



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 07:08 AM EDT

PDB ID : 1EPM  
Title : A STRUCTURAL COMPARISON OF 21 INHIBITOR COMPLEXES OF  
THE ASPARTIC PROTEINASE FROM ENDOTHIA PARASITICA  
Authors : Crawford, M.; Cooper, J.B.; Strop, P.; 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](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
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

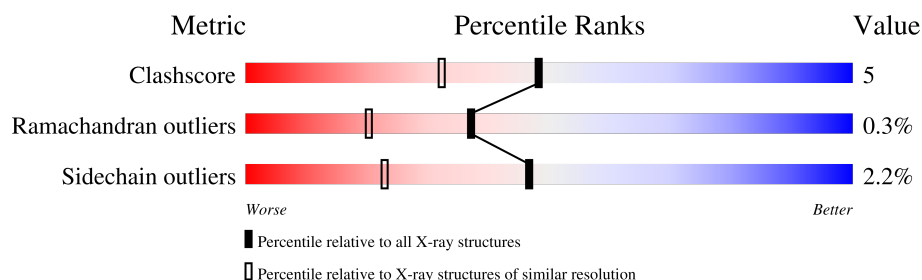
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	
2	I	8	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2759 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 ENDOTHIAPEPSIN.

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 a protein called PS2, THR-PHE-GLN-ALA-PSA-LEU-ARG-GLU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			74	49	12	13			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

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

- Molecule 4 is water.

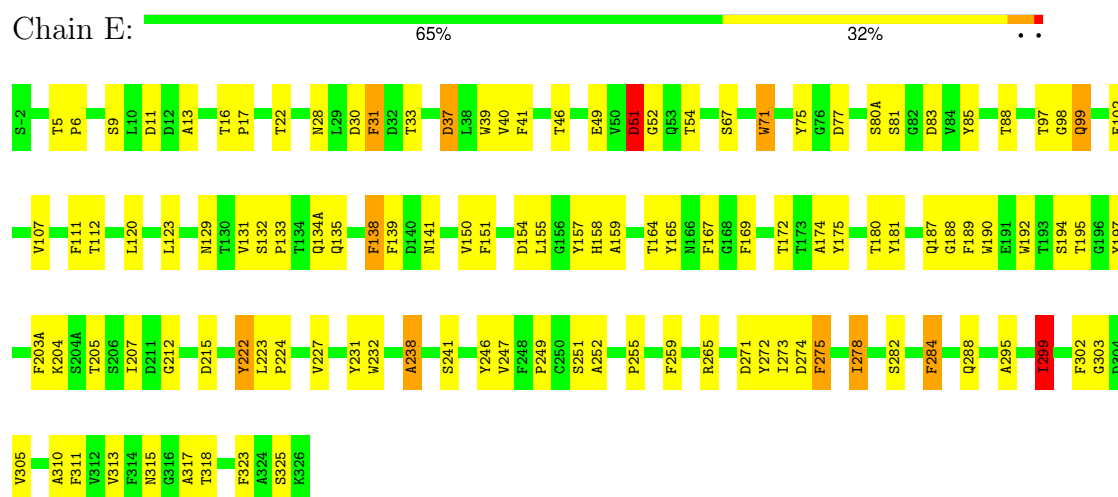
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	274	Total	O	0	0
			274	274		
4	I	7	Total	O	0	0
			7	7		

### 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



#### • Molecule 2: PS2, THR-PHE-GLN-ALA-PSA-LEU-ARG-GLU



## 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, $\alpha$ , $\beta$ , $\gamma$	43.11Å 75.88Å 42.98Å 90.00° 96.76° 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	2759	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: PSA, SO4

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	1.64	22/2445 (0.9%)	2.52	156/3345 (4.7%)
2	I	1.19	1/59 (1.7%)	2.90	7/76 (9.2%)
All	All	1.63	23/2504 (0.9%)	2.53	163/3421 (4.8%)

