



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:42 PM UTC

PDB ID : 4ER2 / pdb_00004er2
Title : The active site of aspartic proteinases
Authors : Bailey, D.; Veerapandian, B.; Cooper, J.B.; Blundell, T.L.
Deposited on : 1990-10-20
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

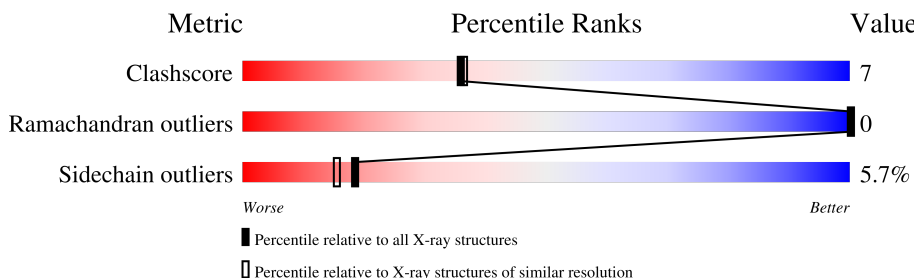
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	51% 42% 7%
2	I	6	67% 17% 17%

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
3	SO4	E	920	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2795 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.

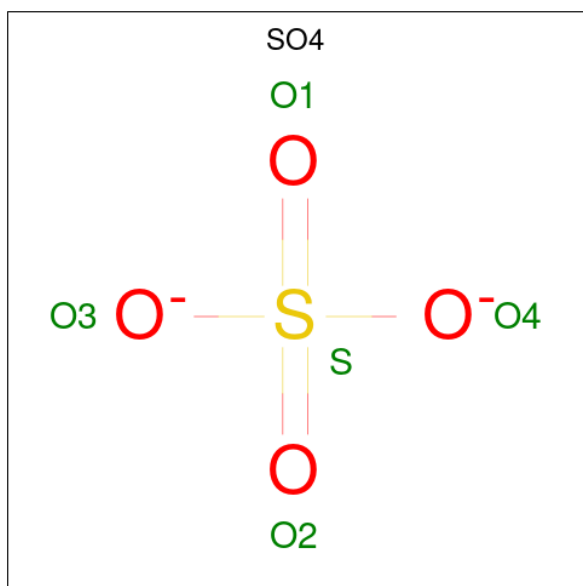
- Molecule 1 is a protein called ENDOTHAPEPSIN.

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 PEPSTATIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			48	34	5	9			

- 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.

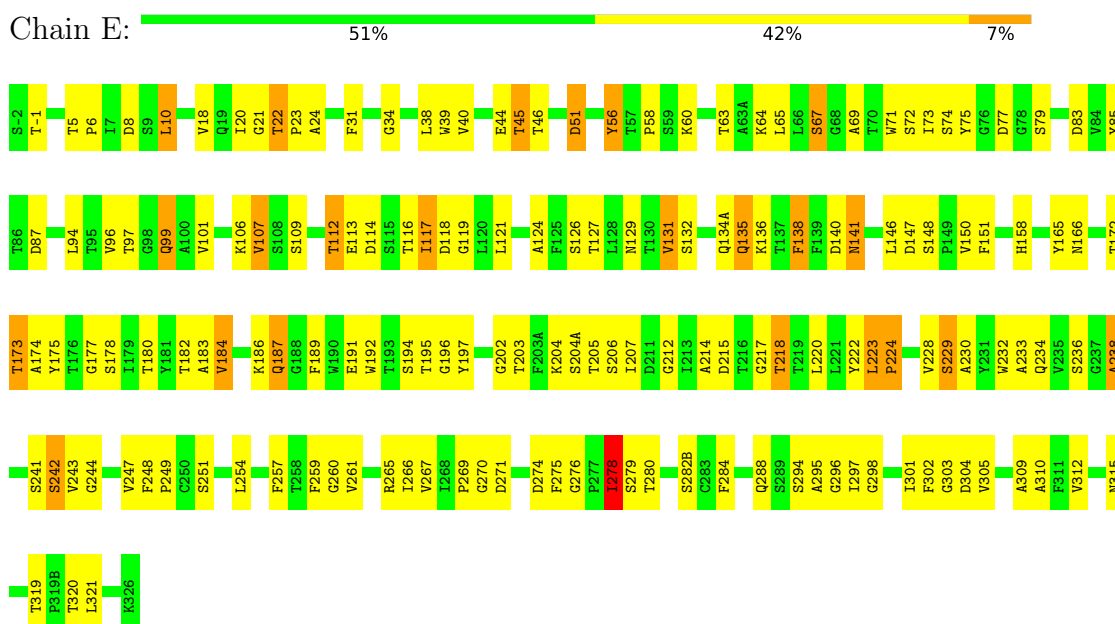
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	338	Total	O	0	0
			338	338		
4	I	5	Total	O	0	0
			5	5		

