



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 04:19 PM EST

PDB ID : 6TMN  
Title : Structures of two thermolysin-inhibitor complexes that differ by a single hydrogen bond  
Authors : Tronrud, D.E.; Holden, H.M.; Matthews, B.W.  
Deposited on : 1987-06-29  
Resolution : 1.60 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

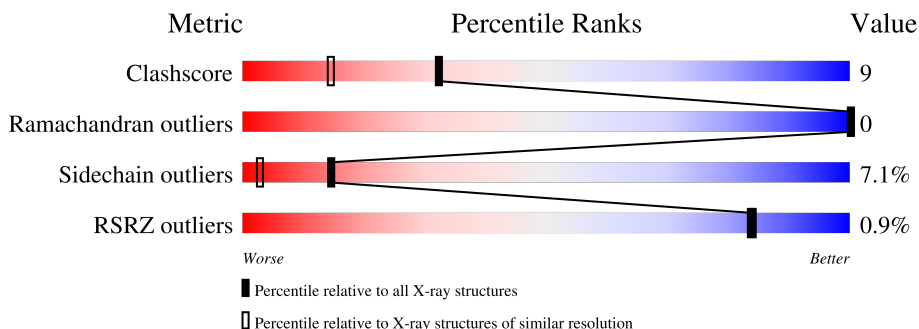
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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 [i](#)

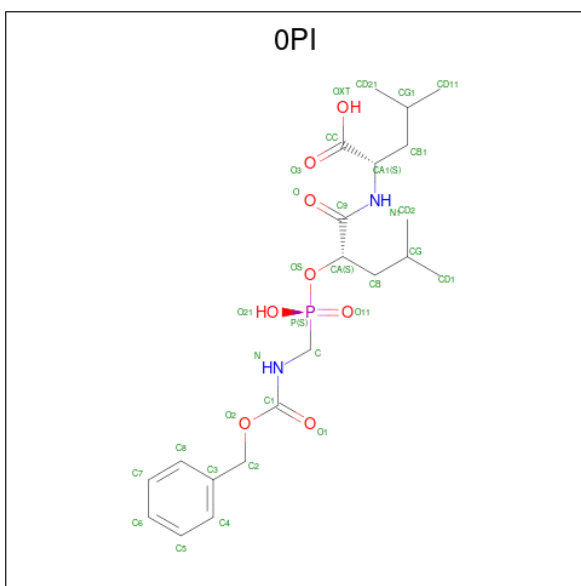
There are 5 unique types of molecules in this entry. The entry contains 2639 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	E	316	2432	1528	408	494	2	0	0	0

- Molecule 2 is N-[(2R,4S)-4-hydroxy-2-(2-methylpropyl)-4-oxido-7-oxo-9-phenyl-3,8-dioxa-6-aza-4-phosphanon-1-yl]-L-leucine (three-letter code: OPI) (formula: C<sub>21</sub>H<sub>33</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	32	21	2	8	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

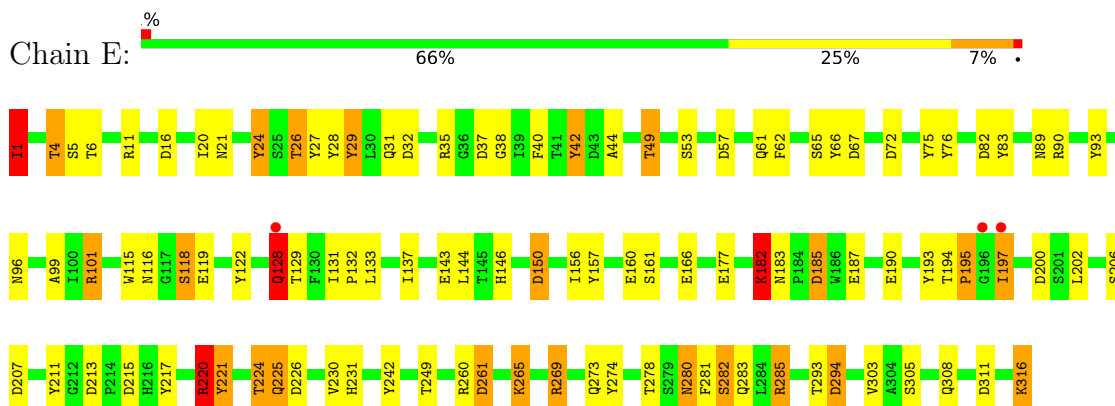
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	170	Total 170	O 170	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: THERMOLYSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.10Å 94.10Å 131.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.60 29.99 – 1.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.60) 70.9 (29.99-1.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 1.61Å)	Xtrriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.171 , (Not available) 0.156 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtrriage
Anisotropy	0.592	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 74.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, ZN, OPI

