



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:54 PM EDT

PDB ID : 3EDZ / pdb_00003edz
Title : Crystal structure of catalytic domain of TACE with hydroxamate inhibitor
Authors : Mazzola, R.D.; Zhu, Z.; Sinning, L.; McKittrick, B.; Lavey, B.; Spitler, J.; Kozlowski, J.; Neng-Yang, S.; Zhou, G.; Guo, Z.; Orth, P.; Madison, V.; Sun, J.; Lundell, D.; Niu, X.
Deposited on : 2008-09-03
Resolution : 1.90 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

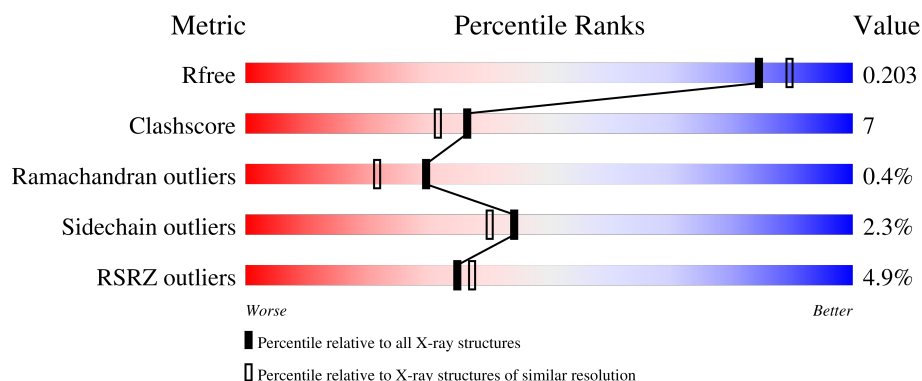
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	271	3% 85% 10% 5%
1	B	271	6% 73% 19% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4575 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 ADAM 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	1	0
			2047	1287	345	401	14			
1	B	254	Total	C	N	O	S	0	1	0
			2012	1267	338	393	14			

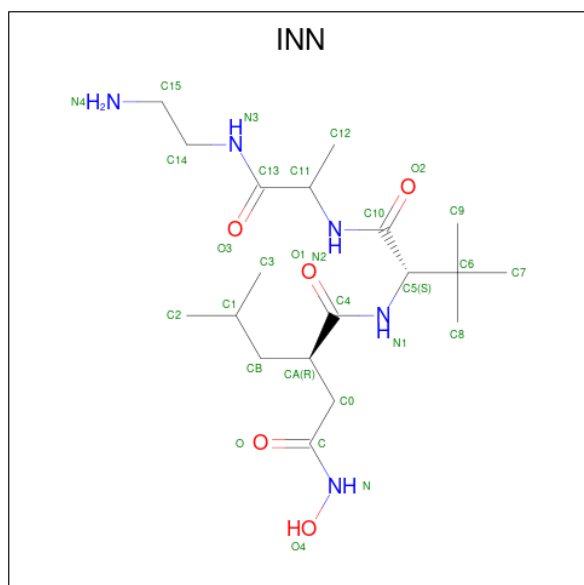
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	engineered mutation	UNP P78536
A	353	GLY	VAL	engineered mutation	UNP P78536
A	452	GLN	ASN	engineered mutation	UNP P78536
A	478	GLY	-	expression tag	UNP P78536
A	479	SER	-	expression tag	UNP P78536
A	480	HIS	-	expression tag	UNP P78536
A	481	HIS	-	expression tag	UNP P78536
A	482	HIS	-	expression tag	UNP P78536
A	483	HIS	-	expression tag	UNP P78536
A	484	HIS	-	expression tag	UNP P78536
A	485	HIS	-	expression tag	UNP P78536
B	266	ALA	SER	engineered mutation	UNP P78536
B	353	GLY	VAL	engineered mutation	UNP P78536
B	452	GLN	ASN	engineered mutation	UNP P78536
B	478	GLY	-	expression tag	UNP P78536
B	479	SER	-	expression tag	UNP P78536
B	480	HIS	-	expression tag	UNP P78536
B	481	HIS	-	expression tag	UNP P78536
B	482	HIS	-	expression tag	UNP P78536
B	483	HIS	-	expression tag	UNP P78536
B	484	HIS	-	expression tag	UNP P78536
B	485	HIS	-	expression tag	UNP P78536

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-3-methyl-L-valyl-N-(2-aminoethyl)-L-alaninamide (CCD ID: INN) (formula: C₁₉H₃₇N₅O₅).