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
2	I	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	134(A)	GLN	CD-OE1	7.21	1.39	1.24
1	E	246	TYR	CD1-CE1	7.08	1.50	1.39
1	E	188	GLY	N-CA	6.71	1.56	1.46
1	E	282	SER	CB-OG	6.51	1.50	1.42
1	E	49	GLU	CD-OE2	6.06	1.32	1.25
1	E	99	GLN	CD-OE1	5.73	1.36	1.24
1	E	212	GLY	CA-C	5.73	1.61	1.51
1	E	71	TRP	CZ3-CH2	5.67	1.49	1.40
1	E	28	ASN	CB-CG	5.43	1.63	1.51
1	E	159	ALA	N-CA	5.36	1.57	1.46
1	E	194	SER	N-CA	5.36	1.57	1.46
1	E	39	TRP	NE1-CE2	-5.36	1.30	1.37
1	E	39	TRP	CB-CG	5.33	1.59	1.50
1	E	81	SER	CB-OG	5.32	1.49	1.42
1	E	158	HIS	ND1-CE1	5.31	1.48	1.34
1	E	232	TRP	CD1-NE1	5.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	GLN	CD-OE1	5.24	1.35	1.24
1	E	71	TRP	CD2-CE2	5.20	1.47	1.41
1	E	33	THR	CB-OG1	5.08	1.53	1.43
1	E	132	SER	CA-CB	5.05	1.60	1.52
1	E	141	ASN	CG-OD1	5.05	1.35	1.24
1	E	231	TYR	CZ-OH	5.04	1.46	1.37
1	E	52	GLY	N-CA	5.02	1.53	1.46

