Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2024 – 01:59 PM EDT

PDB ID	:	8T7D
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)

The following versions of software and data (see references (i)) were used in the production of this report:

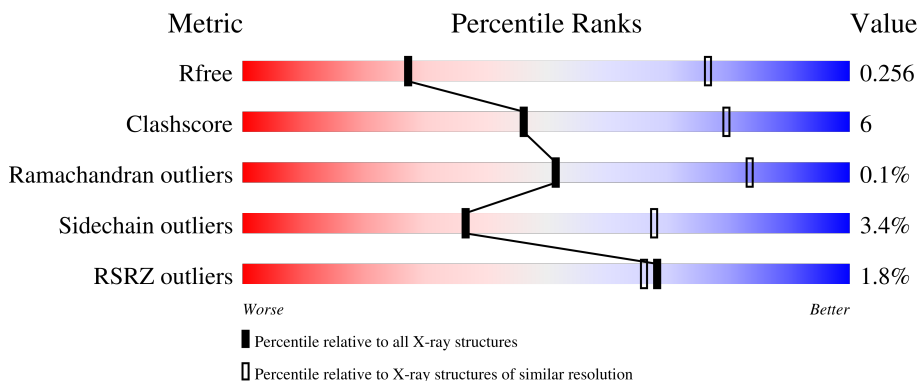|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	Percentile Ranks	Value
Rfree		0.256
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		3.4%
RSRZ outliers		1.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (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 <=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	% 81% 11% · 7%
1	B	424	% 77% 14% · 8%
1	C	424	% 79% 13% 8%
1	D	424	4% 78% 13% · 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 (three-letter code: ZT3) (formula: $C_{25}H_{28}N_4O$) (labeled as "Ligand of Interest" by depositor).

ZT3
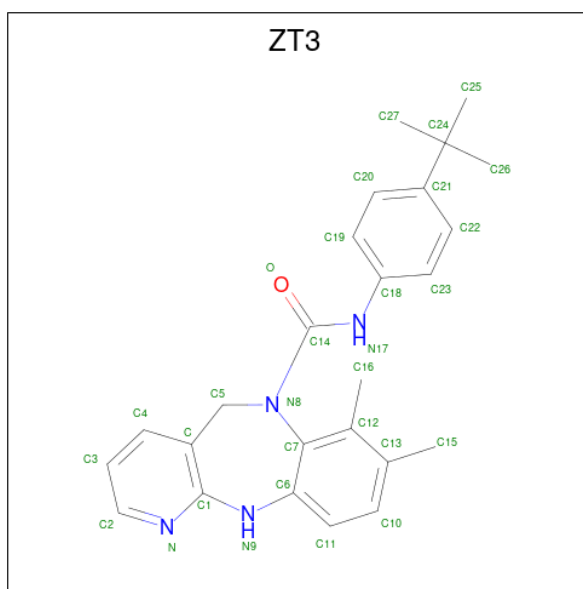
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	25	4	1	0	0

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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		

