



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:43 AM UTC

PDB ID : 4ER1 / pdb_00004er1
Title : THE ACTIVE SITE OF ASPARTIC PROTEINASES
Authors : Quail, J.W.; Cooper, J.B.; Szelke, M.; Blundell, T.L.
Deposited on : 1990-10-14
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

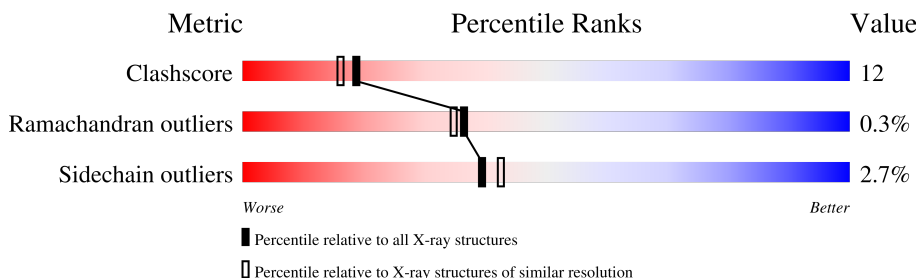
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0ZP	E	327	-	-	X	-

2 Entry composition [i](#)

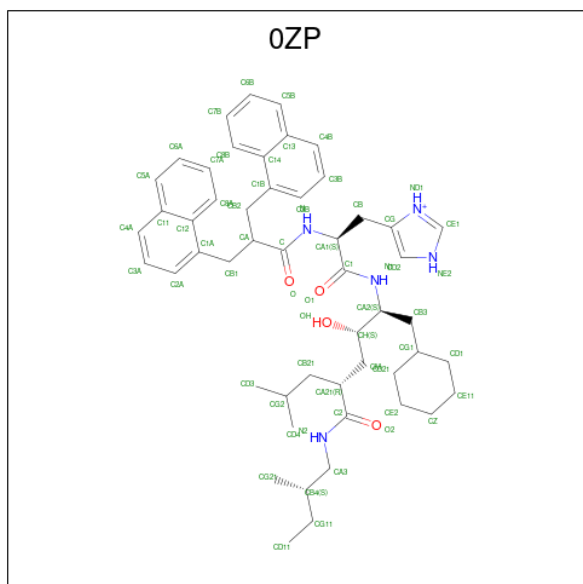
There are 3 unique types of molecules in this entry. The entry contains 2709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOTHAPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	330	Total	C	N	O	S	0	0	0
			2389	1514	366	507	2			

- Molecule 2 is N-[(1R,2R,4R)-1-(cyclohexylmethyl)-2-hydroxy-6-methyl-4-[(2R)-2-methylbutyl]carbonyl]heptyl]-3-(1H-imidazol-3-ium-4-yl)-N 2 -[3-naphthalen-1-yl-2-(naphthalen-1-ylmethyl)propanoyl]-L-alaninamide (CCD ID: 0ZP) (formula: C₅₁H₆₈N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			60	51	5	4		

- Molecule 3 is water.

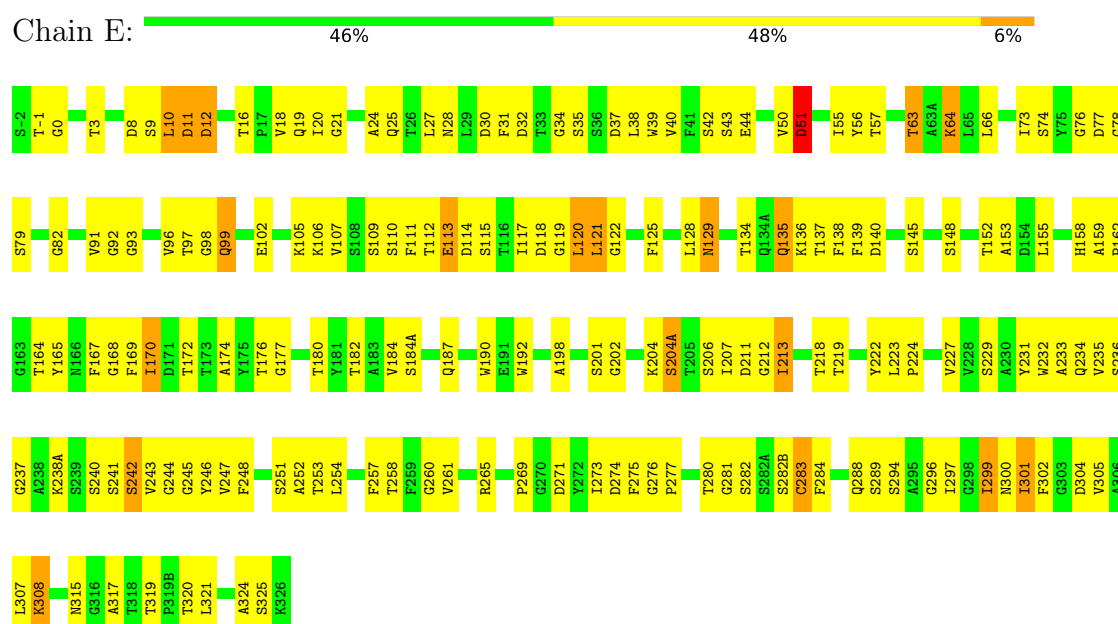
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	260	Total	O	0	0
			260	260		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: ENDOTHIAPEPSIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.10 Å 75.80 Å 43.00 Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.143 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2709	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0ZP