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	PHE	CB-CG-CD1	-17.27	108.71	120.80
1	E	51	ASP	CA-C-O	15.94	153.56	120.10
1	E	265	ARG	NE-CZ-NH1	15.11	127.85	120.30
1	E	157	TYR	CD1-CE1-CZ	-15.00	106.30	119.80
1	E	157	TYR	CG-CD1-CE1	14.64	133.02	121.30
1	E	271	ASP	CB-CG-OD1	14.52	131.37	118.30
1	E	165	TYR	CB-CG-CD1	-12.96	113.23	121.00
1	E	175	TYR	CB-CG-CD2	-12.61	113.43	121.00
1	E	311	PHE	CB-CG-CD1	-12.33	112.17	120.80
1	E	181	TYR	CB-CG-CD2	-12.26	113.64	121.00
1	E	265	ARG	NE-CZ-NH2	-12.11	114.25	120.30
1	E	203(A)	PHE	CB-CG-CD2	-11.94	112.44	120.80
1	E	51	ASP	O-C-N	-11.80	103.14	123.20
1	E	77	ASP	CB-CG-OD1	11.71	128.84	118.30
1	E	157	TYR	CB-CG-CD1	11.63	127.98	121.00
1	E	157	TYR	CB-CG-CD2	-11.61	114.03	121.00
1	E	271	ASP	CB-CG-OD2	-11.06	108.34	118.30
1	E	197	TYR	CB-CG-CD2	-11.02	114.39	121.00
1	E	165	TYR	CG-CD2-CE2	-10.98	112.51	121.30
1	E	167	PHE	CG-CD2-CE2	-10.98	108.72	120.80
1	E	85	TYR	CG-CD2-CE2	-10.81	112.65	121.30
1	E	31	PHE	CB-CG-CD2	-10.41	113.51	120.80
1	E	157	TYR	CG-CD2-CE2	-10.26	113.09	121.30
1	E	222	TYR	CB-CG-CD2	-10.14	114.92	121.00
1	E	246	TYR	CG-CD1-CE1	-10.07	113.25	121.30
2	I	4(A)	GLU	OE1-CD-OE2	-10.00	111.30	123.30
1	E	231	TYR	CZ-CE2-CD2	-9.96	110.83	119.80
1	E	167	PHE	CB-CG-CD2	-9.82	113.93	120.80
1	E	75	TYR	CB-CG-CD2	-9.64	115.21	121.00
1	E	275	PHE	CD1-CG-CD2	9.59	130.76	118.30
1	E	231	TYR	CG-CD2-CE2	9.54	128.93	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	PHE	CZ-CE2-CD2	-9.45	108.76	120.10
1	E	67	SER	O-C-N	9.44	139.24	123.20
1	E	11	ASP	CB-CG-OD1	-9.36	109.88	118.30
1	E	275	PHE	CE1-CZ-CE2	8.99	136.19	120.00
1	E	77	ASP	CB-CG-OD2	-8.75	110.42	118.30
1	E	212	GLY	O-C-N	8.68	136.59	122.70
1	E	259	PHE	CZ-CE2-CD2	-8.43	109.98	120.10
1	E	111	PHE	CB-CG-CD2	-8.37	114.94	120.80
1	E	169	PHE	CG-CD1-CE1	8.33	129.96	120.80
1	E	251	SER	O-C-N	-8.24	109.52	122.70
1	E	98	GLY	O-C-N	8.16	135.76	122.70
1	E	80(A)	SER	O-C-N	-8.15	109.66	122.70
1	E	30	ASP	CB-CG-OD1	8.10	125.59	118.30
1	E	9	SER	O-C-N	8.04	135.56	122.70
1	E	30	ASP	CB-CG-OD2	-7.97	111.12	118.30
1	E	255	PRO	CA-N-CD	7.92	122.79	111.70
1	E	51	ASP	CA-CB-CG	7.90	130.78	113.40
1	E	275	PHE	CG-CD1-CE1	-7.79	112.24	120.80
1	E	295	ALA	O-C-N	-7.79	109.96	123.20
1	E	139	PHE	CB-CG-CD1	7.75	126.23	120.80
1	E	313	VAL	CG1-CB-CG2	-7.74	98.52	110.90
1	E	51	ASP	CB-CG-OD1	7.71	125.24	118.30
1	E	246	TYR	CD1-CG-CD2	7.69	126.36	117.90
1	E	323	PHE	CB-CG-CD2	-7.68	115.42	120.80
1	E	274	ASP	CB-CG-OD2	-7.61	111.45	118.30
2	I	4	PHE	CB-CG-CD2	-7.60	115.48	120.80
1	E	311	PHE	CB-CG-CD2	7.37	125.96	120.80
1	E	71	TRP	CG-CD2-CE3	7.33	140.50	133.90
1	E	85	TYR	CD1-CG-CD2	7.25	125.88	117.90
1	E	37	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	E	246	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	E	189	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	E	167	PHE	CD1-CE1-CZ	-7.09	111.60	120.10
1	E	165	TYR	CZ-CE2-CD2	7.00	126.10	119.80
1	E	259	PHE	CG-CD1-CE1	-6.96	113.14	120.80
1	E	138	PHE	CB-CG-CD2	-6.96	115.93	120.80
1	E	85	TYR	CB-CG-CD2	-6.91	116.86	121.00
1	E	246	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	E	169	PHE	CB-CG-CD1	6.81	125.57	120.80
2	I	4	PHE	CA-C-N	-6.77	102.30	117.20
1	E	192	TRP	CH2-CZ2-CE2	-6.76	110.64	117.40
1	E	139	PHE	CB-CG-CD2	-6.73	116.09	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	39	TRP	CG-CD1-NE1	-6.69	103.41	110.10
1	E	249	PRO	CA-N-CD	6.69	121.06	111.70
1	E	231	TYR	CB-CG-CD2	6.64	124.98	121.00
1	E	51	ASP	CA-C-N	-6.63	102.93	116.20
1	E	317	ALA	N-CA-CB	6.62	119.37	110.10
1	E	197	TYR	CG-CD2-CE2	-6.61	116.01	121.30
1	E	167	PHE	CZ-CE2-CD2	6.58	127.99	120.10
1	E	274	ASP	CB-CG-OD1	6.55	124.20	118.30
1	E	310	ALA	CB-CA-C	-6.52	100.33	110.10
1	E	222	TYR	CB-CG-CD1	6.49	124.90	121.00
1	E	31	PHE	CG-CD2-CE2	-6.43	113.72	120.80
1	E	302	PHE	CZ-CE2-CD2	-6.39	112.43	120.10
1	E	85	TYR	CB-CG-CD1	-6.36	117.19	121.00
1	E	151	PHE	N-CA-CB	6.35	122.02	110.60
1	E	238	ALA	O-C-N	6.33	132.82	122.70
1	E	167	PHE	CD1-CG-CD2	6.32	126.52	118.30
1	E	299	ILE	O-C-N	6.29	132.76	122.70
1	E	39	TRP	CB-CG-CD1	-6.29	118.83	127.00
2	I	4	PHE	CA-C-O	6.23	133.19	120.10
1	E	71	TRP	NE1-CE2-CZ2	-6.19	123.59	130.40
1	E	75	TYR	CD1-CE1-CZ	-6.18	114.24	119.80
1	E	175	TYR	CG-CD2-CE2	-6.13	116.40	121.30
1	E	17	PRO	CA-N-CD	6.11	120.25	111.70
1	E	180	THR	CA-CB-CG2	-6.09	103.88	112.40
1	E	39	TRP	CD1-CG-CD2	6.08	111.16	106.30
1	E	165	TYR	CD1-CG-CD2	6.07	124.58	117.90
1	E	169	PHE	CD1-CE1-CZ	-6.05	112.84	120.10
1	E	81	SER	C-N-CA	-6.04	109.62	122.30
1	E	284	PHE	CG-CD2-CE2	-6.04	114.16	120.80
1	E	204	LYS	CA-CB-CG	-6.02	100.15	113.40
1	E	75	TYR	CG-CD2-CE2	-5.99	116.51	121.30
1	E	272	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	E	132	SER	N-CA-CB	-5.97	101.54	110.50
1	E	123	LEU	O-C-N	5.92	132.17	122.70
1	E	305	VAL	CA-CB-CG1	5.87	119.70	110.90
1	E	51	ASP	OD1-CG-OD2	-5.86	112.16	123.30
1	E	259	PHE	CB-CG-CD1	-5.86	116.70	120.80
1	E	207	ILE	O-C-N	5.84	132.05	122.70
1	E	133	PRO	CA-N-CD	5.80	119.81	111.70
1	E	39	TRP	CE3-CZ3-CH2	-5.78	114.84	121.20
1	E	181	TYR	CD1-CG-CD2	5.76	124.24	117.90
1	E	303	GLY	O-C-N	5.76	131.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	325	SER	CA-CB-OG	-5.76	95.66	111.20
1	E	174	ALA	N-CA-CB	-5.75	102.06	110.10
1	E	154	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	E	284	PHE	O-C-N	-5.69	113.53	123.20
1	E	54	THR	C-N-CA	-5.68	107.51	121.70
1	E	181	TYR	CG-CD2-CE2	-5.67	116.76	121.30
1	E	273	ILE	CA-C-O	5.67	132.01	120.10
1	E	192	TRP	O-C-N	5.66	131.75	122.70
1	E	41	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	E	40	VAL	CG1-CB-CG2	-5.59	101.96	110.90
1	E	227	VAL	CG1-CB-CG2	-5.55	102.03	110.90
1	E	272	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
2	I	3(A)	ARG	CD-NE-CZ	-5.52	115.87	123.60
1	E	22	THR	CA-CB-CG2	-5.51	104.68	112.40
1	E	192	TRP	CB-CG-CD1	5.51	134.16	127.00
1	E	164	THR	CA-CB-CG2	-5.46	104.75	112.40
1	E	46	THR	CA-CB-CG2	-5.46	104.76	112.40
1	E	6	PRO	CA-N-CD	5.44	119.31	111.70
1	E	41	PHE	CZ-CE2-CD2	-5.43	113.59	120.10
1	E	97	THR	CA-CB-CG2	-5.42	104.81	112.40
1	E	190	TRP	CD1-CG-CD2	5.41	110.63	106.30
2	I	4	PHE	CD1-CG-CD2	5.41	125.33	118.30
1	E	49	GLU	CA-CB-CG	-5.39	101.54	113.40
1	E	187	GLN	O-C-N	5.38	132.34	123.20
1	E	195	THR	CA-CB-CG2	-5.37	104.89	112.40
1	E	278	ILE	CA-CB-CG2	5.35	121.60	110.90
1	E	85	TYR	CZ-CE2-CD2	5.33	124.60	119.80
1	E	249	PRO	N-CD-CG	-5.26	95.31	103.20
1	E	154	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	252	ALA	O-C-N	5.20	131.02	122.70
1	E	222	TYR	CD1-CE1-CZ	-5.19	115.12	119.80
1	E	172	THR	CA-CB-CG2	-5.18	105.15	112.40
2	I	2(A)	LEU	C-N-CA	-5.17	108.77	121.70
1	E	155	LEU	C-N-CA	-5.17	111.45	122.30
1	E	88	THR	CA-CB-CG2	-5.16	105.17	112.40
1	E	215	ASP	CB-CG-OD1	5.13	122.91	118.30
1	E	49	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	E	325	SER	CB-CA-C	-5.10	100.40	110.10
1	E	107	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	E	39	TRP	CD1-NE1-CE2	5.08	113.57	109.00
1	E	120	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	E	272	TYR	CE1-CZ-CE2	5.07	127.92	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	11	ASP	N-CA-CB	5.07	119.72	110.60
1	E	67	SER	CA-C-O	-5.06	109.48	120.10
1	E	107	VAL	CA-CB-CG2	5.04	118.47	110.90
1	E	318	THR	CA-CB-CG2	-5.03	105.36	112.40
1	E	83	ASP	CB-CG-OD1	5.01	122.81	118.30
1	E	313	VAL	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	1	PSA	Mainchain,Peptide
2	I	3(A)	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	22	0
2	I	74	0	70	12	0
3	E	15	0	0	0	0
4	E	274	0	0	1	1
4	I	7	0	0	0	0
All	All	2759	0	2350	26	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 5.