3 Residue-property plots

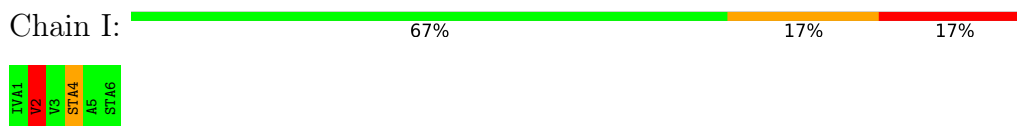
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PEPSTATIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.10 Å 75.60 Å 42.90 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}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2795	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, IVA, STA

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	1.75	38/2445 (1.6%)	2.53	182/3345 (5.4%)
2	I	0.73	0/17	2.50	1/21 (4.8%)
All	All	1.75	38/2462 (1.5%)	2.53	183/3366 (5.4%)

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	4
2	I	0	2
All	All	0	6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	158	HIS	CE1-NE2	9.64	1.42	1.32
1	E	39	TRP	NE1-CE2	-9.35	1.27	1.37
1	E	138	PHE	N-CA	9.29	1.57	1.46
1	E	21	GLY	N-CA	7.09	1.52	1.45
1	E	31	PHE	C-N	-7.00	1.24	1.33
1	E	31	PHE	CA-C	6.86	1.61	1.52
1	E	34	GLY	N-CA	6.69	1.53	1.45
1	E	18	VAL	N-CA	6.56	1.53	1.46
1	E	99	GLN	CD-OE1	6.42	1.35	1.23
1	E	214	ALA	N-CA	6.32	1.54	1.46
1	E	319	THR	N-CA	6.32	1.53	1.45
1	E	158	HIS	ND1-CE1	6.19	1.38	1.32
1	E	134(A)	GLN	CD-OE1	6.17	1.35	1.23
1	E	158	HIS	CD2-NE2	6.16	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	87	ASP	N-CA	6.12	1.53	1.46
1	E	187	GLN	N-CA	6.12	1.53	1.46
1	E	271	ASP	N-CA	6.05	1.53	1.46
1	E	182	THR	N-CA	6.02	1.53	1.45
1	E	124	ALA	N-CA	6.01	1.52	1.46
1	E	65	LEU	N-CA	5.94	1.53	1.46
1	E	166	ASN	CG-OD1	5.83	1.34	1.23
1	E	202	GLY	N-CA	5.68	1.50	1.44
1	E	79	SER	N-CA	5.60	1.52	1.45
1	E	238	ALA	N-CA	5.53	1.53	1.45
1	E	187	GLN	CD-OE1	5.44	1.33	1.23
1	E	116	THR	N-CA	5.38	1.53	1.46
1	E	266	ILE	CA-CB	-5.30	1.47	1.54
1	E	75	TYR	CZ-OH	5.28	1.49	1.38
1	E	234	GLN	CD-OE1	5.26	1.33	1.23
1	E	232	TRP	NE1-CE2	-5.25	1.31	1.37
1	E	233	ALA	N-CA	5.18	1.52	1.46
1	E	136	LYS	N-CA	5.18	1.52	1.45
1	E	218	THR	N-CA	5.15	1.52	1.46
1	E	71	TRP	NE1-CE2	-5.14	1.31	1.37
1	E	266	ILE	N-CA	5.13	1.52	1.46
1	E	180	THR	N-CA	5.10	1.52	1.46
1	E	278	ILE	CA-CB	-5.08	1.47	1.54
1	E	119	GLY	CA-C	-5.07	1.46	1.51