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	1.87	48/2445 (2.0%)	2.78	229/3345 (6.8%)

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 (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	GLU	C-N	-11.23	1.18	1.33
1	E	158	HIS	ND1-CE1	10.01	1.42	1.32
1	E	99	GLN	N-CA	9.78	1.58	1.46
1	E	51	ASP	CA-CB	8.86	1.66	1.52
1	E	55	ILE	C-N	8.51	1.45	1.33
1	E	237	GLY	N-CA	8.03	1.55	1.45
1	E	134	THR	N-CA	7.66	1.55	1.46
1	E	51	ASP	N-CA	7.61	1.57	1.46
1	E	19	GLN	CD-OE1	7.34	1.37	1.23
1	E	158	HIS	CD2-NE2	7.24	1.45	1.37
1	E	129	ASN	CG-OD1	7.03	1.36	1.23
1	E	92	GLY	N-CA	6.88	1.55	1.45
1	E	21	GLY	N-CA	6.87	1.51	1.45
1	E	245	GLY	N-CA	6.79	1.52	1.45
1	E	99	GLN	CD-OE1	6.52	1.35	1.23
1	E	187	GLN	CD-OE1	6.40	1.35	1.23
1	E	119	GLY	N-CA	6.38	1.53	1.45
1	E	294	SER	N-CA	6.37	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	260	GLY	N-CA	6.20	1.55	1.45
1	E	50	VAL	CA-C	6.17	1.60	1.52
1	E	271	ASP	N-CA	6.08	1.53	1.46
1	E	289	SER	N-CA	5.99	1.53	1.46
1	E	50	VAL	C-N	5.97	1.42	1.33
1	E	106	LYS	N-CA	5.86	1.53	1.45
1	E	300	ASN	CG-OD1	5.76	1.34	1.23
1	E	282	SER	N-CA	5.70	1.52	1.45
1	E	110	SER	CA-CB	5.69	1.62	1.53
1	E	121	LEU	N-CA	5.67	1.52	1.46
1	E	218	THR	N-CA	5.65	1.52	1.46
1	E	231	TYR	CA-CB	5.63	1.62	1.53
1	E	288	GLN	CD-OE1	5.57	1.34	1.23
1	E	162	PRO	N-CA	5.55	1.53	1.47
1	E	247	VAL	N-CA	5.50	1.52	1.46
1	E	98	GLY	N-CA	5.46	1.53	1.45
1	E	245	GLY	CA-C	-5.37	1.46	1.52
1	E	234	GLN	CD-OE1	5.30	1.33	1.23
1	E	201	SER	N-CA	5.29	1.52	1.46
1	E	37	ASP	CA-CB	5.28	1.62	1.53
1	E	190	TRP	NE1-CE2	-5.19	1.31	1.37
1	E	28	ASN	CA-CB	5.19	1.59	1.53
1	E	235	VAL	CA-CB	5.18	1.60	1.54
1	E	180	THR	N-CA	5.17	1.52	1.46
1	E	233	ALA	N-CA	5.14	1.53	1.46
1	E	212	GLY	CA-C	5.12	1.57	1.51
1	E	325	SER	N-CA	5.05	1.52	1.45
1	E	182	THR	N-CA	5.04	1.52	1.45
1	E	137	THR	N-CA	5.02	1.52	1.45
1	E	51	ASP	CB-CG	5.00	1.64	1.52

