



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:08 PM UTC

PDB ID : 1EPM / pdb_00001epm
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

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
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

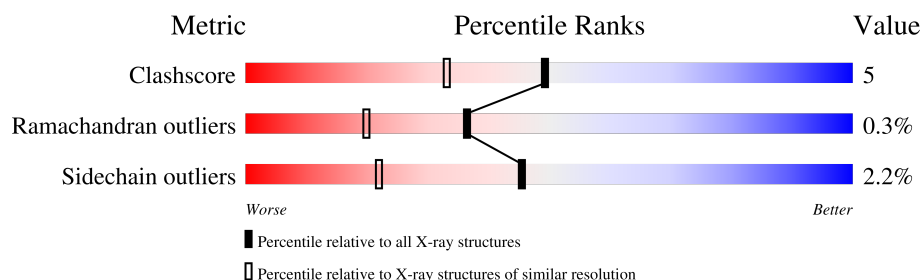
1 Overall quality at a glance

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	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 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 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 (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		

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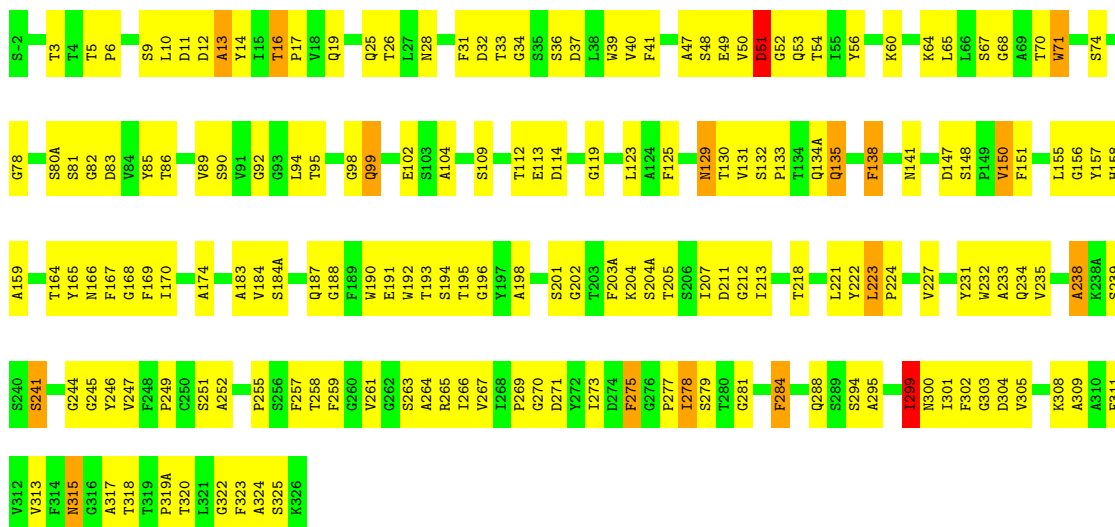
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		

- 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		

Note EDS was not executed.

Chain E: 46% 48% 5%



Chain I: 38% 38% 25%



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 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 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: SO4, PSA

