



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:59 PM UTC

PDB ID : 1ZDP / pdb_00001zdp
Title : Crystal Structure Analysis of Thermolysin Complexed with the Inhibitor (S)-thiorphan
Authors : Roderick, S.L.; Fournie-Zaluski, M.C.; Roques, B.P.; Matthews, B.W.
Deposited on : 2005-04-14
Resolution : 1.70 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

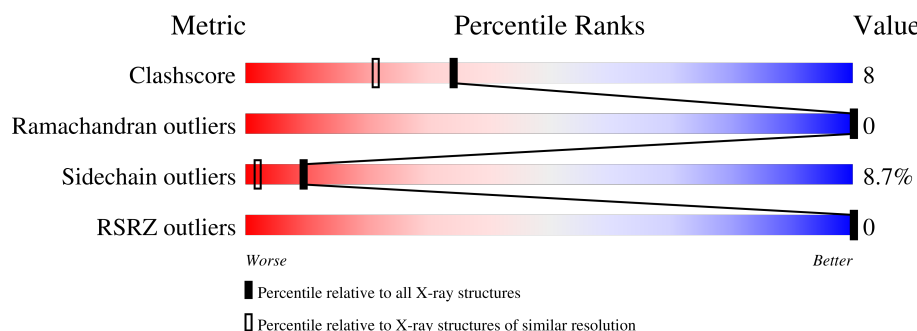
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	E	316	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2615 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 Thermolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	316	Total	C	N	O	S	0	0	0
			2432	1528	408	494	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	37	ASP	ASN	conflict	UNP P00800
E	119	GLU	GLN	conflict	UNP P00800
E	177	GLU	LYS	SEE REMARK 999	UNP P00800

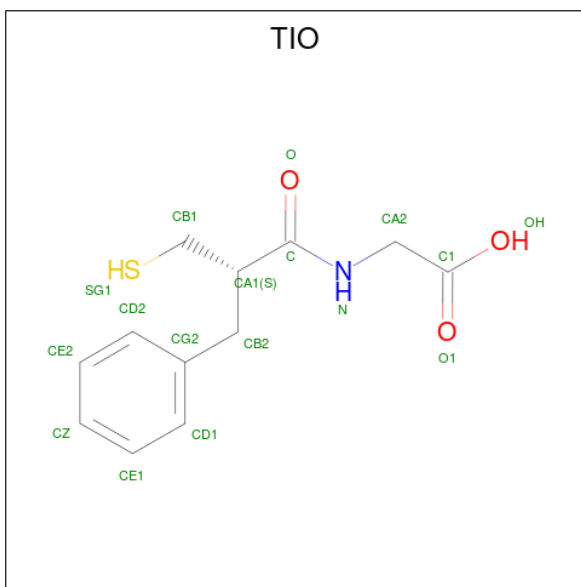
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	4	Total	Ca	0	0
			4	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2-MERCAPTOMETHYL-3-PHENYL-PROPIONYL)-GLYCINE (CCD ID: TIO) (formula: C₁₂H₁₅NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	0
			17	12	1	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	161	Total	O	0	0
			161	161		

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: Thermolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.00Å 94.00Å 132.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.70 10.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	68.0 (10.00-1.70) 67.7 (10.00-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.12 (at 1.70Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.183 , (Not available) 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2615	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: TIO, ZN, CA

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	E	1.63	14/2491 (0.6%)	2.28	119/3391 (3.5%)