All (26) 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:I:2(A):LEU:O	2:I:3(A):ARG:CB	1.76	1.25
2:I:2(A):LEU:O	2:I:3(A):ARG:HB2	0.93	0.80
2:I:2(A):LEU:HG	2:I:3(A):ARG:N	1.97	0.79
1:E:275:PHE:CE2	2:I:4:PHE:HE1	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:ILE:HD11	2:I:3(A):ARG:HD3	1.71	0.73
1:E:5:THR:HG23	4:E:357:HOH:O	1.92	0.69
1:E:51:ASP:OD2	1:E:112:THR:HG22	1.93	0.68
1:E:129:ASN:ND2	1:E:135:GLN:H	1.93	0.66
2:I:4:PHE:CD1	2:I:4:PHE:N	2.59	0.64
1:E:13:ALA:HB2	2:I:3:GLN:NE2	2.16	0.61
1:E:284:PHE:CE2	2:I:4:PHE:CE2	2.96	0.54
1:E:275:PHE:CE2	2:I:4:PHE:CE1	2.91	0.52
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.25	0.52
1:E:284:PHE:CE2	2:I:4:PHE:HE2	2.31	0.48
1:E:205:THR:O	1:E:205:THR:HG23	2.15	0.47
1:E:299:ILE:HD11	2:I:3(A):ARG:CD	2.45	0.45
1:E:150:VAL:HG12	1:E:315:ASN:HA	2.00	0.44
1:E:129:ASN:HD21	1:E:131:VAL:HG23	1.84	0.43
1:E:247:VAL:CG1	1:E:278:ILE:HD11	2.47	0.43
1:E:129:ASN:ND2	1:E:131:VAL:H	2.17	0.42
1:E:16:THR:HB	1:E:31:PHE:CE1	2.54	0.42
1:E:223:LEU:HB3	1:E:224:PRO:HD2	2.02	0.41
1:E:13:ALA:HB2	2:I:3:GLN:HE22	1.82	0.41
1:E:222:TYR:HA	1:E:288:GLN:O	2.21	0.40
1:E:238:ALA:HA	1:E:247:VAL:O	2.21	0.40
1:E:71:TRP:CE2	1:E:102:GLU:HB3	2.57	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)
4:E:564:HOH:O	4:E:575:HOH:O[2_555]	0.29	1.91

