



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:03 AM UTC

PDB ID : 1EPN / pdb_00001epn
Title : A STRUCTURAL COMPARISON OF 21 INHIBITOR COMPLEXES OF
THE ASPARTIC PROTEINASE FROM ENDOTHIA PARASITICA
Authors : Crawford, M.; Cooper, J.B.; Blundell, T.L.
Deposited on : 1994-07-27
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)	:	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

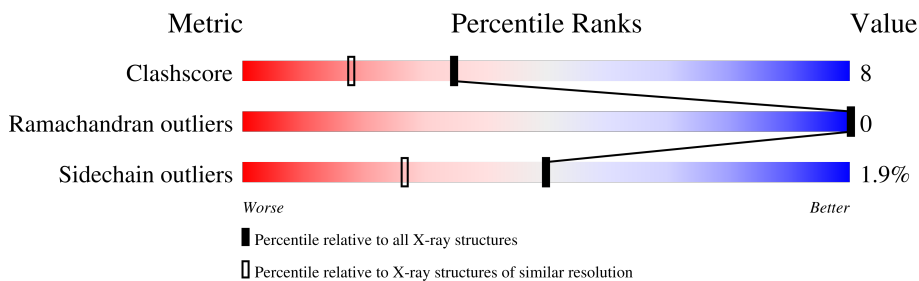
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)

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	

2 Entry composition [i](#)

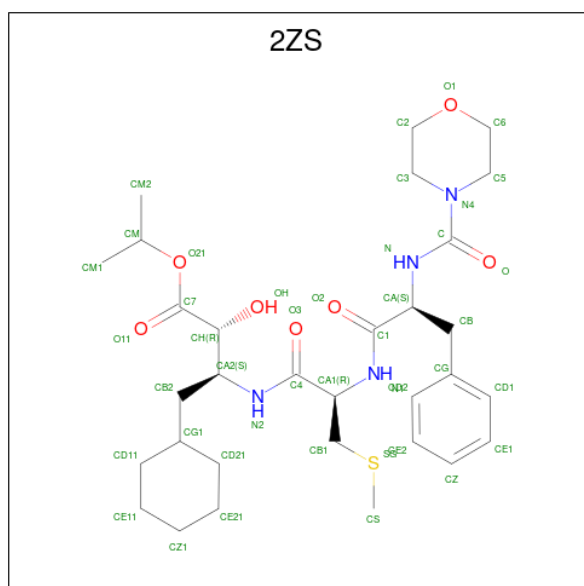
There are 4 unique types of molecules in this entry. The entry contains 2731 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-(morpholin-4-ylcarbonyl)-L-phenylalanyl-N-[(1R,2S)-1-(cyclohexylmethyl)-2-hydroxy-3-(1-methylethoxy)-3-oxopropyl]-S-methyl-L-cysteinamide (CCD ID: 2ZS) (formula: C₃₁H₄₈N₄O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	1
			46	33	4	7	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

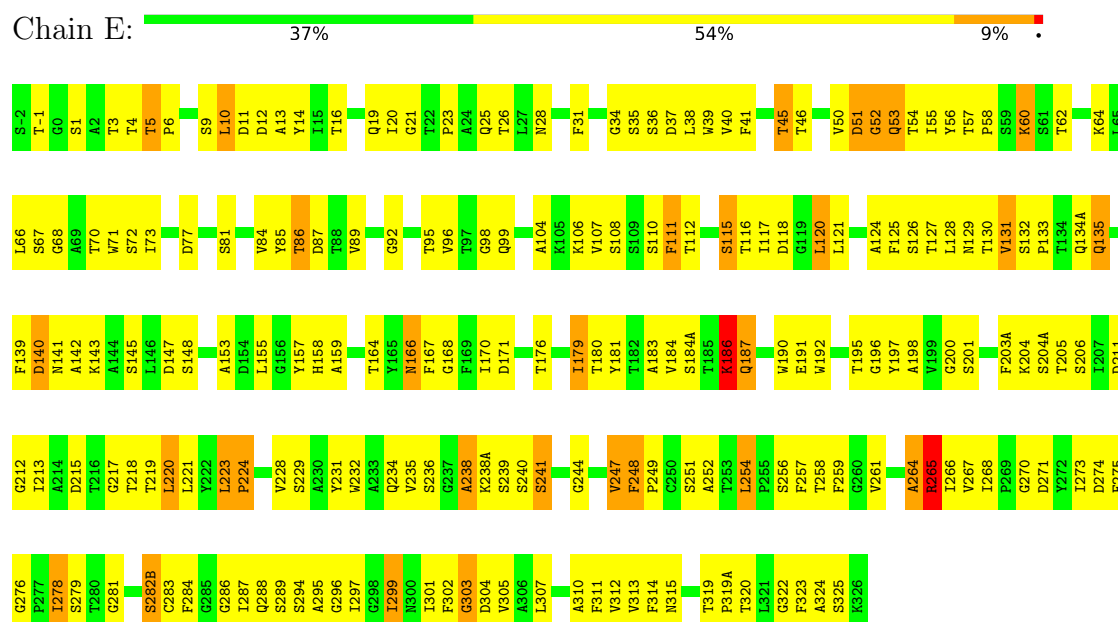
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	281	Total	O	0	0
			281	281		

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: ENDOTHAPEPSIN



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	43.11Å 76.08Å 42.99Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2731	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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: SO4, 2ZS

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	2.55	147/2445 (6.0%)	2.76	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	3

