



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:11 PM UTC

PDB ID : 6TMN / pdb_00006tmn
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

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

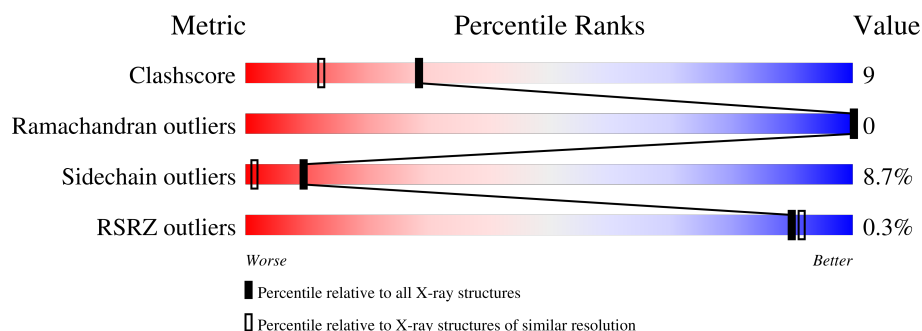
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 ≥ 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	 60% 33% 6% .

2 Entry composition [i](#)

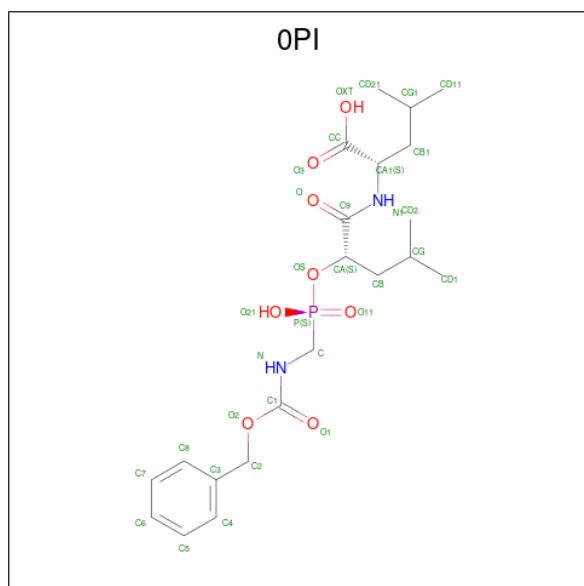
There are 5 unique types of molecules in this entry. The entry contains 2639 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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 (CCD ID: 0PI) (formula: $C_{21}H_{33}N_2O_8P$).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

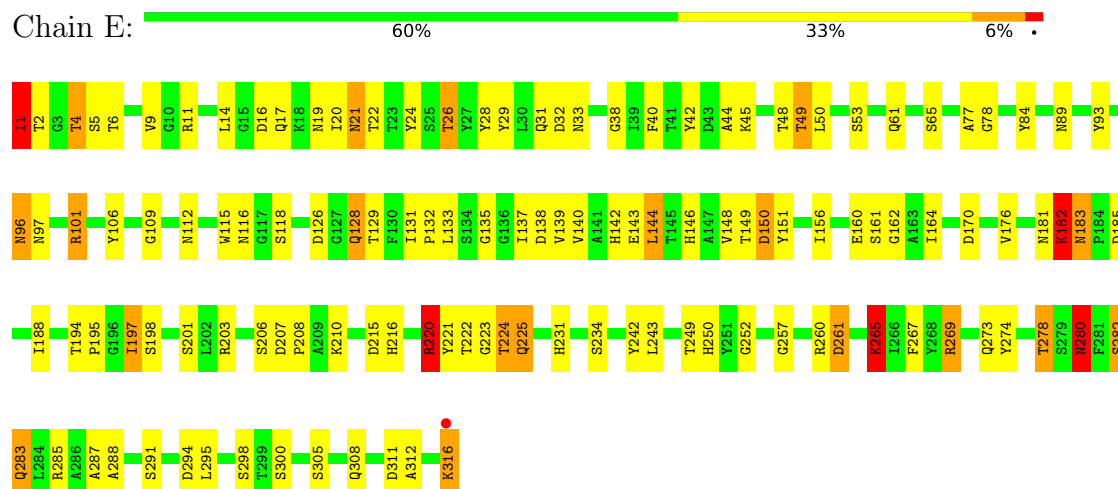
- Molecule 5 is water.

