



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 07:00 PM EST

PDB ID : 4ER1  
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](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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

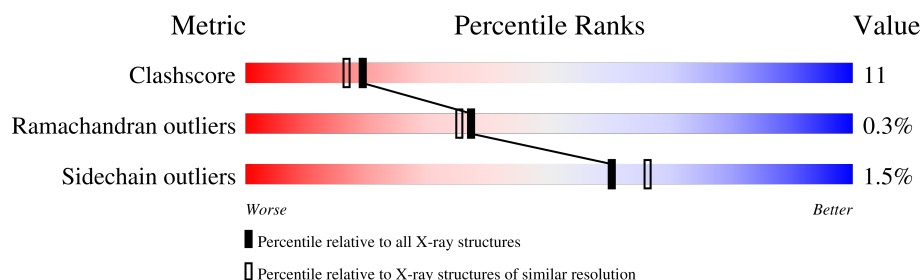
# 1 Overall quality at a glance

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	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (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  $\geq 3$ , 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  $\leq 5\%$ .

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](#)

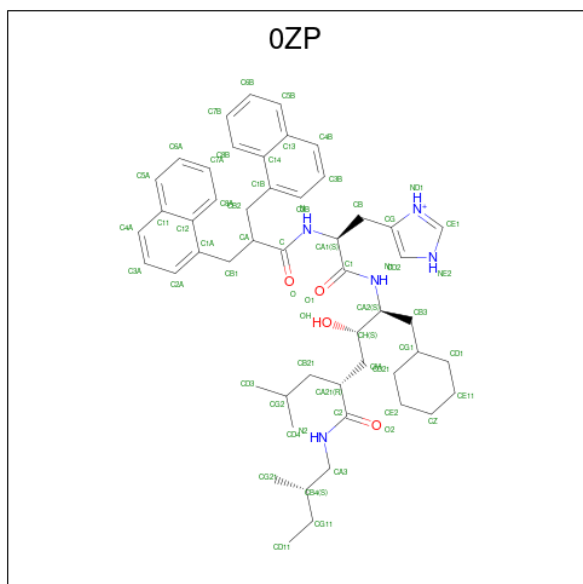
There are 3 unique types of molecules in this entry. The entry contains 2709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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}carbamoyl}heptyl]-3-(1H-imidazol-3-ium-4-yl)-N 2 -[3-naphthalen-1-yl-2-(naphthalen-1-ylmethyl)propanoyl]-L-alaninamide (three-letter code: 0ZP) (formula: C<sub>51</sub>H<sub>68</sub>N<sub>5</sub>O<sub>4</sub>).



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		

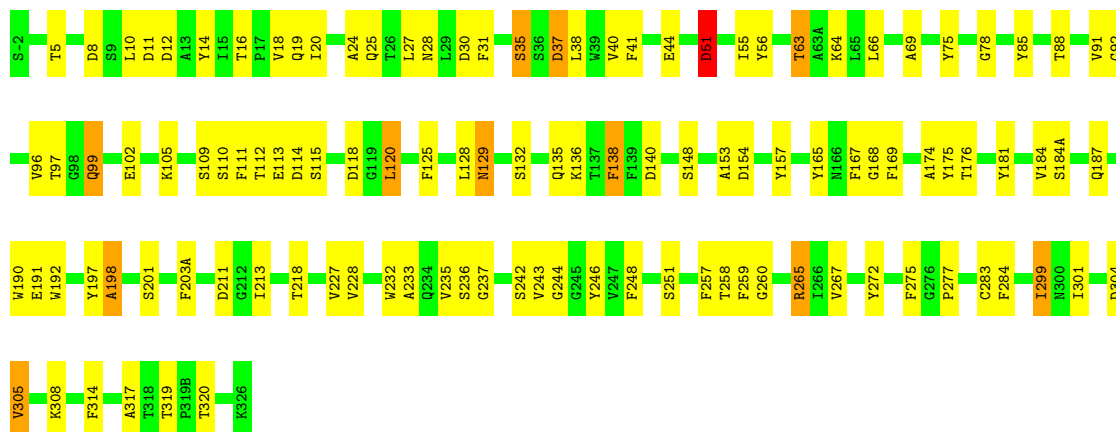
### 3 Residue-property plots [i](#)

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. 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: ENDOTHAPEPSIN

Chain E:  65% 31% .



## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	1.45	17/2445 (0.7%)	2.35	137/3345 (4.1%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	GLU	C-N	-6.70	1.18	1.34
1	E	260	GLY	N-CA	6.30	1.55	1.46
1	E	19	GLN	CD-OE1	6.16	1.37	1.24
1	E	110	SER	CA-CB	6.15	1.62	1.52
1	E	92	GLY	N-CA	6.12	1.55	1.46
1	E	51	ASP	CB-CG	6.10	1.64	1.51
1	E	237	GLY	N-CA	6.02	1.55	1.46
1	E	99	GLN	N-CA	5.96	1.58	1.46
1	E	129	ASN	CG-OD1	5.89	1.36	1.24
1	E	109	SER	CB-OG	5.53	1.49	1.42
1	E	99	GLN	CD-OE1	5.45	1.35	1.24
1	E	51	ASP	CA-CB	5.45	1.66	1.53
1	E	51	ASP	N-CA	5.40	1.57	1.46
1	E	187	GLN	CD-OE1	5.35	1.35	1.24
1	E	165	TYR	CB-CG	5.34	1.59	1.51
1	E	35	SER	CB-OG	5.09	1.48	1.42
1	E	55	ILE	C-N	5.01	1.45	1.34

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	56	TYR	CB-CG-CD1	-15.72	111.57	121.00
1	E	275	PHE	CB-CG-CD1	-13.97	111.02	120.80
1	E	56	TYR	CB-CG-CD2	13.11	128.87	121.00
1	E	246	TYR	CB-CG-CD1	-11.91	113.86	121.00
1	E	56	TYR	CG-CD1-CE1	-11.77	111.88	121.30
1	E	56	TYR	CD1-CE1-CZ	11.66	130.29	119.80
1	E	14	TYR	CB-CG-CD1	11.12	127.67	121.00
1	E	37	ASP	CB-CG-OD1	10.78	128.00	118.30
1	E	181	TYR	CB-CG-CD1	-10.59	114.64	121.00
1	E	248	PHE	CB-CG-CD2	-9.80	113.94	120.80
1	E	75	TYR	CB-CG-CD1	-9.80	115.12	121.00
1	E	44	GLU	OE1-CD-OE2	-9.14	112.33	123.30
1	E	275	PHE	CB-CG-CD2	9.07	127.15	120.80
1	E	154	ASP	CB-CG-OD2	9.01	126.41	118.30
1	E	51	ASP	CB-CG-OD2	8.90	126.31	118.30
1	E	18	VAL	CA-CB-CG1	8.86	124.19	110.90
1	E	14	TYR	CD1-CE1-CZ	8.54	127.49	119.80
1	E	257	PHE	CZ-CE2-CD2	-8.53	109.86	120.10
1	E	175	TYR	CB-CG-CD1	-8.45	115.93	121.00
1	E	191	GLU	OE1-CD-OE2	-8.13	113.55	123.30
1	E	31	PHE	CG-CD2-CE2	-8.01	111.99	120.80
1	E	111	PHE	CD1-CE1-CZ	7.82	129.48	120.10
1	E	78	GLY	O-C-N	-7.80	110.22	122.70
1	E	284	PHE	CB-CG-CD1	-7.74	115.38	120.80
1	E	284	PHE	CG-CD2-CE2	-7.55	112.49	120.80
1	E	37	ASP	OD1-CG-OD2	-7.50	109.06	123.30
1	E	31	PHE	CB-CG-CD1	-7.42	115.61	120.80
1	E	14	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	E	314	PHE	CB-CG-CD1	-7.35	115.66	120.80
1	E	140	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	E	75	TYR	CG-CD1-CE1	-7.10	115.62	121.30
1	E	24	ALA	N-CA-CB	7.09	120.03	110.10
1	E	169	PHE	CB-CG-CD1	6.97	125.68	120.80
1	E	157	TYR	CD1-CE1-CZ	-6.90	113.59	119.80