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	ASP	N-CA	12.84	1.62	1.46
1	E	6	PRO	C-N	12.29	1.48	1.34
1	E	34	GLY	CA-C	9.76	1.61	1.51
1	E	301	ILE	CA-CB	-9.73	1.41	1.53
1	E	132	SER	CA-C	9.63	1.62	1.52
1	E	294	SER	N-CA	9.54	1.58	1.46
1	E	275	PHE	N-CA	-9.14	1.35	1.46
1	E	73	ILE	N-CA	9.11	1.56	1.46
1	E	112	THR	C-O	-8.99	1.13	1.24
1	E	257	PHE	C-O	8.70	1.33	1.24
1	E	181	TYR	N-CA	8.57	1.55	1.45
1	E	196	GLY	N-CA	8.53	1.54	1.45
1	E	200	GLY	N-CA	8.52	1.57	1.45
1	E	325	SER	N-CA	8.51	1.56	1.45
1	E	204(A)	SER	N-CA	8.47	1.56	1.46
1	E	25	GLN	CD-OE1	8.46	1.39	1.23
1	E	131	VAL	N-CA	8.40	1.56	1.46
1	E	158	HIS	ND1-CE1	8.18	1.40	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	135	GLN	CD-OE1	8.13	1.39	1.23
1	E	142	ALA	CA-C	-8.10	1.41	1.52
1	E	223	LEU	C-O	-8.01	1.17	1.24
1	E	229	SER	C-O	7.90	1.34	1.24
1	E	313	VAL	N-CA	7.84	1.56	1.46
1	E	35	SER	N-CA	7.82	1.55	1.46
1	E	307	LEU	CA-C	7.65	1.63	1.52
1	E	95	THR	N-CA	7.49	1.55	1.46
1	E	258	THR	CA-C	7.46	1.61	1.52
1	E	96	VAL	N-CA	7.45	1.54	1.46
1	E	153	ALA	CA-C	7.41	1.61	1.52
1	E	110	SER	N-CA	7.34	1.55	1.46
1	E	284	PHE	N-CA	7.32	1.54	1.46
1	E	219	THR	N-CA	7.29	1.55	1.46
1	E	197	TYR	N-CA	7.27	1.55	1.45
1	E	267	VAL	CA-CB	7.24	1.62	1.54
1	E	312	VAL	N-CA	7.18	1.54	1.46
1	E	81	SER	N-CA	7.15	1.54	1.46
1	E	117	ILE	C-N	-7.10	1.23	1.33
1	E	204	LYS	N-CA	7.02	1.54	1.46
1	E	217	GLY	C-O	-7.00	1.17	1.24
1	E	84	VAL	N-CA	-6.99	1.38	1.46
1	E	55	ILE	N-CA	6.97	1.55	1.46
1	E	134(A)	GLN	CD-OE1	6.91	1.36	1.23
1	E	87	ASP	CA-C	6.88	1.60	1.52
1	E	179	ILE	N-CA	6.88	1.54	1.46
1	E	128	LEU	C-O	-6.83	1.15	1.24
1	E	267	VAL	N-CA	6.79	1.54	1.46
1	E	284	PHE	C-N	6.78	1.43	1.33
1	E	238(A)	LYS	CA-C	6.64	1.60	1.52
1	E	64	LYS	N-CA	6.63	1.54	1.46
1	E	13	ALA	C-O	6.60	1.31	1.23
1	E	28	ASN	CA-CB	6.58	1.62	1.53
1	E	319(A)	PRO	N-CA	6.57	1.54	1.46
1	E	166	ASN	CG-OD1	6.39	1.35	1.23
1	E	220	LEU	CA-C	-6.39	1.44	1.53
1	E	249	PRO	C-O	-6.39	1.16	1.23
1	E	288	GLN	CD-OE1	6.37	1.35	1.23
1	E	164	THR	CB-OG1	6.34	1.53	1.43
1	E	276	GLY	C-N	-6.33	1.25	1.33
1	E	5	THR	C-O	6.27	1.32	1.24
1	E	311	PHE	CA-C	6.17	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	201	SER	N-CA	6.17	1.53	1.46
1	E	186	LYS	CA-C	-6.16	1.44	1.52
1	E	299	ILE	CA-C	6.14	1.60	1.52
1	E	319	THR	N-CA	6.14	1.53	1.45
1	E	252	ALA	C-O	-6.13	1.16	1.23
1	E	303	GLY	N-CA	6.10	1.52	1.45
1	E	198	ALA	CA-C	-6.08	1.45	1.52
1	E	314	PHE	N-CA	6.04	1.54	1.46
1	E	142	ALA	C-N	6.02	1.41	1.33
1	E	282(B)	SER	C-O	-6.02	1.16	1.23
1	E	279	SER	N-CA	6.00	1.53	1.45
1	E	85	TYR	N-CA	5.99	1.53	1.45
1	E	118	ASP	N-CA	5.97	1.53	1.46
1	E	38	LEU	N-CA	5.97	1.53	1.46
1	E	167	PHE	N-CA	5.93	1.53	1.46
1	E	19	GLN	CD-OE1	5.93	1.34	1.23
1	E	134(A)	GLN	N-CA	5.92	1.53	1.45
1	E	319(A)	PRO	CA-CB	-5.91	1.45	1.53
1	E	236	SER	C-O	5.91	1.31	1.24
1	E	56	TYR	N-CA	5.88	1.53	1.46
1	E	240	SER	CA-C	5.88	1.59	1.52
1	E	278	ILE	N-CA	5.86	1.53	1.46
1	E	127	THR	CA-C	-5.86	1.44	1.52
1	E	256	SER	N-CA	5.84	1.53	1.45
1	E	71	TRP	CA-C	5.78	1.59	1.52
1	E	180	THR	CB-OG1	5.78	1.52	1.43
1	E	187	GLN	CD-OE1	5.76	1.34	1.23
1	E	307	LEU	CB-CG	5.76	1.65	1.53
1	E	35	SER	C-N	5.75	1.43	1.34
1	E	310	ALA	CA-C	5.74	1.59	1.52
1	E	322	GLY	N-CA	5.73	1.53	1.46
1	E	311	PHE	N-CA	5.71	1.53	1.46
1	E	158	HIS	CD2-NE2	5.70	1.44	1.37
1	E	224	PRO	N-CD	-5.68	1.39	1.47
1	E	234	GLN	CD-OE1	5.68	1.34	1.23
1	E	184(A)	SER	C-O	-5.67	1.17	1.23
1	E	314	PHE	C-N	-5.67	1.25	1.33
1	E	183	ALA	N-CA	5.65	1.53	1.45
1	E	70	THR	N-CA	5.60	1.53	1.45
1	E	274	ASP	C-O	-5.59	1.16	1.23
1	E	296	GLY	C-N	-5.58	1.26	1.33
1	E	26	THR	N-CA	5.57	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	238	ALA	N-CA	5.57	1.53	1.46
1	E	215	ASP	CA-CB	5.57	1.62	1.53
1	E	72	SER	N-CA	5.56	1.53	1.46
1	E	229	SER	N-CA	5.56	1.53	1.46
1	E	220	LEU	N-CA	5.54	1.52	1.45
1	E	270	GLY	CA-C	-5.50	1.45	1.52
1	E	191	GLU	C-O	-5.49	1.17	1.24
1	E	324	ALA	N-CA	5.49	1.52	1.45
1	E	106	LYS	CA-C	5.44	1.59	1.52
1	E	11	ASP	C-O	5.44	1.30	1.23
1	E	54	THR	N-CA	5.39	1.53	1.46
1	E	66	LEU	C-N	5.38	1.40	1.33
1	E	302	PHE	N-CA	5.37	1.53	1.46
1	E	111	PHE	N-CA	5.35	1.52	1.46
1	E	190	TRP	NE1-CE2	-5.35	1.31	1.37
1	E	187	GLN	C-O	-5.34	1.16	1.24
1	E	127	THR	C-N	5.33	1.41	1.33
1	E	247	VAL	N-CA	5.30	1.52	1.46
1	E	270	GLY	C-O	5.29	1.30	1.23
1	E	108	SER	N-CA	5.29	1.52	1.45
1	E	287	ILE	N-CA	5.28	1.52	1.46
1	E	115	SER	CA-C	-5.25	1.45	1.52
1	E	130	THR	CA-CB	-5.25	1.44	1.53
1	E	191	GLU	C-N	5.25	1.40	1.33
1	E	124	ALA	CA-C	5.24	1.60	1.53
1	E	212	GLY	CA-C	5.23	1.57	1.51
1	E	180	THR	CA-C	5.22	1.58	1.52
1	E	206	SER	C-O	5.22	1.30	1.24
1	E	213	ILE	C-O	-5.21	1.18	1.24
1	E	248	PHE	N-CA	5.21	1.50	1.45
1	E	53	GLN	CD-OE1	5.20	1.33	1.23
1	E	117	ILE	C-O	-5.15	1.18	1.24
1	E	231	TYR	C-O	5.12	1.29	1.24
1	E	236	SER	CA-CB	5.12	1.61	1.53
1	E	16	THR	CA-C	5.11	1.58	1.52
1	E	117	ILE	CA-CB	5.10	1.60	1.54
1	E	171	ASP	N-CA	5.06	1.53	1.46
1	E	320	THR	N-CA	5.04	1.52	1.45
1	E	28	ASN	CG-OD1	5.04	1.33	1.23
1	E	302	PHE	CA-C	5.03	1.59	1.52
1	E	218	THR	N-CA	5.01	1.52	1.46
1	E	201	SER	CB-OG	5.01	1.52	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	261	VAL	C-O	5.00	1.30	1.24
1	E	23	PRO	C-N	-5.00	1.26	1.33
1	E	271	ASP	CA-C	5.00	1.59	1.52