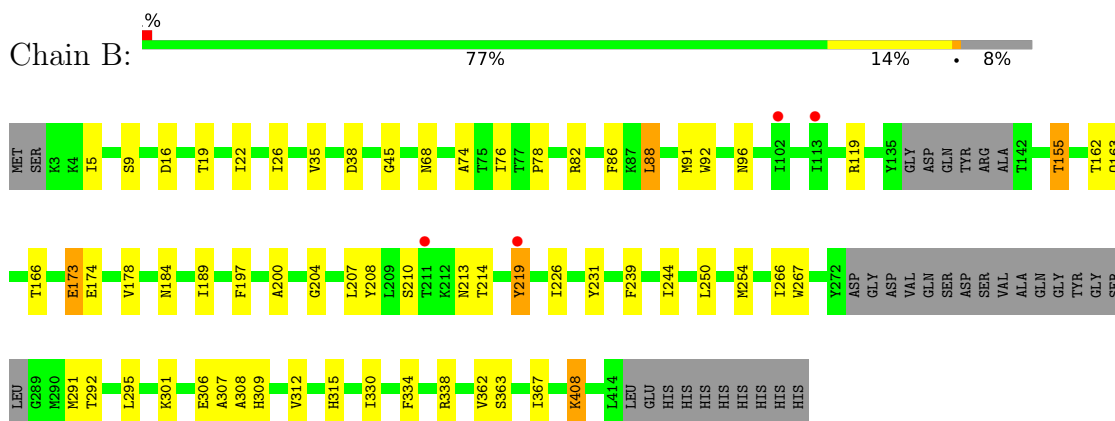# 3 Residue-property plots ⓘ

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.
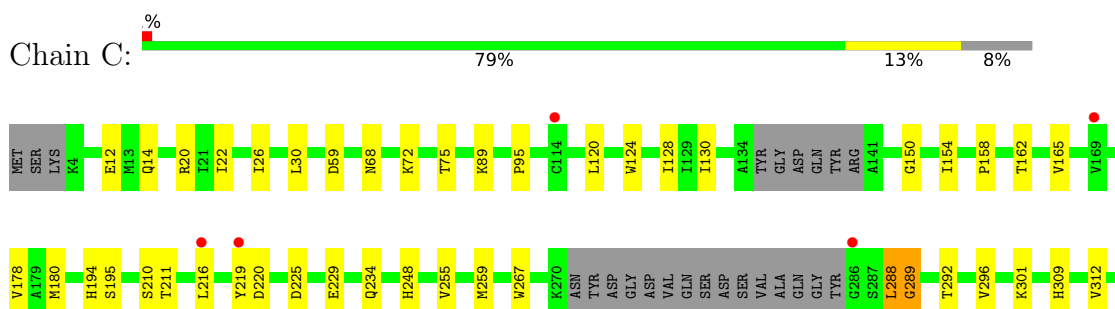
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

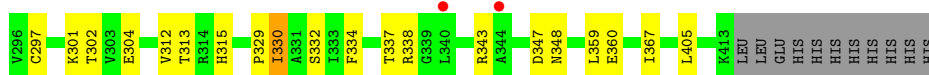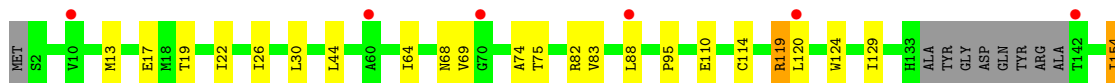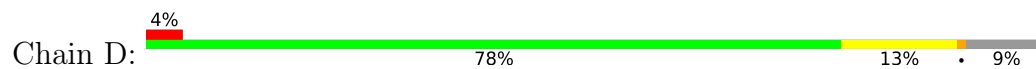- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

H315 I330 A331 R338 L359 V362 S363 I367 N385 D399 L405 L409 L414 LEU GLU HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain D:

4%

78% 13% • 9%

MET S2 V10 M13 E17 M18 T19 I22 I26 L30 L44 A60 I64 N68 V69 G70 A74 T75 R82 V83 L88 P95 E110 C114 R119 L120 W124 I129 H133 ALA TYR GLY ASP GLN TYR ARG ALA T142 I154

T155 Y156 T162 V165 L168 V178 A179 M180 Y183 F197 P206 L207 S210 I215 L216 Y219 F227 I251 D252 S261 GLU GLY GLY F265 I266 W267 K270 ASN TYR ASP GLY ASP VAL GLN SER ASP SER VAL ALA GLN GLY Y285 T292 L295

V296 C297 K301 T302 V303 E304 V312 T313 R314 H315 P329 I330 A331 S332 I333 F334 T337 R338 G339 L340 R343 A344 D347 N348 L359 E360 I367 L405 K413 LEU LEU GLU HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.34 , 73.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

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[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:
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	0.40	0/2989	0.60	1/4072 (0.0%)
1	B	0.37	0/2977	0.58	0/4058
1	C	0.36	0/2957	0.57	0/4029
1	D	0.39	0/2856	0.59	0/3904
All	All	0.38	0/11779	0.59	1/16063 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	TYR	CB-CG-CD2	6.11	124.67	121.00

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	38	0
1	B	2913	0	2678	38	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	0	0
2	D	30	0	0	0	0
All	All	11650	0	10536	140	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 (140) 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: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:C:210:SER:HG	1:C:267:TRP:HE1	1.26	0.80
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:13:MET:HE3	1:D:64:ILE:HD11	1.73	0.69
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:13:MET:CE	1:A:64:ILE:HD11	2.24	0.67
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:76:ILE:HG23	1:A:311:THR:HG21	1.77	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: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:C:210:SER:OG	1:C:267:TRP:NE1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:13:MET:HE1	1:D:64:ILE:HD11	1.85	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:A:13:MET:HE1	1:A:64:ILE:HD11	1.88	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:13:MET:HE2	1:A:64:ILE:HD11	1.92	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HB3	1:A:398:MET:HE2	1.96	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:A:180:MET:HE3	1:A:182:MET:HE3	1.97	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:A:180:MET:HE2	1:A:182:MET:HE1	1.97	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:A:262:GLU:H	1:A:262:GLU:CD	2.20	0.44
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
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	41	75
1	C	384/424 (91%)	365 (95%)	18 (5%)	1 (0%)	41	75
1	D	379/424 (89%)	361 (95%)	18 (5%)	0	100	100
All	All	1536/1696 (91%)	1473 (96%)	61 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	289	GLY
1	B	173	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	282/360 (78%)	273 (97%)	9 (3%)	39	69
1	B	284/360 (79%)	274 (96%)	10 (4%)	36	67
1	C	283/360 (79%)	274 (97%)	9 (3%)	39	69
1	D	261/360 (72%)	251 (96%)	10 (4%)	33	64
All	All	1110/1440 (77%)	1072 (97%)	38 (3%)	37	68