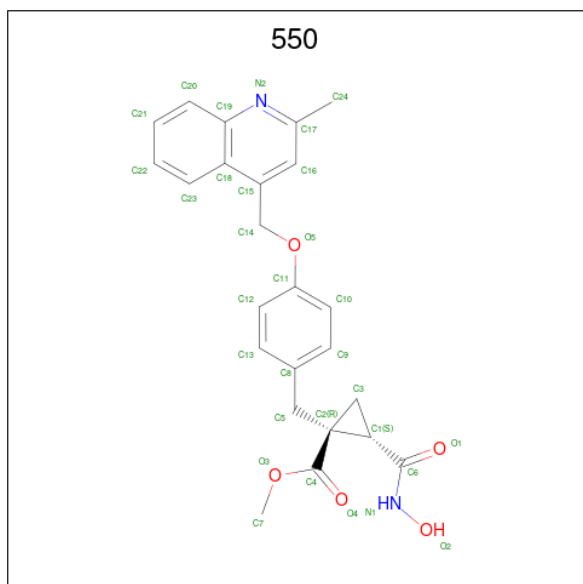
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	19	5	5		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is methyl (1R,2S)-2-(hydroxycarbamoyl)-1-{4-[(2-methylquinolin-4-yl)methoxy]benzyl}cyclopropanecarboxylate (CCD ID: 550) (formula: $C_{24}H_{24}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			31	24	2	5		

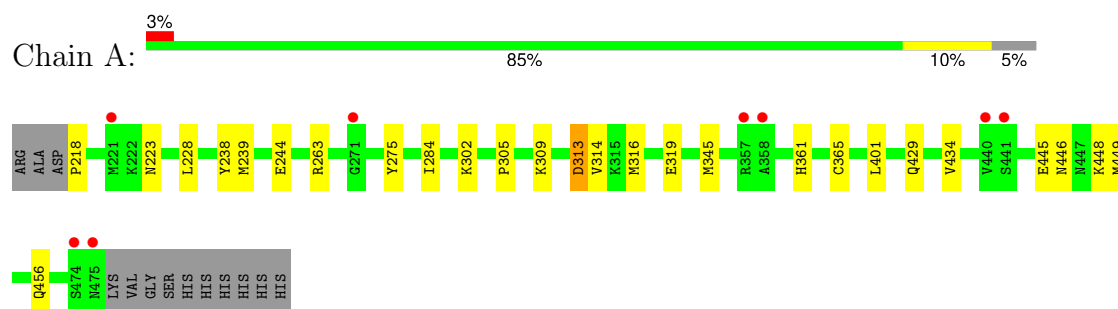
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	217	Total 217	O 217	0	0
6	B	211	Total 211	O 211	0	0

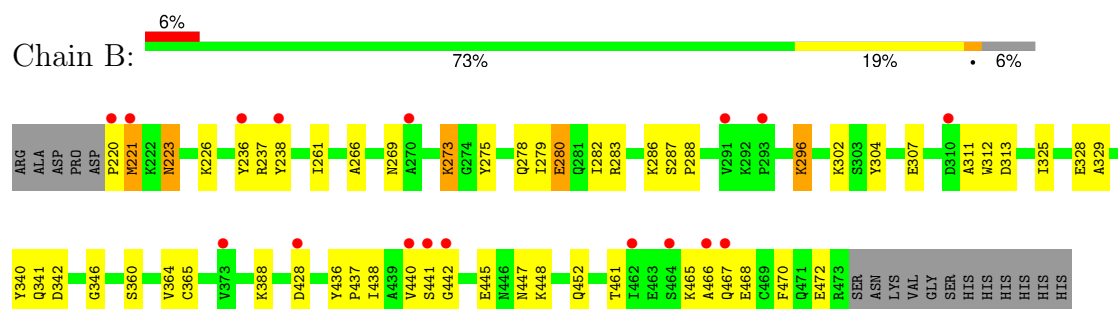
3 Residue-property plots [i](#)