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	SER	O-C-N	13.56	139.61	122.93
1	E	51	ASP	CA-CB-CG	-12.12	100.48	112.60
1	E	66	LEU	CA-C-O	11.63	133.02	120.92
1	E	322	GLY	O-C-N	-10.73	111.69	123.49
1	E	239	SER	CA-C-O	10.68	132.86	120.69
1	E	284	PHE	CA-C-O	10.66	132.64	120.80
1	E	313	VAL	O-C-N	10.49	134.32	123.20
1	E	301	ILE	CA-C-O	-10.34	109.11	120.48
1	E	191	GLU	CA-C-O	9.95	131.27	120.43
1	E	16	THR	CA-C-O	-9.39	109.89	120.03
1	E	281	GLY	O-C-N	-8.83	111.18	122.39
1	E	187	GLN	OE1-CD-NE2	-8.80	113.80	122.60
1	E	67	SER	CA-C-N	-8.77	108.26	122.20
1	E	67	SER	C-N-CA	-8.77	108.26	122.20
1	E	268	ILE	O-C-N	8.65	130.97	121.10
1	E	125	PHE	CA-CB-CG	-8.64	105.16	113.80
1	E	244	GLY	CA-C-O	8.63	128.70	118.86
1	E	258	THR	O-C-N	8.60	133.44	123.29
1	E	266	ILE	CA-C-O	-8.57	111.36	120.53
1	E	92	GLY	O-C-N	8.30	131.37	122.41
1	E	135	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	E	265	ARG	CD-NE-CZ	8.27	135.98	124.40
1	E	299	ILE	O-C-N	8.20	132.02	123.00
1	E	45	THR	OG1-CB-CG2	-8.07	93.16	109.30
1	E	267	VAL	O-C-N	-8.03	114.75	123.18
1	E	60	LYS	O-C-N	-8.01	112.73	122.34
1	E	323	PHE	CE1-CZ-CE2	7.98	134.36	120.00
1	E	307	LEU	N-CA-C	-7.92	102.25	112.23
1	E	13	ALA	CA-C-O	-7.80	112.88	121.23
1	E	87	ASP	O-C-N	-7.75	115.54	123.29
1	E	281	GLY	CA-C-O	7.73	127.60	119.02
1	E	127	THR	O-C-N	-7.68	112.41	122.39
1	E	139	PHE	CA-CB-CG	7.67	121.47	113.80
1	E	241	SER	CA-C-O	7.62	128.50	120.42
1	E	322	GLY	CA-C-O	7.60	128.09	120.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	289	SER	O-C-N	7.58	131.95	123.01
1	E	319	THR	CA-C-O	-7.56	113.01	119.36
1	E	25	GLN	OE1-CD-NE2	-7.48	115.12	122.60
1	E	116	THR	CA-C-N	-7.43	113.21	123.10
1	E	116	THR	C-N-CA	-7.43	113.21	123.10
1	E	258	THR	CA-C-O	-7.41	112.31	120.38
1	E	180	THR	O-C-N	7.36	131.97	123.29
1	E	264	ALA	O-C-N	-7.30	114.53	122.85
1	E	195	THR	CA-C-N	-7.29	112.36	121.83
1	E	195	THR	C-N-CA	-7.29	112.36	121.83
1	E	310	ALA	CA-C-N	-7.26	112.70	122.72
1	E	310	ALA	C-N-CA	-7.26	112.70	122.72
1	E	267	VAL	N-CA-CB	-7.25	101.40	111.25
1	E	20	ILE	CA-C-N	-7.24	110.42	122.43
1	E	20	ILE	C-N-CA	-7.24	110.42	122.43
1	E	112	THR	O-C-N	7.22	129.78	122.12
1	E	133	PRO	CA-N-CD	7.22	121.61	111.50
1	E	249	PRO	CA-N-CD	7.12	121.97	112.00
1	E	84	VAL	N-CA-C	7.11	118.36	108.12
1	E	301	ILE	O-C-N	7.09	130.58	122.99
1	E	155	LEU	CA-C-N	-7.05	113.91	122.15
1	E	155	LEU	C-N-CA	-7.05	113.91	122.15
1	E	34	GLY	N-CA-C	-7.03	103.57	115.80
1	E	121	LEU	CA-C-N	-7.02	114.76	121.57
1	E	121	LEU	C-N-CA	-7.02	114.76	121.57
1	E	131	VAL	O-C-N	7.01	131.22	122.59
1	E	60	LYS	CA-C-O	6.97	127.72	119.56
1	E	204	LYS	O-C-N	6.97	133.84	122.70
1	E	164	THR	O-C-N	6.96	131.75	123.33
1	E	140	ASP	O-C-N	-6.93	114.77	122.12
1	E	192	TRP	CE2-CD2-CE3	6.92	125.72	118.80
1	E	13	ALA	CA-C-N	6.90	132.94	122.93
1	E	13	ALA	C-N-CA	6.90	132.94	122.93
1	E	145	SER	CA-C-O	-6.88	111.31	119.15
1	E	267	VAL	CA-C-O	6.86	127.75	120.48
1	E	134(A)	GLN	CG-CD-NE2	6.84	126.66	116.40
1	E	204	LYS	CA-CB-CG	-6.81	100.47	114.10
1	E	313	VAL	CA-C-N	-6.80	114.00	122.84
1	E	313	VAL	C-N-CA	-6.80	114.00	122.84
1	E	311	PHE	CA-C-N	-6.78	113.52	122.94
1	E	311	PHE	C-N-CA	-6.78	113.52	122.94
1	E	111	PHE	O-C-N	-6.77	114.43	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	ILE	O-C-N	-6.72	115.04	122.83
1	E	254	LEU	CA-C-O	-6.70	114.57	120.60
1	E	315	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	E	191	GLU	O-C-N	-6.66	115.75	123.27
1	E	16	THR	O-C-N	6.62	128.89	121.94
1	E	72	SER	CA-C-N	-6.58	112.28	122.68
1	E	72	SER	C-N-CA	-6.58	112.28	122.68
1	E	325	SER	N-CA-CB	-6.57	100.46	110.45
1	E	37	ASP	CA-C-N	-6.54	114.33	122.84
1	E	37	ASP	C-N-CA	-6.54	114.33	122.84
1	E	268	ILE	CA-C-N	-6.50	113.08	119.78
1	E	268	ILE	C-N-CA	-6.50	113.08	119.78
1	E	53	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	E	120	LEU	CD1-CG-CD2	6.45	124.98	110.80
1	E	240	SER	CA-C-O	-6.42	113.26	120.32
1	E	259	PHE	CA-CB-CG	6.40	120.20	113.80
1	E	134(A)	GLN	CG-CD-OE1	-6.38	108.03	120.80
1	E	159	ALA	CA-C-O	-6.35	114.23	120.26
1	E	257	PHE	CZ-CE2-CD2	-6.34	108.58	120.00
1	E	64	LYS	O-C-N	-6.33	115.77	123.30
1	E	239	SER	O-C-N	-6.30	115.67	123.04
1	E	204(A)	SER	CA-C-N	-6.27	110.90	121.94
1	E	204(A)	SER	C-N-CA	-6.27	110.90	121.94
1	E	5	THR	O-C-N	-6.26	115.78	121.66
1	E	31	PHE	CA-CB-CG	-6.26	107.54	113.80
1	E	270	GLY	O-C-N	-6.26	115.61	122.24
1	E	45	THR	CA-C-O	6.21	128.13	121.05
1	E	143	LYS	O-C-N	-6.19	115.55	122.12
1	E	117	ILE	CB-CA-C	-6.18	102.00	110.77
1	E	135	GLN	CG-CD-NE2	6.16	125.64	116.40
1	E	195	THR	CA-C-O	-6.16	111.83	119.28
1	E	220	LEU	CD1-CG-CD2	6.14	124.31	110.80
1	E	107	VAL	CA-CB-CG2	6.12	120.81	110.40
1	E	171	ASP	CA-CB-CG	-6.12	106.48	112.60
1	E	275	PHE	CB-CG-CD1	-6.09	110.35	120.70
1	E	95	THR	O-C-N	6.08	130.47	123.29
1	E	77	ASP	O-C-N	6.08	129.64	122.34
1	E	295	ALA	CA-C-O	-6.07	114.12	120.55