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	1.36	15/2491 (0.6%)	2.21	124/3391 (3.7%)

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	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	160	GLU	CD-OE1	-8.32	1.16	1.25
1	E	316	LYS	C-OXT	7.78	1.38	1.23
1	E	53	SER	CB-OG	-7.59	1.32	1.42
1	E	187	GLU	CD-OE2	7.34	1.33	1.25
1	E	166	GLU	CD-OE2	7.08	1.33	1.25
1	E	308	GLN	CG-CD	6.32	1.65	1.51
1	E	308	GLN	CD-OE1	6.05	1.37	1.24
1	E	190	GLU	CD-OE2	5.81	1.32	1.25
1	E	119	GLU	CD-OE2	5.74	1.31	1.25
1	E	119	GLU	CD-OE1	-5.66	1.19	1.25
1	E	118	SER	CB-OG	-5.57	1.35	1.42
1	E	261	ASP	CG-OD2	5.41	1.37	1.25
1	E	150	ASP	CG-OD2	5.40	1.37	1.25
1	E	206	SER	CB-OG	-5.27	1.35	1.42
1	E	177	GLU	CD-OE1	-5.25	1.19	1.25

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	ARG	NE-CZ-NH1	-14.62	112.99	120.30
1	E	260	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	E	16	ASP	CB-CG-OD2	-13.90	105.79	118.30
1	E	207	ASP	CB-CG-OD1	13.89	130.80	118.30
1	E	274	TYR	CB-CG-CD2	13.60	129.16	121.00
1	E	207	ASP	CB-CG-OD2	-12.07	107.43	118.30
1	E	269	ARG	CD-NE-CZ	-11.99	106.81	123.60
1	E	101	ARG	CG-CD-NE	-11.60	87.44	111.80
1	E	75	TYR	CB-CG-CD1	-11.17	114.30	121.00
1	E	220	ARG	NE-CZ-NH2	-11.15	114.73	120.30
1	E	29	TYR	CB-CG-CD1	-11.06	114.36	121.00
1	E	4	THR	OG1-CB-CG2	-10.82	85.12	110.00
1	E	211	TYR	CB-CG-CD2	-10.38	114.77	121.00
1	E	200	ASP	CB-CG-OD2	-10.25	109.07	118.30
1	E	285	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	E	197	ILE	CA-CB-CG1	9.97	129.95	111.00
1	E	226	ASP	CB-CG-OD1	9.92	127.22	118.30
1	E	260	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	E	261	ASP	CB-CG-OD2	-9.64	109.63	118.30
1	E	311	ASP	CB-CG-OD2	-9.60	109.66	118.30
1	E	316	LYS	CB-CA-C	9.42	129.24	110.40
1	E	193	TYR	CB-CG-CD1	-9.18	115.49	121.00
1	E	66	TYR	CB-CG-CD1	8.66	126.19	121.00
1	E	274	TYR	CB-CG-CD1	-8.64	115.82	121.00
1	E	311	ASP	CB-CG-OD1	8.57	126.01	118.30
1	E	101	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	E	75	TYR	CG-CD2-CE2	-8.09	114.83	121.30
1	E	6	THR	OG1-CB-CG2	-7.97	91.66	110.00
1	E	269	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	E	27	TYR	CB-CG-CD1	-7.76	116.34	121.00
1	E	57	ASP	CB-CG-OD1	7.72	125.25	118.30
1	E	221	TYR	CB-CG-CD2	-7.67	116.39	121.00
1	E	101	ARG	CD-NE-CZ	7.65	134.30	123.60
1	E	294	ASP	CB-CG-OD1	7.63	125.17	118.30
1	E	215	ASP	CB-CG-OD1	7.60	125.14	118.30
1	E	278	THR	N-CA-CB	-7.59	95.87	110.30
1	E	93	TYR	CB-CG-CD2	-7.54	116.48	121.00
1	E	215	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	E	156	ILE	CA-CB-CG2	7.47	125.84	110.90
1	E	72	ASP	CB-CG-OD1	7.29	124.86	118.30
1	E	28	TYR	CB-CG-CD2	-7.27	116.64	121.00
1	E	35	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	E	217	TYR	CB-CG-CD2	-7.21	116.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	202	LEU	CB-CG-CD1	-7.21	98.74	111.00
1	E	90	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	E	61	GLN	CA-CB-CG	-7.02	97.96	113.40
1	E	161	SER	CB-CA-C	6.97	123.35	110.10
1	E	202	LEU	CB-CG-CD2	-6.94	99.20	111.00
1	E	316	LYS	CB-CG-CD	-6.90	93.67	111.60
1	E	226	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	E	122	TYR	CG-CD2-CE2	6.79	126.73	121.30
1	E	5	SER	N-CA-CB	6.75	120.62	110.50
1	E	220	ARG	CA-CB-CG	6.71	128.16	113.40
1	E	274	TYR	CG-CD2-CE2	6.71	126.66	121.30