1	E	85	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	E	228	VAL	CG1-CB-CG2	-6.87	99.91	110.90
1	E	75	TYR	CD1-CG-CD2	6.82	125.40	117.90
1	E	169	PHE	CG-CD1-CE1	6.78	128.25	120.80
1	E	56	TYR	CG-CD2-CE2	6.76	126.71	121.30
1	E	120	LEU	CB-CG-CD1	6.72	122.43	111.00
1	E	259	PHE	CZ-CE2-CD2	-6.72	112.04	120.10
1	E	304	ASP	CB-CG-OD1	6.65	124.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	284	PHE	CD1-CG-CD2	6.58	126.85	118.30
1	E	305	VAL	CG1-CB-CG2	-6.56	100.40	110.90
1	E	184	VAL	CA-CB-CG2	-6.56	101.06	110.90
1	E	41	PHE	CG-CD2-CE2	6.53	127.98	120.80
1	E	125	PHE	CB-CG-CD1	-6.51	116.25	120.80
1	E	51	ASP	CA-CB-CG	6.50	127.71	113.40
1	E	174	ALA	O-C-N	-6.45	112.39	122.70
1	E	31	PHE	CD1-CG-CD2	6.43	126.66	118.30
1	E	304	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	E	157	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	E	265	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	E	175	TYR	CG-CD1-CE1	-6.24	116.31	121.30
1	E	91	VAL	C-N-CA	-6.18	109.31	122.30
1	E	299	ILE	O-C-N	6.17	132.57	122.70
1	E	320	THR	O-C-N	6.13	132.51	122.70
1	E	111	PHE	CG-CD2-CE2	6.12	127.54	120.80
1	E	115	SER	N-CA-CB	-6.12	101.33	110.50
1	E	85	TYR	CG-CD1-CE1	-6.05	116.46	121.30
1	E	211	ASP	CA-CB-CG	-6.04	100.10	113.40
1	E	184(A)	SER	N-CA-CB	-6.04	101.44	110.50
1	E	251	SER	CA-C-N	5.98	130.35	117.20
1	E	148	SER	N-CA-CB	-5.96	101.56	110.50
1	E	140	ASP	CB-CG-OD2	5.94	123.65	118.30
1	E	197	TYR	CG-CD2-CE2	-5.87	116.60	121.30
1	E	114	ASP	CB-CA-C	-5.86	98.67	110.40
1	E	97	THR	C-N-CA	-5.85	110.02	122.30
1	E	267	VAL	CA-CB-CG1	-5.85	102.13	110.90
1	E	96	VAL	CG1-CB-CG2	5.84	120.24	110.90
1	E	192	TRP	CZ3-CH2-CZ2	-5.83	114.60	121.60
1	E	64	LYS	N-CA-CB	-5.82	100.12	110.60
1	E	267	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	E	203(A)	PHE	CG-CD2-CE2	-5.80	114.42	120.80
1	E	243	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	E	167	PHE	CB-CG-CD1	5.76	124.83	120.80
1	E	136	LYS	CA-CB-CG	-5.74	100.77	113.40
1	E	128	LEU	CB-CG-CD1	-5.74	101.25	111.00
1	E	197	TYR	CZ-CE2-CD2	5.70	124.93	119.80
1	E	257	PHE	CB-CG-CD1	-5.67	116.83	120.80
1	E	25	GLN	CG-CD-NE2	5.67	130.31	116.70
1	E	248	PHE	CG-CD2-CE2	-5.67	114.57	120.80
1	E	190	TRP	CD1-CG-CD2	5.67	110.83	106.30
1	E	111	PHE	CB-CG-CD2	5.65	124.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	132	SER	N-CA-CB	-5.65	102.02	110.50