1	E	68	GLY	N-CA-C	6.04	123.06	115.21
1	E	71	TRP	CE2-CD2-CE3	6.04	124.84	118.80
1	E	238(A)	LYS	CB-CG-CD	6.03	125.18	111.30
1	E	212	GLY	CA-C-O	-6.01	115.29	121.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	SER	CA-C-O	-6.00	113.91	120.81
1	E	106	LYS	CA-C-O	-5.98	114.30	120.99
1	E	275	PHE	O-C-N	5.98	128.54	122.09
1	E	286	GLY	N-CA-C	-5.97	106.34	115.66
1	E	86	THR	CA-C-N	-5.97	110.99	122.09
1	E	86	THR	C-N-CA	-5.97	110.99	122.09
1	E	50	VAL	CA-CB-CG2	5.95	120.51	110.40
1	E	3	THR	CA-C-O	-5.94	113.98	120.81
1	E	197	TYR	CB-CG-CD2	-5.94	111.89	120.80
1	E	257	PHE	CA-C-O	-5.92	113.75	120.32
1	E	319	THR	CB-CA-C	5.90	116.01	110.17
1	E	125	PHE	CA-C-O	5.89	128.43	121.36
1	E	167	PHE	O-C-N	5.86	130.16	123.31
1	E	190	TRP	CE2-CD2-CG	-5.85	100.18	107.20
1	E	139	PHE	CA-C-N	-5.85	112.44	120.28
1	E	139	PHE	C-N-CA	-5.85	112.44	120.28
1	E	297	ILE	CA-C-O	5.85	126.97	120.71
1	E	249	PRO	N-CA-CB	-5.84	97.91	103.34
1	E	236	SER	N-CA-C	5.80	118.55	111.82
1	E	296	GLY	O-C-N	-5.80	114.51	122.68
1	E	273	ILE	CB-CG1-CD1	5.78	125.93	113.80
1	E	21	GLY	O-C-N	-5.76	115.73	122.87
1	E	268	ILE	CA-C-O	-5.76	112.23	119.95
1	E	249	PRO	N-CD-CG	-5.75	94.57	103.20
1	E	157	TYR	CG-CD2-CE2	-5.72	112.63	121.20
1	E	106	LYS	O-C-N	5.71	129.78	123.33
1	E	275	PHE	N-CA-C	5.71	117.30	111.14
1	E	221	LEU	CA-C-N	-5.68	115.10	123.05
1	E	221	LEU	C-N-CA	-5.68	115.10	123.05
1	E	9	SER	CA-C-O	-5.67	111.68	119.05
1	E	187	GLN	CA-C-N	-5.67	111.79	122.05
1	E	187	GLN	C-N-CA	-5.67	111.79	122.05
1	E	133	PRO	CA-C-N	-5.65	115.20	123.00
1	E	133	PRO	C-N-CA	-5.65	115.20	123.00
1	E	10	LEU	CA-C-O	-5.65	112.95	119.56
1	E	184	VAL	O-C-N	5.64	131.72	122.70
1	E	-1	THR	O-C-N	-5.63	116.35	123.17
1	E	41	PHE	CA-C-O	5.62	127.51	121.44
1	E	89	VAL	CA-C-N	-5.60	113.66	122.73
1	E	89	VAL	C-N-CA	-5.60	113.66	122.73
1	E	21	GLY	CA-C-O	5.58	126.93	122.52
1	E	36	SER	CA-C-O	-5.57	114.64	120.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	ILE	N-CA-CB	-5.57	102.87	110.56
1	E	56	TYR	N-CA-CB	-5.54	101.26	110.23
1	E	157	TYR	CZ-CE2-CD2	5.51	129.53	119.60
1	E	294	SER	CA-C-O	-5.50	113.12	119.56
1	E	265	ARG	CA-CB-CG	-5.49	103.11	114.10
1	E	54	THR	CA-C-O	-5.49	114.34	120.54
1	E	159	ALA	CA-C-N	-5.48	114.95	120.21
1	E	159	ALA	C-N-CA	-5.48	114.95	120.21
1	E	35	SER	CA-C-N	-5.48	111.18	121.81
1	E	35	SER	C-N-CA	-5.48	111.18	121.81
1	E	81	SER	CA-C-O	5.46	127.07	121.23
1	E	203(A)	PHE	CA-CB-CG	-5.43	108.37	113.80
1	E	176	THR	CA-C-O	5.41	127.79	121.46
1	E	323	PHE	CZ-CE2-CD2	-5.37	110.33	120.00
1	E	229	SER	N-CA-C	-5.37	105.60	111.82
1	E	206	SER	O-C-N	-5.36	116.43	123.02
1	E	73	ILE	O-C-N	5.35	128.98	123.04
1	E	25	GLN	CG-CD-NE2	5.34	124.41	116.40
1	E	197	TYR	CG-CD2-CE2	-5.33	113.21	121.20
1	E	164	THR	CA-C-O	-5.30	114.23	120.60
1	E	235	VAL	O-C-N	-5.28	117.34	122.99
1	E	23	PRO	CA-N-CD	5.27	118.88	111.50
1	E	168	GLY	CA-C-O	5.27	124.98	119.07
1	E	31	PHE	CE1-CZ-CE2	5.27	129.48	120.00
1	E	304	ASP	OD1-CG-OD2	5.27	135.54	122.90
1	E	62	THR	CA-C-N	-5.25	114.24	122.65
1	E	62	THR	C-N-CA	-5.25	114.24	122.65
1	E	36	SER	N-CA-C	-5.25	104.68	111.71
1	E	170	ILE	O-C-N	5.24	129.24	123.10
1	E	305	VAL	CA-CB-CG2	5.24	119.31	110.40
1	E	104	ALA	CA-C-O	5.22	126.65	120.69
1	E	179	ILE	CA-C-O	5.21	127.63	121.02
1	E	294	SER	N-CA-C	-5.20	106.52	112.92
1	E	211	ASP	OD1-CG-OD2	5.20	135.38	122.90
1	E	302	PHE	CA-C-N	5.20	129.13	121.96
1	E	302	PHE	C-N-CA	5.20	129.13	121.96
1	E	37	ASP	O-C-N	5.19	129.48	123.30
1	E	228	VAL	CA-C-O	5.19	125.85	120.25
1	E	284	PHE	N-CA-CB	-5.18	101.97	110.52
1	E	206	SER	CA-C-O	5.18	126.50	120.49
1	E	141	ASN	CA-CB-CG	5.17	117.77	112.60
1	E	238	ALA	O-C-N	-5.16	114.44	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	107	VAL	CA-C-N	-5.15	111.78	121.66
1	E	107	VAL	C-N-CA	-5.15	111.78	121.66
1	E	251	SER	O-C-N	-5.14	115.54	122.43
1	E	203(A)	PHE	CE1-CZ-CE2	5.14	129.25	120.00
1	E	257	PHE	CA-CB-CG	-5.14	108.66	113.80
1	E	166	ASN	O-C-N	5.13	129.87	123.19
1	E	275	PHE	CZ-CE2-CD2	-5.13	110.76	120.00
1	E	40	VAL	CA-CB-CG2	5.13	119.12	110.40
1	E	232	TRP	CZ3-CH2-CZ2	-5.13	114.83	121.50
1	E	239	SER	CA-CB-OG	-5.12	100.87	111.10
1	E	77	ASP	CA-CB-CG	5.11	117.71	112.60
1	E	54	THR	CA-C-N	-5.08	115.13	122.45
1	E	54	THR	C-N-CA	-5.08	115.13	122.45
1	E	145	SER	N-CA-C	-5.08	107.13	113.38
1	E	58	PRO	CA-CB-CG	5.08	114.14	104.50
1	E	39	TRP	CE3-CZ3-CH2	-5.07	114.50	121.10
1	E	57	THR	CA-C-O	5.06	125.05	120.09
1	E	283	CYS	N-CA-CB	-5.05	102.76	111.55
1	E	204	LYS	N-CA-CB	-5.04	102.65	110.57
1	E	39	TRP	O-C-N	-5.04	117.42	123.27
1	E	35	SER	N-CA-CB	-5.04	103.28	111.24
1	E	117	ILE	CA-CB-CG2	-5.03	101.95	110.50
1	E	180	THR	CA-CB-OG1	-5.02	102.07	109.60
1	E	98	GLY	CA-C-N	-5.01	114.25	121.42
1	E	98	GLY	C-N-CA	-5.01	114.25	121.42
1	E	159	ALA	O-C-N	5.01	126.27	121.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	LEU	Mainchain
1	E	265	ARG	Sidechain
1	E	52	GLY	Peptide

