



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:02 PM UTC

PDB ID : 1ESC / pdb_00001esc
Title : THE MOLECULAR MECHANISM OF ENANTIORECOGNITION BY ESTERASES
Authors : Wei, Y.; Schottel, J.L.; Derewenda, U.; Swenson, L.; Patkar, S.; Derewenda, Z.S.
Deposited on : 1994-10-07
Resolution : 2.10 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
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

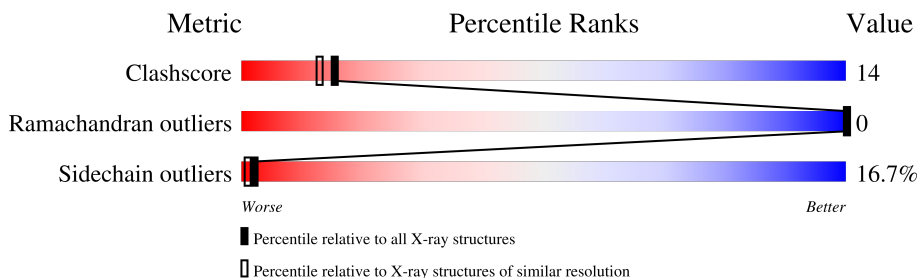
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	A	306	 44% 36% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2518 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 ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2295	1442	390	456	7			

- Molecule 2 is water.

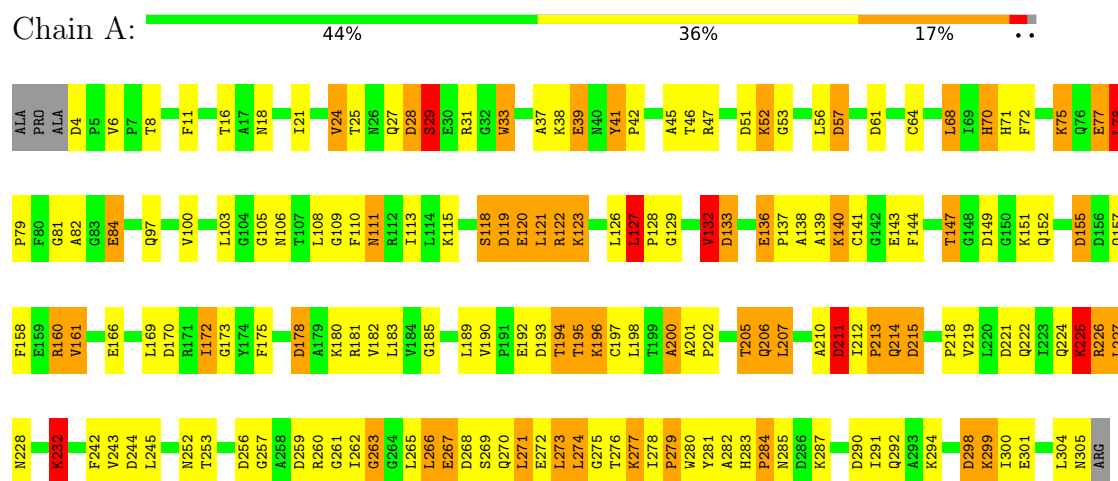
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	223	Total	O	0	0
			223	223		

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: ESTERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.03Å 48.50Å 70.31Å 90.00° 118.09° 90.00°	Depositor
Resolution (Å)	7.50 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2518	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	A	1.01	1/2344 (0.0%)	2.53	182/3185 (5.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	LEU	N-CA	5.50	1.53	1.46