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	PHE	CA-CB-CG	-13.26	100.54	113.80
1	E	196	GLY	CA-C-O	-11.84	112.74	120.91
1	E	302	PHE	CA-C-N	11.51	137.84	121.96
1	E	302	PHE	C-N-CA	11.51	137.84	121.96
1	E	288	GLN	CG-CD-NE2	9.89	131.23	116.40
1	E	51	ASP	CA-CB-CG	9.87	122.47	112.60
1	E	295	ALA	CA-C-N	9.15	130.28	120.03
1	E	295	ALA	C-N-CA	9.15	130.28	120.03
1	E	260	GLY	CA-C-O	-9.14	113.13	121.18
1	E	298	GLY	CA-C-N	-8.94	109.36	122.23
1	E	298	GLY	C-N-CA	-8.94	109.36	122.23
1	E	223	LEU	CA-C-O	-8.83	111.57	120.66
1	E	73	ILE	CA-C-O	-8.79	111.50	120.90
1	E	206	SER	CA-C-N	-8.65	111.18	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	SER	C-N-CA	-8.65	111.18	123.11
1	E	150	VAL	CA-CB-CG1	8.61	125.04	110.40
1	E	304	ASP	CA-CB-CG	-8.61	103.99	112.60
1	E	288	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	E	236	SER	O-C-N	-8.27	112.55	122.22
1	E	241	SER	CA-C-N	8.18	131.24	120.28
1	E	241	SER	C-N-CA	8.18	131.24	120.28
1	E	58	PRO	N-CA-C	-8.13	103.69	113.86
1	E	278	ILE	CA-C-N	8.06	136.60	121.69
1	E	278	ILE	C-N-CA	8.06	136.60	121.69
1	E	305	VAL	O-C-N	-7.78	114.27	121.89
1	E	280	THR	CA-C-O	7.74	129.40	120.96
1	E	284	PHE	CA-C-N	7.66	128.12	120.31
1	E	284	PHE	C-N-CA	7.66	128.12	120.31
1	E	296	GLY	CA-C-O	7.62	128.27	120.80
1	E	56	TYR	O-C-N	-7.55	114.45	123.13
1	E	269	PRO	O-C-N	-7.54	113.81	123.00
1	E	229	SER	CA-C-N	7.45	130.26	120.28
1	E	229	SER	C-N-CA	7.45	130.26	120.28
1	E	138	PHE	CA-C-O	-7.40	112.57	120.42
1	E	186	LYS	CA-C-N	-7.29	111.05	122.49
1	E	186	LYS	C-N-CA	-7.29	111.05	122.49
1	E	274	ASP	CA-C-O	7.27	129.38	121.02
1	E	269	PRO	CB-CA-C	-7.26	101.43	110.95
1	E	97	THR	CA-C-O	-7.24	113.18	121.72
1	E	39	TRP	CG-CD2-CE3	7.24	141.14	133.90
1	E	135	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	E	315	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	E	269	PRO	CA-C-O	7.06	131.11	122.08
1	E	214	ALA	O-C-N	6.96	131.28	122.93