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ASP	CA-CB-CG	15.11	127.71	112.60
1	E	276	GLY	CA-C-N	-12.92	107.64	120.31
1	E	276	GLY	C-N-CA	-12.92	107.64	120.31
1	E	211	ASP	CA-CB-CG	-12.50	100.10	112.60
1	E	25	GLN	OE1-CD-NE2	-12.34	110.26	122.60
1	E	28	ASN	OD1-CG-ND2	-12.21	110.39	122.60
1	E	159	ALA	CA-C-N	-11.97	108.67	120.52
1	E	159	ALA	C-N-CA	-11.97	108.67	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	PHE	CA-CB-CG	-11.62	102.18	113.80
1	E	78	GLY	O-C-N	-11.00	110.22	122.65
1	E	275	PHE	CA-CB-CG	-10.67	103.13	113.80
1	E	21	GLY	CA-C-O	-9.35	115.13	122.52
1	E	165	TYR	CA-C-O	-9.28	110.31	120.43
1	E	25	GLN	CG-CD-NE2	9.27	130.31	116.40
1	E	40	VAL	CA-C-O	8.95	130.49	121.63
1	E	315	ASN	OD1-CG-ND2	-8.82	113.78	122.60
1	E	223	LEU	CA-C-N	-8.72	111.40	120.03
1	E	223	LEU	C-N-CA	-8.72	111.40	120.03
1	E	299	ILE	O-C-N	8.71	132.57	123.00
1	E	158	HIS	CA-CB-CG	-8.66	105.14	113.80
1	E	78	GLY	CA-C-O	8.65	128.52	119.27
1	E	176	THR	CA-C-O	-8.62	111.37	121.11
1	E	16	THR	O-C-N	8.58	130.95	121.94
1	E	122	GLY	CA-C-O	-8.55	113.78	121.64
1	E	254	LEU	CA-C-N	-8.36	112.25	120.52
1	E	254	LEU	C-N-CA	-8.36	112.25	120.52
1	E	300	ASN	OD1-CG-ND2	8.27	130.87	122.60
1	E	37	ASP	CA-CB-CG	-8.23	104.37	112.60
1	E	18	VAL	CA-CB-CG1	8.11	124.19	110.40
1	E	176	THR	CA-C-N	8.05	133.43	120.07
1	E	176	THR	C-N-CA	8.05	133.43	120.07
1	E	218	THR	O-C-N	-8.02	113.83	123.29
1	E	289	SER	CA-C-N	-7.97	109.41	122.65
1	E	289	SER	C-N-CA	-7.97	109.41	122.65
1	E	248	PHE	CA-C-N	-7.88	111.63	119.90
1	E	248	PHE	C-N-CA	-7.88	111.63	119.90
1	E	42	SER	CA-C-O	7.87	129.88	121.45
1	E	169	PHE	O-C-N	-7.82	115.05	123.42
1	E	135	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	E	302	PHE	CA-CB-CG	-7.76	106.04	113.80
1	E	118	ASP	O-C-N	7.70	131.97	122.34
1	E	113	GLU	CA-C-N	-7.63	112.36	123.05
1	E	113	GLU	C-N-CA	-7.63	112.36	123.05
1	E	187	GLN	N-CA-C	-7.60	103.08	112.88
1	E	320	THR	O-C-N	7.58	132.51	122.96
1	E	304	ASP	CA-CB-CG	-7.47	105.13	112.60
1	E	27	LEU	CA-C-O	-7.42	112.44	121.11
1	E	55	ILE	O-C-N	7.42	131.14	122.69
1	E	12	ASP	CA-CB-CG	-7.41	105.19	112.60
1	E	244	GLY	O-C-N	-7.40	113.79	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	235	VAL	N-CA-CB	-7.29	102.17	111.64
1	E	19	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	E	207	ILE	N-CA-CB	-7.23	102.79	111.90
1	E	248	PHE	O-C-N	7.16	126.88	121.65
1	E	20	ILE	CA-C-N	-7.12	110.61	122.43
1	E	20	ILE	C-N-CA	-7.12	110.61	122.43
1	E	55	ILE	CA-C-N	-7.10	112.19	122.19
1	E	55	ILE	C-N-CA	-7.10	112.19	122.19
1	E	106	LYS	CA-C-O	-7.09	112.84	121.06
1	E	107	VAL	CA-C-O	-7.09	113.77	121.28
1	E	114	ASP	CB-CA-C	-7.02	98.67	110.19
1	E	168	GLY	O-C-N	-6.99	114.28	122.60
1	E	66	LEU	CA-C-O	6.95	128.15	120.92
1	E	66	LEU	CA-C-N	6.95	130.99	121.05
1	E	66	LEU	C-N-CA	6.95	130.99	121.05
1	E	241	SER	CA-C-N	6.84	129.78	120.54
1	E	241	SER	C-N-CA	6.84	129.78	120.54
1	E	24	ALA	N-CA-CB	6.80	120.03	109.48
1	E	167	PHE	CA-C-N	-6.80	111.83	122.51
1	E	167	PHE	C-N-CA	-6.80	111.83	122.51
1	E	174	ALA	O-C-N	-6.76	112.39	122.39
1	E	204(A)	SER	O-C-N	-6.74	115.38	123.13
1	E	252	ALA	O-C-N	-6.69	114.97	122.86
1	E	136	LYS	CA-CB-CG	-6.67	100.77	114.10
1	E	140	ASP	CA-CB-CG	-6.65	105.95	112.60
