



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:43 AM UTC

PDB ID : 1ESE / pdb_00001ese
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 : 2.40 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

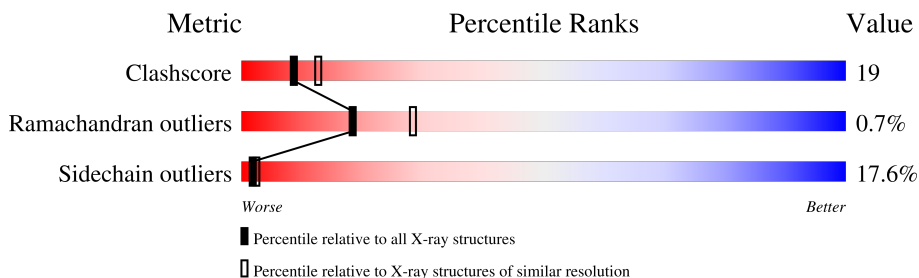
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	

2 Entry composition [i](#)

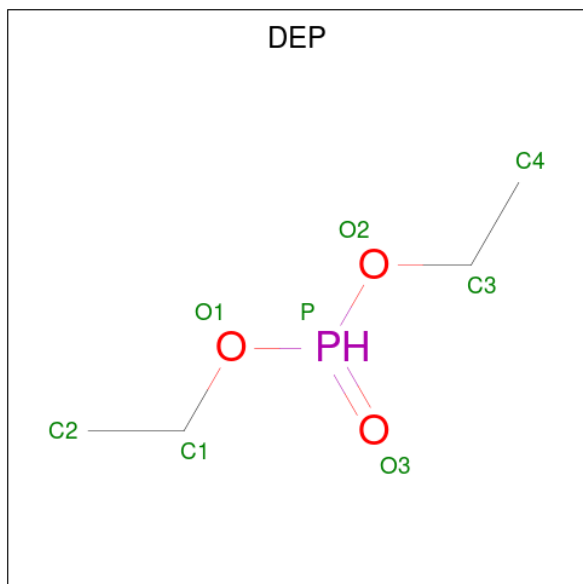
There are 3 unique types of molecules in this entry. The entry contains 2476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIETHYL PHOSPHONATE (CCD ID: DEP) (formula: $C_4H_{11}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			8	4	3	1		

- Molecule 3 is water.

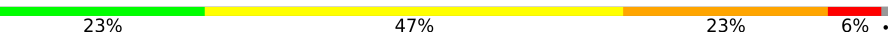
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total	O	0	0
			173	173		

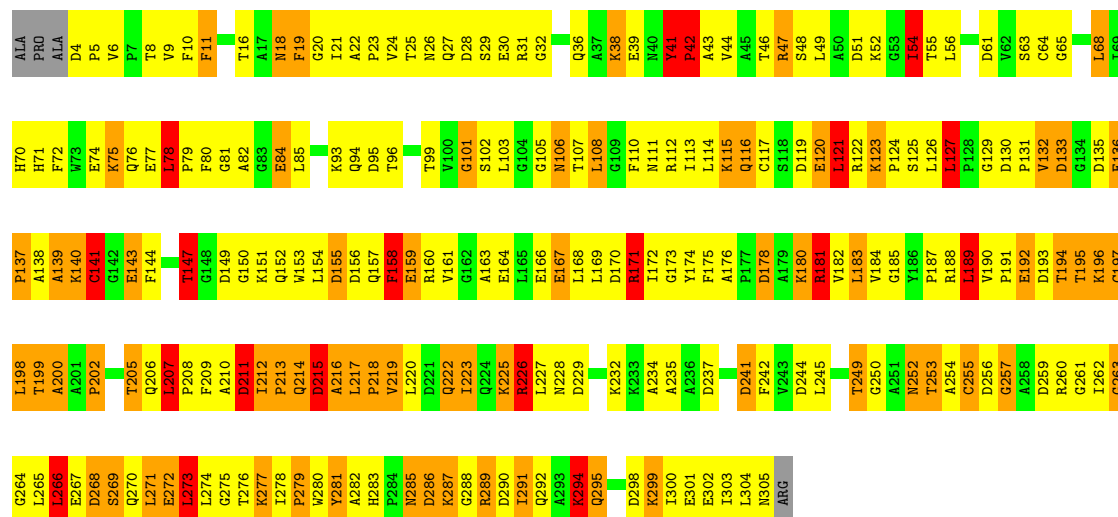
3 Residue-property plots

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

Chain A: 



