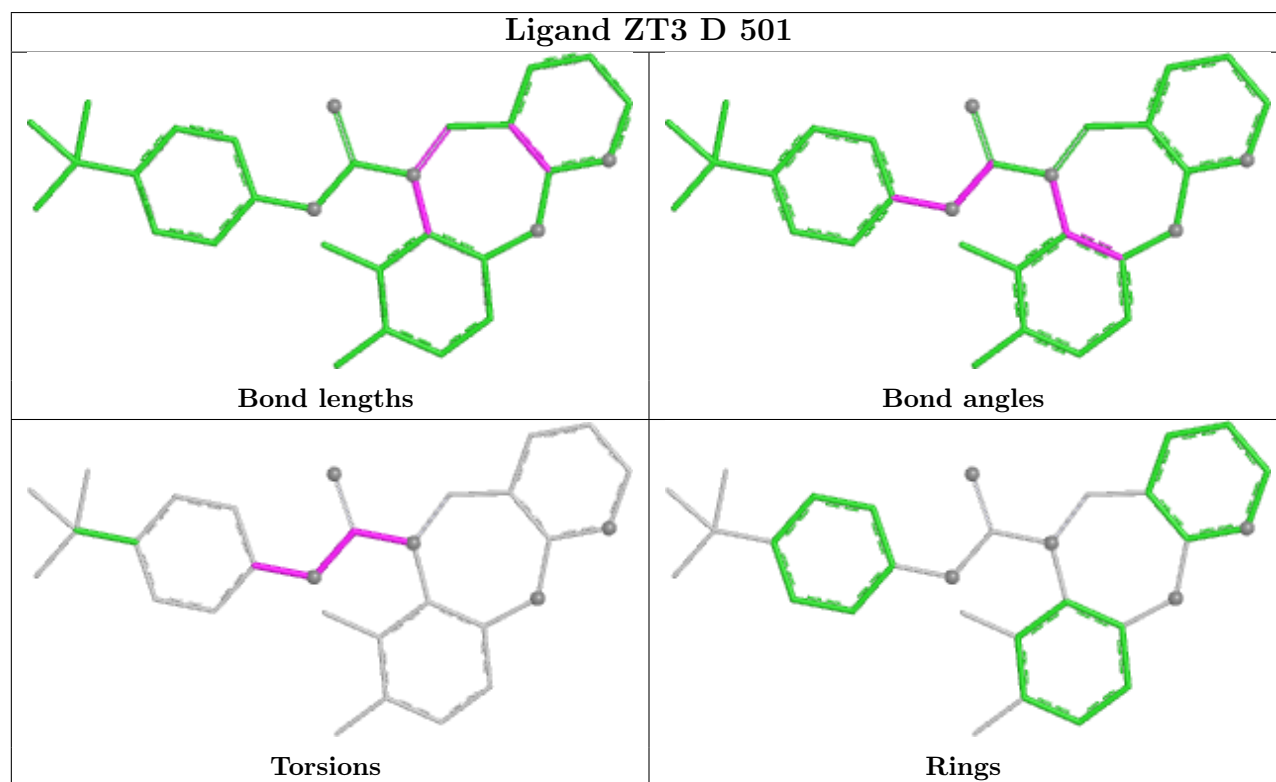
There are no ring outliers.

1 monomer is involved in 1 short contact:

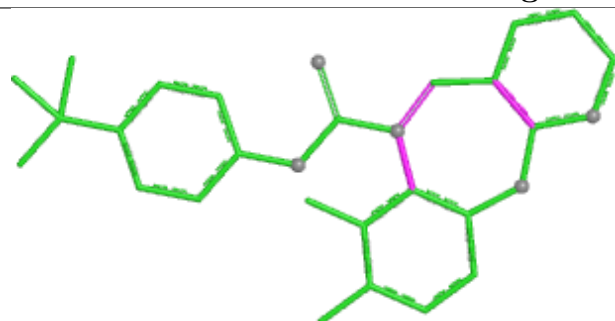
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ZT3	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

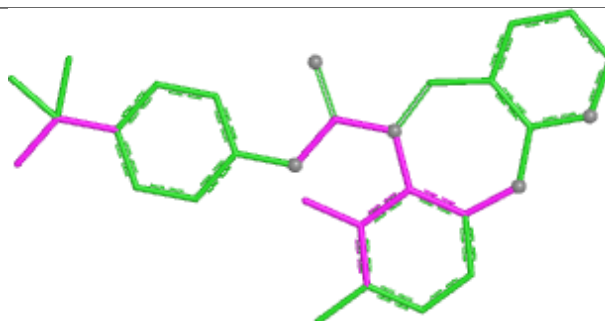
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