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: ADAM 17



• Molecule 1: ADAM 17



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.80Å 75.70Å 102.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.83 – 1.90 28.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.6 (28.83-1.90) 92.0 (28.83-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 1.91Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.174 , 0.204 0.172 , 0.203	Depositor DCC
R_{free} test set	823 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4575	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 550, CIT, ZN, INN

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	0.55	0/2097	0.88	8/2829 (0.3%)
1	B	0.49	0/2063	0.89	5/2782 (0.2%)
All	All	0.52	0/4160	0.88	13/5611 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ASP	N-CA-C	-7.50	97.83	109.76
1	A	313	ASP	N-CA-C	-6.94	98.73	109.76
1	A	434	VAL	N-CA-C	6.61	117.36	110.62
1	B	445	GLU	N-CA-C	6.24	118.60	111.11
1	B	472	GLU	N-CA-C	-6.12	102.28	110.55
1	A	228	LEU	N-CA-C	-5.69	99.45	108.73
1	A	238	TYR	N-CA-C	5.69	119.40	112.23
1	A	445	GLU	N-CA-C	5.62	118.13	111.33
1	A	345	MET	N-CA-C	5.37	118.85	111.54
1	B	468	GLU	N-CA-C	5.24	116.80	111.14
1	B	441	SER	N-CA-C	5.23	116.47	108.30
1	A	239	MET	N-CA-C	-5.21	107.47	113.88
1	A	314	VAL	N-CA-C	5.19	115.91	110.62

There are no chirality outliers.

There are no planarity outliers.