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	130.39Å 48.52Å 70.19Å 90.00° 117.74° 90.00°	Depositor
Resolution (Å)	7.50 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2476	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: DEP

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	1.29	7/2344 (0.3%)	3.13	357/3185 (11.2%)

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	A	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	GLY	N-CA	6.37	1.52	1.45
1	A	263	GLY	CA-C	5.87	1.57	1.52
1	A	242	PHE	N-CA	5.57	1.52	1.46
1	A	132	VAL	N-CA	5.51	1.53	1.46
1	A	275	GLY	N-CA	5.21	1.52	1.45
1	A	207	LEU	N-CA	5.07	1.53	1.45
1	A	30	GLU	CD-OE1	5.03	1.34	1.25

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	GLU	CA-CB-CG	13.94	141.97	114.10
1	A	292	GLN	N-CA-C	-12.13	98.04	111.14
1	A	232	LYS	CA-CB-CG	11.87	137.84	114.10
1	A	206	GLN	OE1-CD-NE2	11.82	134.42	122.60
1	A	206	GLN	CA-CB-CG	-11.20	91.70	114.10
1	A	170	ASP	CA-CB-CG	11.18	123.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	LYS	CA-C-O	11.18	132.73	121.00
1	A	121	LEU	CA-C-O	-10.94	107.39	119.97
1	A	187	PRO	CB-CA-C	10.61	125.25	110.60
1	A	285	ASN	OD1-CG-ND2	-10.44	112.17	122.60
1	A	292	GLN	O-C-N	10.40	133.32	122.09
1	A	222	GLN	CA-CB-CG	10.15	134.41	114.10
1	A	292	GLN	CA-C-O	-10.14	110.25	120.70
1	A	256	ASP	CA-CB-CG	-10.04	102.56	112.60
1	A	213	PRO	CA-C-N	9.94	136.50	120.60
1	A	213	PRO	C-N-CA	9.94	136.50	120.60
1	A	302	GLU	CA-C-N	9.81	136.70	120.62
1	A	302	GLU	C-N-CA	9.81	136.70	120.62
1	A	209	PHE	CA-C-O	-9.80	109.02	121.17
1	A	225	LYS	CA-C-N	9.79	134.40	120.79
1	A	225	LYS	C-N-CA	9.79	134.40	120.79
1	A	18	ASN	CB-CG-ND2	9.67	130.91	116.40
1	A	64	CYS	O-C-N	9.63	134.45	123.48
1	A	19	PHE	O-C-N	9.62	134.71	122.97
1	A	52	LYS	CA-C-N	9.60	138.05	120.87
1	A	52	LYS	C-N-CA	9.60	138.05	120.87
1	A	160	ARG	CD-NE-CZ	9.37	137.52	124.40
1	A	132	VAL	CB-CA-C	9.36	126.64	111.29
1	A	226	ARG	CA-C-O	9.32	131.33	121.07
1	A	130	ASP	O-C-N	9.29	129.24	121.35
1	A	166	GLU	CB-CG-CD	9.28	128.38	112.60
1	A	18	ASN	OD1-CG-ND2	-9.18	113.42	122.60
1	A	38	LYS	CA-C-O	9.17	130.61	119.79
1	A	273	LEU	CA-C-O	-9.12	107.47	120.51
1	A	164	GLU	O-C-N	-9.10	111.83	122.20
1	A	291	ILE	CA-C-N	9.07	132.77	120.44
1	A	291	ILE	C-N-CA	9.07	132.77	120.44
1	A	159	GLU	CA-C-O	-8.96	109.21	119.79
1	A	232	LYS	CA-C-O	-8.92	111.45	120.82
1	A	108	LEU	N-CA-C	-8.89	101.67	111.36
1	A	116	GLN	N-CA-CB	8.88	122.95	110.07
1	A	121	LEU	O-C-N	8.76	133.05	122.27
1	A	215	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	270	GLN	CG-CD-NE2	-8.73	103.30	116.40
1	A	270	GLN	CG-CD-OE1	8.58	137.96	120.80
1	A	294	LYS	CA-C-N	8.56	132.11	120.38