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	36	1
2	E	46	0	11	0	0
3	E	15	0	0	1	0
4	E	281	0	0	3	0
All	All	2731	0	2291	36	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ASP:O	1:E:53:GLN:OE1	1.75	1.04
1:E:51:ASP:C	1:E:51:ASP:OD1	2.06	0.97
1:E:187:GLN:NE2	4:E:607:HOH:O	2.22	0.72
1:E:5:THR:HG23	4:E:357:HOH:O	1.89	0.71
1:E:205:THR:O	1:E:205:THR:HG23	1.90	0.71
1:E:51:ASP:O	1:E:51:ASP:OD1	2.13	0.65
1:E:179:ILE:N	3:E:329:SO4:O2	2.26	0.64
1:E:51:ASP:O	1:E:53:GLN:CD	2.45	0.58
1:E:129:ASN:ND2	1:E:131:VAL:H	2.05	0.55
1:E:205:THR:O	1:E:205:THR:CG2	2.56	0.53
1:E:129:ASN:ND2	1:E:135:GLN:H	2.09	0.51
1:E:264:ALA:C	1:E:265:ARG:HG2	2.35	0.49
1:E:1:SER:OG	1:E:166:ASN:ND2	2.48	0.47
1:E:220:LEU:O	1:E:303:GLY:HA3	2.15	0.46
1:E:223:LEU:HB3	1:E:224:PRO:HD2	1.97	0.46
1:E:126:SER:OG	1:E:140:ASP:OD2	2.23	0.45
1:E:52:GLY:HA3	1:E:115:SER:HB2	1.99	0.44
1:E:248:PHE:CZ	1:E:254:LEU:HD11	2.52	0.44
1:E:86:THR:HA	1:E:99:GLN:O	2.19	0.43
1:E:4:THR:OG1	1:E:14:TYR:HB3	2.19	0.42
1:E:45:THR:O	1:E:46:THR:C	2.62	0.42
1:E:223:LEU:HB3	1:E:224:PRO:CD	2.50	0.42
1:E:51:ASP:C	1:E:53:GLN:H	2.29	0.41
1:E:186:LYS:HD2	4:E:605:HOH:O	2.20	0.41
1:E:278:ILE:HD12	1:E:282(B):SER:CB	2.51	0.41
1:E:238:ALA:HA	1:E:247:VAL:O	2.21	0.40