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	2047	0	1955	14	0
1	B	2012	0	1925	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	36	1	0
4	A	13	0	5	1	0
4	B	13	0	5	0	0
5	B	31	0	23	2	0
6	A	217	0	0	2	0
6	B	211	0	0	3	0
All	All	4575	0	3949	58	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 7.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:VAL:HG23	1:B:465:LYS:HD3	1.47	0.96
1:A:446:ASN:HA	1:A:449[A]:MET:HE2	1.53	0.88
1:B:448:LYS:HG3	6:B:831:HOH:O	1.82	0.80
1:B:237:ARG:HD2	1:B:238:TYR:CZ	2.18	0.79
1:A:305:PRO:HG3	1:A:316:MET:HE1	1.66	0.78
1:B:461:THR:HG23	1:B:465:LYS:HD2	1.67	0.75
1:A:302:LYS:HG2	6:A:506:HOH:O	1.85	0.75
1:B:360:SER:HB3	6:B:856:HOH:O	1.92	0.69
1:B:364:VAL:CG2	1:B:465:LYS:HD3	2.21	0.68
1:B:438:ILE:HG22	1:B:440:VAL:HB	1.74	0.67
1:A:218:PRO:HB3	1:A:275:TYR:HE1	1.62	0.63
1:B:226:LYS:HE3	1:B:278:GLN:NE2	2.13	0.63
1:B:311:ALA:HB2	1:B:341:GLN:HB2	1.80	0.62
1:A:313:ASP:CB	1:A:316:MET:HE3	2.29	0.62
1:A:361:HIS:HD2	4:A:4:CIT:O6	1.83	0.61
1:B:221:MET:HE1	1:B:467:GLN:NE2	2.15	0.61
1:B:302:LYS:HD2	1:B:307:GLU:HG3	1.80	0.61
1:B:438:ILE:CG2	1:B:440:VAL:HB	2.30	0.61
1:B:266:ALA:HB2	1:B:273:LYS:HZ3	1.66	0.60
1:A:218:PRO:HB3	1:A:275:TYR:CE1	2.38	0.58
1:B:221:MET:HE1	1:B:467:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASP:HB3	1:A:316:MET:HE3	1.88	0.56
1:B:236:TYR:CZ	1:B:286:LYS:HG2	2.41	0.55
1:B:287:SER:HB2	1:B:288:PRO:HD2	1.89	0.55
1:A:218:PRO:HA	1:A:275:TYR:OH	2.06	0.54
1:B:283:ARG:HH22	1:B:328:GLU:HG3	1.72	0.54
1:B:283:ARG:NH2	1:B:328:GLU:HG3	2.24	0.53
1:B:269:ASN:ND2	1:B:452:GLN:OE1	2.42	0.52
1:A:319:GLU:HG3	6:A:659:HOH:O	2.10	0.52
1:B:266:ALA:HB2	1:B:273:LYS:NZ	2.26	0.51
1:B:279:ILE:HG21	1:B:282:ILE:HG13	1.95	0.49
1:B:436:TYR:CG	1:B:437:PRO:HD2	2.48	0.48
1:B:340:TYR:CE2	1:B:388:LYS:HD2	2.49	0.47
1:B:223:ASN:C	1:B:223:ASN:HD22	2.22	0.46
1:B:226:LYS:HB3	1:B:280:GLU:HB2	1.98	0.46
1:A:309:LYS:HB3	1:A:309:LYS:HE3	1.56	0.45
3:A:2:INN:O3	3:A:2:INN:H152	2.15	0.45
1:B:342:ASP:HB2	1:B:388:LYS:HE2	1.99	0.45
1:B:436:TYR:CD1	1:B:437:PRO:HD2	2.52	0.44
1:B:261:ILE:HD13	6:B:823:HOH:O	2.17	0.44
1:B:220:PRO:HG2	1:B:275:TYR:OH	2.17	0.44
1:B:296:LYS:HE2	1:B:296:LYS:HB2	1.85	0.44
1:A:446:ASN:HA	1:A:449[A]:MET:CE	2.38	0.43
1:B:237:ARG:HD2	1:B:238:TYR:CE1	2.53	0.43
1:B:273:LYS:NZ	1:B:273:LYS:HB3	2.33	0.43
1:B:346:GLY:O	5:B:1:550:H7A	2.18	0.43
1:B:237:ARG:CD	1:B:238:TYR:CE1	3.02	0.43
1:B:311:ALA:CB	1:B:341:GLN:HB2	2.48	0.43
1:B:466:ALA:HA	1:B:470:PHE:CG	2.54	0.42
1:A:401:LEU:HD21	1:A:448:LYS:HG2	2.02	0.42
1:B:325:ILE:HG23	1:B:329:ALA:HB2	2.02	0.42
1:B:442:GLY:N	1:B:447:ASN:OD1	2.51	0.41
1:B:307:GLU:O	1:B:307:GLU:HG2	2.20	0.41
1:A:244:GLU:HG3	1:A:284:ILE:HD13	2.02	0.41
5:B:1:550:H5	5:B:1:550:O1	2.21	0.41
1:B:304:TYR:O	1:B:312:TRP:HA	2.21	0.41
1:B:237:ARG:CD	1:B:238:TYR:CZ	2.96	0.41
1:B:223:ASN:C	1:B:223:ASN:ND2	2.79	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	257/271 (95%)	250 (97%)	6 (2%)	1 (0%)	30	22
1	B	253/271 (93%)	245 (97%)	7 (3%)	1 (0%)	30	22
All	All	510/542 (94%)	495 (97%)	13 (2%)	2 (0%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	CYS
1	B	365	CYS