1	A	294	LYS	C-N-CA	8.56	132.11	120.38
1	A	110	PHE	CA-C-N	8.56	131.57	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	PHE	C-N-CA	8.56	131.57	120.44
1	A	229	ASP	CA-C-O	-8.43	111.62	120.55
1	A	163	ALA	CB-CA-C	8.42	123.92	110.96
1	A	48	SER	CB-CA-C	-8.28	96.61	110.68
1	A	250	GLY	CA-C-N	8.27	135.11	122.37
1	A	250	GLY	C-N-CA	8.27	135.11	122.37
1	A	302	GLU	O-C-N	-8.24	111.63	122.59
1	A	160	ARG	NE-CZ-NH1	8.23	129.73	121.50
1	A	242	PHE	CA-CB-CG	8.23	122.03	113.80
1	A	106	ASN	CA-CB-CG	-8.23	104.37	112.60
1	A	255	CYS	N-CA-C	8.22	121.86	112.57
1	A	232	LYS	N-CA-CB	8.22	121.93	110.01
1	A	36	GLN	OE1-CD-NE2	-8.21	114.39	122.60
1	A	143	GLU	CA-CB-CG	8.20	130.50	114.10
1	A	292	GLN	N-CA-CB	8.20	121.96	110.07
1	A	298	ASP	CA-CB-CG	8.16	120.76	112.60
1	A	119	ASP	N-CA-CB	8.07	121.99	110.12
1	A	152	GLN	CA-C-N	8.07	131.09	120.28
1	A	152	GLN	C-N-CA	8.07	131.09	120.28
1	A	184	VAL	CA-C-O	7.98	129.10	120.57
1	A	151	LYS	CA-C-O	-7.95	112.13	120.55
1	A	61	ASP	O-C-N	7.94	133.30	123.14
1	A	250	GLY	CA-C-O	-7.90	112.39	120.45
1	A	28	ASP	N-CA-CB	-7.90	99.65	110.56
1	A	171	ARG	CD-NE-CZ	-7.90	113.34	124.40
1	A	111	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	27	GLN	CA-CB-CG	7.86	129.82	114.10
1	A	159	GLU	N-CA-C	-7.86	102.33	112.23
1	A	254	ALA	CA-C-O	-7.85	112.23	120.55
1	A	173	GLY	CA-C-N	7.83	133.79	120.71
1	A	173	GLY	C-N-CA	7.83	133.79	120.71
1	A	279	PRO	O-C-N	-7.79	113.50	123.00
1	A	263	GLY	N-CA-C	-7.79	102.98	111.93
1	A	274	LEU	CB-CA-C	7.75	125.88	112.00
1	A	159	GLU	CB-CG-CD	-7.75	99.42	112.60
1	A	158	PHE	CA-C-O	7.71	128.59	120.42
1	A	141	CYS	CA-C-O	-7.71	109.49	120.51
1	A	30	GLU	CA-C-O	-7.71	112.73	120.82
1	A	55	THR	CA-C-O	7.71	128.71	120.46
1	A	160	ARG	CG-CD-NE	7.70	128.94	112.00
1	A	270	GLN	CA-C-O	7.69	128.35	119.35
1	A	42	PRO	CA-C-N	7.65	130.87	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	PRO	C-N-CA	7.65	130.87	120.54
1	A	25	THR	CA-CB-OG1	-7.62	98.17	109.60
1	A	298	ASP	CA-C-N	7.61	130.48	120.28
1	A	298	ASP	C-N-CA	7.61	130.48	120.28
1	A	149	ASP	CA-CB-CG	7.61	120.20	112.60
1	A	206	GLN	CG-CD-NE2	-7.58	105.02	116.40
1	A	94	GLN	CB-CG-CD	-7.58	99.71	112.60
1	A	289	ARG	NE-CZ-NH2	-7.57	112.39	119.20
1	A	26	ASN	OD1-CG-ND2	7.53	130.13	122.60
1	A	283	HIS	O-C-N	7.53	127.97	121.20
1	A	19	PHE	N-CA-C	-7.50	99.66	110.24
1	A	20	GLY	O-C-N	7.50	129.82	122.77
1	A	20	GLY	CA-C-O	-7.45	113.08	119.56
1	A	112	ARG	CA-C-N	7.44	132.46	120.55
1	A	112	ARG	C-N-CA	7.44	132.46	120.55
1	A	108	LEU	N-CA-CB	7.43	121.16	110.16
1	A	216	ALA	N-CA-C	-7.40	103.30	111.36
1	A	291	ILE	CA-C-O	7.35	128.64	120.85
1	A	170	ASP	CA-C-O	-7.33	111.03	119.60