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, α , β , γ	94.10Å 94.10Å 131.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.60 81.49 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.60) 70.9 (81.49-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 1.61Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.171 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2639	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage'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.*

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: 0PI, 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	1.75	20/2491 (0.8%)	2.39	143/3391 (4.2%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	316	LYS	C-OXT	7.29	1.38	1.23
1	E	308	GLN	CD-OE1	7.22	1.37	1.23
1	E	261	ASP	CG-OD2	6.54	1.37	1.25
1	E	150	ASP	CG-OD2	6.54	1.37	1.25
1	E	242	TYR	CA-C	6.26	1.60	1.52
1	E	22	THR	CA-C	6.10	1.61	1.53
1	E	139	VAL	CA-C	6.05	1.60	1.52
1	E	109	GLY	CA-C	5.85	1.57	1.51
1	E	252	GLY	C-N	5.72	1.41	1.33
1	E	77	ALA	C-N	5.64	1.41	1.33
1	E	308	GLN	CG-CD	5.42	1.65	1.52
1	E	203	ARG	NE-CZ	5.39	1.39	1.33
1	E	11	ARG	NE-CZ	5.34	1.39	1.33
1	E	139	VAL	C-N	5.33	1.40	1.33
1	E	170	ASP	CG-OD2	5.24	1.35	1.25
1	E	267	PHE	CA-C	5.11	1.59	1.52
1	E	216	HIS	CA-CB	5.09	1.62	1.53
1	E	140	VAL	N-CA	5.06	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	78	GLY	CA-C	5.02	1.57	1.52
1	E	142	HIS	N-CA	5.01	1.52	1.46