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	E	2	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	183	ASN	C-O	-7.62	1.20	1.23
1	E	294	ASP	N-CA	-6.67	1.38	1.46
1	E	150	ASP	CG-OD2	6.44	1.37	1.25
1	E	125	GLY	N-CA	6.39	1.52	1.45
1	E	242	TYR	CA-C	6.35	1.61	1.52
1	E	153	ALA	N-CA	5.85	1.53	1.46
1	E	140	VAL	N-CA	5.83	1.53	1.46
1	E	313	VAL	CA-C	-5.70	1.45	1.53
1	E	78	GLY	N-CA	5.63	1.52	1.45
1	E	216	HIS	CA-CB	5.62	1.63	1.53
1	E	187	GLU	CD-OE2	5.58	1.35	1.25
1	E	85	LYS	C-O	-5.41	1.17	1.24
1	E	213	ASP	CG-OD2	5.27	1.35	1.25
1	E	77	ALA	N-CA	5.03	1.52	1.46

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	260	ARG	N-CA-C	13.79	126.31	111.28
1	E	269	ARG	CD-NE-CZ	-11.56	108.22	124.40
1	E	89	ASN	CA-CB-CG	-10.73	101.87	112.60
1	E	183	ASN	CB-CA-C	-10.26	102.07	111.00
1	E	278	THR	N-CA-CB	-9.40	96.15	110.73
1	E	269	ARG	NE-CZ-NH1	-9.07	112.43	121.50
1	E	282	SER	CB-CA-C	8.67	125.18	110.79
1	E	129	THR	N-CA-C	-8.60	101.11	111.69
1	E	133	LEU	N-CA-C	8.23	121.17	111.71
1	E	316	LYS	CB-CA-C	8.19	125.66	110.10
1	E	89	ASN	OD1-CG-ND2	8.04	130.64	122.60
1	E	84	TYR	N-CA-C	8.02	120.02	111.28
1	E	86	ASN	N-CA-C	7.98	120.06	111.36
1	E	4	THR	OG1-CB-CG2	-7.96	93.37	109.30
1	E	61	GLN	CA-CB-CG	-7.86	98.39	114.10
1	E	214	PRO	N-CA-CB	7.83	110.62	103.34
1	E	220	ARG	CD-NE-CZ	7.76	135.26	124.40
1	E	53	SER	CB-CA-C	-7.76	95.42	109.38
1	E	156	ILE	CA-CB-CG2	7.71	123.60	110.50
1	E	261	ASP	N-CA-CB	-7.64	98.94	110.01
1	E	96	ASN	CB-CG-ND2	-7.61	104.98	116.40
1	E	6	THR	OG1-CB-CG2	-7.28	94.75	109.30
1	E	48	THR	CA-C-O	7.28	127.98	119.32
1	E	316	LYS	N-CA-CB	7.26	122.84	110.50
1	E	281	PHE	CA-CB-CG	7.21	121.01	113.80
1	E	26	THR	N-CA-CB	7.19	122.64	110.49
1	E	58	ALA	N-CA-C	7.12	120.08	111.82
1	E	49	THR	CA-CB-OG1	-7.10	98.95	109.60
1	E	65	SER	CA-CB-OG	-7.09	96.92	111.10
1	E	101	ARG	CG-CD-NE	-7.02	96.56	112.00
1	E	220	ARG	CA-CB-CG	6.91	127.91	114.10
1	E	233	ASN	CA-CB-CG	-6.84	105.76	112.60
1	E	195	PRO	CA-C-N	-6.76	108.17	121.41
1	E	195	PRO	C-N-CA	-6.76	108.17	121.41
1	E	14	LEU	CD1-CG-CD2	-6.75	95.94	110.80
1	E	203	ARG	O-C-N	6.74	130.94	123.25
1	E	298	SER	N-CA-C	6.73	121.09	112.34
1	E	114	PHE	CA-CB-CG	6.70	120.50	113.80
1	E	224	THR	OG1-CB-CG2	6.68	122.66	109.30
1	E	143	GLU	N-CA-C	6.61	118.14	111.07
1	E	26	THR	CB-CA-C	6.58	123.52	110.42
1	E	257	GLY	CA-C-O	-6.57	115.67	121.58
1	E	21	ASN	OD1-CG-ND2	-6.50	116.10	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	TYR	CB-CG-CD2	-6.49	111.07	120.80
1	E	249	THR	CA-C-N	-6.49	113.62	122.77
1	E	249	THR	C-N-CA	-6.49	113.62	122.77
1	E	67	ASP	CA-CB-CG	6.46	119.06	112.60
1	E	160	GLU	N-CA-CB	6.46	119.38	110.01
1	E	32	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	131	ILE	N-CA-CB	6.39	120.16	111.21
1	E	57	ASP	CB-CG-OD1	6.38	133.07	118.40
1	E	294	ASP	CB-CA-C	-6.38	100.20	110.79