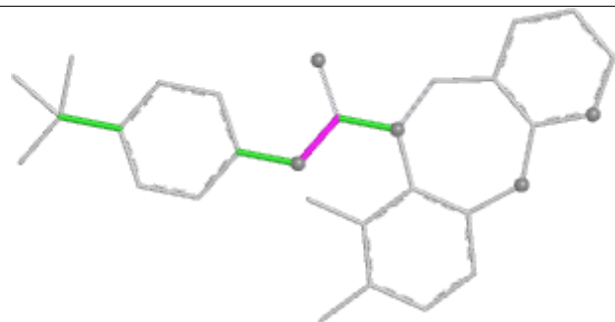
Ligand ZT3 C 501



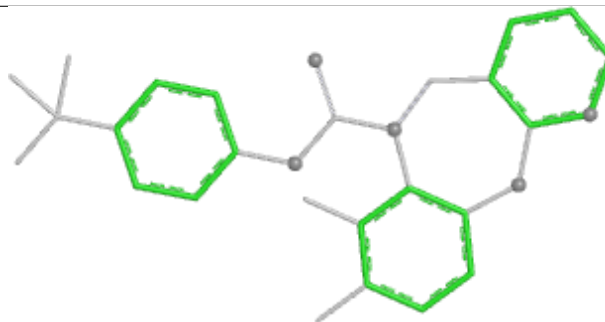
Bond lengths



Bond angles

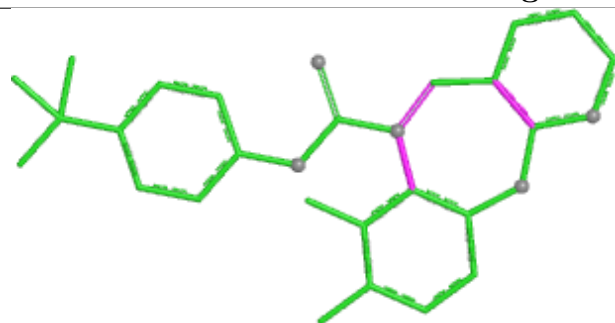


Torsions

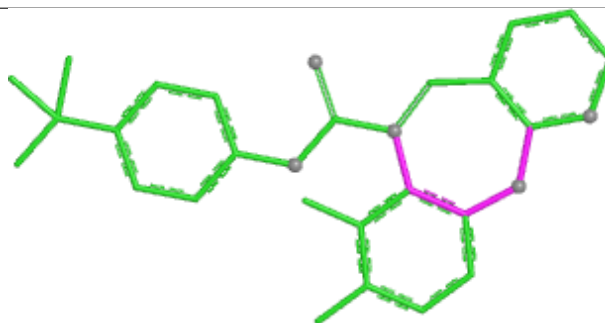


Rings

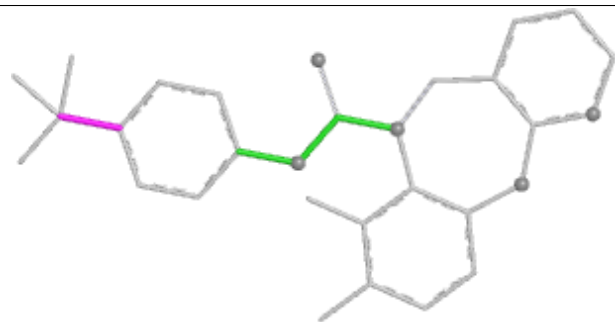
Ligand ZT3 B 501



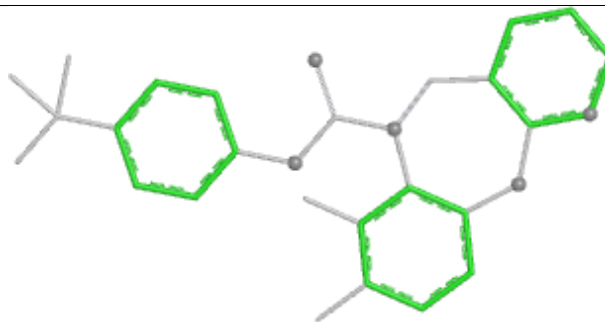
Bond lengths



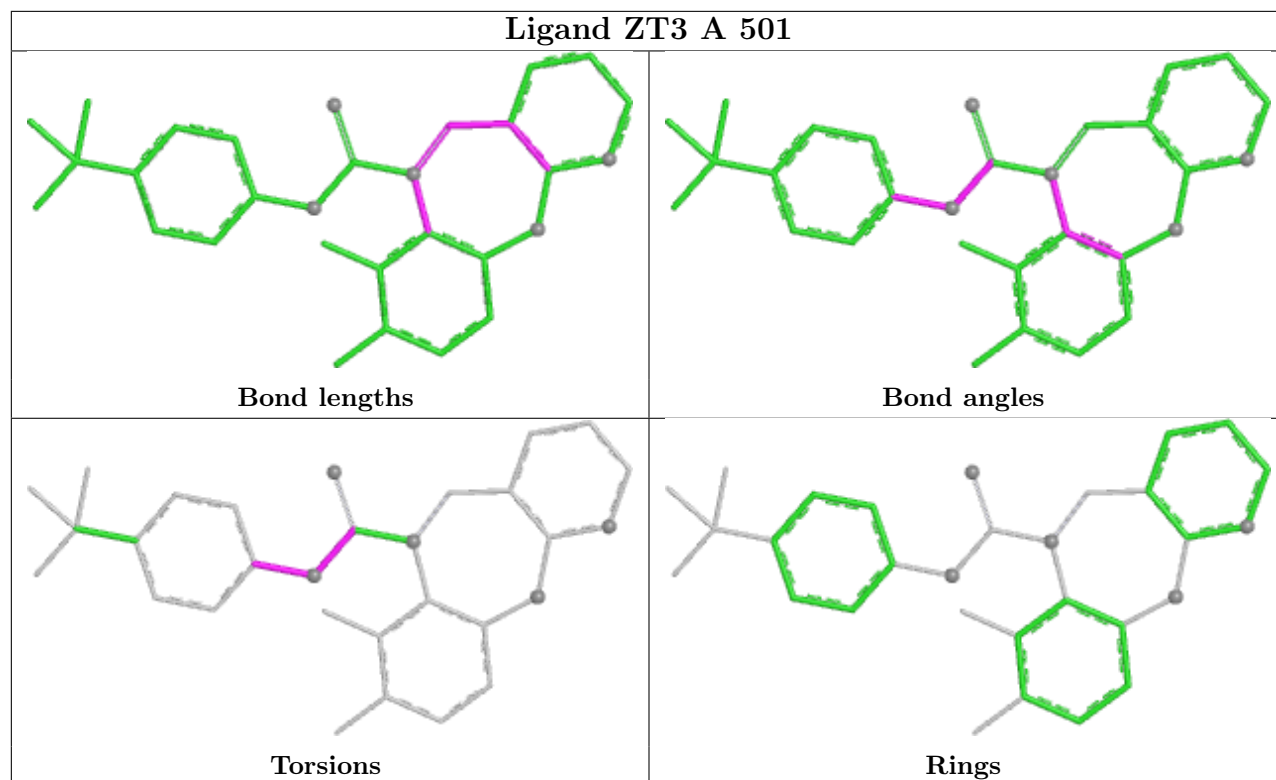
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	395/424 (93%)	0.26	6 (1%)	72 52	42, 79, 111, 135	0
1	B	390/424 (91%)	0.26	1 (0%)	90 80	40, 86, 120, 137	0
1	C	390/424 (91%)	0.26	3 (0%)	82 64	50, 88, 118, 130	0
1	D	387/424 (91%)	0.37	6 (1%)	70 50	56, 98, 125, 156	0
All	All	1562/1696 (92%)	0.29	16 (1%)	79 60	40, 88, 120, 156	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	LEU	4.1
1	C	288	LEU	3.3
1	B	120	LEU	3.3
1	A	286	GLY	3.0
1	A	120	LEU	2.9
1	D	207	LEU	2.9
1	C	216	LEU	2.8
1	A	285	TYR	2.3
1	A	163	GLN	2.3
1	C	213	ASN	2.3
1	D	290	MET	2.2
1	A	270	LYS	2.2
1	A	240	GLU	2.1
1	D	133	HIS	2.1
1	D	270	LYS	2.1
1	D	247	GLU	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](#)