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	117	ILE
1	A	119	ARG
1	A	182	MET
1	A	213	ASN
1	A	262	GLU
1	A	314	ARG
1	A	399	ASP
1	A	409	LEU

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Mol	Chain	Res	Type
1	B	88	LEU
1	B	119	ARG
1	B	155	THR
1	B	173	GLU
1	B	174	GLU
1	B	184	ASN
1	B	213	ASN
1	B	219	TYR
1	B	295	LEU
1	B	408	LYS
1	C	20	ARG
1	C	59	ASP
1	C	89	LYS
1	C	165	VAL
1	C	180	MET
1	C	288	LEU
1	C	385	ASN
1	C	399	ASP
1	C	409	LEU
1	D	114	CYS
1	D	119	ARG
1	D	154	ILE
1	D	162	THR
1	D	165	VAL
1	D	168	LEU
1	D	252	ASP
1	D	330	ILE
1	D	332	SER
1	D	348	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	198	GLN
1	C	198	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 monosaccharides 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	B	501	-	33,33,33	1.37	3 (9%)	38,49,49	0.84	1 (2%)
2	ZT3	C	501	-	33,33,33	1.29	3 (9%)	38,49,49	1.31	4 (10%)
2	ZT3	A	501	-	33,33,33	1.42	3 (9%)	38,49,49	1.41	2 (5%)
2	ZT3	D	501	-	33,33,33	1.40	3 (9%)	38,49,49	1.04	2 (5%)

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	B	501	-	-	6/12/26/26	0/3/4/4
2	ZT3	C	501	-	-	2/12/26/26	0/3/4/4
2	ZT3	A	501	-	-	4/12/26/26	0/3/4/4
2	ZT3	D	501	-	-	4/12/26/26	0/3/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ZT3	C7-N8	-4.76	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ZT3	C7-N8	-4.31	1.39	1.43
2	B	501	ZT3	C7-N8	-4.02	1.39	1.43
2	C	501	ZT3	C5-N8	-3.91	1.43	1.47
2	D	501	ZT3	C5-N8	-3.85	1.43	1.47
2	B	501	ZT3	C5-N8	-3.55	1.43	1.47
2	A	501	ZT3	C5-N8	-3.39	1.43	1.47
2	C	501	ZT3	C7-N8	-3.00	1.40	1.43
2	B	501	ZT3	C-C1	-2.78	1.38	1.41
2	C	501	ZT3	C-C1	-2.52	1.38	1.41
2	D	501	ZT3	C-C1	-2.48	1.38	1.41
2	A	501	ZT3	C-C1	-2.30	1.38	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ZT3	C18-N17-C14	-6.19	113.69	126.12
2	D	501	ZT3	C18-N17-C14	-3.48	119.14	126.12
2	C	501	ZT3	C6-C7-N8	-3.29	117.15	121.44
2	C	501	ZT3	C16-C12-C13	-2.85	114.47	119.71
2	A	501	ZT3	C6-C7-N8	-2.34	118.39	121.44
2	C	501	ZT3	C16-C12-C7	2.26	125.57	121.29
2	B	501	ZT3	C6-C7-N8	-2.21	118.56	121.44
2	D	501	ZT3	C6-C7-N8	-2.10	118.70	121.44
2	C	501	ZT3	C27-C24-C21	-2.03	105.49	110.36

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	501	ZT3	C20-C21-C24-C25
2	B	501	ZT3	C20-C21-C24-C27
2	B	501	ZT3	C22-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 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 ZT3 B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ZT3 C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ZT3 A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ZT3 D 501