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	CD-NE-CZ	20.34	152.87	124.40
1	A	215	ASP	CA-CB-CG	16.06	128.66	112.60
1	A	160	ARG	CD-NE-CZ	13.50	143.30	124.40
1	A	127	LEU	O-C-N	11.89	132.36	121.19
1	A	136	GLU	CB-CA-C	10.08	125.51	109.27
1	A	28	ASP	CA-CB-CG	9.70	122.30	112.60
1	A	28	ASP	N-CA-CB	-9.68	96.27	110.70
1	A	213	PRO	CA-C-N	9.27	133.91	120.38
1	A	213	PRO	C-N-CA	9.27	133.91	120.38
1	A	57	ASP	CA-CB-CG	9.15	121.75	112.60
1	A	192	GLU	CA-CB-CG	9.11	132.33	114.10
1	A	149	ASP	CA-CB-CG	9.08	121.68	112.60
1	A	31	ARG	NE-CZ-NH2	-8.98	111.12	119.20
1	A	151	LYS	CA-C-O	-8.94	110.97	120.63
1	A	262	ILE	CA-C-O	-8.90	110.69	120.48
1	A	206	GLN	OE1-CD-NE2	8.61	131.21	122.60
1	A	232	LYS	CA-CB-CG	8.60	131.29	114.10
1	A	178	ASP	CA-CB-CG	8.55	121.15	112.60
1	A	6	VAL	N-CA-C	-8.42	99.81	108.15
1	A	256	ASP	CA-CB-CG	-8.42	104.18	112.60
1	A	173	GLY	CA-C-N	8.42	131.89	120.44
1	A	173	GLY	C-N-CA	8.42	131.89	120.44
1	A	206	GLN	CA-CB-CG	-8.34	97.42	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	THR	CA-C-O	-8.26	111.44	121.11
1	A	136	GLU	N-CA-C	-8.11	98.88	110.08
1	A	147	THR	N-CA-CB	-8.11	98.36	111.18
1	A	27	GLN	CA-CB-CG	8.07	130.24	114.10
1	A	225	LYS	CA-C-N	7.99	131.33	120.54
1	A	225	LYS	C-N-CA	7.99	131.33	120.54
1	A	82	ALA	O-C-N	7.96	130.60	122.08
1	A	274	LEU	CB-CA-C	7.93	124.92	110.88
1	A	298	ASP	CA-C-N	7.93	131.24	120.38
1	A	298	ASP	C-N-CA	7.93	131.24	120.38
1	A	61	ASP	N-CA-C	-7.91	92.17	107.44
1	A	292	GLN	O-C-N	7.83	130.17	122.03
1	A	52	LYS	N-CA-C	-7.80	102.82	112.88
1	A	31	ARG	NE-CZ-NH1	7.73	129.23	121.50
1	A	81	GLY	O-C-N	7.62	130.44	122.51
1	A	205	THR	N-CA-C	-7.62	104.51	113.88
1	A	143	GLU	CB-CG-CD	7.59	125.50	112.60
1	A	72	PHE	N-CA-C	-7.58	103.10	111.36
1	A	155	ASP	CA-C-O	-7.52	111.32	119.97
1	A	270	GLN	CG-CD-OE1	7.49	135.78	120.80
1	A	161	VAL	CA-C-N	7.45	128.25	119.98
1	A	161	VAL	C-N-CA	7.45	128.25	119.98
1	A	211	ASP	CA-CB-CG	7.44	120.04	112.60
1	A	172	ILE	CA-C-N	7.42	128.34	120.03
1	A	172	ILE	C-N-CA	7.42	128.34	120.03
1	A	132	VAL	CB-CA-C	7.24	123.16	111.29
1	A	194	THR	CA-CB-OG1	-7.19	98.81	109.60
1	A	147	THR	CB-CA-C	7.14	118.78	109.28
1	A	123	LYS	N-CA-CB	7.11	117.99	109.74
1	A	11	PHE	CA-C-O	-6.98	113.98	121.45
1	A	277	LYS	O-C-N	6.96	131.23	123.01
1	A	242	PHE	CA-CB-CG	6.90	120.70	113.80
1	A	283	HIS	N-CA-CB	6.88	119.64	109.88
1	A	133	ASP	N-CA-CB	6.79	120.54	110.49
1	A	228	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	305	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	206	GLN	O-C-N	6.71	130.61	123.03