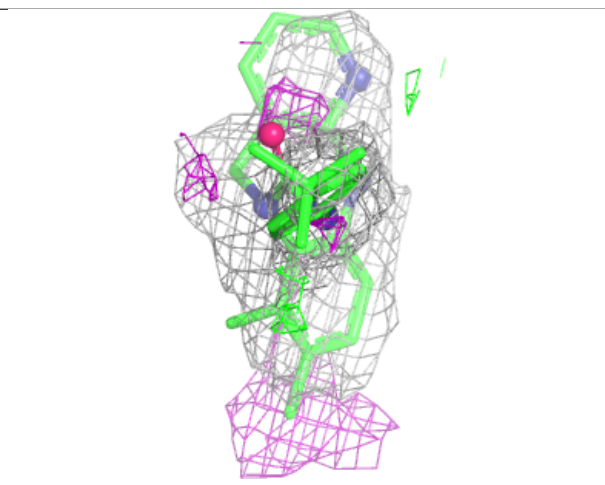
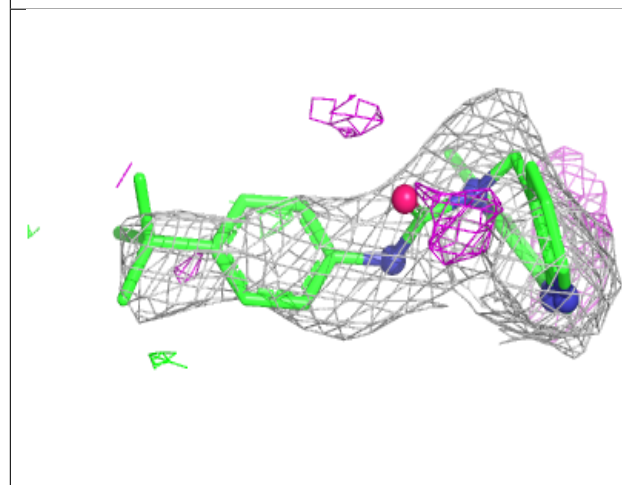
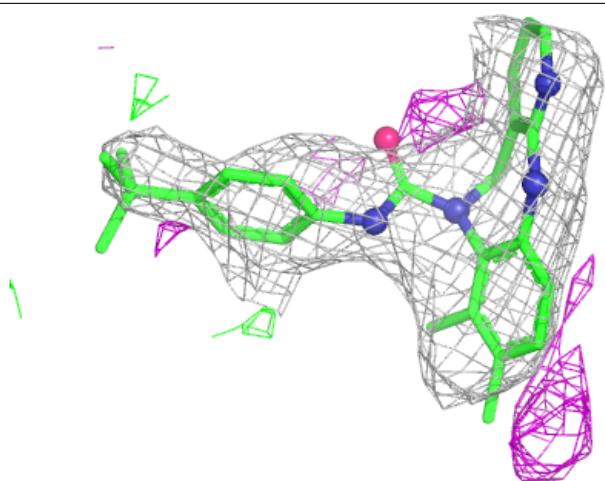
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ZT3	A	501	30/30	0.82	0.21	88,100,113,115	0
2	ZT3	D	501	30/30	0.83	0.21	113,121,127,129	0
2	ZT3	B	501	30/30	0.93	0.12	76,88,95,96	0
2	ZT3	C	501	30/30	0.94	0.11	72,89,98,103	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.