Bond lengths

Bond angles

Torsions

Rings
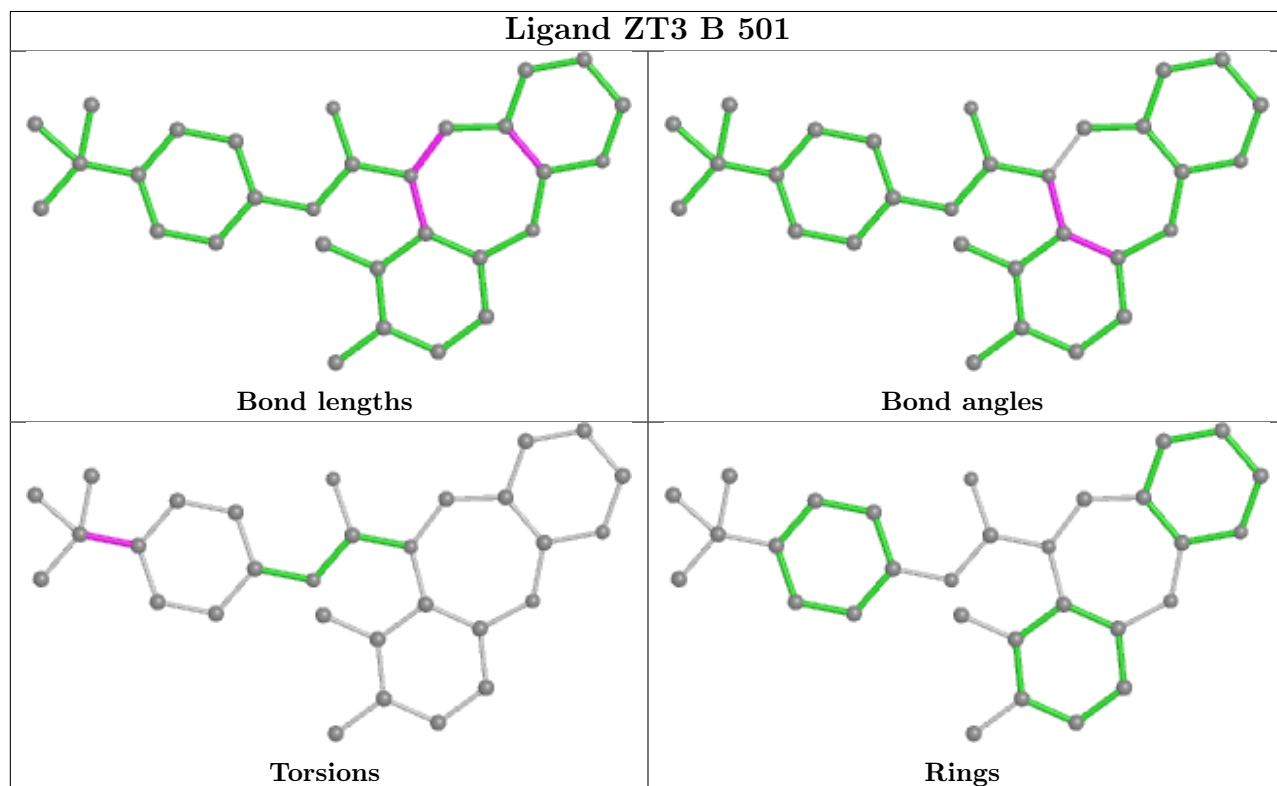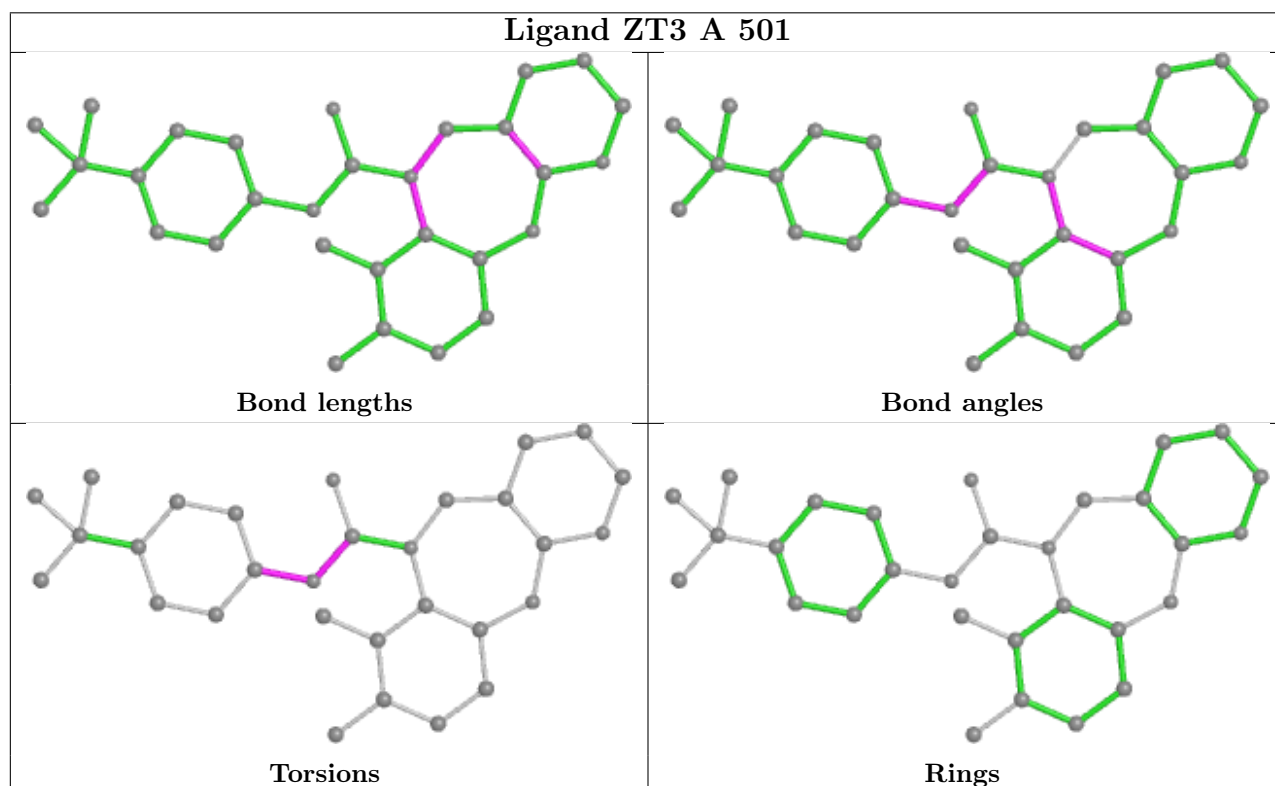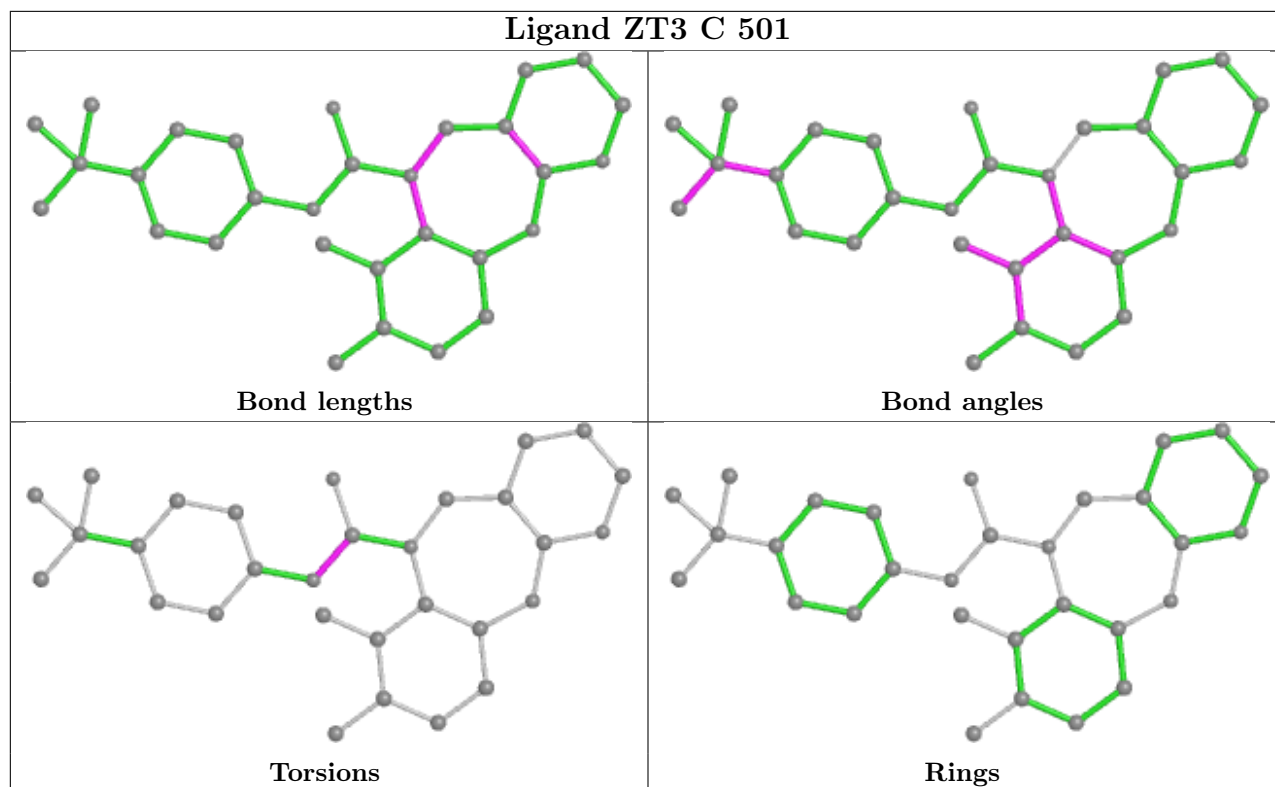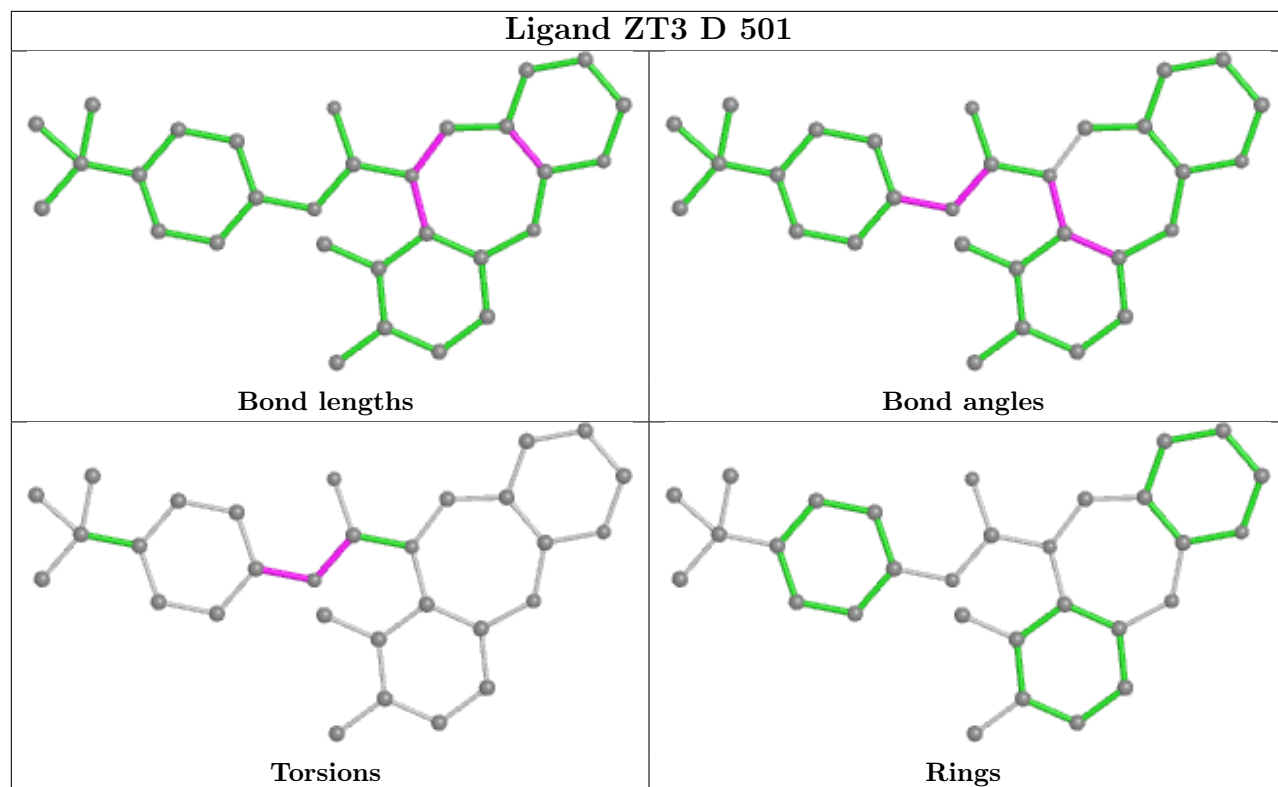
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	395/424 (93%)	0.42	3 (0%)	86	83	42, 79, 111, 135	0
1	B	390/424 (91%)	0.45	4 (1%)	82	79	40, 86, 120, 137	0
1	C	390/424 (91%)	0.48	5 (1%)	77	74	50, 88, 118, 130	0
1	D	387/424 (91%)	0.49	16 (4%)	37	36	56, 98, 125, 156	0
All	All	1562/1696 (92%)	0.46	28 (1%)	68	66	40, 88, 120, 156	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	VAL	3.3
1	D	165	VAL	3.2
1	D	197	PHE	3.2
1	D	227	PHE	3.1
1	D	70	GLY	2.9
1	D	207	LEU	2.7
1	C	286	GLY	2.7
1	D	10	VAL	2.7
1	D	206	PRO	2.6
1	C	114	CYS	2.5
1	B	211	THR	2.5
1	C	219	TYR	2.4
1	D	120	LEU	2.3
1	A	7	GLY	2.3
1	C	216	LEU	2.2
1	B	219	TYR	2.2
1	D	162	THR	2.2
1	D	344	ALA	2.1
1	B	102	ILE	2.1
1	A	340	LEU	2.1
1	D	142	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	340	LEU	2.1
1	D	88	LEU	2.1
1	A	154	ILE	2.1
1	D	183	TYR	2.1
1	D	60	ALA	2.0
1	B	113	ILE	2.0
1	D	292	THR	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 ⓘ