1	E	282	SER	CB-CA-C	6.67	122.77	110.10
1	E	200	ASP	CB-CG-OD1	6.64	124.27	118.30
1	E	260	ARG	CD-NE-CZ	6.59	132.82	123.60
1	E	308	GLN	CG-CD-OE1	6.54	134.69	121.60
1	E	67	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	E	76	TYR	CZ-CE2-CD2	-6.54	113.91	119.80
1	E	221	TYR	CG-CD2-CE2	-6.54	116.07	121.30
1	E	182	LYS	CD-CE-NZ	6.53	126.71	111.70
1	E	76	TYR	CG-CD1-CE1	-6.38	116.19	121.30
1	E	133	LEU	CB-CG-CD2	-6.26	100.36	111.00
1	E	242	TYR	CG-CD2-CE2	-6.15	116.38	121.30
1	E	221	TYR	CD1-CG-CD2	6.12	124.63	117.90
1	E	11	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	E	242	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	E	128	GLN	N-CA-CB	-6.03	99.75	110.60
1	E	293	THR	CA-CB-CG2	-6.03	103.96	112.40
1	E	281	PHE	CB-CG-CD2	-6.03	116.58	120.80
1	E	305	SER	N-CA-CB	5.89	119.34	110.50
1	E	274	TYR	CD1-CE1-CZ	5.88	125.09	119.80
1	E	75	TYR	CD1-CG-CD2	5.86	124.34	117.90
1	E	220	ARG	N-CA-CB	-5.86	100.06	110.60
1	E	75	TYR	CD1-CE1-CZ	-5.85	114.53	119.80
1	E	89	ASN	CA-CB-CG	-5.85	100.53	113.40
1	E	150	ASP	CB-CG-OD1	-5.85	113.04	118.30
1	E	82	ASP	CB-CG-OD1	5.83	123.55	118.30
1	E	185	ASP	CB-CG-OD1	5.75	123.48	118.30
1	E	213	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	E	11	ARG	CD-NE-CZ	-5.73	115.58	123.60
1	E	24	TYR	CG-CD2-CE2	-5.71	116.73	121.30
1	E	195	PRO	C-N-CA	-5.69	110.36	122.30
1	E	42	TYR	CZ-CE2-CD2	-5.62	114.74	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	83	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	E	261	ASP	CB-CA-C	-5.60	99.21	110.40
1	E	303	VAL	CG1-CB-CG2	-5.59	101.96	110.90
1	E	273	GLN	CB-CA-C	-5.57	99.26	110.40
1	E	26	THR	N-CA-CB	5.56	120.87	110.30
1	E	182	LYS	CG-CD-CE	5.56	128.58	111.90
1	E	285	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	E	26	THR	CA-CB-OG1	5.52	120.60	109.00
1	E	265	LYS	CA-CB-CG	-5.51	101.27	113.40
1	E	65	SER	CB-CA-C	5.51	120.56	110.10
1	E	224	THR	OG1-CB-CG2	5.50	122.65	110.00
1	E	242	TYR	CD1-CG-CD2	5.50	123.95	117.90
1	E	1	ILE	O-C-N	-5.46	113.96	122.70
1	E	37	ASP	CB-CG-OD1	5.46	123.21	118.30
1	E	157	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	E	99	ALA	CB-CA-C	-5.43	101.95	110.10
1	E	1	ILE	CA-CB-CG2	5.39	121.68	110.90
1	E	29	TYR	CG-CD2-CE2	-5.39	116.99	121.30
1	E	231	HIS	N-CA-CB	5.37	120.26	110.60
1	E	11	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	E	62	PHE	CB-CG-CD2	5.34	124.53	120.80
1	E	6	THR	CA-CB-CG2	-5.33	104.93	112.40
1	E	76	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	E	42	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	E	249	THR	CA-CB-CG2	-5.32	104.96	112.40
1	E	57	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	E	260	ARG	CG-CD-NE	-5.29	100.70	111.80
1	E	67	ASP	CB-CG-OD1	5.23	123.00	118.30
1	E	101	ARG	CA-CB-CG	-5.22	101.91	113.40
1	E	44	ALA	O-C-N	-5.21	114.37	122.70
1	E	230	VAL	CG1-CB-CG2	5.20	119.21	110.90
1	E	49	THR	N-CA-CB	-5.18	100.45	110.30
1	E	16	ASP	CB-CG-OD1	5.16	122.95	118.30
1	E	160	GLU	OE1-CD-OE2	-5.09	117.20	123.30
1	E	129	THR	OG1-CB-CG2	5.06	121.64	110.00
1	E	101	ARG	CB-CA-C	-5.05	100.31	110.40
1	E	157	TYR	CZ-CE2-CD2	-5.03	115.28	119.80
1	E	76	TYR	CD1-CG-CD2	5.02	123.42	117.90
1	E	157	TYR	CB-CG-CD2	5.01	124.00	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	21	ASN	Sidechain