All (1) 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)
1:E:51:ASP:CB	1:E:147:ASP:O[1_556]	1.99	0.21

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%)	323 (98%)	5 (2%)	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	263/263 (100%)	258 (98%)	5 (2%)	50	27

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	60	LYS
1	E	148	SER
1	E	186	LYS
1	E	241	SER
1	E	299	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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	300	ASN
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 ⓘ

5 ligands are 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	2ZS	E	327[B]	-	45,45,45	2.21	13 (28%)	55,59,59	3.17	21 (38%)
3	SO4	E	328	-	4,4,4	0.29	0	6,6,6	0.67	0
3	SO4	E	329	-	4,4,4	0.27	0	6,6,6	0.61	0
2	2ZS	E	327[A]	-	45,45,45	2.20	13 (28%)	55,59,59	3.51	25 (45%)
3	SO4	E	330	-	4,4,4	0.21	0	6,6,6	0.35	0

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	2ZS	E	327[A]	-	-	11/47/63/63	0/3/3/3
2	2ZS	E	327[B]	-	-	9/47/63/63	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	327[A]	2ZS	C4-N2	6.68	1.48	1.34
2	E	327[B]	2ZS	C4-N2	6.68	1.48	1.34
2	E	327[A]	2ZS	CB2-CG1	5.30	1.61	1.53
2	E	327[B]	2ZS	CB2-CG1	5.30	1.61	1.53
2	E	327[A]	2ZS	O21-C7	4.01	1.43	1.34
2	E	327[B]	2ZS	O21-C7	4.01	1.43	1.34
2	E	327[A]	2ZS	CB1-SG	3.78	1.90	1.81
2	E	327[B]	2ZS	CB1-SG	-3.72	1.72	1.81
2	E	327[A]	2ZS	CB2-CA2	3.35	1.57	1.53
2	E	327[B]	2ZS	CB2-CA2	3.35	1.57	1.53
2	E	327[A]	2ZS	CH-CA2	3.33	1.58	1.54
2	E	327[B]	2ZS	CH-CA2	3.33	1.58	1.54
2	E	327[A]	2ZS	O21-CM	3.02	1.54	1.47
2	E	327[B]	2ZS	O21-CM	3.02	1.54	1.47
2	E	327[A]	2ZS	C5-N4	-2.96	1.41	1.47
2	E	327[B]	2ZS	C5-N4	-2.96	1.41	1.47
2	E	327[A]	2ZS	CZ-CE2	-2.90	1.31	1.38
2	E	327[B]	2ZS	CZ-CE2	-2.90	1.31	1.38
2	E	327[A]	2ZS	CD21-CG1	-2.87	1.44	1.52
2	E	327[B]	2ZS	CD21-CG1	-2.87	1.44	1.52
2	E	327[A]	2ZS	C1-N1	2.63	1.39	1.34
2	E	327[B]	2ZS	C1-N1	2.63	1.39	1.34
2	E	327[A]	2ZS	CD2-CG	-2.47	1.34	1.38
2	E	327[B]	2ZS	CD2-CG	-2.47	1.34	1.38
2	E	327[A]	2ZS	O11-C7	2.13	1.26	1.21
2	E	327[B]	2ZS	O11-C7	2.13	1.26	1.21