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	ARG	CD-NE-CZ	-12.56	106.81	124.40
1	E	4	THR	OG1-CB-CG2	-12.09	85.12	109.30
1	E	89	ASN	CA-CB-CG	-12.06	100.53	112.60
1	E	197	ILE	CA-CB-CG1	11.50	129.95	110.40
1	E	101	ARG	CG-CD-NE	-11.16	87.44	112.00
1	E	316	LYS	CB-CA-C	10.07	129.24	110.10
1	E	278	THR	N-CA-CB	-9.41	95.87	110.92
1	E	156	ILE	CA-CB-CG2	9.03	125.84	110.50
1	E	96	ASN	OD1-CG-ND2	8.89	131.49	122.60
1	E	6	THR	OG1-CB-CG2	-8.82	91.66	109.30
1	E	183	ASN	OD1-CG-ND2	8.63	131.23	122.60
1	E	133	LEU	N-CA-C	8.52	121.51	111.71
1	E	269	ARG	NE-CZ-NH1	-8.51	112.99	121.50
1	E	21	ASN	OD1-CG-ND2	-8.51	114.09	122.60
1	E	112	ASN	OD1-CG-ND2	-8.48	114.12	122.60
1	E	260	ARG	N-CA-C	8.46	121.64	111.82
1	E	183	ASN	CB-CA-C	-8.25	105.34	111.20
1	E	61	GLN	CA-CB-CG	-8.07	97.96	114.10
1	E	215	ASP	CA-CB-CG	-7.80	104.80	112.60
1	E	183	ASN	N-CA-CB	-7.76	103.04	111.66
1	E	316	LYS	CB-CG-CD	-7.67	93.67	111.30
1	E	161	SER	CB-CA-C	7.57	123.35	110.79
1	E	182	LYS	CG-CD-CE	7.51	128.58	111.30
1	E	261	ASP	CB-CA-C	-7.40	99.21	110.90
1	E	96	ASN	CB-CG-ND2	-7.37	105.35	116.40
1	E	26	THR	CA-CB-OG1	7.33	120.60	109.60
1	E	49	THR	CA-CB-OG1	-7.21	98.79	109.60
1	E	176	VAL	N-CA-C	-7.20	103.45	110.72
1	E	5	SER	N-CA-CB	7.15	120.62	109.69
1	E	250	HIS	CA-C-O	-7.11	112.71	120.24
1	E	101	ARG	CD-NE-CZ	7.07	134.30	124.40
1	E	220	ARG	CA-CB-CG	7.03	128.16	114.10
1	E	308	GLN	CG-CD-OE1	6.94	134.69	120.80
1	E	33	ASN	OD1-CG-ND2	6.86	129.46	122.60
1	E	220	ARG	N-CA-CB	-6.79	100.06	110.04
1	E	224	THR	OG1-CB-CG2	6.68	122.65	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	280	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	E	14	LEU	CD1-CG-CD2	-6.63	96.22	110.80
1	E	182	LYS	CA-C-O	-6.59	114.79	122.37
1	E	1	ILE	CA-CB-CG2	6.58	121.68	110.50
1	E	260	ARG	NE-CZ-NH2	-6.56	113.30	119.20
1	E	216	HIS	CA-CB-CG	-6.55	107.25	113.80
1	E	156	ILE	CB-CG1-CD1	-6.52	100.11	113.80
1	E	181	ASN	CA-C-O	6.50	129.01	121.28
1	E	183	ASN	CA-CB-CG	6.48	119.08	112.60
1	E	45	LYS	CB-CA-C	-6.47	102.54	111.73
1	E	161	SER	CA-CB-OG	-6.47	98.17	111.10
1	E	65	SER	CA-CB-OG	-6.46	98.18	111.10
1	E	61	GLN	OE1-CD-NE2	6.44	129.04	122.60
1	E	265	LYS	CA-CB-CG	-6.42	101.27	114.10
1	E	156	ILE	O-C-N	-6.37	115.88	122.63
1	E	17	GLN	CG-CD-NE2	-6.35	106.87	116.40
1	E	282	SER	CB-CA-C	6.30	122.77	110.67
1	E	11	ARG	CD-NE-CZ	-6.30	115.58	124.40
1	E	288	ALA	CA-C-N	6.28	128.47	120.56
1	E	288	ALA	C-N-CA	6.28	128.47	120.56
1	E	305	SER	N-CA-CB	6.27	119.34	110.12
1	E	257	GLY	CA-C-O	-6.25	115.96	121.58
1	E	231	HIS	N-CA-CB	6.24	120.26	110.46
1	E	160	GLU	N-CA-CB	6.22	119.03	110.01
1	E	298	SER	N-CA-C	6.21	119.96	112.38
1	E	149	THR	CA-C-O	6.21	127.13	120.55
1	E	249	THR	CA-CB-OG1	-6.21	100.29	109.60
1	E	129	THR	OG1-CB-CG2	6.17	121.64	109.30
1	E	288	ALA	O-C-N	-6.15	115.61	122.12
1	E	26	THR	N-CA-CB	6.14	120.87	110.49
1	E	49	THR	N-CA-CB	-6.13	100.45	109.95
1	E	50	LEU	CD1-CG-CD2	6.12	124.26	110.80
1	E	101	ARG	CA-CB-CG	-6.10	101.91	114.10
1	E	44	ALA	CA-C-O	6.05	126.60	119.28
1	E	138	ASP	CA-CB-CG	6.02	118.62	112.60