1	E	320	THR	CA-CB-CG2	-5.65	104.49	112.40
1	E	153	ALA	CB-CA-C	-5.64	101.64	110.10
1	E	197	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	E	169	PHE	CZ-CE2-CD2	5.61	126.83	120.10
1	E	20	ILE	C-N-CA	-5.57	110.61	122.30
1	E	218	THR	O-C-N	-5.55	113.83	122.70
1	E	105	LYS	CA-CB-CG	-5.54	101.20	113.40
1	E	154	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	E	138	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	E	244	GLY	O-C-N	-5.53	113.79	123.20
1	E	140	ASP	N-CA-CB	-5.50	100.69	110.60
1	E	284	PHE	CD1-CE1-CZ	-5.50	113.50	120.10
1	E	190	TRP	NE1-CE2-CZ2	-5.46	124.39	130.40
1	E	165	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	E	40	VAL	CA-CB-CG1	-5.44	102.75	110.90
1	E	56	TYR	CZ-CE2-CD2	-5.40	114.94	119.80
1	E	235	VAL	CG1-CB-CG2	-5.39	102.27	110.90
1	E	75	TYR	CG-CD2-CE2	-5.35	117.02	121.30
1	E	257	PHE	CG-CD2-CE2	5.34	126.67	120.80
1	E	69	ALA	N-CA-CB	-5.32	102.65	110.10
1	E	110	SER	N-CA-CB	-5.32	102.52	110.50
1	E	248	PHE	CD1-CG-CD2	5.32	125.21	118.30
1	E	63	THR	O-C-N	-5.31	114.20	122.70
1	E	176	THR	C-N-CA	5.30	133.43	122.30
1	E	190	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	E	55	ILE	O-C-N	5.28	131.14	122.70
1	E	44	GLU	CG-CD-OE2	5.28	128.85	118.30
1	E	168	GLY	O-C-N	-5.26	114.28	122.70
1	E	181	TYR	CG-CD2-CE2	-5.25	117.10	121.30
1	E	248	PHE	C-N-CD	5.22	139.36	128.40
1	E	16	THR	O-C-N	5.18	130.95	121.10
1	E	27	LEU	CB-CG-CD2	5.18	119.81	111.00
1	E	5	THR	CA-CB-CG2	-5.18	105.15	112.40
1	E	232	TRP	NE1-CE2-CZ2	-5.18	124.70	130.40
1	E	192	TRP	CB-CG-CD2	5.17	133.32	126.60
1	E	201	SER	N-CA-CB	-5.17	102.74	110.50
1	E	88	THR	CA-CB-CG2	-5.17	105.17	112.40
1	E	198	ALA	CB-CA-C	-5.16	102.36	110.10
1	E	118	ASP	O-C-N	5.16	131.97	123.20
1	E	37	ASP	CB-CG-OD2	5.15	122.94	118.30
1	E	227	VAL	CA-CB-CG2	5.14	118.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	157	TYR	CD1-CG-CD2	5.13	123.54	117.90
1	E	41	PHE	CB-CG-CD2	5.11	124.37	120.80
1	E	319	THR	O-C-N	5.08	130.76	121.10
1	E	236	SER	C-N-CA	-5.07	111.66	122.30
1	E	25	GLN	OE1-CD-NE2	-5.06	110.26	121.90
1	E	272	TYR	CB-CG-CD1	5.06	124.03	121.00
1	E	233	ALA	O-C-N	-5.03	114.65	122.70
1	E	233	ALA	CB-CA-C	-5.03	102.55	110.10
1	E	66	LEU	O-C-N	-5.02	114.66	122.70
1	E	102	GLU	CA-CB-CG	-5.01	102.37	113.40
1	E	28	ASN	OD1-CG-ND2	-5.00	110.39	121.90