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327[A]	2ZS	O3-C4-N2	-9.85	105.33	122.96
2	E	327[B]	2ZS	O3-C4-N2	-9.85	105.33	122.96
2	E	327[A]	2ZS	O21-C7-O11	-9.44	106.90	123.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327[B]	2ZS	O21-C7-O11	-9.44	106.90	123.95
2	E	327[A]	2ZS	CA1-CB1-SG	8.33	127.52	114.04
2	E	327[A]	2ZS	CA1-C4-N2	7.32	132.25	116.63
2	E	327[B]	2ZS	CA1-C4-N2	7.32	132.25	116.63
2	E	327[A]	2ZS	CA2-N2-C4	7.25	135.85	123.25
2	E	327[B]	2ZS	CA2-N2-C4	7.25	135.85	123.25
2	E	327[A]	2ZS	O21-C7-CH	6.52	121.47	111.13
2	E	327[B]	2ZS	O21-C7-CH	6.52	121.47	111.13
2	E	327[A]	2ZS	CB1-CA1-N1	6.34	127.65	111.06
2	E	327[A]	2ZS	CM-O21-C7	-5.20	110.31	117.71
2	E	327[B]	2ZS	CM-O21-C7	-5.20	110.31	117.71
2	E	327[A]	2ZS	C5-N4-C3	4.55	121.96	112.68
2	E	327[B]	2ZS	C5-N4-C3	4.55	121.96	112.68
2	E	327[A]	2ZS	O3-C4-CA1	-4.06	111.98	120.48
2	E	327[B]	2ZS	O3-C4-CA1	-4.06	111.98	120.48
2	E	327[A]	2ZS	CE1-CD1-CG	-4.03	114.94	120.61
2	E	327[B]	2ZS	CE1-CD1-CG	-4.03	114.94	120.61
2	E	327[A]	2ZS	CD2-CG-CD1	3.61	123.61	118.23
2	E	327[B]	2ZS	CD2-CG-CD1	3.61	123.61	118.23
2	E	327[A]	2ZS	CB1-CA1-C4	3.55	117.47	109.46
2	E	327[A]	2ZS	CZ-CE2-CD2	-3.38	116.06	120.24
2	E	327[B]	2ZS	CZ-CE2-CD2	-3.38	116.06	120.24
2	E	327[A]	2ZS	CE2-CZ-CE1	3.38	124.49	119.87
2	E	327[B]	2ZS	CE2-CZ-CE1	3.38	124.49	119.87
2	E	327[A]	2ZS	CB-CG-CD2	-3.35	114.67	120.90
2	E	327[B]	2ZS	CB-CG-CD2	-3.35	114.67	120.90
2	E	327[A]	2ZS	O11-C7-CH	3.34	131.62	123.11
2	E	327[B]	2ZS	O11-C7-CH	3.34	131.62	123.11
2	E	327[A]	2ZS	O-C-N4	-3.15	117.28	121.67
2	E	327[B]	2ZS	O-C-N4	-3.15	117.28	121.67
2	E	327[A]	2ZS	C6-C5-N4	2.98	116.08	109.82
2	E	327[B]	2ZS	C6-C5-N4	2.98	116.08	109.82
2	E	327[A]	2ZS	CB2-CG1-CD21	2.71	118.02	111.71
2	E	327[B]	2ZS	CB2-CG1-CD21	2.71	118.02	111.71
2	E	327[A]	2ZS	O21-CM-CM2	2.24	113.09	107.13
2	E	327[B]	2ZS	O21-CM-CM2	2.24	113.09	107.13
2	E	327[A]	2ZS	O21-CM-CM1	2.24	113.08	107.13
2	E	327[B]	2ZS	O21-CM-CM1	2.24	113.08	107.13
2	E	327[A]	2ZS	CS-SG-CB1	-2.20	89.88	101.71
2	E	327[A]	2ZS	O1-C2-C3	-2.15	107.14	111.77
2	E	327[B]	2ZS	O1-C2-C3	-2.15	107.14	111.77
2	E	327[A]	2ZS	C5-N4-C	-2.02	114.48	121.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327[B]	2ZS	C5-N4-C	-2.02	114.48	121.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	327[A]	2ZS	CA1-CB1-SG-CS
2	E	327[A]	2ZS	CB2-CA2-N2-C4
2	E	327[A]	2ZS	CH-CA2-N2-C4
2	E	327[A]	2ZS	CA2-CB2-CG1-CD21
2	E	327[B]	2ZS	CB2-CA2-N2-C4
2	E	327[B]	2ZS	CH-CA2-N2-C4
2	E	327[B]	2ZS	CA2-CB2-CG1-CD21
2	E	327[A]	2ZS	O3-C4-N2-CA2
2	E	327[B]	2ZS	O3-C4-N2-CA2
2	E	327[A]	2ZS	C4-CA1-CB1-SG
2	E	327[A]	2ZS	N1-CA1-CB1-SG
2	E	327[A]	2ZS	CA2-CB2-CG1-CD11
2	E	327[B]	2ZS	CA2-CB2-CG1-CD11
2	E	327[B]	2ZS	CA1-CB1-SG-CS
2	E	327[A]	2ZS	O11-C7-CH-CA2
2	E	327[A]	2ZS	O21-C7-CH-CA2
2	E	327[B]	2ZS	O11-C7-CH-CA2
2	E	327[B]	2ZS	O21-C7-CH-CA2
2	E	327[A]	2ZS	O3-C4-CA1-N1
2	E	327[B]	2ZS	O3-C4-CA1-N1