1	E	78	GLY	N-CA-C	-6.64	106.79	114.69
1	E	232	TRP	N-CA-C	-6.64	105.14	113.18
1	E	319	THR	CA-C-O	-6.53	113.88	119.36
1	E	227	VAL	CA-C-N	-6.50	111.19	120.42
1	E	227	VAL	C-N-CA	-6.50	111.19	120.42
1	E	105	LYS	CA-CB-CG	-6.45	101.20	114.10
1	E	73	ILE	O-C-N	-6.41	116.14	123.07
1	E	140	ASP	N-CA-CB	-6.41	100.69	110.12
1	E	57	THR	CA-C-N	-6.36	113.08	119.56
1	E	57	THR	C-N-CA	-6.36	113.08	119.56
1	E	315	ASN	CB-CG-ND2	6.33	125.89	116.40
1	E	66	LEU	O-C-N	-6.31	114.66	122.68
1	E	145	SER	CA-C-O	-6.27	112.00	119.15
1	E	56	TYR	CG-CD1-CE1	-6.21	111.88	121.20
1	E	236	SER	CA-C-N	-6.20	111.66	122.83
1	E	236	SER	C-N-CA	-6.20	111.66	122.83
1	E	97	THR	CA-C-N	-6.17	110.02	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	97	THR	C-N-CA	-6.17	110.02	121.07
1	E	288	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	E	56	TYR	CB-CG-CD1	-6.16	111.57	120.80
1	E	93	GLY	O-C-N	-6.15	115.70	122.65
1	E	64	LYS	N-CA-CB	-6.15	100.12	111.13
1	E	213	ILE	O-C-N	6.15	129.49	123.03
1	E	74	SER	CA-CB-OG	-6.14	98.82	111.10
1	E	19	GLN	CG-CD-NE2	6.13	125.59	116.40
1	E	281	GLY	CA-C-O	6.12	125.77	119.10
1	E	118	ASP	CA-C-O	-6.12	112.19	119.35
1	E	242	SER	O-C-N	-6.11	115.74	122.09
1	E	167	PHE	CA-CB-CG	-6.10	107.70	113.80
1	E	219	THR	N-CA-CB	-6.04	101.20	110.20
1	E	202	GLY	CA-C-O	-6.03	116.25	122.28
1	E	107	VAL	CA-C-N	-6.02	111.93	121.86
1	E	107	VAL	C-N-CA	-6.02	111.93	121.86
1	E	296	GLY	O-C-N	-6.01	115.93	122.54
1	E	324	ALA	CA-C-O	-5.98	114.12	121.11
1	E	32	ASP	CA-CB-CG	-5.96	106.64	112.60
1	E	275	PHE	N-CA-CB	5.96	118.62	109.98
1	E	42	SER	O-C-N	-5.95	116.26	123.10
1	E	39	TRP	CA-C-N	-5.94	114.25	122.69
1	E	39	TRP	C-N-CA	-5.94	114.25	122.69
1	E	56	TYR	CD1-CE1-CZ	5.94	130.29	119.60
1	E	119	GLY	N-CA-C	-5.91	102.77	110.45
1	E	321	LEU	N-CA-CB	-5.91	101.17	110.69
1	E	164	THR	CA-C-O	-5.91	114.20	121.11
1	E	120	LEU	CA-C-N	-5.90	114.69	123.00
1	E	120	LEU	C-N-CA	-5.90	114.69	123.00
1	E	3	THR	O-C-N	5.90	130.00	123.16
1	E	222	TYR	O-C-N	5.90	130.11	123.27
1	E	240	SER	CA-CB-OG	-5.89	99.33	111.10
1	E	297	ILE	N-CA-CB	-5.88	104.23	112.35
1	E	11	ASP	CA-C-O	-5.87	114.30	121.28
1	E	102	GLU	CA-CB-CG	-5.87	102.37	114.10
1	E	152	THR	CA-C-O	-5.84	114.63	121.46
1	E	115	SER	N-CA-CB	-5.82	101.33	110.46
1	E	251	SER	CA-C-O	-5.81	111.50	119.05
1	E	91	VAL	CA-C-N	-5.80	109.31	120.80
1	E	91	VAL	C-N-CA	-5.80	109.31	120.80
1	E	243	VAL	N-CA-C	-5.79	104.89	113.39
1	E	37	ASP	OD1-CG-OD2	-5.77	109.06	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	ILE	N-CA-CB	-5.77	103.41	111.25
1	E	98	GLY	N-CA-C	-5.75	106.23	115.08
1	E	77	ASP	CA-C-N	-5.73	114.49	122.86
1	E	77	ASP	C-N-CA	-5.73	114.49	122.86
1	E	0	GLY	O-C-N	5.73	128.81	123.54
1	E	40	VAL	O-C-N	-5.72	116.55	123.02
1	E	271	ASP	CA-CB-CG	-5.71	106.89	112.60
1	E	121	LEU	N-CA-CB	-5.71	101.75	110.65
1	E	119	GLY	O-C-N	-5.69	117.77	124.15
1	E	275	PHE	CB-CG-CD1	-5.69	111.02	120.70
1	E	10	LEU	N-CA-C	5.69	120.21	113.16
1	E	206	SER	CA-CB-OG	-5.68	99.74	111.10
1	E	19	GLN	CA-C-N	-5.68	116.15	123.19
1	E	19	GLN	C-N-CA	-5.68	116.15	123.19
1	E	307	LEU	N-CA-C	5.67	117.47	111.28
1	E	233	ALA	O-C-N	-5.66	114.65	122.46
1	E	257	PHE	CZ-CE2-CD2	-5.63	109.86	120.00
1	E	43	SER	O-C-N	-5.60	114.98	122.43