## 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	E	2432	0	2267	24	0
2	E	32	0	31	18	0
3	E	4	0	0	0	0
4	E	1	0	0	0	0
5	E	170	0	0	3	2
All	All	2639	0	2298	42	2

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 9.

All (42) 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)
2:E:317:0PI:CD21	2:E:317:0PI:HD25	0.97	1.11
2:E:317:0PI:HD16	2:E:317:0PI:CD11	0.97	1.11
2:E:317:0PI:CD21	2:E:317:0PI:HD26	0.97	1.11
1:E:285:ARG:HD3	1:E:316:LYS:HD3	1.33	1.08
2:E:317:0PI:CD11	2:E:317:0PI:HD15	0.97	1.07
2:E:317:0PI:CD21	2:E:317:0PI:HD24	0.97	1.07
2:E:317:0PI:CD11	2:E:317:0PI:HD14	0.97	1.05
2:E:317:0PI:HD25	2:E:317:0PI:CG1	2.04	0.88
2:E:317:0PI:HD16	2:E:317:0PI:CG1	2.05	0.87
2:E:317:0PI:HD15	2:E:317:0PI:CG1	2.05	0.86
2:E:317:0PI:HD14	2:E:317:0PI:CG1	2.05	0.86
2:E:317:0PI:HD24	2:E:317:0PI:CG1	2.04	0.86
2:E:317:0PI:HD25	2:E:317:0PI:HD24	1.58	0.86
2:E:317:0PI:HD26	2:E:317:0PI:CG1	2.04	0.85
2:E:317:0PI:HD26	2:E:317:0PI:HD24	1.58	0.85
2:E:317:0PI:HD15	2:E:317:0PI:HD14	1.58	0.84
2:E:317:0PI:HD16	2:E:317:0PI:HD14	1.58	0.83
2:E:317:0PI:HD25	2:E:317:0PI:HD26	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:317:0PI:HD16	2:E:317:0PI:HD15	1.58	0.82
1:E:269:ARG:NH1	1:E:294:ASP:OD2	2.16	0.77
1:E:116:ASN:O	5:E:323:HOH:O	2.06	0.72
1:E:285:ARG:HD3	1:E:316:LYS:CD	2.19	0.69
1:E:4:THR:HG22	1:E:24:TYR:HB3	1.80	0.63
1:E:1:ILE:HG21	1:E:29:TYR:CD2	2.36	0.61
1:E:42:TYR:HE2	1:E:101:ARG:HG2	1.65	0.61
1:E:220:ARG:HD2	5:E:480:HOH:O	2.02	0.60
1:E:280:ASN:HD22	1:E:283:GLN:H	1.50	0.60
1:E:221:TYR:OH	1:E:225:GLN:HG3	2.03	0.58
1:E:137:ILE:HG22	1:E:182:LYS:HZ3	1.75	0.51
1:E:42:TYR:CE2	1:E:101:ARG:HG2	2.47	0.50
1:E:280:ASN:ND2	1:E:283:GLN:H	2.09	0.50
1:E:137:ILE:H	1:E:182:LYS:NZ	2.11	0.47
1:E:137:ILE:CG2	1:E:182:LYS:HD3	2.44	0.47
1:E:194:THR:HA	1:E:195:PRO:HD2	1.72	0.44
1:E:32:ASP:O	1:E:38:GLY:HA2	2.18	0.43
1:E:128:GLN:O	1:E:195:PRO:HD2	2.18	0.43
1:E:131:ILE:HB	1:E:132:PRO:CD	2.49	0.43
1:E:143:GLU:O	1:E:146:HIS:HB2	2.19	0.43
1:E:131:ILE:HG23	1:E:195:PRO:HG3	2.01	0.43