1	E	161	SER	CA-CB-OG	-6.31	98.49	111.10
1	E	286	ALA	N-CA-CB	-6.30	100.52	110.22
1	E	2	THR	CA-C-O	-6.20	113.73	120.36
1	E	130	PHE	CA-CB-CG	6.18	119.98	113.80
1	E	93	TYR	N-CA-C	6.15	118.95	111.82
1	E	308	GLN	OE1-CD-NE2	-6.14	116.45	122.60
1	E	292	ALA	N-CA-C	-6.11	104.70	111.36
1	E	224	THR	CA-CB-CG2	6.04	120.77	110.50
1	E	265	LYS	CB-CA-C	-5.97	101.50	110.88
1	E	182	LYS	CG-CD-CE	5.95	124.99	111.30
1	E	84	TYR	CA-C-O	5.94	126.84	120.55
1	E	215	ASP	CA-CB-CG	-5.90	106.70	112.60
1	E	172	PHE	CA-CB-CG	-5.89	107.91	113.80
1	E	117	GLY	N-CA-C	-5.88	107.69	114.69
1	E	224	THR	CA-C-O	-5.85	112.71	118.97
1	E	140	VAL	N-CA-CB	5.84	117.39	110.55
1	E	183	ASN	N-CA-CB	-5.81	103.20	111.51
1	E	135	GLY	O-C-N	-5.79	114.72	122.48
1	E	193	TYR	CA-C-O	-5.76	114.30	120.92
1	E	184	PRO	N-CA-C	5.75	120.03	111.41
1	E	103	SER	N-CA-CB	5.75	120.34	110.68
1	E	104	VAL	CA-C-O	-5.72	116.22	121.72
1	E	37	ASP	CA-CB-CG	5.72	118.32	112.60
1	E	274	TYR	N-CA-C	5.72	120.92	113.88
1	E	213	ASP	CA-C-O	-5.68	115.49	120.60
1	E	74	HIS	CG-CD2-NE2	-5.68	101.52	107.20
1	E	37	ASP	N-CA-CB	5.66	119.18	110.46
1	E	172	PHE	O-C-N	-5.65	115.32	122.27
1	E	224	THR	N-CA-CB	-5.63	102.84	110.67
1	E	207	ASP	O-C-N	5.62	125.17	121.23
1	E	156	ILE	O-C-N	-5.62	116.68	122.63
1	E	220	ARG	CA-C-N	5.56	129.44	121.50
1	E	220	ARG	C-N-CA	5.56	129.44	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	E	65	SER	CB-CA-C	5.52	120.84	110.63
1	E	190	GLU	N-CA-C	5.48	117.96	111.33
1	E	52	GLY	O-C-N	-5.48	115.58	122.70
1	E	19	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	E	114	PHE	CA-C-N	5.42	130.64	123.05
1	E	114	PHE	C-N-CA	5.42	130.64	123.05
1	E	142	HIS	N-CA-C	-5.40	105.29	111.07
1	E	61	GLN	CB-CG-CD	-5.39	103.44	112.60
1	E	308	GLN	CA-CB-CG	5.34	124.77	114.10
1	E	74	HIS	ND1-CG-CD2	5.33	111.43	106.10
1	E	311	ASP	CB-CG-OD1	5.28	130.53	118.40
1	E	16	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	21	ASN	CB-CG-ND2	5.26	124.29	116.40
1	E	174	THR	CA-CB-OG1	-5.26	101.72	109.60
1	E	256	VAL	CB-CA-C	-5.25	104.94	111.08
1	E	1	ILE	CA-CB-CG2	5.24	119.41	110.50
1	E	123	GLY	N-CA-C	-5.20	104.48	112.85
1	E	184	PRO	CA-C-O	-5.19	115.44	122.08
1	E	33	ASN	CA-C-O	5.14	125.30	119.18
1	E	274	TYR	CB-CG-CD2	5.14	128.51	120.80
1	E	261	ASP	CB-CA-C	-5.13	102.82	110.88
1	E	124	ASP	CA-C-N	-5.13	115.49	121.85
1	E	124	ASP	C-N-CA	-5.13	115.49	121.85
1	E	311	ASP	CB-CG-OD2	-5.12	106.61	118.40
1	E	129	THR	OG1-CB-CG2	5.11	119.52	109.30
1	E	81	TYR	N-CA-C	-5.10	105.61	111.07
1	E	118	SER	N-CA-CB	5.09	118.58	111.15
1	E	89	ASN	N-CA-CB	-5.08	104.46	112.13
1	E	305	SER	N-CA-CB	5.08	117.58	110.12
1	E	53	SER	CA-C-O	-5.06	115.34	120.71
1	E	118	SER	N-CA-C	5.04	121.11	114.75
1	E	231	HIS	ND1-CG-CD2	5.03	111.13	106.10
1	E	234	SER	N-CA-C	-5.02	106.00	111.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	224	THR	CB
1	E	316	LYS	CA