1	E	105	LYS	CA-C-O	-5.59	113.20	119.79
1	E	139	PHE	CA-C-O	5.56	126.43	120.70
1	E	158	HIS	CB-CA-C	-5.56	103.68	111.80
1	E	34	GLY	O-C-N	-5.55	115.94	122.27
1	E	129	ASN	N-CA-C	5.54	118.27	110.23
1	E	288	GLN	CG-CD-NE2	5.54	124.71	116.40
1	E	153	ALA	CA-C-N	-5.52	114.74	123.24
1	E	153	ALA	C-N-CA	-5.52	114.74	123.24
1	E	301	ILE	O-C-N	5.50	128.88	122.99
1	E	284	PHE	CD1-CG-CD2	5.50	126.85	118.60
1	E	184	VAL	CA-CB-CG2	-5.50	101.06	110.40
1	E	76	GLY	N-CA-C	-5.49	106.01	113.37
1	E	134	THR	N-CA-CB	-5.43	102.04	110.57
1	E	79	SER	N-CA-C	-5.43	102.72	110.59
1	E	261	VAL	O-C-N	5.41	127.95	122.71
1	E	172	THR	O-C-N	-5.40	115.19	122.43
1	E	246	TYR	CA-C-O	5.38	126.83	120.69
1	E	31	PHE	CD1-CG-CD2	5.38	126.66	118.60
1	E	56	TYR	CB-CG-CD2	5.38	128.87	120.80
1	E	248	PHE	CA-C-O	-5.36	115.41	120.34
1	E	-1	THR	CA-C-N	-5.35	113.66	121.26
1	E	-1	THR	C-N-CA	-5.35	113.66	121.26
1	E	148	SER	N-CA-CB	-5.35	101.56	111.18
1	E	187	GLN	OE1-CD-NE2	-5.34	117.26	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	SER	N-CA-CB	-5.34	102.74	110.70
1	E	269	PRO	CA-C-N	-5.33	113.45	120.22
1	E	269	PRO	C-N-CA	-5.33	113.45	120.22
1	E	320	THR	CA-C-O	-5.33	115.54	121.51
1	E	110	SER	O-C-N	-5.33	116.47	122.12
1	E	117	ILE	N-CA-CB	-5.31	104.73	111.64
1	E	63	THR	O-C-N	-5.31	114.20	122.70
1	E	192	TRP	CZ3-CH2-CZ2	-5.31	114.60	121.50
1	E	235	VAL	CA-C-O	5.31	125.91	120.39
1	E	129	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	E	248	PHE	N-CA-C	5.31	114.41	108.25
1	E	244	GLY	CA-C-O	5.30	124.25	118.95
1	E	184(A)	SER	N-CA-CB	-5.28	101.44	110.16
1	E	235	VAL	O-C-N	-5.28	117.61	123.20
1	E	184(A)	SER	O-C-N	-5.27	117.21	123.22
1	E	111	PHE	CD1-CE1-CZ	5.27	129.48	120.00
1	E	99	GLN	CG-CD-NE2	5.26	124.30	116.40
1	E	27	LEU	O-C-N	5.26	129.71	123.24
1	E	308	LYS	CB-CG-CD	-5.26	99.20	111.30
1	E	9	SER	N-CA-C	-5.24	106.66	113.16
1	E	109	SER	CA-CB-OG	-5.24	100.62	111.10
1	E	82	GLY	CA-C-O	-5.23	116.91	121.04
1	E	110	SER	N-CA-CB	-5.17	102.52	110.12
1	E	304	ASP	CB-CA-C	-5.16	101.08	110.63
1	E	162	PRO	O-C-N	-5.15	116.86	123.04
1	E	224	PRO	N-CA-CB	-5.15	97.97	103.38
1	E	280	THR	O-C-N	-5.15	116.57	122.95
1	E	96	VAL	O-C-N	5.13	128.38	123.14
1	E	273	ILE	N-CA-C	-5.13	105.52	113.16
1	E	282(B)	SER	CA-CB-OG	-5.13	100.84	111.10
1	E	31	PHE	CG-CD2-CE2	-5.12	111.99	120.70
1	E	274	ASP	CA-C-O	5.12	126.50	120.98
1	E	129	ASN	CA-CB-CG	5.11	117.71	112.60
1	E	240	SER	CB-CA-C	-5.11	101.81	110.19
1	E	177	GLY	N-CA-C	-5.11	102.68	111.47
1	E	204(A)	SER	N-CA-C	-5.11	100.83	108.96
1	E	128	LEU	CA-C-N	-5.10	113.46	120.71
1	E	128	LEU	C-N-CA	-5.10	113.46	120.71
1	E	229	SER	CA-C-N	5.09	127.52	120.29
1	E	229	SER	C-N-CA	5.09	127.52	120.29
1	E	25	GLN	N-CA-CB	-5.09	102.58	110.57
1	E	158	HIS	CA-C-N	-5.09	114.12	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	158	HIS	C-N-CA	-5.09	114.12	122.26
1	E	271	ASP	CA-C-O	-5.08	114.35	120.10
1	E	238(A)	LYS	O-C-N	-5.08	117.46	123.25
1	E	319	THR	O-C-N	5.08	130.76	121.10
1	E	56	TYR	N-CA-CB	-5.05	101.83	110.16
1	E	283	CYS	N-CA-CB	-5.04	103.04	111.20
1	E	28	ASN	N-CA-CB	-5.03	102.08	110.37
1	E	253	THR	O-C-N	-5.02	116.29	122.82
1	E	92	GLY	N-CA-C	-5.02	107.16	114.90
1	E	99	GLN	O-C-N	-5.02	117.16	123.04
1	E	155	LEU	O-C-N	-5.02	117.44	123.06