1	A	291	ILE	CA-C-N	6.69	129.48	120.65
1	A	291	ILE	C-N-CA	6.69	129.48	120.65
1	A	45	ALA	CA-C-O	-6.65	113.83	120.82
1	A	267	GLU	CA-C-O	-6.65	114.31	121.56
1	A	111	ASN	CA-CB-CG	-6.65	105.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	GLU	CA-C-O	-6.60	113.52	120.58
1	A	170	ASP	CA-C-O	-6.55	112.06	119.79
1	A	155	ASP	N-CA-CB	6.55	120.43	110.28
1	A	252	ASN	CA-CB-CG	-6.54	106.06	112.60
1	A	119	ASP	N-CA-CB	6.51	120.25	110.22
1	A	61	ASP	N-CA-CB	6.48	122.16	110.95
1	A	206	GLN	N-CA-CB	6.47	120.65	110.56
1	A	259	ASP	CA-C-N	6.37	129.75	120.71
1	A	259	ASP	C-N-CA	6.37	129.75	120.71
1	A	252	ASN	N-CA-CB	6.36	120.76	111.54
1	A	214	GLN	CA-C-N	6.34	131.46	120.68
1	A	214	GLN	C-N-CA	6.34	131.46	120.68
1	A	279	PRO	CA-C-N	6.33	129.05	120.44
1	A	279	PRO	C-N-CA	6.33	129.05	120.44
1	A	71	HIS	CA-CB-CG	-6.29	107.50	113.80
1	A	292	GLN	N-CA-C	-6.27	104.14	110.97
1	A	118	SER	CA-C-N	6.26	129.30	120.28
1	A	118	SER	C-N-CA	6.26	129.30	120.28
1	A	178	ASP	N-CA-CB	-6.26	101.16	110.61
1	A	16	THR	CA-C-O	6.25	126.30	119.24
1	A	18	ASN	CB-CG-ND2	6.24	125.76	116.40
1	A	263	GLY	O-C-N	-6.19	114.90	122.76
1	A	275	GLY	N-CA-C	-6.14	98.63	113.18
1	A	270	GLN	CG-CD-NE2	-6.11	107.24	116.40
1	A	53	GLY	N-CA-C	6.10	123.78	115.30
1	A	205	THR	CA-C-N	-6.09	111.66	122.74
1	A	205	THR	C-N-CA	-6.09	111.66	122.74
1	A	232	LYS	CA-C-N	6.08	128.34	120.44
1	A	232	LYS	C-N-CA	6.08	128.34	120.44
1	A	57	ASP	CB-CA-C	6.04	121.46	111.31
1	A	29	SER	CA-C-O	-6.03	114.71	121.40
1	A	21	ILE	CB-CA-C	6.00	119.43	111.21
1	A	228	ASN	CA-C-O	-6.00	114.52	120.82
1	A	155	ASP	N-CA-C	-5.97	104.89	111.82
1	A	183	LEU	CA-C-O	-5.92	113.80	120.43
1	A	84	GLU	O-C-N	5.92	130.34	123.30
1	A	122	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	11	PHE	O-C-N	5.90	129.89	123.10
1	A	110	PHE	CA-C-N	5.90	128.19	120.28
1	A	110	PHE	C-N-CA	5.90	128.19	120.28
1	A	227	LEU	N-CA-C	-5.88	104.87	111.28
1	A	277	LYS	N-CA-C	-5.87	100.92	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	GLU	CA-C-O	-5.84	114.05	120.36
1	A	290	ASP	CA-C-O	-5.82	112.92	119.79
1	A	195	THR	CB-CA-C	5.81	120.56	110.68
1	A	155	ASP	O-C-N	5.80	129.40	122.27
1	A	273	LEU	CA-C-O	-5.80	112.22	120.51
1	A	25	THR	CA-CB-OG1	-5.78	100.94	109.60
1	A	180	LYS	N-CA-C	-5.75	100.62	109.76
1	A	285	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	84	GLU	CA-CB-CG	5.72	125.53	114.10
1	A	219	VAL	CA-C-O	5.68	126.79	120.71
1	A	143	GLU	O-C-N	5.68	129.76	122.03
1	A	75	LYS	N-CA-CB	5.66	118.29	109.85
1	A	39	GLU	CA-CB-CG	5.66	125.42	114.10
1	A	175	PHE	CA-C-N	5.66	129.07	122.85