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	2.15	70/2445 (2.9%)	2.74	223/3345 (6.7%)
2	I	1.37	1/59 (1.7%)	3.14	8/76 (10.5%)
All	All	2.13	71/2504 (2.8%)	2.75	231/3421 (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
2	I	0	3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	158	HIS	ND1-CE1	15.48	1.48	1.32
1	E	159	ALA	N-CA	11.23	1.57	1.46
1	E	223	LEU	N-CA	9.84	1.52	1.46
1	E	194	SER	N-CA	8.78	1.57	1.45
1	E	134(A)	GLN	CD-OE1	8.55	1.39	1.23
1	E	212	GLY	CA-C	8.47	1.61	1.51
1	E	138	PHE	N-CA	7.88	1.55	1.46
1	E	10	LEU	N-CA	7.62	1.56	1.46
1	E	158	HIS	CD2-NE2	7.37	1.46	1.37
1	E	32	ASP	C-O	7.27	1.32	1.24
1	E	188	GLY	N-CA	7.15	1.56	1.45
1	E	311	PHE	N-CA	7.00	1.54	1.46
1	E	318	THR	C-N	-7.00	1.24	1.33
1	E	317	ALA	CA-CB	-6.87	1.43	1.53
1	E	32	ASP	N-CA	6.86	1.55	1.46
1	E	99	GLN	CD-OE1	6.84	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	74	SER	C-O	6.82	1.32	1.23
1	E	278	ILE	CA-CB	-6.74	1.46	1.54
1	E	41	PHE	CA-C	6.67	1.61	1.52
1	E	192	TRP	CA-C	6.46	1.60	1.52
1	E	184	VAL	N-CA	6.36	1.53	1.46
2	I	3	GLN	CD-OE1	6.28	1.35	1.23
1	E	39	TRP	NE1-CE2	-6.24	1.30	1.37
1	E	227	VAL	N-CA	6.19	1.53	1.46
1	E	213	ILE	N-CA	6.16	1.53	1.46
1	E	89	VAL	N-CA	6.14	1.53	1.46
1	E	141	ASN	CG-OD1	6.06	1.35	1.23
1	E	119	GLY	N-CA	6.04	1.50	1.45
1	E	33	THR	CB-OG1	6.03	1.53	1.43
1	E	82	GLY	N-CA	5.99	1.52	1.45
1	E	234	GLN	CD-OE1	5.91	1.34	1.23
1	E	135	GLN	CD-OE1	5.86	1.34	1.23
1	E	301	ILE	C-N	-5.86	1.25	1.33
1	E	233	ALA	N-CA	5.84	1.53	1.46
1	E	221	LEU	CA-C	5.78	1.60	1.52
1	E	261	VAL	CA-C	5.72	1.60	1.52
1	E	235	VAL	CA-CB	5.67	1.61	1.54
1	E	90	SER	CA-C	5.67	1.59	1.52
1	E	187	GLN	CD-OE1	5.65	1.34	1.23
1	E	71	TRP	NE1-CE2	-5.64	1.31	1.37
1	E	166	ASN	CG-OD1	5.64	1.34	1.23
1	E	19	GLN	C-N	-5.59	1.26	1.33
1	E	114	ASP	N-CA	5.59	1.53	1.46
1	E	258	THR	N-CA	5.52	1.52	1.46
1	E	52	GLY	N-CA	5.48	1.53	1.44
1	E	261	VAL	N-CA	5.47	1.53	1.46
1	E	28	ASN	N-CA	5.45	1.53	1.46
1	E	89	VAL	C-O	5.42	1.29	1.24
1	E	40	VAL	CA-CB	5.39	1.64	1.55
1	E	211	ASP	N-CA	5.39	1.52	1.46
1	E	232	TRP	NE1-CE2	-5.34	1.31	1.37
1	E	191	GLU	C-N	5.32	1.40	1.33
1	E	273	ILE	CA-CB	-5.29	1.47	1.54
1	E	231	TYR	CA-CB	5.29	1.61	1.53
1	E	130	THR	C-O	5.28	1.30	1.24
1	E	191	GLU	N-CA	5.26	1.52	1.46
1	E	202	GLY	N-CA	5.26	1.51	1.45
1	E	325	SER	CA-C	5.25	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	3	THR	N-CA	5.23	1.52	1.46
1	E	257	PHE	N-CA	5.23	1.52	1.46
1	E	193	THR	N-CA	5.22	1.52	1.46
1	E	270	GLY	N-CA	5.21	1.52	1.45
1	E	39	TRP	CA-C	-5.18	1.46	1.52
1	E	47	ALA	C-O	-5.18	1.18	1.24
1	E	14	TYR	C-O	-5.18	1.17	1.24
1	E	86	THR	CA-C	5.15	1.58	1.52
1	E	257	PHE	C-O	5.13	1.29	1.24
1	E	323	PHE	C-N	-5.11	1.26	1.33
1	E	53	GLN	CD-OE1	5.07	1.33	1.23
1	E	158	HIS	CG-CD2	5.03	1.41	1.35
1	E	125	PHE	C-O	5.00	1.30	1.23