1	E	44	GLU	OE1-CD-OE2	-6.94	106.25	122.90
1	E	151	PHE	CA-CB-CG	6.89	120.69	113.80
1	E	265	ARG	NE-CZ-NH2	6.84	125.36	119.20
1	E	205	THR	CB-CA-C	6.81	121.37	109.80
1	E	107	VAL	CA-CB-CG1	6.79	121.94	110.40
1	E	217	GLY	O-C-N	6.77	131.50	122.70
1	E	224	PRO	N-CA-CB	-6.73	97.07	103.33
1	E	229	SER	CA-C-O	-6.69	113.46	120.55
1	E	296	GLY	O-C-N	-6.68	115.69	122.17
1	E	280	THR	O-C-N	-6.67	115.05	123.06
1	E	140	ASP	CA-CB-CG	-6.64	105.96	112.60
1	E	75	TYR	CA-C-N	6.63	134.40	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	75	TYR	C-N-CA	6.63	134.40	121.41
1	E	138	PHE	N-CA-CB	-6.62	100.36	110.16
1	E	296	GLY	N-CA-C	6.59	120.87	112.83
1	E	135	GLN	CG-CD-NE2	6.58	126.27	116.40
1	E	165	TYR	CA-C-O	6.57	127.54	120.38
1	E	31	PHE	CA-C-O	-6.56	113.19	120.60
1	E	278	ILE	CA-CB-CG2	6.54	121.63	110.50
1	E	203	THR	N-CA-C	-6.50	100.86	110.48
1	E	243	VAL	N-CA-CB	-6.47	100.79	111.98
1	E	45	THR	O-C-N	-6.42	115.03	122.93
1	E	158	HIS	CE1-NE2-CD2	-6.42	102.58	109.00
1	E	60	LYS	N-CA-C	-6.41	104.71	113.30
1	E	173	THR	CA-C-N	-6.39	110.81	122.38
1	E	173	THR	C-N-CA	-6.39	110.81	122.38
1	E	121	LEU	CA-C-N	6.39	126.83	120.31
1	E	121	LEU	C-N-CA	6.39	126.83	120.31
1	E	158	HIS	N-CA-CB	6.31	121.89	112.30
1	E	85	TYR	CA-C-O	-6.27	114.13	121.46
1	E	20	ILE	CA-C-O	-6.25	113.88	120.57
1	E	222	TYR	O-C-N	6.25	130.53	123.27
1	E	320	THR	N-CA-CB	6.25	122.57	111.69
1	E	23	PRO	CA-N-CD	6.23	120.22	111.50
1	E	20	ILE	N-CA-C	6.20	117.23	108.36
1	E	312	VAL	CA-CB-CG2	6.18	120.91	110.40
1	E	44	GLU	CG-CD-OE1	6.14	132.51	118.40
1	E	202	GLY	CA-C-O	-6.13	115.52	122.33
1	E	172	THR	CA-C-N	6.11	130.93	120.72
1	E	172	THR	C-N-CA	6.11	130.93	120.72
1	E	259	PHE	O-C-N	6.11	130.75	123.24
1	E	109	SER	CA-C-O	-6.10	114.08	120.55
1	E	276	GLY	O-C-N	-6.10	115.67	121.77
1	E	230	ALA	N-CA-CB	6.10	119.09	110.12
1	E	172	THR	O-C-N	-6.05	114.11	122.46
1	E	158	HIS	CG-CD2-NE2	6.05	113.25	107.20