1:E:115:TRP:NE1	1:E:150:ASP:OD2	2.53	0.42
1:E:31:GLN:HG3	1:E:40:PHE:CE1	2.55	0.41
1:E:265:LYS:HE2	5:E:404:HOH:O	2.20	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:434:HOH:O	5:E:434:HOH:O[7_555]	1.80	0.40
5:E:387:HOH:O	5:E:387:HOH:O[12_565]	2.07	0.13

## 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%)	301 (96%)	13 (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%)	234 (93%)	18 (7%)	14	3

All (18) 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	96	ASN
1	E	118	SER
1	E	128	GLN
1	E	144	LEU
1	E	182	LYS
1	E	183	ASN
1	E	185	ASP
1	E	197	ILE
1	E	220	ARG
1	E	224	THR
1	E	225	GLN
1	E	261	ASP
1	E	280	ASN
1	E	282	SER

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	31	GLN
1	E	33	ASN
1	E	97	ASN
1	E	280	ASN
1	E	290	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](#)

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
2	OPI	E	317	4	30,32,32	1.65	3 (10%)	38,43,43	2.35	17 (44%)

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	OPI	E	317	4	-	10/35/36/36	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	317	0PI	P-O21	-6.32	1.41	1.56
2	E	317	0PI	P-OS	3.14	1.62	1.57
2	E	317	0PI	C2-C3	3.11	1.57	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	317	0PI	OS-P-O11	-6.14	104.89	115.39
2	E	317	0PI	C2-O2-C1	4.33	125.59	115.93
2	E	317	0PI	O1-C1-N	3.92	130.98	124.96
2	E	317	0PI	C6-C5-C4	-3.87	114.29	120.19
2	E	317	0PI	O21-P-C	3.58	115.88	106.71
2	E	317	0PI	C5-C4-C3	3.51	126.02	120.63
2	E	317	0PI	O11-P-C	3.44	118.19	108.62
2	E	317	0PI	CB1-CA1-CC	2.85	119.05	110.23
2	E	317	0PI	OXT-CC-O3	-2.69	117.98	124.09
2	E	317	0PI	OXT-CC-CA1	2.62	122.12	113.40
2	E	317	0PI	O2-C2-C3	2.41	115.18	109.39
2	E	317	0PI	CD2-CG-CB	-2.36	102.42	111.11
2	E	317	0PI	O-C9-CA	2.27	123.31	119.74
2	E	317	0PI	O2-C1-O1	-2.22	119.99	124.25
2	E	317	0PI	CB1-CA1-N1	2.18	115.60	110.58
2	E	317	0PI	CG-CB-CA	-2.17	111.84	115.25
2	E	317	0PI	C7-C8-C3	-2.07	117.46	120.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