1	A	222	GLN	OE1-CD-NE2	7.33	129.93	122.60
1	A	11	PHE	CA-C-O	-7.28	113.35	121.51
1	A	139	ALA	N-CA-C	7.21	121.18	112.38
1	A	200	ALA	CA-C-N	7.18	130.68	120.49
1	A	200	ALA	C-N-CA	7.18	130.68	120.49
1	A	288	GLY	N-CA-C	-7.14	104.16	112.73
1	A	78	LEU	O-C-N	7.13	129.15	121.60
1	A	130	ASP	CA-C-O	-7.12	113.33	120.66
1	A	6	VAL	O-C-N	7.11	129.21	121.10
1	A	249	THR	CA-C-N	7.11	129.08	120.13
1	A	249	THR	C-N-CA	7.11	129.08	120.13
1	A	114	LEU	N-CA-C	-7.09	103.16	111.03
1	A	27	GLN	CA-C-N	7.09	134.42	122.65
1	A	27	GLN	C-N-CA	7.09	134.42	122.65
1	A	19	PHE	CA-C-O	-7.08	113.36	121.15
1	A	96	THR	CA-C-N	7.07	133.50	122.26
1	A	96	THR	C-N-CA	7.07	133.50	122.26
1	A	143	GLU	CB-CG-CD	7.06	124.61	112.60
1	A	190	VAL	N-CA-C	7.06	115.59	107.89
1	A	127	LEU	CB-CA-C	7.05	118.26	110.15
1	A	272	GLU	CB-CG-CD	-7.05	100.62	112.60
1	A	149	ASP	N-CA-C	-7.04	103.37	112.23
1	A	288	GLY	CA-C-O	-7.04	113.50	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CYS	CA-C-O	-6.99	112.19	120.43
1	A	189	LEU	CA-C-N	6.97	131.09	123.43
1	A	189	LEU	C-N-CA	6.97	131.09	123.43
1	A	211	ASP	CB-CA-C	-6.96	98.77	110.81
1	A	49	LEU	N-CA-C	-6.95	103.76	111.82
1	A	212	ILE	O-C-N	6.92	128.99	121.10
1	A	290	ASP	CA-C-O	-6.92	112.01	119.97
1	A	41	TYR	N-CA-C	-6.88	104.30	113.25
1	A	275	GLY	N-CA-C	-6.87	96.90	113.18
1	A	126	LEU	N-CA-CB	-6.84	101.11	110.56
1	A	21	ILE	CB-CA-C	6.84	120.58	111.21
1	A	32	GLY	N-CA-C	-6.83	104.53	112.73
1	A	237	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	205	THR	CA-C-O	6.79	127.09	119.41
1	A	99	THR	CA-C-N	6.79	132.43	122.99
1	A	99	THR	C-N-CA	6.79	132.43	122.99
1	A	192	GLU	CG-CD-OE1	6.74	133.91	118.40
1	A	11	PHE	CA-CB-CG	6.72	120.52	113.80
1	A	273	LEU	CB-CA-C	6.72	123.79	110.42
1	A	269	SER	CA-C-N	6.71	133.61	122.54
1	A	269	SER	C-N-CA	6.71	133.61	122.54
1	A	124	PRO	CA-C-N	6.66	133.27	121.75
1	A	124	PRO	C-N-CA	6.66	133.27	121.75
1	A	95	ASP	CB-CG-OD2	-6.65	103.11	118.40
1	A	172	ILE	CA-C-N	6.60	128.45	120.13
1	A	172	ILE	C-N-CA	6.60	128.45	120.13
1	A	77	GLU	CB-CG-CD	-6.58	101.42	112.60
1	A	167	GLU	O-C-N	-6.56	115.16	122.12
1	A	9	VAL	CA-C-O	-6.55	113.51	120.39
1	A	295	GLN	CA-C-O	-6.55	113.55	120.63
1	A	178	ASP	N-CA-CB	-6.54	100.81	110.49
1	A	44	VAL	CA-C-O	-6.53	113.93	120.85
1	A	56	LEU	CA-C-O	-6.51	113.18	120.54
1	A	6	VAL	CA-C-O	-6.49	111.26	119.95
1	A	167	GLU	CA-C-N	6.47	128.86	120.44
1	A	167	GLU	C-N-CA	6.47	128.86	120.44
1	A	36	GLN	O-C-N	6.46	130.74	123.05
1	A	113	ILE	CA-C-O	-6.46	113.80	120.71
1	A	155	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	160	ARG	CA-CB-CG	6.45	127.00	114.10
1	A	147	THR	N-CA-CB	-6.43	101.01	111.18