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	2279	23	0
2	E	60	0	67	40	0
3	E	260	0	0	1	0
All	All	2709	0	2346	55	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 11.

All (55) 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:299:ILE:HD11	1:E:301:ILE:HD11	1.89	0.54
1:E:51:ASP:CG	1:E:112:THR:O	2.48	0.52
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: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:38:LEU:C	1:E:38:LEU:HD23	2.35	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:301:ILE:HD13	2:E:327:OZP:HD32	2.02	0.42

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%)	37	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%)	259 (98%)	4 (2%)	60	66

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	37	ASP
1	E	51	ASP
1	E	63	THR
1	E	242	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	28	ASN
1	E	99	GLN
1	E	129	ASN
1	E	134(A)	GLN
1	E	135	GLN
1	E	141	ASN
1	E	166	ASN
1	E	300	ASN

### 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](#)

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	-	61,65,65	1.91	6 (9%)	74,88,88	1.59	11 (14%)

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	-5.70	95.71	110.30
2	E	327	0ZP	C1B-C14-C13	-4.18	113.74	119.01
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	3.27	117.60	110.83
2	E	327	0ZP	C5B-C13-C14	-3.06	115.18	119.12
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	CD2-NE2-CE1	2.53	109.72	105.72
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:

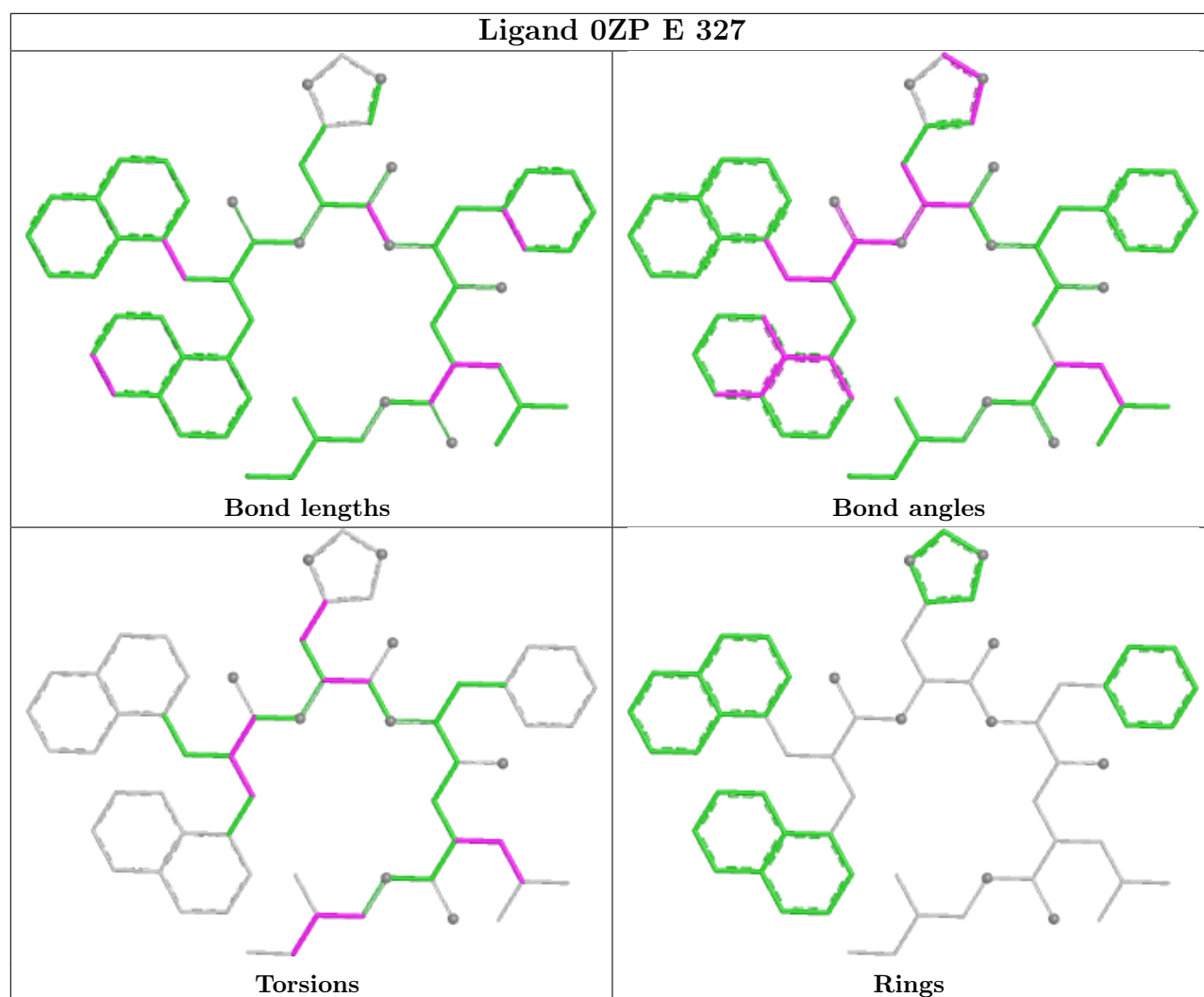
Mol	Chain	Res	Type	Atoms
2	E	327	0ZP	CA1-CB-CG-ND1
2	E	327	0ZP	CA1-CB-CG-CD2
2	E	327	0ZP	CM-CA21-CB21-CG2
2	E	327	0ZP	C2-CA21-CB21-CG2
2	E	327	0ZP	CA3-CB4-CG11-CD11
2	E	327	0ZP	CB1-CA-CB2-C1B
2	E	327	0ZP	CG21-CB4-CG11-CD11
2	E	327	0ZP	N2-CA3-CB4-CG21
2	E	327	0ZP	N2-CA3-CB4-CG11
2	E	327	0ZP	CA21-CB21-CG2-CD3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