1	E	294	SER	CA-C-N	6.04	128.70	120.54
1	E	294	SER	C-N-CA	6.04	128.70	120.54
1	E	83	ASP	CA-C-O	-6.02	114.50	121.49
1	E	87	ASP	CA-CB-CG	-5.99	106.61	112.60
1	E	236	SER	N-CA-C	5.97	118.58	111.71
1	E	5	THR	N-CA-CB	-5.97	99.15	110.49
1	E	77	ASP	CA-C-N	-5.95	113.17	122.51
1	E	77	ASP	C-N-CA	-5.95	113.17	122.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	312	VAL	O-C-N	5.94	129.62	123.20
1	E	305	VAL	CA-C-O	5.90	127.18	121.05
1	E	77	ASP	O-C-N	-5.86	114.87	122.37
1	E	275	PHE	CB-CG-CD1	-5.83	110.79	120.70
1	E	315	ASN	CB-CG-ND2	5.81	125.11	116.40
1	E	243	VAL	O-C-N	-5.74	116.61	122.23
1	E	223	LEU	N-CA-CB	5.71	120.61	110.39
2	I	2	VAL	CA-CB-CG2	5.71	120.11	110.40
1	E	205	THR	O-C-N	-5.68	116.45	123.44
1	E	175	TYR	O-C-N	-5.68	115.23	122.78
1	E	40	VAL	N-CA-C	5.67	116.91	108.46
1	E	109	SER	CA-C-N	-5.67	111.69	120.31
1	E	109	SER	C-N-CA	-5.67	111.69	120.31
1	E	244	GLY	CA-C-N	-5.67	114.46	121.83
1	E	244	GLY	C-N-CA	-5.67	114.46	121.83
1	E	147	ASP	CA-CB-CG	-5.65	106.95	112.60
1	E	295	ALA	CA-C-O	-5.65	114.85	120.90
1	E	282(B)	SER	CA-C-O	-5.64	114.54	120.80
1	E	309	ALA	N-CA-CB	-5.64	101.81	110.44
1	E	6	PRO	N-CA-C	5.63	119.93	111.14
1	E	127	THR	CA-C-O	5.61	126.28	119.38
1	E	261	VAL	O-C-N	5.61	128.99	122.99
1	E	228	VAL	N-CA-C	5.60	115.79	110.42
1	E	67	SER	CA-C-N	-5.57	114.33	122.46
1	E	67	SER	C-N-CA	-5.57	114.33	122.46
1	E	22	THR	C-N-CD	-5.57	108.36	120.60
1	E	267	VAL	CA-CB-CG2	5.56	119.85	110.40
1	E	242	SER	N-CA-CB	5.55	118.28	110.12
1	E	138	PHE	N-CA-C	-5.54	105.32	111.36
1	E	126	SER	CA-C-O	5.52	126.05	119.10
1	E	195	THR	O-C-N	-5.51	114.59	122.41
1	E	24	ALA	CA-C-N	5.50	130.09	122.77
1	E	24	ALA	C-N-CA	5.50	130.09	122.77
1	E	131	VAL	O-C-N	5.50	129.21	122.72
1	E	112	THR	N-CA-C	-5.49	105.38	111.36
1	E	173	THR	N-CA-CB	5.47	119.48	110.39
1	E	34	GLY	O-C-N	-5.46	116.05	122.27
1	E	18	VAL	CA-CB-CG1	5.46	119.67	110.40
1	E	310	ALA	N-CA-C	5.45	118.14	109.81