1	E	260	ARG	CD-NE-CZ	6.02	132.82	124.40
1	E	280	ASN	CB-CG-ND2	6.00	125.39	116.40
1	E	222	THR	CA-C-O	5.99	126.25	119.18
1	E	28	TYR	CA-C-O	-5.96	113.98	120.36
1	E	265	LYS	CG-CD-CE	-5.88	97.76	111.30
1	E	84	TYR	N-CA-CB	5.86	118.73	110.12
1	E	300	SER	CA-C-N	5.83	128.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	300	SER	C-N-CA	5.83	128.02	120.44
1	E	44	ALA	O-C-N	-5.80	114.37	122.37
1	E	49	THR	CB-CA-C	5.79	119.28	109.84
1	E	2	THR	CA-C-O	-5.78	114.17	120.36
1	E	298	SER	O-C-N	5.78	129.91	122.39
1	E	17	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	E	283	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	E	1	ILE	O-C-N	-5.65	113.96	123.00
1	E	308	GLN	OE1-CD-NE2	-5.64	116.95	122.60
1	E	208	PRO	O-C-N	-5.61	114.98	122.22
1	E	4	THR	CB-CA-C	5.59	118.97	109.75
1	E	291	SER	O-C-N	5.58	127.82	122.07
1	E	269	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	E	274	TYR	CB-CG-CD2	5.57	129.16	120.80
1	E	273	GLN	CB-CA-C	-5.55	99.26	109.15
1	E	148	VAL	N-CA-CB	5.54	117.03	110.55
1	E	140	VAL	CA-C-O	5.52	127.01	121.27
1	E	16	ASP	CB-CG-OD2	-5.48	105.79	118.40
1	E	84	TYR	CA-C-O	5.46	126.34	120.55
1	E	243	LEU	O-C-N	-5.46	116.45	122.07
1	E	26	THR	CB-CA-C	5.41	121.19	110.42
1	E	308	GLN	CG-CD-NE2	-5.41	108.29	116.40
1	E	207	ASP	CB-CG-OD1	5.39	130.80	118.40
1	E	65	SER	CB-CA-C	5.37	120.56	110.63
1	E	48	THR	CA-C-O	5.35	125.91	119.59
1	E	188	ILE	N-CA-C	5.34	115.27	107.37
1	E	135	GLY	O-C-N	-5.33	116.66	122.84
1	E	197	ILE	CA-C-O	5.31	126.11	120.48
1	E	201	SER	N-CA-C	-5.29	101.23	108.38
1	E	278	THR	OG1-CB-CG2	5.26	119.82	109.30
1	E	295	LEU	N-CA-C	5.26	118.16	111.69
1	E	210	LYS	CA-C-N	5.26	130.75	122.49
1	E	210	LYS	C-N-CA	5.26	130.75	122.49
1	E	198	SER	N-CA-C	5.24	118.23	110.48
1	E	11	ARG	CA-C-O	-5.24	115.05	120.70
1	E	305	SER	CA-CB-OG	-5.23	100.64	111.10
1	E	53	SER	CB-CA-C	-5.22	100.69	109.72
1	E	162	GLY	O-C-N	-5.21	117.14	122.19
1	E	287	ALA	CA-C-O	-5.21	115.33	120.70
1	E	312	ALA	N-CA-C	5.21	117.70	111.71
1	E	278	THR	CA-CB-CG2	5.20	119.34	110.50
1	E	206	SER	CA-C-N	5.19	126.84	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	SER	C-N-CA	5.19	126.84	122.28
1	E	106	TYR	N-CA-CB	-5.16	101.95	109.95
1	E	144	LEU	CB-CA-C	5.16	119.61	110.85
1	E	223	GLY	CA-C-O	5.15	129.53	120.57
1	E	164	ILE	N-CA-CB	5.14	116.56	110.55
1	E	260	ARG	CG-CD-NE	-5.14	100.70	112.00
1	E	311	ASP	CA-C-O	-5.13	115.11	120.55
1	E	126	ASP	N-CA-C	-5.11	106.73	113.17
1	E	215	ASP	CA-C-O	5.10	125.50	119.48
1	E	93	TYR	CA-C-N	-5.10	114.13	122.54
1	E	93	TYR	C-N-CA	-5.10	114.13	122.54
1	E	151	TYR	CA-CB-CG	-5.09	104.74	113.90
1	E	234	SER	N-CA-C	-5.09	106.17	112.38
1	E	33	ASN	CA-C-O	5.07	125.42	119.28
1	E	160	GLU	CA-CB-CG	-5.07	103.95	114.10
1	E	308	GLN	O-C-N	5.07	127.29	122.07
1	E	26	THR	OG1-CB-CG2	5.05	119.40	109.30
1	E	150	ASP	CA-CB-CG	5.03	117.63	112.60
1	E	224	THR	N-CA-C	5.03	120.06	113.88
1	E	197	ILE	O-C-N	-5.00	117.93	123.18
1	E	19	ASN	CA-C-N	-5.00	114.74	122.69
1	E	19	ASN	C-N-CA	-5.00	114.74	122.69
1	E	144	LEU	CD1-CG-CD2	-5.00	99.80	110.80