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ASP	CA-C-O	19.12	153.56	122.20
1	E	51	ASP	CA-CB-CG	18.18	130.78	112.60
1	E	80(A)	SER	O-C-N	-12.86	109.66	123.42
1	E	67	SER	O-C-N	11.80	139.24	123.07
1	E	295	ALA	O-C-N	-11.66	109.96	122.09
1	E	212	GLY	O-C-N	11.34	136.59	123.44
1	E	98	GLY	O-C-N	11.00	135.76	122.34
2	I	4	PHE	CA-CB-CG	-10.88	102.92	113.80
1	E	251	SER	O-C-N	-10.86	109.52	122.22
1	E	303	GLY	O-C-N	10.58	131.91	122.81
1	E	67	SER	CA-C-O	-10.48	109.48	120.80
1	E	54	THR	CA-C-N	-10.38	107.51	122.45
1	E	54	THR	C-N-CA	-10.38	107.51	122.45
1	E	273	ILE	CA-C-O	10.27	132.01	119.58
2	I	4	PHE	CA-C-O	9.76	133.19	121.87
1	E	51	ASP	O-C-N	-9.68	103.14	122.22
1	E	207	ILE	O-C-N	9.63	132.05	122.71
1	E	155	LEU	CA-C-N	-9.15	111.45	122.15
1	E	155	LEU	C-N-CA	-9.15	111.45	122.15
1	E	9	SER	O-C-N	8.99	135.56	122.43
1	E	275	PHE	CE1-CZ-CE2	8.99	136.19	120.00
1	E	299	ILE	O-C-N	8.88	132.76	123.00
1	E	51	ASP	N-CA-C	8.71	123.53	107.60
1	E	123	LEU	CA-C-O	-8.61	111.54	120.32
1	E	241	SER	CA-C-O	8.59	129.93	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	113	GLU	CA-C-N	-8.55	110.97	123.11
1	E	113	GLU	C-N-CA	-8.55	110.97	123.11
1	E	187	GLN	OE1-CD-NE2	-8.41	114.19	122.60
1	E	16	THR	CA-C-N	-8.37	110.95	119.99
1	E	16	THR	C-N-CA	-8.37	110.95	119.99
1	E	81	SER	CA-C-N	-8.35	109.62	120.72
1	E	81	SER	C-N-CA	-8.35	109.62	120.72
1	E	284	PHE	O-C-N	-8.30	113.53	123.16
1	E	56	TYR	CA-C-O	8.22	129.83	120.54
1	E	192	TRP	CA-C-O	-8.19	112.68	121.45
1	E	275	PHE	CD1-CG-CD2	8.11	130.76	118.60
1	E	123	LEU	O-C-N	8.03	132.17	122.21
1	E	187	GLN	O-C-N	8.00	132.34	122.34
1	E	277	PRO	CA-C-O	7.96	130.79	121.56
1	E	157	TYR	CG-CD1-CE1	7.88	133.02	121.20
1	E	25	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	E	325	SER	CA-CB-OG	-7.72	95.66	111.10
1	E	255	PRO	CA-N-CD	7.71	122.79	112.00
1	E	99	GLN	CG-CD-NE2	7.64	127.86	116.40
1	E	299	ILE	CA-C-O	-7.58	113.38	121.19
1	E	295	ALA	CA-C-O	7.54	128.97	120.90
1	E	192	TRP	O-C-N	7.52	131.75	123.10
1	E	80(A)	SER	CA-C-O	7.50	129.25	121.23
1	E	157	TYR	CD1-CE1-CZ	-7.39	106.30	119.60
1	E	50	VAL	CA-C-O	-7.30	112.76	120.57
1	E	271	ASP	CA-CB-CG	-7.28	105.32	112.60
1	E	141	ASN	CA-CB-CG	-7.14	105.45	112.60
1	E	11	ASP	CA-CB-CG	7.12	119.72	112.60
1	E	275	PHE	CB-CG-CD1	-7.05	108.71	120.70
1	E	167	PHE	CG-CD2-CE2	-7.05	108.72	120.70
1	E	204	LYS	CA-CB-CG	-6.98	100.15	114.10
1	E	202	GLY	O-C-N	-6.92	116.86	122.81
1	E	252	ALA	O-C-N	6.91	131.02	122.86
1	E	168	GLY	N-CA-C	6.90	124.84	115.32
1	E	279	SER	CA-C-N	-6.83	111.01	120.71
1	E	279	SER	C-N-CA	-6.83	111.01	120.71
1	E	56	TYR	O-C-N	-6.83	115.44	123.22
1	E	150	VAL	CA-C-O	6.80	128.25	121.45