1	E	-1	THR	CA-C-O	5.44	127.44	121.40
1	E	119	GLY	CA-C-O	-5.43	116.30	121.83
1	E	58	PRO	O-C-N	5.41	129.66	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	69	ALA	CA-C-N	5.40	132.70	123.03
1	E	69	ALA	C-N-CA	5.40	132.70	123.03
1	E	148	SER	CA-C-O	-5.40	114.72	120.28
1	E	72	SER	CA-C-N	-5.35	113.85	122.25
1	E	72	SER	C-N-CA	-5.35	113.85	122.25
1	E	284	PHE	CB-CG-CD1	-5.32	111.66	120.70
1	E	74	SER	CA-C-O	5.28	127.62	121.44
1	E	197	TYR	N-CA-C	5.28	117.11	108.76
1	E	305	VAL	CA-C-N	5.28	129.44	120.88
1	E	305	VAL	C-N-CA	5.28	129.44	120.88
1	E	302	PHE	CA-C-O	-5.25	115.51	121.66
1	E	174	ALA	N-CA-C	-5.23	106.68	113.16
1	E	118	ASP	N-CA-C	-5.22	106.59	113.17
1	E	212	GLY	O-C-N	5.22	129.76	123.55
1	E	65	LEU	CA-C-O	-5.21	114.82	120.81
1	E	319	THR	N-CA-CB	-5.20	102.42	110.07
1	E	39	TRP	CE2-CD2-CE3	-5.18	113.62	118.80
1	E	6	PRO	O-C-N	-5.18	116.76	123.03
1	E	126	SER	O-C-N	-5.17	115.55	122.43
1	E	73	ILE	CA-C-N	-5.17	114.48	122.59
1	E	73	ILE	C-N-CA	-5.17	114.48	122.59
1	E	321	LEU	N-CA-CB	-5.16	102.38	110.69
1	E	207	ILE	N-CA-CB	-5.16	105.50	112.10
1	E	24	ALA	O-C-N	-5.16	116.50	122.89
1	E	234	GLN	OE1-CD-NE2	5.14	127.74	122.60
1	E	165	TYR	O-C-N	-5.14	117.23	123.29
1	E	113	GLU	CA-C-O	5.13	125.69	119.38
1	E	121	LEU	CA-C-O	-5.12	115.02	120.40
1	E	184	VAL	N-CA-CB	-5.12	102.49	111.39
1	E	183	ALA	CA-C-N	-5.11	116.01	123.06
1	E	183	ALA	C-N-CA	-5.11	116.01	123.06
1	E	113	GLU	CA-C-N	-5.10	115.59	123.14
1	E	113	GLU	C-N-CA	-5.10	115.59	123.14
1	E	113	GLU	O-C-N	-5.05	115.66	122.43
1	E	224	PRO	CA-C-N	5.04	128.39	120.82
1	E	224	PRO	C-N-CA	5.04	128.39	120.82
1	E	270	GLY	CA-C-N	-5.03	113.03	120.28
1	E	270	GLY	C-N-CA	-5.03	113.03	120.28
1	E	117	ILE	CB-CG1-CD1	5.03	124.36	113.80
1	E	94	LEU	CA-C-O	-5.03	115.22	120.80
1	E	215	ASP	O-C-N	-5.02	115.44	122.87
1	E	8	ASP	CA-C-N	5.02	131.98	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	ASP	C-N-CA	5.02	131.98	121.94