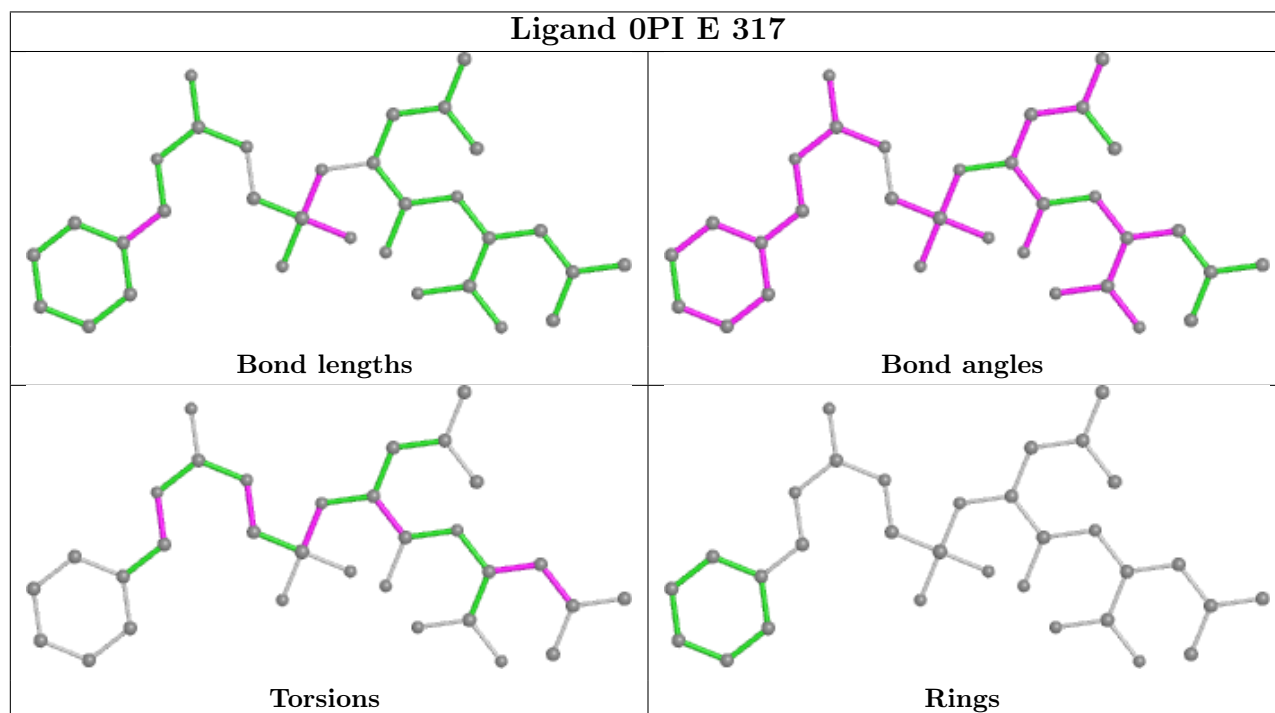
Mol	Chain	Res	Type	Atoms
2	E	317	0PI	CA-OS-P-O11
2	E	317	0PI	CA1-CB1-CG1-CD21
2	E	317	0PI	CA-OS-P-C
2	E	317	0PI	CA1-CB1-CG1-CD11
2	E	317	0PI	O-C9-CA-CB
2	E	317	0PI	N1-C9-CA-OS
2	E	317	0PI	C3-C2-O2-C1
2	E	317	0PI	P-C-N-C1
2	E	317	0PI	N1-C9-CA-CB
2	E	317	0PI	CC-CA1-CB1-CG1

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	317	OPI	18	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	316/316 (100%)	-0.67	3 (0%) 84   84	6, 12, 26, 36	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	197	ILE	3.1
1	E	128	GLN	2.7
1	E	196	GLY	2.3

### 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 monosaccharides 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, 95<sup>th</sup> 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.