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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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:137:ILE:H	1:E:182:LYS:HZ2	1.35	0.73
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:ILE:CG2	1:E:182:LYS:HD3	2.44	0.47
1:E:137:ILE:H	1:E:182:LYS:NZ	2.11	0.45
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 ⓘ

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	E	307/316 (97%)	296 (96%)	11 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	E	252/252 (100%)	230 (91%)	22 (9%)	9 1

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

Mol	Chain	Res	Type
1	E	1	ILE
1	E	9	VAL
1	E	20	ILE
1	E	26	THR
1	E	49	THR
1	E	96	ASN
1	E	97	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	265	LYS
1	E	278	THR
1	E	280	ASN
1	E	282	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	21	ASN
1	E	31	GLN
1	E	33	ASN
1	E	97	ASN
1	E	159	ASN
1	E	183	ASN
1	E	227	ASN
1	E	246	GLN

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Mol	Chain	Res	Type
1	E	280	ASN
1	E	290	GLN
1	E	301	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, 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	5 (16%)	38,43,43	2.42	18 (47%)

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	-	5/35/36/36	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	317	0PI	P-O21	-6.08	1.41	1.56
2	E	317	0PI	C2-C3	3.14	1.57	1.50
2	E	317	0PI	P-OS	2.98	1.62	1.57
2	E	317	0PI	CB-CA	2.07	1.56	1.53
2	E	317	0PI	P-O11	2.02	1.56	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	317	0PI	OS-P-O11	-5.59	104.89	115.27
2	E	317	0PI	C6-C5-C4	-4.82	114.29	120.24
2	E	317	0PI	C2-O2-C1	4.29	125.59	115.93
2	E	317	0PI	O1-C1-N	4.02	130.98	124.93
2	E	317	0PI	C5-C4-C3	3.85	126.02	120.61
2	E	317	0PI	O21-P-C	3.79	115.88	106.78
2	E	317	0PI	O11-P-C	3.59	118.19	108.66
2	E	317	0PI	CB1-CA1-CC	2.91	119.05	110.28
2	E	317	0PI	OXT-CC-O3	-2.69	117.98	124.08
2	E	317	0PI	OXT-CC-CA1	2.55	122.12	113.51
2	E	317	0PI	CD2-CG-CB	-2.41	102.42	111.08
2	E	317	0PI	O-C9-CA	2.39	123.31	119.58
2	E	317	0PI	O2-C2-C3	2.38	115.18	109.40
2	E	317	0PI	CG-CB-CA	-2.29	111.84	115.28
2	E	317	0PI	C7-C8-C3	-2.24	117.46	120.61
2	E	317	0PI	O2-C1-O1	-2.23	119.99	124.26
2	E	317	0PI	CB1-CA1-N1	2.22	115.60	110.58
2	E	317	0PI	C6-C7-C8	2.04	122.75	120.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

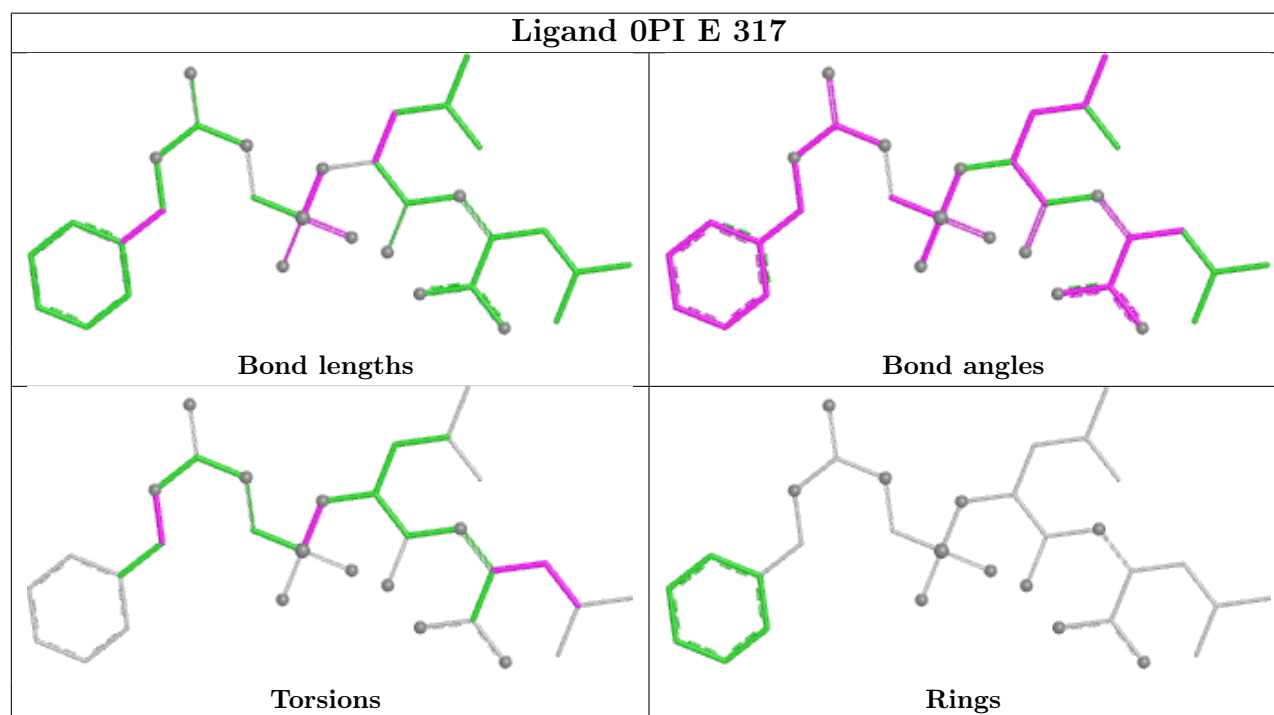
Mol	Chain	Res	Type	Atoms
2	E	317	0PI	CA-OS-P-O11
2	E	317	0PI	CA1-CB1-CG1-CD21
2	E	317	0PI	CA1-CB1-CG1-CD11
2	E	317	0PI	C3-C2-O2-C1
2	E	317	0PI	CC-CA1-CB1-CG1