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	220/231 (95%)	216 (98%)	4 (2%)	51	50
1	B	216/231 (94%)	210 (97%)	6 (3%)	38	32
All	All	436/462 (94%)	426 (98%)	10 (2%)	44	40

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	263	ARG
1	A	429	GLN
1	A	456	GLN

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Mol	Chain	Res	Type
1	B	221	MET
1	B	223	ASN
1	B	273	LYS
1	B	280	GLU
1	B	296	LYS
1	B	428	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	269	ASN
1	A	361	HIS
1	A	377	ASN
1	A	410	ASN
1	A	429	GLN
1	A	452	GLN
1	A	467	GLN
1	B	223	ASN
1	B	281	GLN
1	B	410	ASN
1	B	467	GLN
1	B	471	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	CIT	A	4	-	12,12,12	1.06	0	17,17,17	1.30	1 (5%)
4	CIT	B	3	-	12,12,12	0.84	0	17,17,17	1.41	4 (23%)
3	INN	A	2	2	28,28,28	0.60	0	35,38,38	0.97	2 (5%)
5	550	B	1	2	33,34,34	1.11	3 (9%)	39,49,49	1.20	6 (15%)

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
4	CIT	A	4	-	-	2/16/16/16	-
4	CIT	B	3	-	-	2/16/16/16	-
3	INN	A	2	2	-	3/40/40/40	-
5	550	B	1	2	-	6/24/32/32	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	550	C16-C15	2.21	1.42	1.38
5	B	1	550	C22-C23	2.16	1.41	1.36
5	B	1	550	C21-C20	2.15	1.41	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	INN	O4-N-C	-2.71	115.79	119.79
4	B	3	CIT	C2-C3-C6	2.70	116.01	110.03
4	A	4	CIT	O6-C6-C3	2.66	118.25	113.14
5	B	1	550	O4-C4-C2	-2.41	120.26	125.08
4	B	3	CIT	O6-C6-C3	2.40	117.74	113.14
5	B	1	550	C3-C2-C1	2.28	60.59	58.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	550	C23-C18-C19	2.27	120.89	118.36
5	B	1	550	C2-C5-C8	-2.27	112.71	116.17
4	B	3	CIT	C3-C4-C5	-2.21	107.88	113.92
4	B	3	CIT	C4-C3-C2	-2.13	103.85	109.31
3	A	2	INN	O1-C4-CA	-2.12	118.92	122.19
5	B	1	550	C13-C8-C9	2.05	121.28	118.23
5	B	1	550	C24-C17-C16	-2.04	118.79	121.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	INN	N3-C14-C15-N4
5	B	1	550	C3-C2-C4-O3
3	A	2	INN	C15-C14-N3-C13
5	B	1	550	C2-C5-C8-C9
5	B	1	550	C2-C5-C8-C13
5	B	1	550	O5-C14-C15-C16
5	B	1	550	O5-C14-C15-C18
5	B	1	550	C3-C2-C4-O4
4	B	3	CIT	O2-C1-C2-C3
4	A	4	CIT	O2-C1-C2-C3
4	B	3	CIT	O1-C1-C2-C3
4	A	4	CIT	O1-C1-C2-C3
3	A	2	INN	N-C-C0-CA