1	E	9	SER	CA-C-O	-6.80	110.41	119.11
1	E	14	TYR	CA-C-N	-6.73	111.36	122.67
1	E	14	TYR	C-N-CA	-6.73	111.36	122.67
1	E	104	ALA	N-CA-C	6.73	119.48	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184(A)	SER	O-C-N	-6.70	115.70	123.27
2	I	2(A)	LEU	CA-C-N	-6.68	108.77	121.54
2	I	2(A)	LEU	C-N-CA	-6.68	108.77	121.54
1	E	317	ALA	N-CA-CB	6.67	119.37	110.29
1	E	311	PHE	N-CA-C	-6.67	98.37	109.24
1	E	159	ALA	N-CA-C	-6.62	102.17	108.13
1	E	158	HIS	CA-CB-CG	-6.61	107.19	113.80
1	E	71	TRP	CG-CD2-CE3	6.60	140.50	133.90
1	E	212	GLY	CA-C-O	-6.57	114.71	121.61
1	E	264	ALA	O-C-N	6.55	130.34	122.68
1	E	212	GLY	CA-C-N	-6.54	111.67	122.67
1	E	212	GLY	C-N-CA	-6.54	111.67	122.67
1	E	278	ILE	CA-CB-CG2	6.53	121.60	110.50
1	E	313	VAL	O-C-N	6.50	130.70	123.10
1	E	249	PRO	CA-N-CD	6.47	121.06	112.00
2	I	3	GLN	CG-CD-NE2	6.45	126.07	116.40
1	E	10	LEU	N-CA-CB	-6.42	100.99	110.49
1	E	302	PHE	CA-CB-CG	-6.38	107.42	113.80
1	E	196	GLY	O-C-N	-6.37	116.83	123.58
1	E	265	ARG	NE-CZ-NH1	6.35	127.85	121.50
1	E	40	VAL	CA-C-O	6.33	127.90	121.63
1	E	238	ALA	O-C-N	6.33	132.82	122.70
1	E	304	ASP	N-CA-C	6.30	118.95	111.71
1	E	322	GLY	O-C-N	-6.29	116.58	123.49
1	E	49	GLU	CA-CB-CG	-6.28	101.54	114.10
1	E	251	SER	CA-C-N	6.27	130.78	120.94
1	E	251	SER	C-N-CA	6.27	130.78	120.94
1	E	37	ASP	CA-CB-CG	-6.27	106.33	112.60
1	E	235	VAL	N-CA-CB	-6.26	104.08	112.10
1	E	47	ALA	N-CA-C	6.26	118.62	111.11
1	E	275	PHE	CZ-CE2-CD2	-6.25	108.76	120.00
1	E	125	PHE	CA-C-O	6.23	128.63	121.47
1	E	125	PHE	CA-CB-CG	-6.22	107.58	113.80
1	E	147	ASP	CA-CB-CG	-6.21	106.39	112.60
1	E	170	ILE	CA-C-O	-6.21	113.88	120.53
1	E	267	VAL	CA-C-N	6.18	126.80	122.60
1	E	267	VAL	C-N-CA	6.18	126.80	122.60
1	E	148	SER	O-C-N	-6.17	115.46	121.94
1	E	304	ASP	CA-CB-CG	6.17	118.77	112.60
1	E	315	ASN	CA-C-O	6.16	127.63	120.98
1	E	246	TYR	CA-C-N	6.16	132.48	122.69
1	E	246	TYR	C-N-CA	6.16	132.48	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	315	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	E	159	ALA	N-CA-CB	-6.12	105.52	111.27
1	E	300	ASN	CA-CB-CG	-6.12	106.48	112.60
1	E	92	GLY	O-C-N	-6.11	117.56	122.51
1	E	203(A)	PHE	CA-C-O	6.11	127.44	120.54
1	E	263	SER	CA-C-O	6.09	127.10	119.12
2	I	3(A)	ARG	CD-NE-CZ	-6.09	115.87	124.40
1	E	309	ALA	CA-C-N	-6.08	112.63	122.36
1	E	309	ALA	C-N-CA	-6.08	112.63	122.36
1	E	308	LYS	CG-CD-CE	6.07	125.25	111.30
1	E	53	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	E	301	ILE	O-C-N	6.02	128.87	123.03
1	E	109	SER	N-CA-C	6.01	118.32	111.11
1	E	65	LEU	O-C-N	-6.00	115.93	123.01
1	E	11	ASP	O-C-N	5.96	130.34	122.47
1	E	133	PRO	CA-N-CD	5.94	119.81	111.50