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, 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%)	-0.64	1 (0%) 90 91	6, 12, 26, 36	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	316	LYS	2.4

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](#)

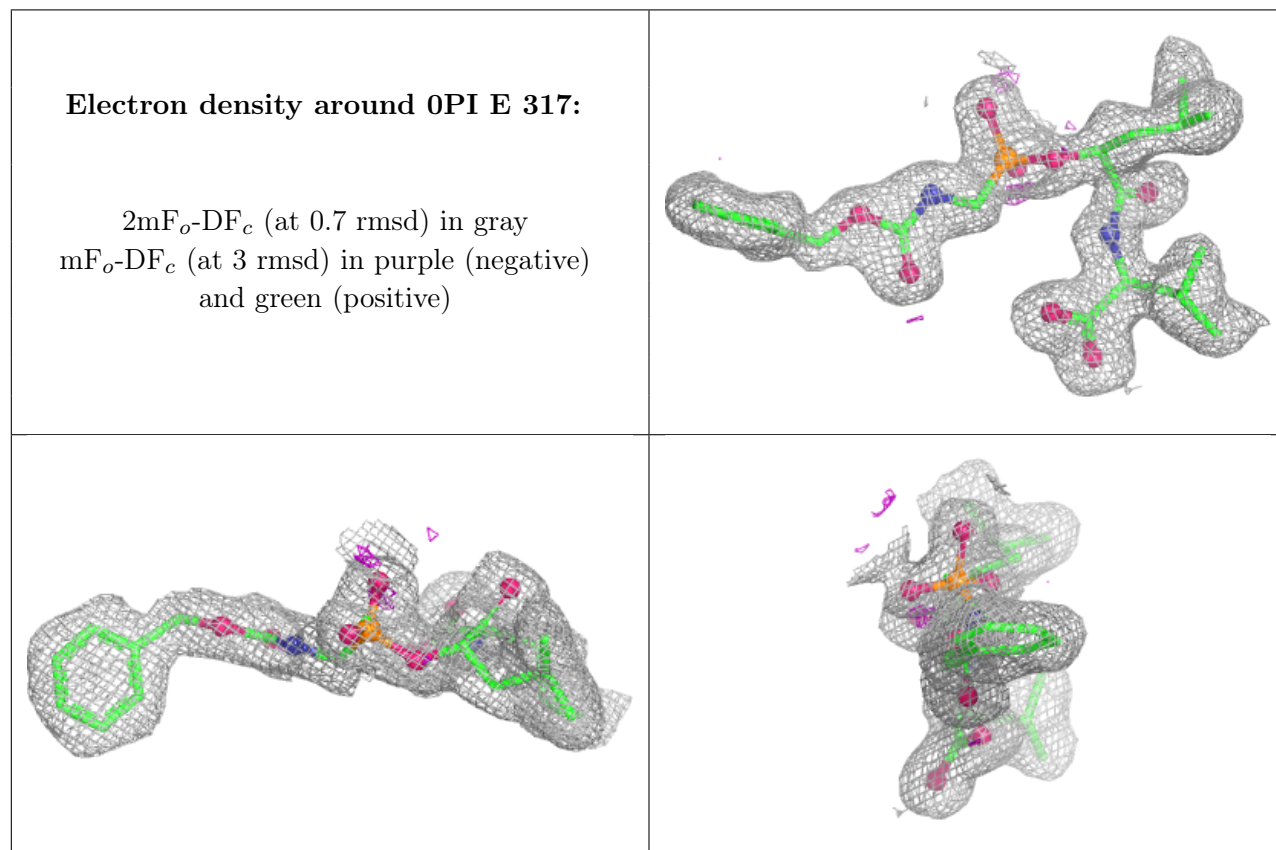
There are no oligosaccharides in this entry.

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
2	OPI	E	317	32/32	0.98	0.06	5,17,29,30	0
3	CA	E	321	1/1	0.98	0.03	16,16,16,16	0
3	CA	E	318	1/1	0.99	0.05	8,8,8,8	0
3	CA	E	320	1/1	1.00	0.01	11,11,11,11	0
3	CA	E	319	1/1	1.00	0.02	13,13,13,13	0
4	ZN	E	322	1/1	1.00	0.01	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.