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	101	VAL	Mainchain
1	E	22	THR	Peptide
1	E	257	PHE	Mainchain
1	E	56	TYR	Mainchain
2	I	4	STA	Peptide,Mainchain

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	35	1
2	I	48	0	60	1	0
3	E	15	0	0	2	5
4	E	338	0	0	2	7
4	I	5	0	0	0	0
All	All	2795	0	2340	35	8

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 7.

All (35) 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:187:GLN:HG3	1:E:187:GLN:O	1.54	1.03
1:E:51:ASP:OD1	1:E:112:THR:HG22	1.76	0.86
1:E:187:GLN:HG2	1:E:189:PHE:CD1	2.15	0.81
1:E:129:ASN:ND2	1:E:135:GLN:H	1.86	0.73
1:E:106:LYS:HE2	4:E:1264:HOH:O	1.91	0.69
1:E:220:LEU:O	1:E:303:GLY:HA3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LEU:N	1:E:10:LEU:HD23	2.11	0.66
1:E:187:GLN:HG2	1:E:189:PHE:HD1	1.57	0.64
1:E:248:PHE:CZ	1:E:254:LEU:HD11	2.38	0.59
1:E:192:TRP:CH2	1:E:194:SER:HB2	2.39	0.57
1:E:51:ASP:OD1	1:E:112:THR:CG2	2.53	0.55
1:E:129:ASN:HD22	1:E:135:GLN:H	1.55	0.55
1:E:10:LEU:N	1:E:10:LEU:CD2	2.70	0.54
1:E:187:GLN:HG2	1:E:189:PHE:CE1	2.42	0.54
1:E:96:VAL:HG11	1:E:141:ASN:HB3	1.92	0.51
1:E:10:LEU:HD22	4:E:967:HOH:O	2.11	0.50
1:E:38:LEU:C	1:E:38:LEU:HD23	2.38	0.49
1:E:297:ILE:HG21	1:E:301:ILE:HD11	1.95	0.48
1:E:187:GLN:CG	1:E:189:PHE:CD1	2.94	0.47
1:E:297:ILE:HD13	1:E:301:ILE:HD12	1.97	0.46
1:E:238:ALA:HA	1:E:247:VAL:O	2.16	0.46
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.31	0.46
1:E:132:SER:OG	3:E:920:SO4:O4	2.32	0.45
1:E:187:GLN:CG	1:E:189:PHE:CE1	3.00	0.45
1:E:249:PRO:C	1:E:251:SER:H	2.24	0.44
1:E:247:VAL:CG1	1:E:278:ILE:HD11	2.48	0.44
1:E:247:VAL:HG12	1:E:278:ILE:HD11	2.00	0.43
1:E:178:SER:HA	3:E:930:SO4:O2	2.19	0.42
1:E:249:PRO:C	1:E:251:SER:N	2.75	0.42
1:E:223:LEU:HB3	1:E:224:PRO:CD	2.50	0.41
1:E:114:ASP:OD2	1:E:117:ILE:HD12	2.19	0.41
1:E:184:VAL:HA	1:E:191:GLU:O	2.20	0.41
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.86	0.41
1:E:45:THR:O	1:E:46:THR:C	2.63	0.40
1:E:218:THR:HA	2:I:2:VAL:O	2.22	0.40

All (8) 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)
3:E:920:SO4:S	4:E:1087:HOH:O[2_556]	0.61	1.59
3:E:920:SO4:O2	4:E:1087:HOH:O[2_556]	0.97	1.23
3:E:920:SO4:O3	4:E:1087:HOH:O[2_556]	1.60	0.60
3:E:920:SO4:O4	4:E:1087:HOH:O[2_556]	1.61	0.59
4:E:1033:HOH:O	4:E:1119:HOH:O[2_545]	1.85	0.35
4:E:1084:HOH:O	4:E:1190:HOH:O[2_555]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:920:SO4:O1	4:E:1087:HOH:O[2_556]	1.96	0.24
1:E:64:LYS:NZ	1:E:177:GLY:O[2_655]	2.16	0.04

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%)	318 (97%)	10 (3%)	0	100	100
2	I	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	331/336 (98%)	320 (97%)	11 (3%)	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	242/263 (92%)	229 (95%)	13 (5%)	20	17
2	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	244/265 (92%)	230 (94%)	14 (6%)	18	15

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	10	LEU

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Mol	Chain	Res	Type
1	E	63	THR
1	E	67	SER
1	E	107	VAL
1	E	141	ASN
1	E	146	LEU
1	E	173	THR
1	E	204	LYS
1	E	204(A)	SER
1	E	229	SER
1	E	242	SER
1	E	278	ILE
1	E	279	SER
2	I	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) 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	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	STA	I	4	2	10,10,11	1.24	1 (10%)	9,12,14	1.83	1 (11%)
2	STA	I	6	2	11,11,11	0.89	0	11,14,14	0.43	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	STA	I	4	2	-	3/11/11/12	-
2	STA	I	6	2	-	1/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	STA	CD2-CG	2.86	1.66	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	STA	O-C-CM	-4.37	112.66	125.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	4	STA	CA-CH-CM-C
2	I	4	STA	OH-CH-CM-C
2	I	4	STA	O-C-CM-CH
2	I	6	STA	N-CA-CB-CG

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	920	-	4,4,4	0.23	0	6,6,6	0.29	0
3	SO4	E	910	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	E	930	-	4,4,4	0.33	0	6,6,6	0.31	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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	920	SO4	1	5
3	E	930	SO4	1	0

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.