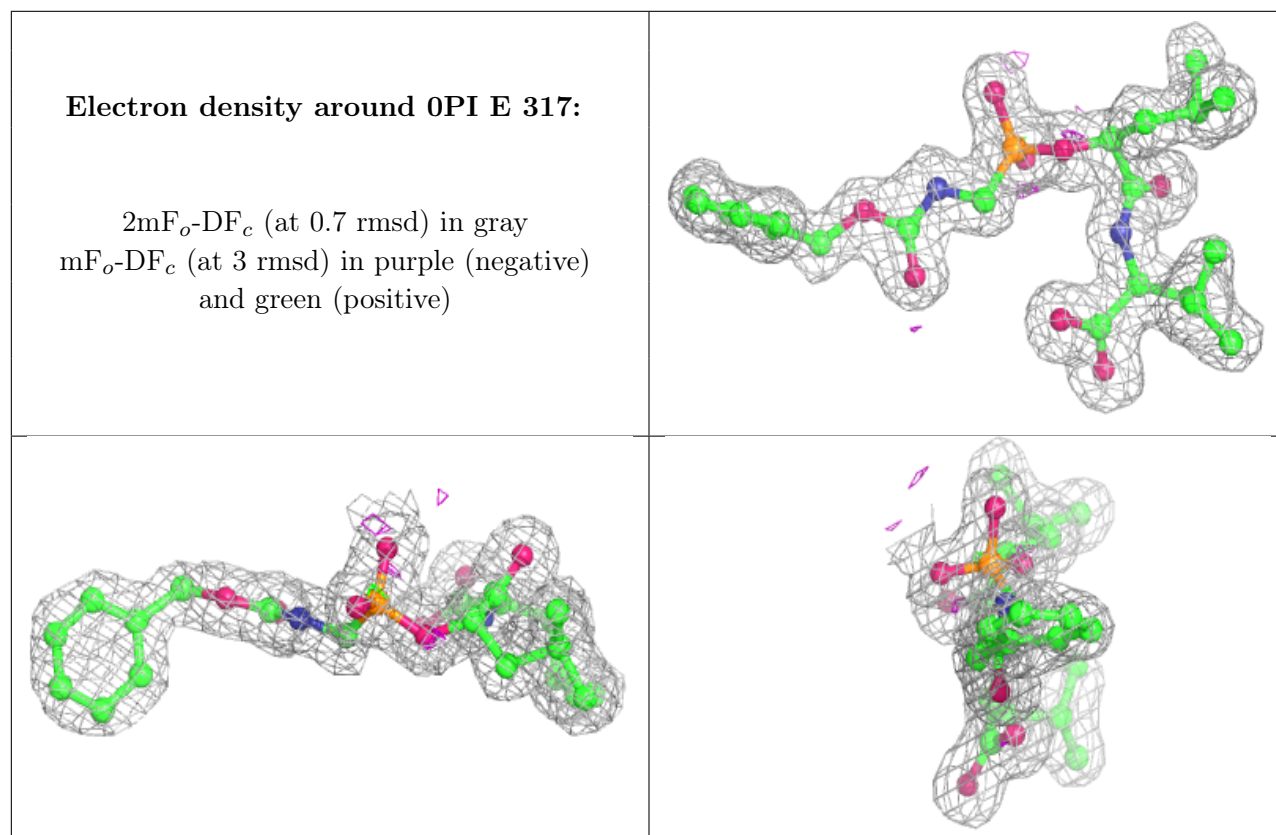
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OPI	E	317	32/32	0.98	0.06	5,17,29,30	0
3	CA	E	321	1/1	0.99	0.04	16,16,16,16	0
3	CA	E	319	1/1	1.00	0.06	13,13,13,13	0
3	CA	E	320	1/1	1.00	0.05	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	E	318	1/1	1.00	0.03	8,8,8,8	0
4	ZN	E	322	1/1	1.00	0.06	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 [i](#)

There are no such residues in this entry.