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	E	2432	0	2267	36	0
2	E	4	0	0	0	0
3	E	1	0	0	0	0
4	E	17	0	13	2	0
5	E	161	0	0	3	0
All	All	2615	0	2280	36	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.

All (36) 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:E:285:ARG:HD3	1:E:316:LYS:HD3	1.28	1.05
1:E:269:ARG:NH1	1:E:294:ASP:OD2	2.16	0.79
1:E:280:ASN:ND2	1:E:283:GLN:H	1.83	0.77
1:E:221:TYR:OH	1:E:225:GLN:HG3	1.90	0.70
1:E:139:VAL:HG22	4:E:1006:TIO:CZ	2.25	0.66
1:E:280:ASN:HD22	1:E:283:GLN:H	1.45	0.64
1:E:285:ARG:HD3	1:E:316:LYS:CD	2.18	0.62
1:E:220:ARG:HD2	5:E:542:HOH:O	2.03	0.59
1:E:120:MET:SD	1:E:144:LEU:HD23	2.45	0.57
1:E:265:LYS:HE2	5:E:446:HOH:O	2.04	0.57
1:E:280:ASN:HD22	1:E:280:ASN:C	2.13	0.56
1:E:4:THR:HG22	1:E:24:TYR:HB3	1.87	0.56
1:E:68:ALA:HB3	1:E:69:PRO:HD3	1.87	0.55
1:E:120:MET:CE	1:E:144:LEU:HD23	2.36	0.55
1:E:143:GLU:OE2	4:E:1006:TIO:HB22	2.06	0.55
1:E:191:ASP:HB2	5:E:350:HOH:O	2.09	0.52
1:E:31:GLN:HG3	1:E:40:PHE:CE1	2.45	0.52
1:E:131:ILE:HB	1:E:132:PRO:HD2	1.92	0.50
1:E:32:ASP:O	1:E:38:GLY:HA2	2.11	0.50
1:E:144:LEU:O	1:E:147:ALA:HB3	2.14	0.48
1:E:128:GLN:O	1:E:195:PRO:HD2	2.13	0.48
1:E:276:THR:HB	1:E:277:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:ILE:HG21	1:E:29:TYR:CD2	2.49	0.47
1:E:194:THR:HA	1:E:195:PRO:HD2	1.51	0.47
1:E:137:ILE:HG22	1:E:182:LYS:HZ3	1.81	0.46
1:E:182:LYS:NZ	1:E:191:ASP:OD2	2.49	0.46
1:E:120:MET:HE2	1:E:144:LEU:HD23	1.98	0.46
1:E:175:LEU:HD23	1:E:175:LEU:HA	1.76	0.45
1:E:97:ASN:HD22	1:E:97:ASN:HA	1.65	0.44
1:E:269:ARG:HH11	1:E:269:ARG:HD3	1.21	0.44
1:E:300:SER:OG	1:E:303:VAL:HG23	2.18	0.44
1:E:29:TYR:CE1	1:E:56:ALA:HB2	2.54	0.43
1:E:161:SER:HB3	1:E:279:SER:O	2.19	0.42
1:E:131:ILE:HB	1:E:132:PRO:CD	2.50	0.42
1:E:279:SER:HA	1:E:283:GLN:OE1	2.20	0.41
1:E:194:THR:C	1:E:196:GLY:N	2.74	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	E	314/316 (99%)	302 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	E	252/252 (100%)	230 (91%)	22 (9%)	9 2