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	265	ARG	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	2389	0	2280	25	0
2	E	60	0	67	40	0
3	E	260	0	0	1	0
All	All	2709	0	2347	57	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 12.

All (57) 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:327:0ZP:CD11	2:E:327:0ZP:HD3	0.97	1.14
2:E:327:0ZP:CD11	2:E:327:0ZP:HD21	0.97	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:327:0ZP:HD22	2:E:327:0ZP:CD21	0.97	1.14
1:E:213:ILE:HD11	2:E:327:0ZP:HD31	1.27	1.13
2:E:327:0ZP:CE11	2:E:327:0ZP:HE12	0.97	1.11
2:E:327:0ZP:CA21	2:E:327:0ZP:HA21	0.97	1.10
2:E:327:0ZP:CE11	2:E:327:0ZP:HE13	0.97	1.10
2:E:327:0ZP:C2	2:E:327:0ZP:CB21	2.25	1.05
2:E:327:0ZP:CD21	2:E:327:0ZP:HD23	0.97	1.05
2:E:327:0ZP:CD11	2:E:327:0ZP:HD11	0.97	1.04
2:E:327:0ZP:HA21	2:E:327:0ZP:C2	1.89	1.03
2:E:327:0ZP:C2	2:E:327:0ZP:CM	2.31	0.96
2:E:327:0ZP:HD23	2:E:327:0ZP:CG1	1.96	0.95
2:E:327:0ZP:HD22	2:E:327:0ZP:CG1	1.96	0.94
1:E:213:ILE:CD1	2:E:327:0ZP:HD31	2.01	0.90
2:E:327:0ZP:HA21	2:E:327:0ZP:CM	2.01	0.90
1:E:213:ILE:HD11	2:E:327:0ZP:CD3	2.02	0.88
2:E:327:0ZP:HA21	2:E:327:0ZP:CB21	2.04	0.88
2:E:327:0ZP:HE12	2:E:327:0ZP:HE13	1.56	0.86
2:E:327:0ZP:HD22	2:E:327:0ZP:HD23	1.56	0.86
2:E:327:0ZP:HE12	2:E:327:0ZP:CZ	2.06	0.85
2:E:327:0ZP:HD21	2:E:327:0ZP:HD11	1.58	0.85
2:E:327:0ZP:HE13	2:E:327:0ZP:CZ	2.07	0.85
2:E:327:0ZP:HD21	2:E:327:0ZP:CG11	2.06	0.84
2:E:327:0ZP:HE13	2:E:327:0ZP:CD1	2.07	0.84
2:E:327:0ZP:HD11	2:E:327:0ZP:CG11	2.06	0.84
2:E:327:0ZP:HD23	2:E:327:0ZP:CE2	2.07	0.84
2:E:327:0ZP:HD3	2:E:327:0ZP:HD11	1.58	0.84
2:E:327:0ZP:HD22	2:E:327:0ZP:CE2	2.07	0.84
2:E:327:0ZP:HD3	2:E:327:0ZP:CG11	2.06	0.84
2:E:327:0ZP:HE12	2:E:327:0ZP:CD1	2.07	0.83
2:E:327:0ZP:HD3	2:E:327:0ZP:HD21	1.58	0.82
1:E:299:ILE:HD12	1:E:301:ILE:HG12	1.66	0.75
1:E:12:ASP:HB3	2:E:327:0ZP:H3B	1.74	0.69
1:E:51:ASP:OD1	1:E:113:GLU:HA	1.93	0.69
1:E:299:ILE:HD12	1:E:301:ILE:CG1	2.26	0.66
1:E:299:ILE:CD1	1:E:301:ILE:HG12	2.29	0.63
1:E:129:ASN:ND2	1:E:135:GLN:H	1.97	0.62
2:E:327:0ZP:CB21	2:E:327:0ZP:CM	2.44	0.62
1:E:30:ASP:OD2	2:E:327:0ZP:HE23	2.02	0.59
1:E:51:ASP:CG	1:E:112:THR:O	2.48	0.56
1:E:299:ILE:HD11	1:E:301:ILE:HD11	1.89	0.54
2:E:327:0ZP:HA21	2:E:327:0ZP:N2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LEU:HD21	2:E:327:OZP:HD23	1.91	0.51
1:E:38:LEU:C	1:E:38:LEU:HD23	2.35	0.51
1:E:277:PRO:HA	1:E:283:CYS:HA	1.93	0.49
1:E:10:LEU:O	1:E:11:ASP:HB2	2.12	0.48
2:E:327:OZP:HA21	2:E:327:OZP:CG2	2.43	0.47
1:E:35:SER:HB3	2:E:327:OZP:HA11	1.96	0.46
1:E:305:VAL:HA	1:E:308:LYS:HE2	1.99	0.44
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.32	0.44
1:E:299:ILE:CD1	1:E:301:ILE:CG1	2.93	0.43
1:E:8:ASP:HB2	3:E:359:HOH:O	2.19	0.43
1:E:198:ALA:HB3	1:E:258:THR:HB	2.02	0.42
1:E:121:LEU:C	1:E:121:LEU:HD23	2.45	0.42
1:E:301:ILE:HD13	2:E:327:OZP:HD32	2.02	0.42
1:E:38:LEU:C	1:E:38:LEU:CD2	2.93	0.41