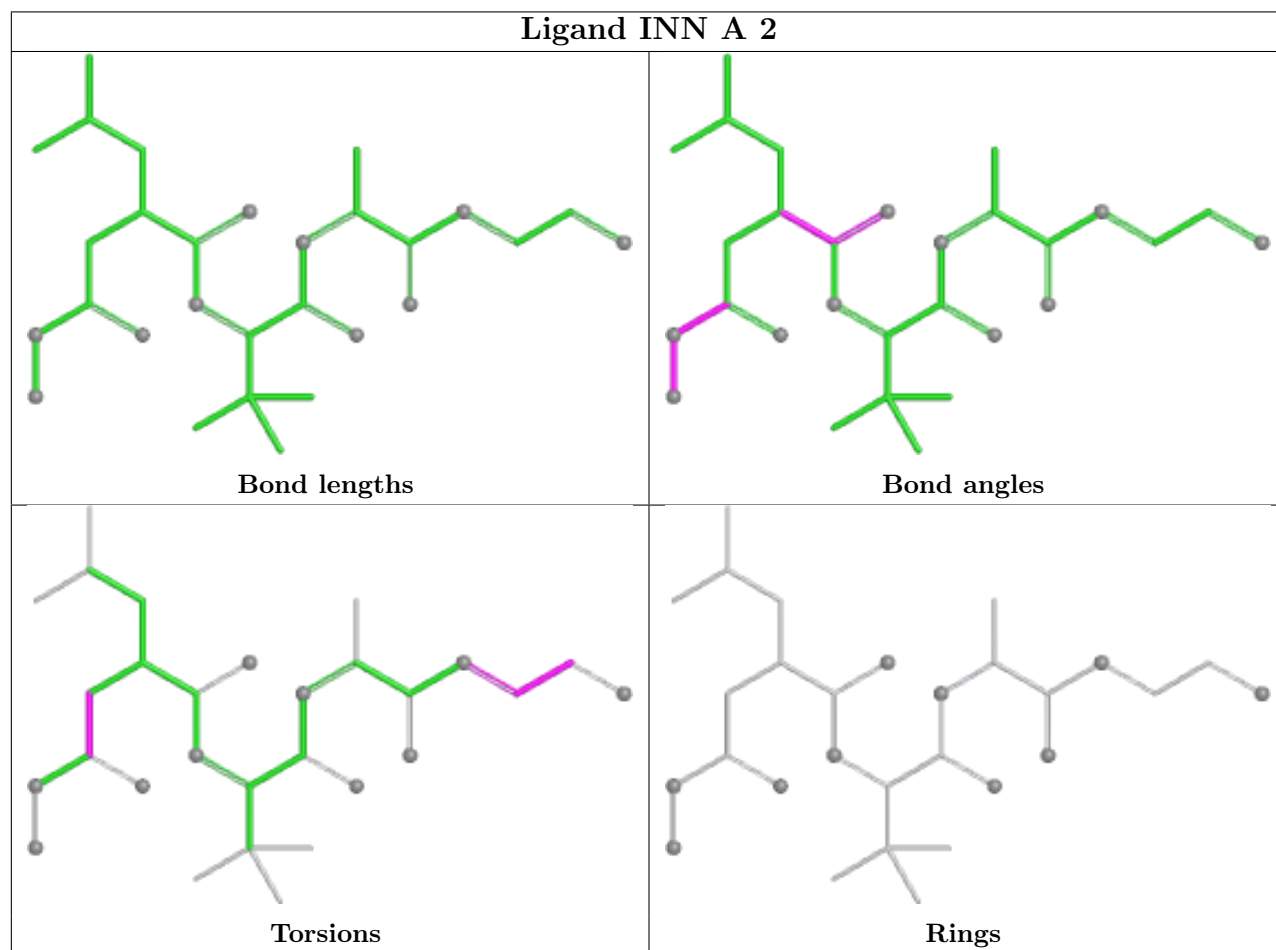
There are no ring outliers.