1	A	175	PHE	C-N-CA	5.66	129.07	122.85
1	A	284	PRO	CA-C-O	5.65	127.78	121.34
1	A	228	ASN	O-C-N	5.65	127.89	122.07
1	A	270	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	268	ASP	O-C-N	5.60	129.59	123.04
1	A	273	LEU	CA-C-N	-5.60	113.75	122.42
1	A	273	LEU	C-N-CA	-5.60	113.75	122.42
1	A	78	LEU	O-C-N	5.59	127.80	121.53
1	A	205	THR	CB-CA-C	5.58	118.06	109.03
1	A	275	GLY	CA-C-N	-5.57	113.11	122.29
1	A	275	GLY	C-N-CA	-5.57	113.11	122.29
1	A	28	ASP	N-CA-C	5.54	119.04	112.72
1	A	292	GLN	N-CA-CB	5.51	117.95	109.91
1	A	274	LEU	N-CA-C	-5.49	104.21	111.96
1	A	64	CYS	O-C-N	5.48	129.73	123.48
1	A	33	TRP	CA-CB-CG	-5.47	103.21	113.60
1	A	6	VAL	N-CA-CB	5.46	116.98	111.36
1	A	75	LYS	CB-CA-C	-5.45	101.17	109.89
1	A	212	ILE	O-C-N	5.43	127.29	121.10
1	A	214	GLN	CA-C-O	5.42	126.27	120.20
1	A	268	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	127	LEU	CA-C-O	-5.38	114.84	119.36
1	A	56	LEU	CA-C-O	-5.36	114.58	120.69
1	A	290	ASP	N-CA-CB	5.36	118.55	110.30
1	A	224	GLN	N-CA-CB	5.35	118.17	110.20
1	A	133	ASP	CB-CA-C	-5.33	102.72	111.68
1	A	37	ALA	CA-C-N	5.33	127.42	120.28
1	A	37	ALA	C-N-CA	5.33	127.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CB-CA-C	5.30	118.75	111.23
1	A	79	PRO	CA-C-N	5.29	131.64	121.54
1	A	79	PRO	C-N-CA	5.29	131.64	121.54
1	A	290	ASP	O-C-N	5.29	129.42	122.33
1	A	29	SER	O-C-N	5.29	129.81	122.78
1	A	120	GLU	CA-CB-CG	5.28	124.65	114.10
1	A	214	GLN	N-CA-CB	-5.28	101.80	110.14
1	A	291	ILE	CA-C-O	5.28	126.44	120.95
1	A	105	GLY	CA-C-O	-5.27	115.63	120.80
1	A	51	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	108	LEU	CA-C-O	5.23	126.31	120.82
1	A	222	GLN	N-CA-C	-5.23	105.48	111.07
1	A	56	LEU	CA-C-N	-5.21	115.60	122.85
1	A	56	LEU	C-N-CA	-5.21	115.60	122.85
1	A	27	GLN	CA-C-N	5.21	131.11	122.73
1	A	27	GLN	C-N-CA	5.21	131.11	122.73
1	A	97	GLN	CA-CB-CG	5.20	124.51	114.10
1	A	82	ALA	N-CA-C	-5.20	104.67	111.02
1	A	77	GLU	CA-CB-CG	5.19	124.47	114.10
1	A	190	VAL	CA-C-O	-5.18	115.86	119.38
1	A	147	THR	CA-CB-OG1	-5.14	101.88	109.60
1	A	270	GLN	CB-CG-CD	5.14	121.33	112.60
1	A	79	PRO	N-CA-CB	5.13	107.81	103.35
1	A	218	PRO	CA-C-N	5.12	128.74	120.55
1	A	218	PRO	C-N-CA	5.12	128.74	120.55
1	A	152	GLN	N-CA-CB	5.09	117.97	110.33
1	A	160	ARG	N-CA-C	-5.06	105.85	111.36
1	A	173	GLY	O-C-N	-5.05	117.27	122.17
1	A	221	ASP	CA-C-N	5.05	127.01	120.44
1	A	221	ASP	C-N-CA	5.05	127.01	120.44
1	A	200	ALA	N-CA-C	-5.04	102.30	110.32
1	A	46	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	24	VAL	N-CA-CB	-5.00	101.64	110.95