There are no monosaccharides 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, 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(Å^2)	Q<0.9
2	ZT3	D	501	30/30	0.86	0.42	113,121,127,129	0
2	ZT3	A	501	30/30	0.88	0.53	88,100,113,115	0
2	ZT3	C	501	30/30	0.95	0.47	72,89,98,103	0
2	ZT3	B	501	30/30	0.95	0.40	76,88,95,96	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.
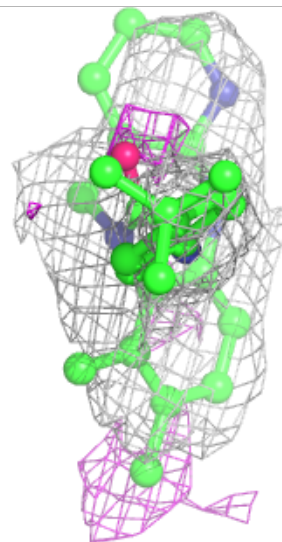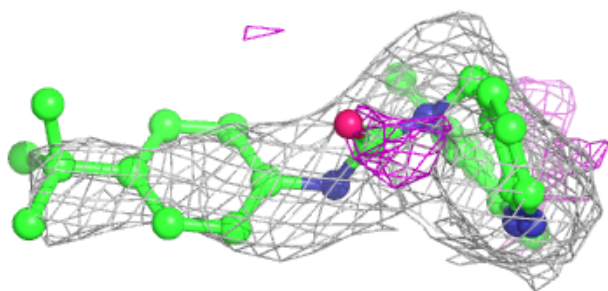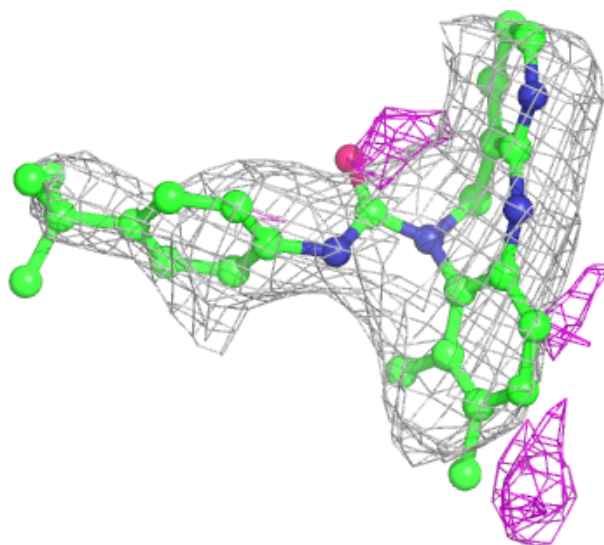
WORLDWIDE
wwPDB
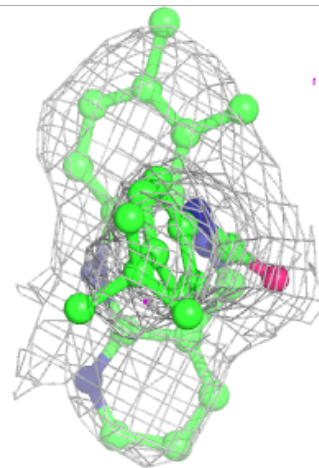PROTEIN DATA BANK