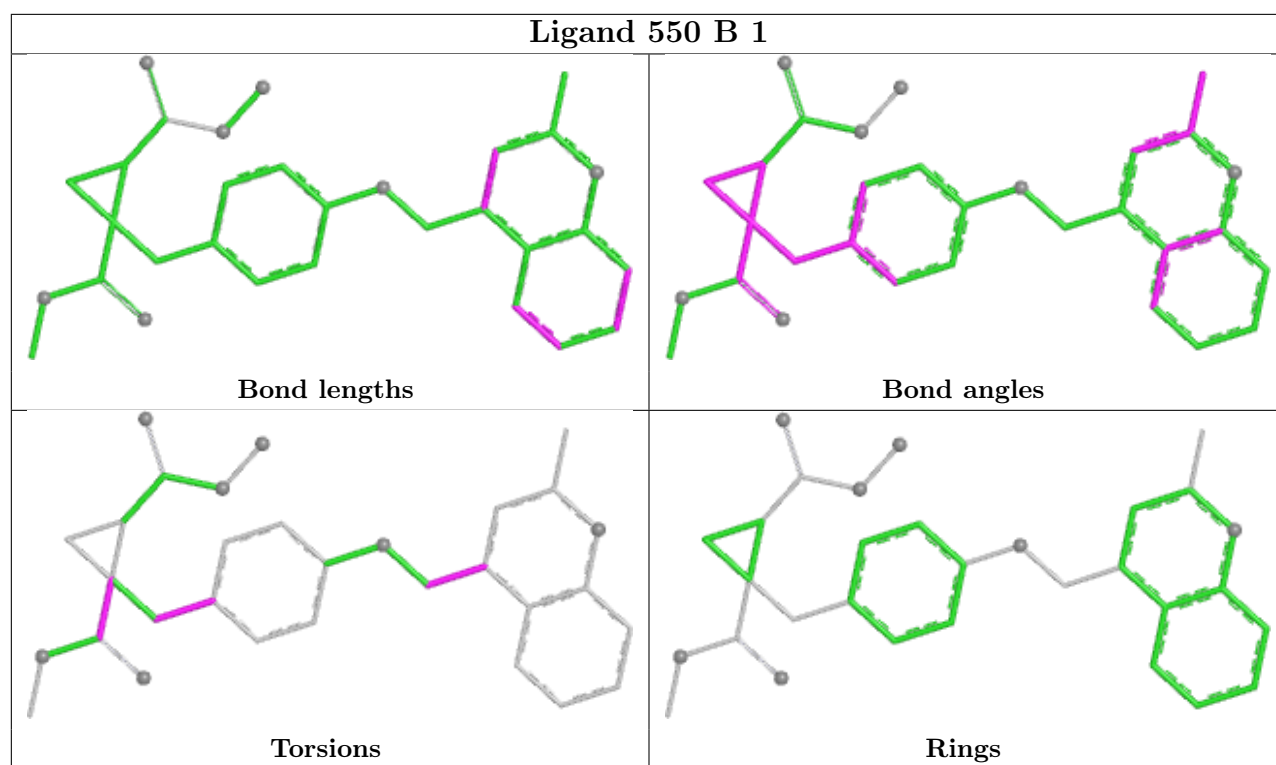
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4	CIT	1	0
3	A	2	INN	1	0
5	B	1	550	2	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	258/271 (95%)	-0.29	8 (3%) 51 55	13, 22, 48, 76	1 (0%)
1	B	254/271 (93%)	0.30	17 (6%) 24 25	16, 29, 54, 72	1 (0%)
All	All	512/542 (94%)	0.00	25 (4%) 35 37	13, 25, 51, 76	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	VAL	5.6
1	B	220	PRO	4.5
1	B	466	ALA	4.4
1	B	221	MET	3.7
1	A	441	SER	3.3
1	B	428	ASP	3.1
1	A	358	ALA	3.0
1	A	475	ASN	2.9
1	B	291	VAL	2.8
1	B	467	GLN	2.7
1	B	464	SER	2.6
1	B	310	ASP	2.6
1	A	271	GLY	2.5
1	B	442	GLY	2.4
1	B	270	ALA	2.4
1	B	441	SER	2.4
1	B	462	ILE	2.3
1	B	238	TYR	2.3
1	A	221	MET	2.2
1	B	236	TYR	2.1
1	A	474	SER	2.1
1	B	373	VAL	2.1
1	B	293	PRO	2.0
1	A	357	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	440	VAL	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](#)