1	A	294	LYS	O-C-N	-6.40	115.38	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLY	CA-C-O	-6.39	117.85	122.45
1	A	27	GLN	CA-C-O	6.38	128.49	121.02
1	A	136	GLU	CB-CG-CD	-6.38	101.76	112.60
1	A	133	ASP	N-CA-CB	6.37	120.90	110.39
1	A	268	ASP	O-C-N	6.37	130.48	123.22
1	A	153	TRP	CA-C-O	-6.37	113.80	120.55
1	A	191	PRO	O-C-N	6.36	130.67	123.04
1	A	205	THR	N-CA-C	-6.35	105.67	113.41
1	A	25	THR	N-CA-C	-6.32	100.63	110.42
1	A	252	ASN	OD1-CG-ND2	6.31	128.91	122.60
1	A	202	PRO	CA-C-O	-6.29	109.14	120.60
1	A	232	LYS	CB-CA-C	-6.29	101.01	110.88
1	A	194	THR	CA-CB-OG1	-6.27	100.20	109.60
1	A	175	PHE	CA-C-N	6.23	129.34	122.74
1	A	175	PHE	C-N-CA	6.23	129.34	122.74
1	A	71	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	A	22	ALA	CB-CA-C	6.21	118.50	108.87
1	A	136	GLU	CB-CA-C	6.21	119.65	109.46
1	A	102	SER	CA-C-O	-6.20	113.44	120.32
1	A	209	PHE	CA-C-N	6.18	133.34	121.54
1	A	209	PHE	C-N-CA	6.18	133.34	121.54
1	A	110	PHE	CA-C-O	-6.17	113.13	120.10
1	A	292	GLN	CB-CA-C	-6.17	101.15	110.90
1	A	72	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	103	LEU	CA-C-O	-6.16	112.97	120.54
1	A	252	ASN	N-CA-CB	6.15	121.35	111.20
1	A	111	ASN	N-CA-CB	6.15	118.92	110.01
1	A	164	GLU	CA-C-N	6.13	128.99	120.29
1	A	164	GLU	C-N-CA	6.13	128.99	120.29
1	A	137	PRO	N-CA-CB	-6.12	96.23	102.72
1	A	198	LEU	CA-C-O	-6.12	111.85	119.38
1	A	219	VAL	CA-C-N	6.12	128.81	120.54
1	A	219	VAL	C-N-CA	6.12	128.81	120.54
1	A	195	THR	CB-CA-C	6.11	121.07	110.68
1	A	8	THR	CA-C-O	-6.10	113.64	120.66
1	A	158	PHE	CB-CA-C	6.10	121.22	110.85
1	A	226	ARG	N-CA-C	6.10	118.46	111.02
1	A	156	ASP	CB-CG-OD2	-6.08	104.42	118.40
1	A	47	ARG	N-CA-CB	6.08	119.05	109.82
1	A	277	LYS	O-C-N	6.06	130.16	123.01
1	A	182	VAL	N-CA-CB	6.05	119.51	111.64
1	A	234	ALA	O-C-N	-6.04	115.80	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLN	CB-CG-CD	6.03	122.85	112.60
1	A	38	LYS	CA-CB-CG	6.03	126.15	114.10
1	A	43	ALA	O-C-N	-6.03	115.82	122.09
1	A	41	TYR	CB-CA-C	6.01	125.43	112.38
1	A	274	LEU	CA-C-O	-6.01	114.09	120.71
1	A	79	PRO	O-C-N	6.00	130.43	123.06
1	A	256	ASP	CA-C-O	5.99	127.79	120.55
1	A	188	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A	164	GLU	N-CA-CB	-5.97	100.71	110.14
1	A	227	LEU	N-CA-C	-5.96	103.96	111.11
1	A	244	ASP	CA-C-O	5.95	128.25	121.58
1	A	215	ASP	N-CA-C	-5.92	105.14	112.90
1	A	108	LEU	CA-C-O	-5.92	114.15	120.42
1	A	169	LEU	CA-C-O	-5.88	113.46	120.10
1	A	205	THR	CB-CA-C	5.84	119.47	109.24
1	A	79	PRO	N-CA-CB	5.83	108.75	103.33
1	A	197	CYS	CA-C-O	5.81	126.09	119.18
1	A	71	HIS	CA-C-O	5.80	126.59	119.05
1	A	135	ASP	OD1-CG-OD2	5.80	136.82	122.90
1	A	211	ASP	N-CA-C	5.79	119.42	112.93