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	ILE
1	E	20	ILE
1	E	26	THR
1	E	49	THR
1	E	89	ASN
1	E	96	ASN
1	E	97	ASN
1	E	101	ARG
1	E	128	GLN
1	E	144	LEU
1	E	174	THR
1	E	182	LYS
1	E	183	ASN
1	E	197	ILE
1	E	198	SER
1	E	224	THR
1	E	225	GLN
1	E	261	ASP
1	E	265	LYS
1	E	278	THR
1	E	280	ASN
1	E	316	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	21	ASN
1	E	97	ASN
1	E	280	ASN
1	E	290	GLN
1	E	301	GLN

5.3.3 RNA ⓘ

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, 5 are monoatomic - leaving 1 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	TIO	E	1006	3	17,17,17	1.56	3 (17%)	19,21,21	2.82	11 (57%)

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	TIO	E	1006	3	-	5/15/15/15	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1006	TIO	CA1-C	3.65	1.57	1.51
4	E	1006	TIO	O-C	2.65	1.28	1.23
4	E	1006	TIO	CA2-C1	2.62	1.57	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1006	TIO	CB1-CA1-C	6.13	121.09	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1006	TIO	CG2-CB2-CA1	-5.98	102.37	113.74
4	E	1006	TIO	CA1-C-N	-3.57	111.42	115.99
4	E	1006	TIO	CD2-CG2-CD1	3.39	123.27	118.23
4	E	1006	TIO	CA1-CB1-SG1	-3.09	108.39	114.31
4	E	1006	TIO	CE2-CD2-CG2	-2.48	117.13	120.61
4	E	1006	TIO	O-C-CA1	2.45	125.98	122.19
4	E	1006	TIO	CZ-CE1-CD1	-2.40	117.28	120.24
4	E	1006	TIO	CA2-N-C	2.35	127.32	121.38
4	E	1006	TIO	C1-CA2-N	-2.33	105.83	113.06
4	E	1006	TIO	CE2-CZ-CE1	2.21	122.90	119.87

There are no chirality outliers.

All (5) torsion outliers are listed below:

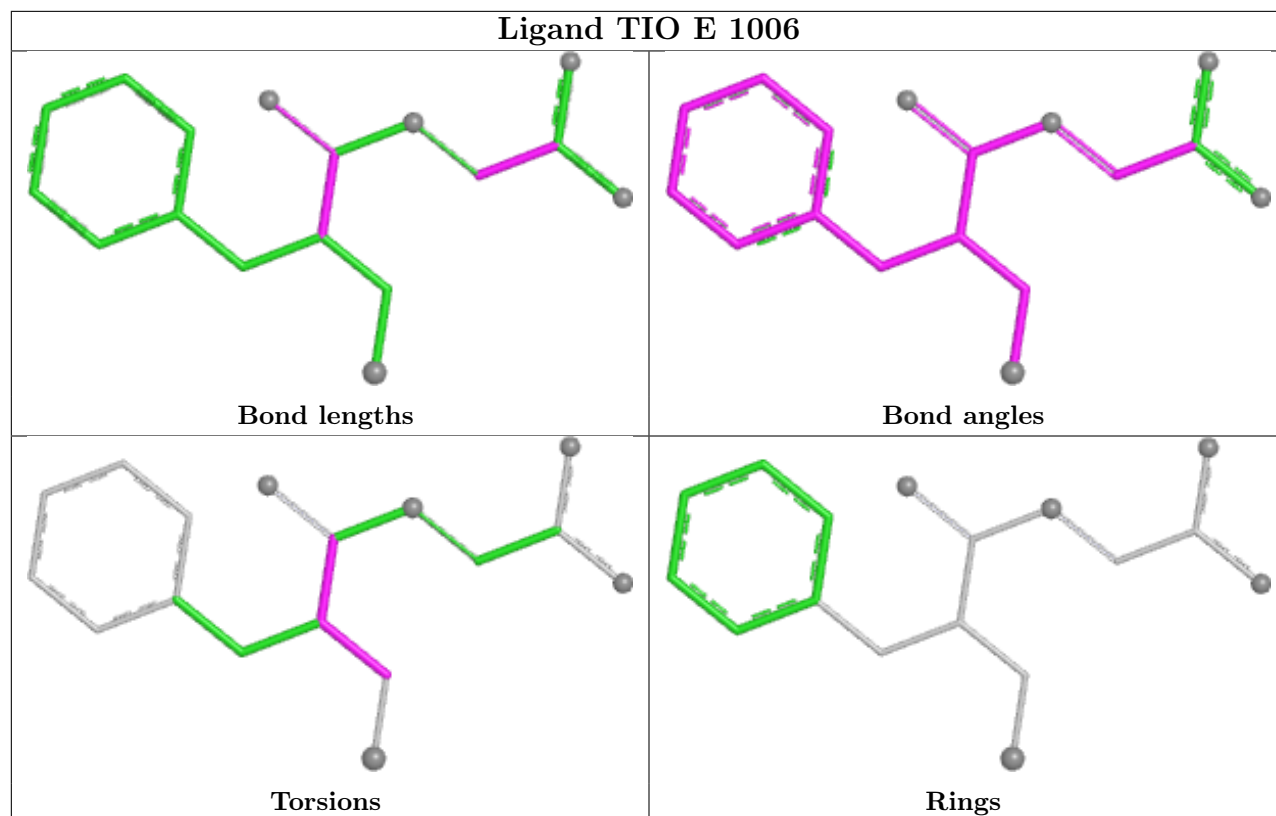
Mol	Chain	Res	Type	Atoms
4	E	1006	TIO	C-CA1-CB1-SG1
4	E	1006	TIO	O-C-CA1-CB1
4	E	1006	TIO	N-C-CA1-CB1
4	E	1006	TIO	O-C-CA1-CB2
4	E	1006	TIO	N-C-CA1-CB2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1006	TIO	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 [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	E	316/316 (100%)	-0.72	0 100 100	6, 14, 26, 37	0

There are no RSRZ outliers to report.

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.