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)
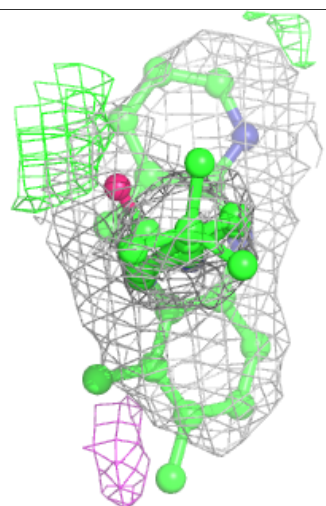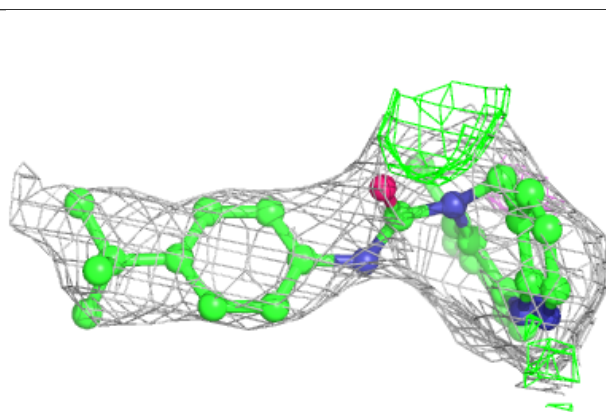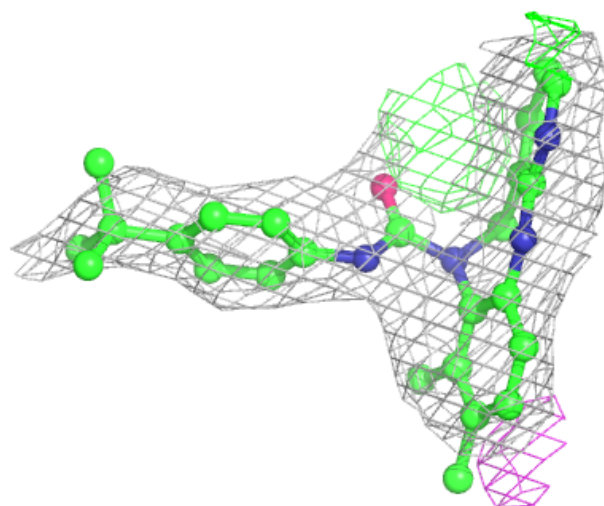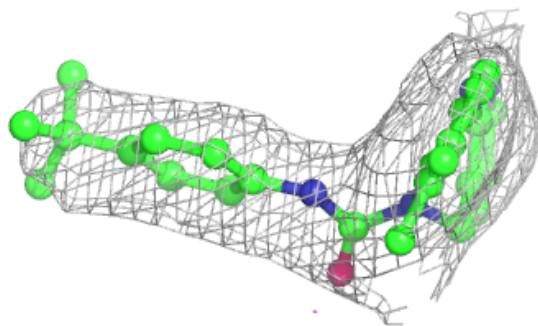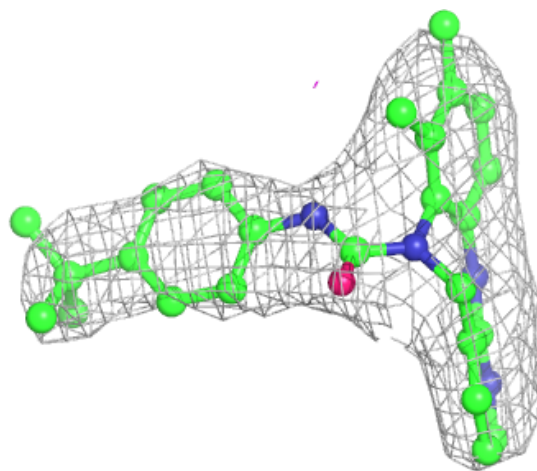
Electron density around ZT3 A 501:

$2mF_o$-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 C 501:

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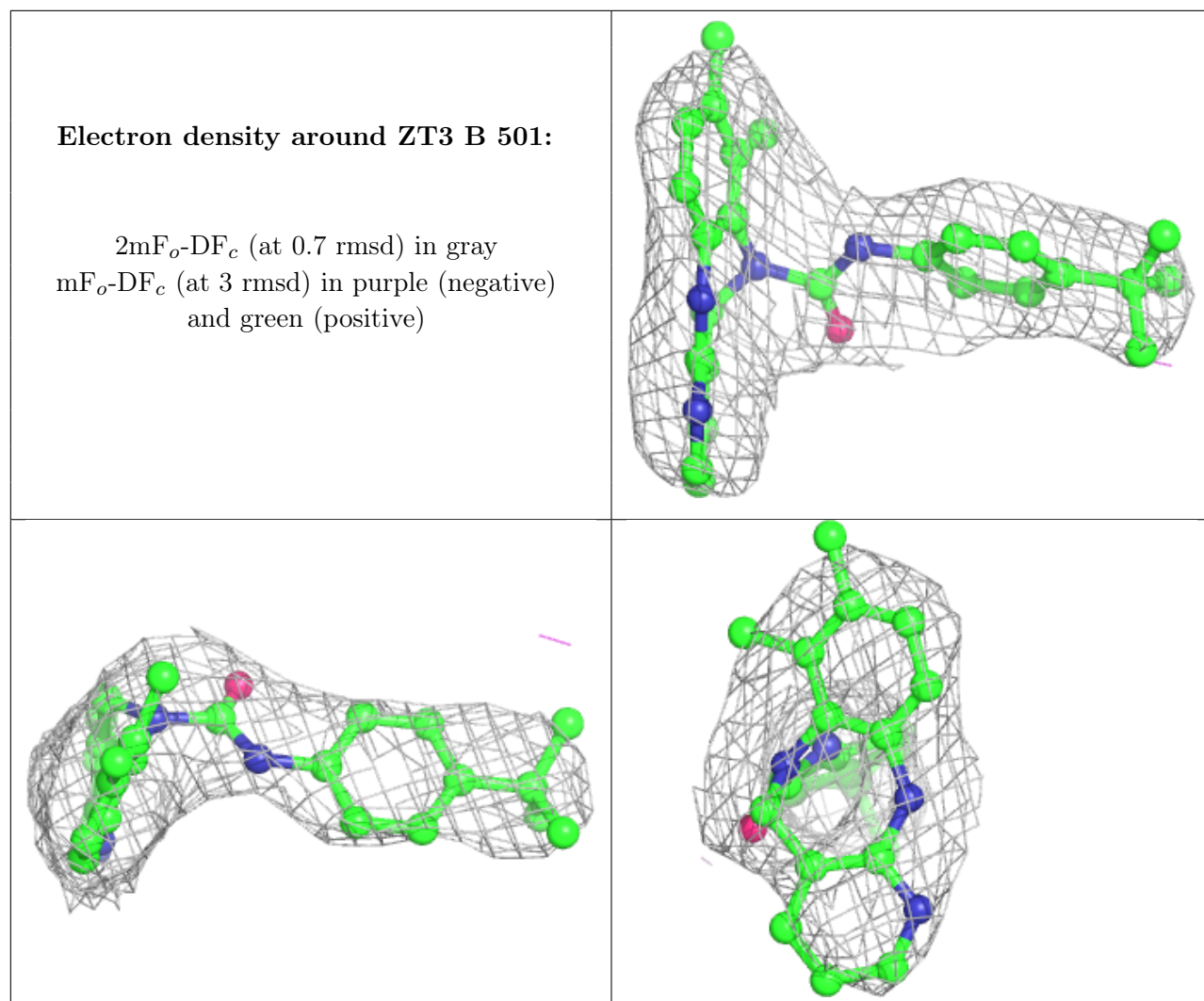and green (positive)

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)

6.5 Other polymers ⓘ

There are no such residues in this entry.