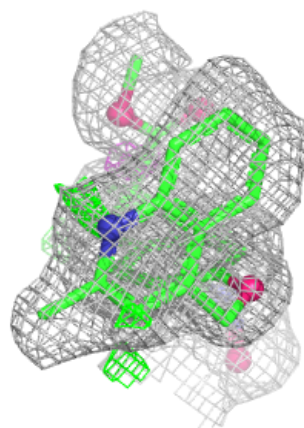
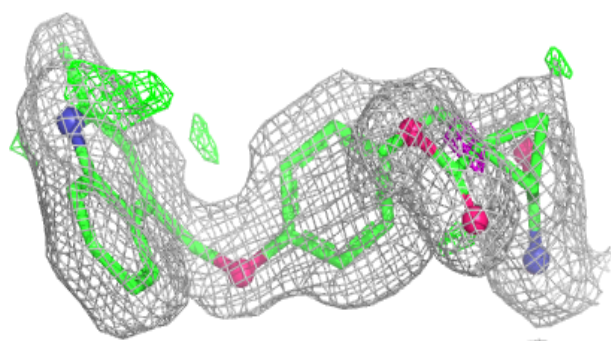
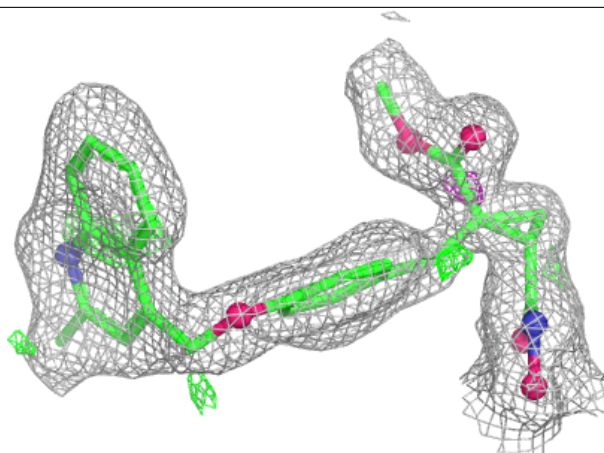
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	A	4	13/13	0.87	0.10	33,35,37,39	0
4	CIT	B	3	13/13	0.91	0.08	31,32,38,39	0
5	550	B	1	31/31	0.92	0.09	19,27,35,35	0
3	INN	A	2	29/29	0.93	0.11	15,23,52,96	0
2	ZN	A	1	1/1	1.00	0.01	16,16,16,16	0
2	ZN	B	2	1/1	1.00	0.01	20,20,20,20	0

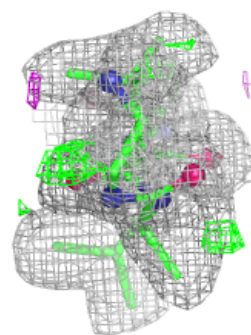
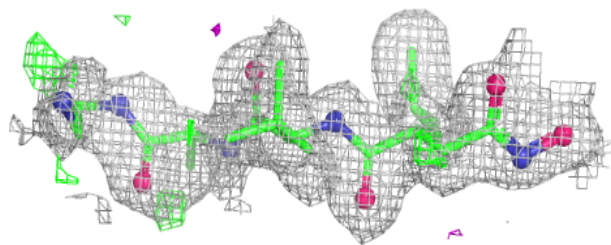
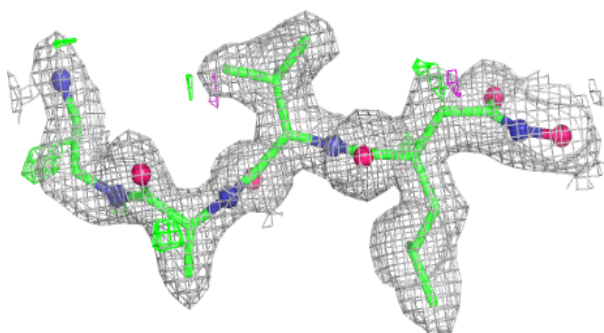
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 550 B 1:

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

**Electron density around INN A 2:**

$2mF_o-DF_c$ (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.