There are no chirality outliers.

There are no planarity outliers.

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	A	2295	0	2211	61	0
2	A	223	0	0	7	0
All	All	2518	0	2211	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (61) 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:A:272:GLU:HA	1:A:276:THR:O	1.77	0.82
1:A:195:THR:HA	1:A:198:LEU:HD12	1.69	0.74
1:A:172:ILE:HG21	1:A:181:ARG:HG2	1.79	0.64
1:A:158:PHE:CZ	1:A:226:ARG:HD2	2.37	0.60
1:A:225:LYS:HD3	2:A:437:HOH:O	2.02	0.58
1:A:257:GLY:O	1:A:260:ARG:NH1	2.31	0.58
1:A:169:LEU:O	1:A:181:ARG:NH1	2.37	0.58
1:A:263:GLY:HA3	1:A:280:TRP:CD1	2.38	0.58
1:A:121:LEU:HD22	1:A:265:LEU:HD21	1.85	0.57
1:A:133:ASP:HB3	1:A:136:GLU:HB2	1.86	0.57
1:A:300:ILE:O	1:A:304:LEU:HG	2.09	0.53
1:A:193:ASP:O	1:A:196:LYS:HG3	2.07	0.53
1:A:200:ALA:HB3	2:A:621:HOH:O	2.08	0.53
1:A:195:THR:O	1:A:198:LEU:HB2	2.10	0.52
1:A:267:GLU:O	1:A:279:PRO:HA	2.09	0.52
1:A:29:SER:HA	2:A:573:HOH:O	2.10	0.52
1:A:269:SER:OG	1:A:271:LEU:HB2	2.10	0.52
1:A:178:ASP:HB2	2:A:500:HOH:O	2.09	0.52
1:A:194:THR:HG22	1:A:214:GLN:OE1	2.11	0.50
1:A:197:CYS:O	1:A:207:LEU:HD13	2.12	0.50
1:A:115:LYS:NZ	1:A:127:LEU:O	2.38	0.50
1:A:158:PHE:CE2	1:A:226:ARG:HD2	2.47	0.49
1:A:185:GLY:O	1:A:245:LEU:HD12	2.11	0.49
1:A:111:ASN:HD22	1:A:129:GLY:HA3	1.76	0.49
1:A:41:TYR:CG	1:A:42:PRO:HD3	2.48	0.49
1:A:33:TRP:HB2	1:A:78:LEU:HG	1.93	0.49
1:A:158:PHE:CZ	1:A:226:ARG:HB3	2.49	0.48
1:A:226:ARG:HD3	2:A:609:HOH:O	2.14	0.47
1:A:276:THR:HG22	1:A:277:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASP:OD1	1:A:195:THR:OG1	2.29	0.47
1:A:137:PRO:O	1:A:138:ALA:C	2.58	0.46
1:A:120:GLU:HB2	1:A:211:ASP:OD2	2.15	0.46
1:A:39:GLU:OE1	1:A:47:ARG:NH2	2.48	0.46
1:A:206:GLN:HG2	1:A:207:LEU:H	1.81	0.45
1:A:119:ASP:HA	1:A:122:ARG:HG3	1.98	0.45
1:A:133:ASP:HB2	1:A:144:PHE:CE1	2.52	0.45
1:A:263:GLY:HA3	1:A:280:TRP:CG	2.52	0.45
1:A:70:HIS:C	1:A:70:HIS:CD2	2.95	0.45
1:A:132:VAL:HG22	1:A:144:PHE:CZ	2.51	0.45
1:A:68:LEU:HD22	1:A:106:ASN:HB3	1.99	0.45
1:A:126:LEU:HD12	1:A:278:ILE:HD12	1.98	0.45
1:A:157:GLN:O	1:A:161:VAL:HG23	2.18	0.44
1:A:139:ALA:HA	1:A:213:PRO:HG3	1.99	0.44
1:A:157:GLN:NE2	2:A:512:HOH:O	2.47	0.44
1:A:201:ALA:O	1:A:202:PRO:C	2.61	0.43
1:A:243:VAL:HG22	1:A:299:LYS:HG2	2.01	0.43
1:A:298:ASP:O	1:A:301:GLU:HB3	2.20	0.42
1:A:52:LYS:HD2	2:A:552:HOH:O	2.20	0.41
1:A:120:GLU:HG2	1:A:266:LEU:HD21	2.02	0.41
1:A:232:LYS:NZ	1:A:244:ASP:OD2	2.53	0.41
1:A:210:ALA:HB2	1:A:266:LEU:CD2	2.51	0.41
1:A:127:LEU:HD22	1:A:128:PRO:HD2	2.03	0.41
1:A:158:PHE:HE1	1:A:227:LEU:HA	1.86	0.41
1:A:140:LYS:HE3	1:A:140:LYS:HB3	1.94	0.40
1:A:261:GLY:O	1:A:284:PRO:HA	2.21	0.40
1:A:281:TYR:O	1:A:282:ALA:HB3	2.21	0.40
1:A:210:ALA:HB2	1:A:266:LEU:HD22	2.02	0.40
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.95	0.40
1:A:109:GLY:O	1:A:113:ILE:HG13	2.20	0.40
1:A:100:VAL:HG22	1:A:182:VAL:HB	2.02	0.40
1:A:253:THR:O	1:A:260:ARG:HA	2.22	0.40

There are no symmetry-related clashes.

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	A	300/306 (98%)	275 (92%)	25 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	A	239/241 (99%)	199 (83%)	40 (17%)	2	1

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	24	VAL
1	A	28	ASP
1	A	29	SER
1	A	38	LYS
1	A	41	TYR
1	A	57	ASP
1	A	68	LEU
1	A	70	HIS
1	A	75	LYS
1	A	77	GLU
1	A	78	LEU
1	A	84	GLU
1	A	118	SER
1	A	121	LEU
1	A	123	LYS
1	A	127	LEU
1	A	132	VAL
1	A	140	LYS

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Mol	Chain	Res	Type
1	A	141	CYS
1	A	147	THR
1	A	155	ASP
1	A	160	ARG
1	A	166	GLU
1	A	189	LEU
1	A	196	LYS
1	A	205	THR
1	A	207	LEU
1	A	211	ASP
1	A	215	ASP
1	A	225	LYS
1	A	226	ARG
1	A	232	LYS
1	A	266	LEU
1	A	271	LEU
1	A	273	LEU
1	A	274	LEU
1	A	287	LYS
1	A	294	LYS
1	A	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN

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

There are no ligands in this entry.

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.