1	A	255	CYS	CB-CA-C	-5.76	102.13	111.06
1	A	51	ASP	OD1-CG-OD2	5.75	136.71	122.90
1	A	212	ILE	CB-CG1-CD1	5.74	125.86	113.80
1	A	136	GLU	CA-CB-CG	-5.73	102.64	114.10
1	A	157	GLN	CA-C-N	5.73	128.43	120.29
1	A	157	GLN	C-N-CA	5.73	128.43	120.29
1	A	281	TYR	CA-CB-CG	5.73	124.21	113.90
1	A	64	CYS	CA-C-N	-5.72	114.91	120.34
1	A	64	CYS	C-N-CA	-5.72	114.91	120.34
1	A	115	LYS	CA-C-O	-5.71	113.80	120.20
1	A	5	PRO	O-C-N	-5.71	115.93	123.01
1	A	157	GLN	CB-CG-CD	5.71	122.31	112.60
1	A	116	GLN	O-C-N	5.70	128.25	122.09
1	A	61	ASP	CA-C-O	-5.69	112.79	120.47
1	A	216	ALA	CB-CA-C	5.68	120.50	110.85
1	A	218	PRO	CA-C-N	5.67	128.48	120.42
1	A	218	PRO	C-N-CA	5.67	128.48	120.42
1	A	102	SER	O-C-N	5.67	129.94	123.31
1	A	254	ALA	O-C-N	5.67	128.12	122.12
1	A	81	GLY	O-C-N	5.65	128.77	122.50
1	A	285	ASN	CB-CG-ND2	5.65	124.88	116.40
1	A	192	GLU	N-CA-CB	5.64	118.91	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	CA-C-N	5.64	128.40	120.28
1	A	156	ASP	C-N-CA	5.64	128.40	120.28
1	A	152	GLN	CA-C-O	5.63	126.43	119.79
1	A	227	LEU	N-CA-CB	5.62	118.31	109.94
1	A	61	ASP	N-CA-C	-5.61	96.61	107.44
1	A	153	TRP	O-C-N	5.60	128.06	122.12
1	A	127	LEU	O-C-N	5.60	128.23	121.29
1	A	259	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	116	GLN	CA-C-O	-5.58	114.96	120.70
1	A	199	THR	CA-C-O	-5.58	114.86	121.16
1	A	47	ARG	CD-NE-CZ	-5.57	116.60	124.40
1	A	10	PHE	N-CA-CB	5.56	119.64	110.69
1	A	215	ASP	CA-C-O	5.54	126.08	119.60
1	A	99	THR	CA-CB-CG2	5.53	119.91	110.50
1	A	266	LEU	N-CA-CB	-5.53	102.30	110.49
1	A	132	VAL	CA-C-O	-5.52	113.88	120.78
1	A	286	ASP	CB-CA-C	5.52	119.64	110.81
1	A	214	GLN	CA-C-O	5.51	126.16	119.49
1	A	122	ARG	O-C-N	-5.51	115.27	122.59
1	A	61	ASP	N-CA-CB	5.46	120.40	110.95
1	A	135	ASP	CB-CG-OD2	-5.45	105.86	118.40
1	A	269	SER	N-CA-C	-5.45	101.29	109.79
1	A	265	LEU	CA-C-N	5.44	131.51	122.54
1	A	265	LEU	C-N-CA	5.44	131.51	122.54
1	A	27	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	241	ASP	CA-C-N	-5.42	113.94	122.73
1	A	241	ASP	C-N-CA	-5.42	113.94	122.73
1	A	262	ILE	CB-CG1-CD1	5.42	125.19	113.80
1	A	72	PHE	N-CA-C	-5.41	105.54	111.82
1	A	219	VAL	CA-CB-CG1	5.41	119.60	110.40
1	A	273	LEU	CA-C-N	-5.41	114.19	121.71
1	A	273	LEU	C-N-CA	-5.41	114.19	121.71
1	A	74	GLU	CA-C-N	5.40	128.51	120.95
1	A	74	GLU	C-N-CA	5.40	128.51	120.95
1	A	8	THR	CA-CB-CG2	5.39	119.67	110.50
1	A	253	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	278	ILE	O-C-N	5.39	127.24	121.10
1	A	84	GLU	CA-CB-CG	5.38	124.87	114.10
1	A	192	GLU	CA-C-N	5.37	129.98	122.41
1	A	192	GLU	C-N-CA	5.37	129.98	122.41
1	A	184	VAL	O-C-N	-5.36	117.08	123.03