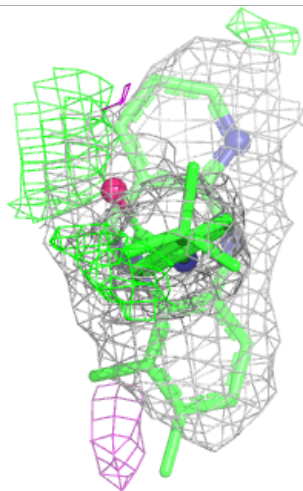
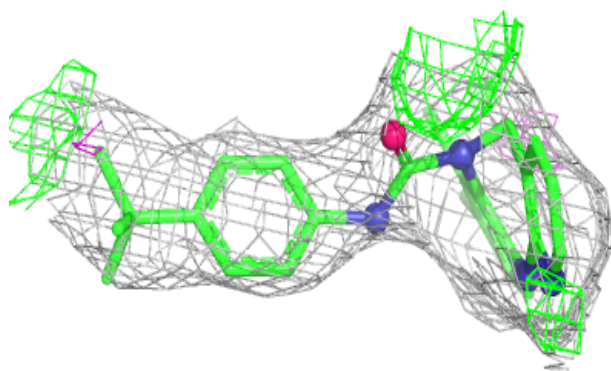
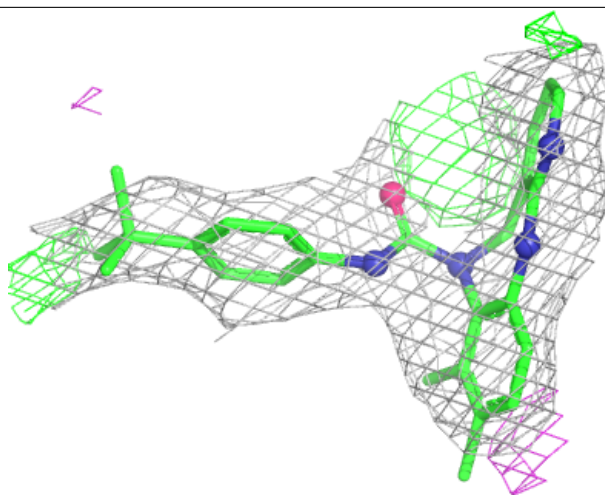
Electron density around ZT3 A 501:

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



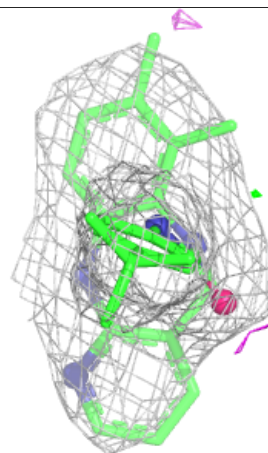
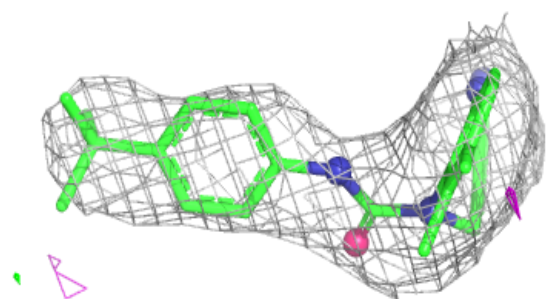
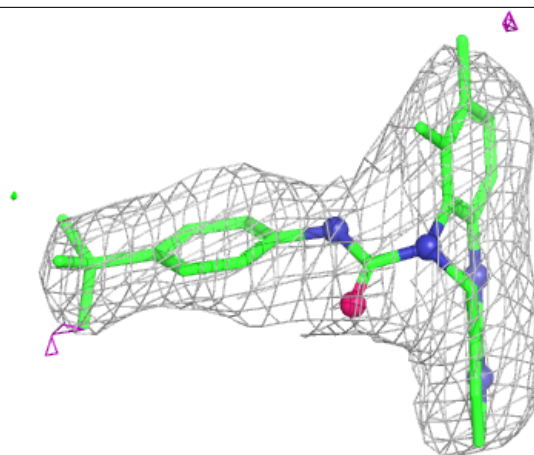
Electron density around ZT3 D 501:

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



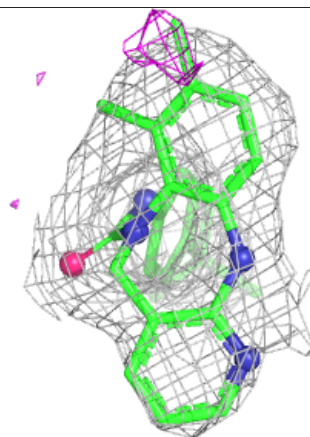
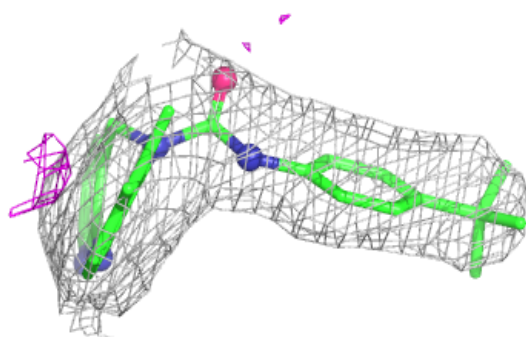
Electron density around ZT3 B 501:

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



Electron density around ZT3 C 501:

$2mF_o-DF_c$ (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.