## 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	328/330 (99%)	326 (99%)	2 (1%)	0	100	100
2	I	5/8 (62%)	4 (80%)	0	1 (20%)	0	0
All	All	333/338 (98%)	330 (99%)	2 (1%)	1 (0%)	37	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	3(A)	ARG

### 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	263/263 (100%)	259 (98%)	4 (2%)	60	39
2	I	6/6 (100%)	4 (67%)	2 (33%)	0	0
All	All	269/269 (100%)	263 (98%)	6 (2%)	47	23

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	37	ASP
1	E	51	ASP
1	E	241	SER
1	E	299	ILE
2	I	3	GLN
2	I	3(A)	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	99	GLN
1	E	129	ASN
1	E	134(A)	GLN
1	E	135	GLN

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Mol	Chain	Res	Type
1	E	141	ASN
1	E	166	ASN
1	E	187	GLN
1	E	300	ASN
2	I	3	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	PSA	I	1	2	14,14,15	1.29	1 (7%)	15,17,19	1.77	5 (33%)

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	PSA	I	1	2	-	3/11/11/12	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	PSA	CZ-CE2	3.18	1.45	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	PSA	CB-CA-CH	-3.01	107.07	111.86
2	I	1	PSA	CE1-CD1-CG	2.97	124.80	120.61
2	I	1	PSA	CE2-CD2-CG	2.97	124.79	120.61
2	I	1	PSA	CD2-CG-CD1	-2.26	114.87	118.23
2	I	1	PSA	CH-CM-C	2.04	116.50	113.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	PSA	CA-CB-CG-CD1
2	I	1	PSA	CA-CB-CG-CD2
2	I	1	PSA	O-C-CM-CH

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
3	SO4	E	327	-	4,4,4	0.20	0	6,6,6	0.49	0
3	SO4	E	328	-	4,4,4	0.16	0	6,6,6	0.69	0
3	SO4	E	329	-	4,4,4	0.27	0	6,6,6	0.54	0

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.