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	328/330 (99%)	325 (99%)	2 (1%)	1 (0%)	36 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	317	ALA

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	263/263 (100%)	256 (97%)	7 (3%)	39	42

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	51	ASP
1	E	63	THR
1	E	64	LYS
1	E	170	ILE
1	E	204	LYS
1	E	204(A)	SER
1	E	242	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	99	GLN
1	E	129	ASN
1	E	141	ASN
1	E	166	ASN
1	E	187	GLN
1	E	315	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	0ZP	E	327	-	65,65,65	1.85	6 (9%)	79,88,88	1.63	11 (13%)

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	0ZP	E	327	-	-	15/55/63/63	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	327	0ZP	CA21-C2	-11.28	1.32	1.51
2	E	327	0ZP	CD21-CG1	-3.74	1.41	1.52
2	E	327	0ZP	C1-N1	-3.65	1.26	1.34
2	E	327	0ZP	CB1-C1A	3.08	1.59	1.51
2	E	327	0ZP	C6B-C5B	2.49	1.42	1.36
2	E	327	0ZP	CB21-CA21	-2.41	1.48	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327	0ZP	CB-CA1-C1	-6.30	95.71	110.57
2	E	327	0ZP	C1B-C14-C13	-4.18	113.74	119.01
2	E	327	0ZP	CA1-CB-CG	3.85	122.78	113.75
2	E	327	0ZP	C1A-CB1-CA	-3.81	109.40	113.99
2	E	327	0ZP	C8B-C14-C13	3.72	122.73	117.92
2	E	327	0ZP	CB-CA1-N	3.65	117.60	110.64
2	E	327	0ZP	C5B-C13-C14	-3.06	115.18	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327	0ZP	C2B-C1B-C14	2.90	123.37	119.06
2	E	327	0ZP	CA-C-N	-2.88	111.22	116.19
2	E	327	0ZP	O-C-N	2.82	128.01	122.96
2	E	327	0ZP	CA21-CB21-CG2	-2.27	110.88	115.60