1	E	26	THR	CA-C-O	5.92	127.24	120.54
1	E	94	LEU	CA-C-O	5.91	126.69	120.36
1	E	17	PRO	CA-N-CD	5.89	120.25	112.00
1	E	95	THR	CA-C-O	5.86	126.92	120.71
1	E	315	ASN	O-C-N	-5.86	114.72	122.57
1	E	70	THR	O-C-N	-5.84	114.94	122.94
1	E	40	VAL	O-C-N	-5.83	116.43	123.02
1	E	266	ILE	O-C-N	5.82	129.37	123.20
1	E	165	TYR	CG-CD2-CE2	-5.79	112.51	121.20
1	E	303	GLY	CA-C-N	-5.74	112.02	120.28
1	E	303	GLY	C-N-CA	-5.74	112.02	120.28
1	E	183	ALA	CA-C-N	-5.72	115.16	123.06
1	E	183	ALA	C-N-CA	-5.72	115.16	123.06
1	E	134(A)	GLN	CG-CD-NE2	5.71	124.97	116.40
1	E	324	ALA	O-C-N	-5.71	116.65	123.27
1	E	85	TYR	CG-CD2-CE2	-5.70	112.65	121.20
1	E	98	GLY	CA-C-N	-5.67	113.30	121.42
1	E	98	GLY	C-N-CA	-5.67	113.30	121.42
1	E	170	ILE	O-C-N	5.67	129.73	123.10
1	E	64	LYS	O-C-N	5.66	129.93	123.31
1	E	34	GLY	O-C-N	-5.65	115.83	122.27
1	E	151	PHE	N-CA-CB	5.64	122.02	111.53
1	E	271	ASP	CB-CG-OD1	5.64	131.37	118.40
1	E	190	TRP	O-C-N	5.61	129.13	122.46
1	E	48	SER	CA-C-O	-5.60	111.77	119.05
1	E	195	THR	CA-C-O	-5.59	112.67	119.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	284	PHE	CA-C-O	5.59	127.34	120.92
1	E	313	VAL	CG1-CB-CG2	-5.58	98.52	110.80
1	E	259	PHE	CZ-CE2-CD2	-5.57	109.98	120.00
1	E	83	ASP	CA-CB-CG	-5.55	107.05	112.60
1	E	201	SER	CA-C-O	-5.54	112.78	119.59
1	E	244	GLY	O-C-N	-5.53	116.36	122.55
1	E	241	SER	O-C-N	-5.52	114.93	122.33
1	E	132	SER	CA-C-O	-5.51	114.23	120.46
1	E	138	PHE	N-CA-C	-5.51	105.28	111.28
1	E	246	TYR	CD1-CG-CD2	5.50	126.36	118.10
1	E	265	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	E	156	GLY	CA-C-N	-5.49	114.89	122.30
1	E	156	GLY	C-N-CA	-5.49	114.89	122.30
1	E	174	ALA	N-CA-CB	-5.48	102.06	110.44
1	E	158	HIS	CA-C-N	-5.48	113.91	122.56
1	E	158	HIS	C-N-CA	-5.48	113.91	122.56
1	E	305	VAL	CA-CB-CG1	5.47	119.70	110.40
1	E	119	GLY	CA-C-O	-5.46	116.26	121.83
1	E	169	PHE	CG-CD1-CE1	5.45	129.96	120.70
1	E	52	GLY	O-C-N	-5.44	116.50	122.65
1	E	233	ALA	N-CA-C	-5.44	105.90	112.54
1	E	68	GLY	CA-C-N	-5.44	114.04	122.09
1	E	68	GLY	C-N-CA	-5.44	114.04	122.09
1	E	281	GLY	CA-C-N	-5.44	111.08	120.97
1	E	281	GLY	C-N-CA	-5.44	111.08	120.97
1	E	218	THR	O-C-N	5.43	129.76	123.30
1	E	257	PHE	CA-C-O	-5.42	114.49	120.24
1	E	158	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	E	315	ASN	CB-CG-ND2	5.41	124.51	116.40
1	E	157	TYR	CG-CD2-CE2	-5.41	113.09	121.20
1	E	204(A)	SER	CA-C-O	5.40	126.36	120.58
1	E	39	TRP	CB-CG-CD1	-5.38	118.83	126.90
1	E	284	PHE	CA-CB-CG	-5.36	108.44	113.80
1	E	129	ASN	OD1-CG-ND2	-5.35	117.25	122.60
2	I	3	GLN	O-C-N	5.35	129.82	123.24
1	E	239	SER	CA-CB-OG	-5.34	100.42	111.10
1	E	269	PRO	CB-CA-C	-5.33	104.41	111.23