1	A	302	GLU	CA-C-O	5.36	128.17	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	LEU	O-C-N	5.36	128.26	122.15
1	A	252	ASN	CA-CB-CG	-5.36	107.24	112.60
1	A	120	GLU	CA-C-N	5.34	128.43	120.31
1	A	120	GLU	C-N-CA	5.34	128.43	120.31
1	A	183	LEU	CA-C-O	-5.33	114.66	120.36
1	A	283	HIS	CA-C-O	-5.33	114.96	120.87
1	A	125	SER	N-CA-CB	5.31	120.53	111.66
1	A	161	VAL	CA-C-O	-5.31	115.15	121.05
1	A	48	SER	N-CA-C	5.30	117.75	111.33
1	A	65	GLY	CA-C-O	5.30	127.63	121.90
1	A	188	ARG	CD-NE-CZ	-5.30	116.98	124.40
1	A	259	ASP	N-CA-C	-5.30	106.40	112.92
1	A	48	SER	CA-CB-OG	-5.29	100.52	111.10
1	A	244	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	46	THR	CA-C-N	5.28	128.13	120.79
1	A	46	THR	C-N-CA	5.28	128.13	120.79
1	A	137	PRO	CB-CA-C	5.25	118.45	110.21
1	A	157	GLN	N-CA-C	5.22	117.72	111.71
1	A	174	TYR	N-CA-C	5.22	117.78	111.40
1	A	191	PRO	CA-C-N	5.22	127.80	120.28
1	A	191	PRO	C-N-CA	5.22	127.80	120.28
1	A	190	VAL	N-CA-CB	-5.22	106.03	111.61
1	A	106	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	272	GLU	O-C-N	5.21	129.50	123.30
1	A	227	LEU	CA-C-N	5.20	127.20	120.44
1	A	227	LEU	C-N-CA	5.20	127.20	120.44
1	A	169	LEU	N-CA-C	-5.20	105.73	111.71
1	A	29	SER	O-C-N	5.17	129.87	122.74
1	A	93	LYS	CG-CD-CE	5.17	123.18	111.30
1	A	22	ALA	CA-C-O	-5.16	114.63	120.46
1	A	295	GLN	O-C-N	5.16	127.59	122.12
1	A	249	THR	N-CA-C	-5.13	105.74	112.41
1	A	262	ILE	N-CA-CB	-5.12	105.22	111.21
1	A	164	GLU	N-CA-C	5.11	118.30	111.75
1	A	10	PHE	N-CA-C	-5.11	101.37	109.59
1	A	54	ILE	N-CA-CB	5.10	116.82	111.00
1	A	184	VAL	CA-C-N	5.10	127.07	120.64
1	A	184	VAL	C-N-CA	5.10	127.07	120.64
1	A	52	LYS	N-CA-C	-5.10	106.90	113.02
1	A	28	ASP	N-CA-C	5.09	118.64	112.93
1	A	222	GLN	CB-CA-C	5.09	118.96	110.81
1	A	70	HIS	N-CA-CB	5.09	119.30	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	127	LEU	N-CA-C	-5.07	100.69	109.15
1	A	290	ASP	O-C-N	5.07	128.50	122.27
1	A	190	VAL	O-C-N	5.06	125.97	121.41
1	A	285	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	181	ARG	CA-CB-CG	-5.06	103.99	114.10
1	A	235	ALA	N-CA-CB	-5.06	102.44	110.28
1	A	301	GLU	CB-CA-C	-5.05	102.95	110.88
1	A	223	ILE	O-C-N	-5.05	116.77	121.87
1	A	228	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	180	LYS	O-C-N	-5.04	117.14	123.04
1	A	176	ALA	CA-C-O	5.03	127.06	121.22
1	A	136	GLU	N-CA-C	-5.02	102.87	109.84
1	A	215	ASP	CB-CA-C	5.02	119.75	109.67
1	A	46	THR	CA-CB-OG1	-5.00	102.09	109.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	31	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	A	2295	0	2210	85	1
2	A	8	0	10	1	0
3	A	173	0	0	12	1
All	All	2476	0	2220	85	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 19.