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	327	0ZP	CM-CA21-CB21-CG2
2	E	327	0ZP	C2-CA21-CB21-CG2
2	E	327	0ZP	CA3-CB4-CG11-CD11
2	E	327	0ZP	CA1-CB-CG-CD2
2	E	327	0ZP	CA1-CB-CG-ND1
2	E	327	0ZP	CB1-CA-CB2-C1B
2	E	327	0ZP	CG21-CB4-CG11-CD11
2	E	327	0ZP	N2-CA3-CB4-CG21
2	E	327	0ZP	N2-CA3-CB4-CG11
2	E	327	0ZP	CA21-CB21-CG2-CD3
2	E	327	0ZP	O-C-CA-CB1
2	E	327	0ZP	O1-C1-CA1-N
2	E	327	0ZP	CA21-CB21-CG2-CD4
2	E	327	0ZP	N1-C1-CA1-N
2	E	327	0ZP	O-C-CA-CB2

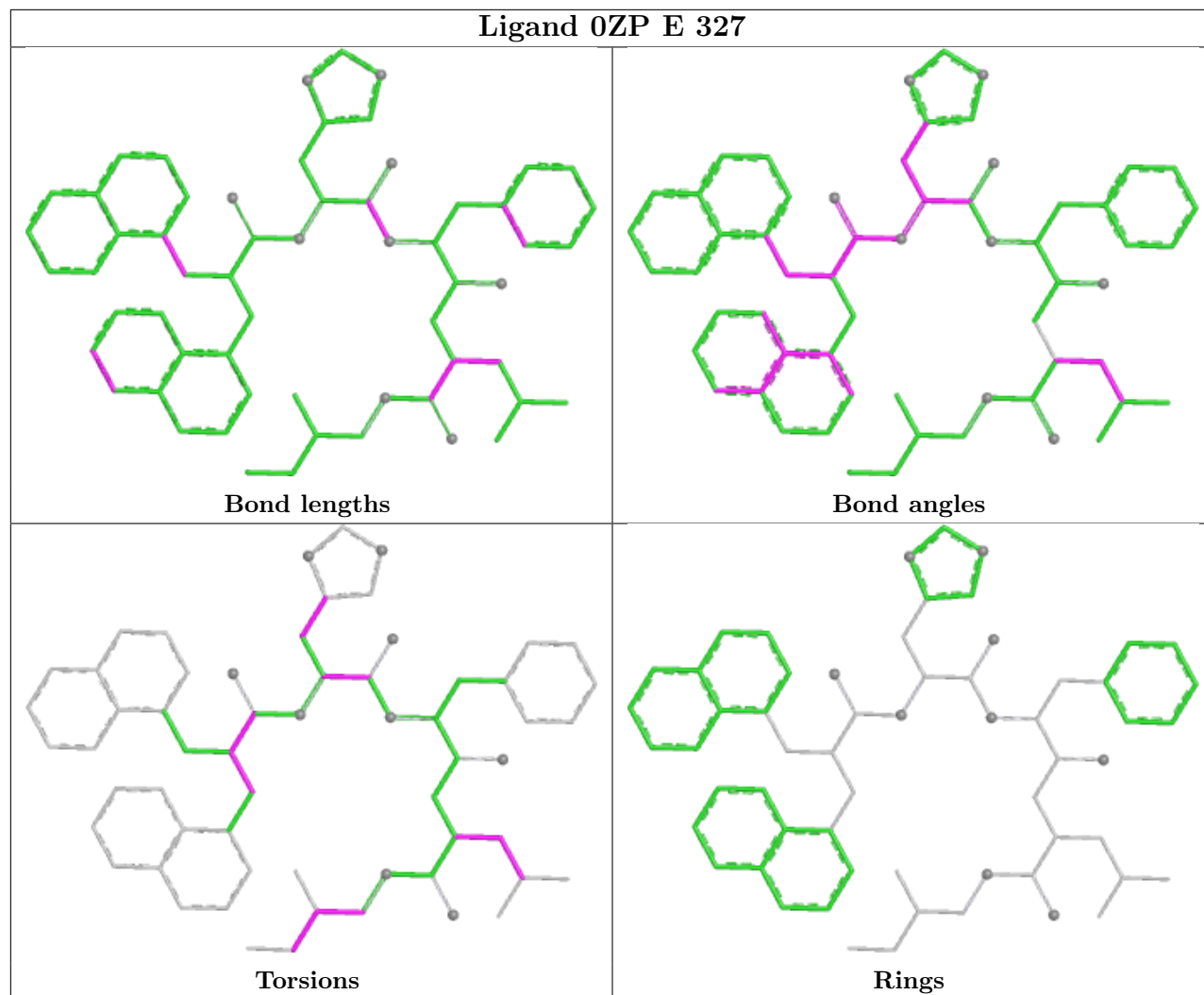
There are no ring outliers.

1 monomer is involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	327	0ZP	40	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	44:GLU	C	45:THR	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.