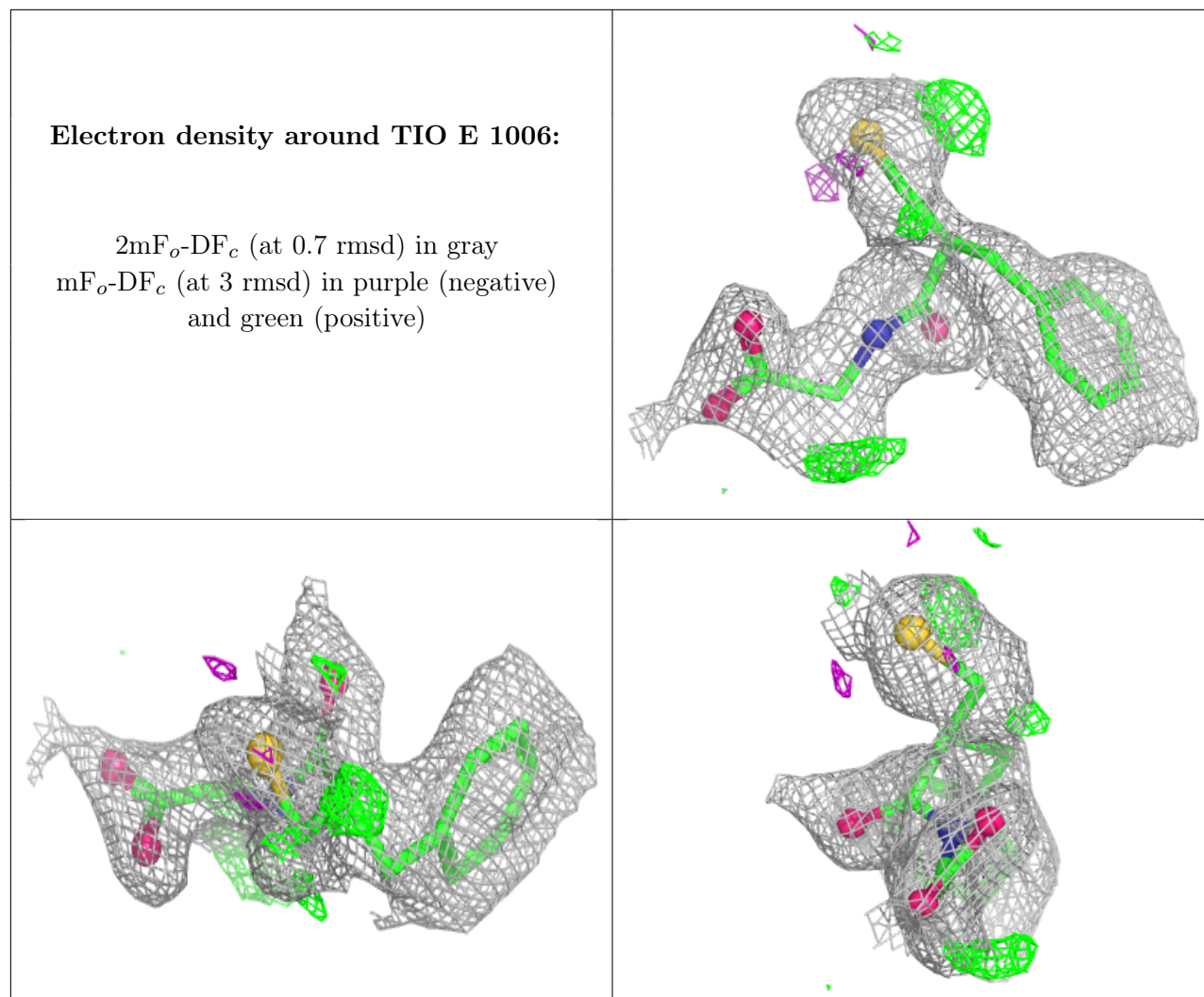
6.4 Ligands [i](#)

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	TIO	E	1006	17/17	0.93	0.07	20,23,30,37	0
2	CA	E	1004	1/1	0.98	0.02	17,17,17,17	0
2	CA	E	1001	1/1	0.99	0.02	13,13,13,13	0
3	ZN	E	1005	1/1	0.99	0.02	12,12,12,12	0
2	CA	E	1002	1/1	0.99	0.01	15,15,15,15	0
2	CA	E	1003	1/1	1.00	0.04	10,10,10,10	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.