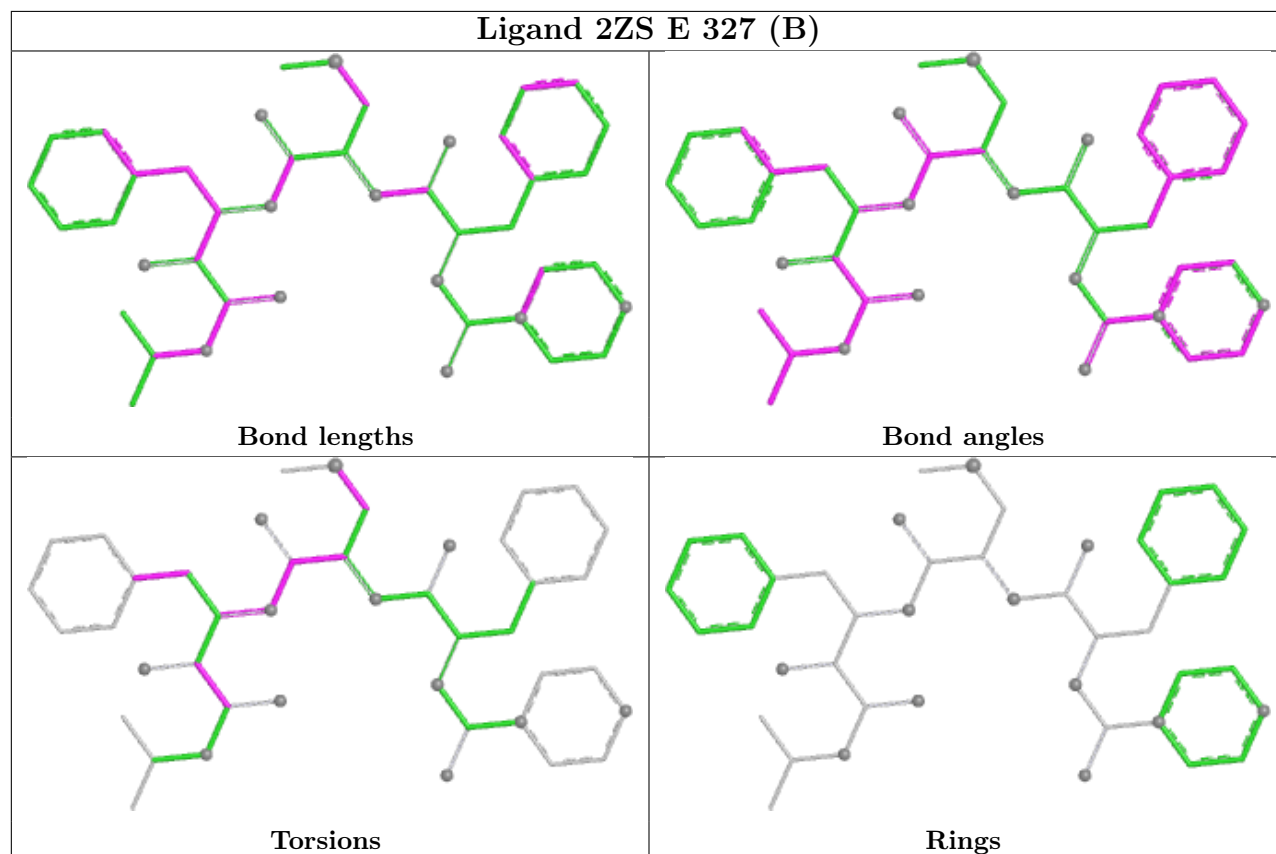
There are no ring outliers.

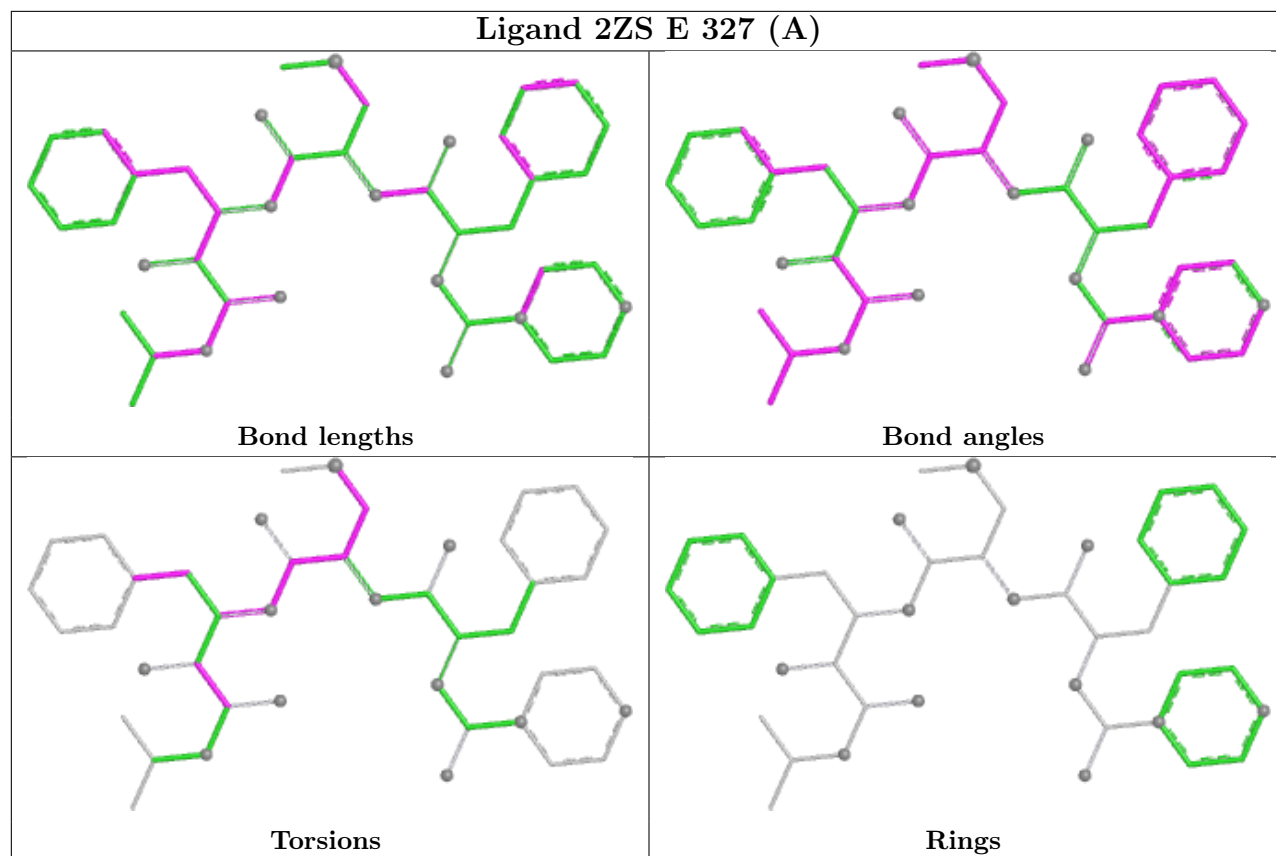
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	329	SO4	1	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

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.