1	E	278	ILE	CB-CA-C	5.31	119.31	112.14
1	E	246	TYR	CG-CD1-CE1	-5.30	113.25	121.20
1	E	99	GLN	CA-C-N	-5.30	113.92	121.50
1	E	99	GLN	C-N-CA	-5.30	113.92	121.50
1	E	294	SER	N-CA-C	-5.29	106.60	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	194	SER	N-CA-C	-5.28	103.06	110.50
1	E	192	TRP	CH2-CZ2-CE2	-5.28	110.64	117.50
1	E	167	PHE	CD1-CG-CD2	5.28	126.52	118.60
1	E	190	TRP	CE2-CD2-CE3	5.27	124.07	118.80
1	E	135	GLN	CB-CG-CD	5.26	121.55	112.60
1	E	249	PRO	N-CD-CG	-5.26	95.31	103.20
1	E	202	GLY	CA-C-O	5.26	128.15	122.47
1	E	36	SER	CA-CB-OG	-5.23	100.64	111.10
1	E	6	PRO	CA-N-CD	5.22	119.31	112.00
1	E	39	TRP	CG-CD1-NE1	-5.22	103.41	110.20
1	E	132	SER	N-CA-CB	-5.21	101.54	110.72
1	E	85	TYR	CD1-CG-CD2	5.19	125.88	118.10
1	E	132	SER	O-C-N	5.18	126.26	121.80
1	E	231	TYR	CG-CD2-CE2	5.15	128.93	121.20
1	E	12	ASP	CA-C-O	5.15	126.00	120.55
1	E	232	TRP	O-C-N	5.15	129.33	122.43
1	E	320	THR	O-C-N	-5.14	116.48	122.96
1	E	125	PHE	O-C-N	-5.14	117.15	122.96
1	E	198	ALA	CA-C-N	-5.13	116.82	123.19
1	E	198	ALA	C-N-CA	-5.13	116.82	123.19
1	E	49	GLU	CA-C-O	5.12	125.35	119.35
1	E	13	ALA	CA-C-O	-5.12	115.96	121.38
1	E	299	ILE	CA-C-N	-5.11	112.91	121.39
1	E	299	ILE	C-N-CA	-5.11	112.91	121.39
1	E	302	PHE	CA-C-N	5.09	128.98	121.96
1	E	302	PHE	C-N-CA	5.09	128.98	121.96
1	E	141	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	E	98	GLY	CA-C-O	-5.07	113.00	119.58
1	E	78	GLY	CA-C-O	-5.06	113.58	119.10
1	E	165	TYR	CB-CG-CD1	-5.05	113.23	120.80
1	E	32	ASP	N-CA-CB	-5.05	102.36	110.69
1	E	164	THR	N-CA-CB	-5.04	102.16	111.53
1	E	319(A)	PRO	O-C-N	5.04	129.29	123.14
1	E	67	SER	N-CA-C	5.03	117.85	110.30
1	E	245	GLY	CA-C-N	-5.02	113.74	120.87
1	E	245	GLY	C-N-CA	-5.02	113.74	120.87
1	E	311	PHE	CB-CG-CD1	-5.02	112.17	120.70
2	I	3	GLN	CA-CB-CG	-5.02	104.07	114.10

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 [i](#)

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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	3(A)	ARG

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%)	57	35
2	I	6/6 (100%)	4 (67%)	2 (33%)	0	0
All	All	269/269 (100%)	263 (98%)	6 (2%)	45	22

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

Mol	Chain	Res	Type
1	E	51	ASP
1	E	60	LYS
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 (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	315	ASN
2	I	3	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	329	-	4,4,4	0.27	0	6,6,6	0.54	0
3	SO4	E	328	-	4,4,4	0.16	0	6,6,6	0.69	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 [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.