All (85) 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:120:GLU:HG2	1:A:266:LEU:HD21	1.50	0.93
1:A:193:ASP:OD1	1:A:195:THR:OG1	2.02	0.75
1:A:193:ASP:O	1:A:196:LYS:HG3	1.86	0.75
1:A:213:PRO:O	1:A:216:ALA:HB3	1.90	0.72
1:A:194:THR:HG23	1:A:217:LEU:HD12	1.71	0.70
1:A:158:PHE:CZ	1:A:226:ARG:HB3	2.28	0.69
1:A:75:LYS:HG3	1:A:85:LEU:O	1.93	0.68
1:A:138:ALA:O	1:A:141:CYS:HB3	1.95	0.67
1:A:105:GLY:HA3	2:A:400:DEP:H41	1.78	0.65
1:A:120:GLU:HB2	1:A:211:ASP:OD2	1.95	0.65
1:A:139:ALA:HA	1:A:213:PRO:HG3	1.79	0.64
1:A:263:GLY:HA3	1:A:280:TRP:CG	2.33	0.63
1:A:210:ALA:HB2	1:A:266:LEU:HD22	1.80	0.63
1:A:281:TYR:O	1:A:282:ALA:HB3	1.98	0.62
1:A:195:THR:O	1:A:198:LEU:HB2	2.00	0.61
1:A:180:LYS:HE3	3:A:648:HOH:O	1.99	0.61
1:A:255:CYS:HA	3:A:548:HOH:O	2.00	0.60
1:A:141:CYS:SG	1:A:216:ALA:HB1	2.42	0.59
1:A:257:GLY:O	1:A:260:ARG:NH1	2.35	0.59
1:A:54:ILE:HG13	3:A:640:HOH:O	2.03	0.59
1:A:269:SER:OG	1:A:271:LEU:HB2	2.01	0.58
1:A:193:ASP:HB3	1:A:196:LYS:HD2	1.85	0.58
1:A:291:ILE:O	1:A:295:GLN:HG2	2.03	0.58
1:A:143:GLU:O	1:A:147:THR:N	2.37	0.57
1:A:272:GLU:HA	1:A:276:THR:O	2.04	0.57
1:A:39:GLU:OE1	1:A:47:ARG:NH2	2.37	0.57
1:A:300:ILE:O	1:A:304:LEU:HG	2.05	0.56
1:A:195:THR:HA	1:A:198:LEU:HD12	1.87	0.55
1:A:16:THR:HA	1:A:41:TYR:CE2	2.43	0.54
1:A:219:VAL:O	1:A:223:ILE:HG13	2.08	0.53
1:A:263:GLY:HA3	1:A:280:TRP:CD1	2.45	0.52
1:A:41:TYR:CG	1:A:42:PRO:HD3	2.45	0.52
1:A:140:LYS:HA	1:A:143:GLU:OE2	2.09	0.52
1:A:214:GLN:HA	1:A:217:LEU:HG	1.91	0.51
1:A:47:ARG:NH2	3:A:532:HOH:O	2.32	0.51
1:A:4:ASP:N	3:A:642:HOH:O	2.44	0.51
1:A:117:CYS:HB3	1:A:212:ILE:HG23	1.94	0.50
1:A:200:ALA:HB2	1:A:207:LEU:HD23	1.94	0.49
1:A:185:GLY:O	1:A:245:LEU:HD12	2.12	0.48
1:A:68:LEU:HB3	1:A:107:THR:OG1	2.14	0.48
1:A:75:LYS:HG2	1:A:84:GLU:HB3	1.96	0.48
1:A:76:GLN:O	1:A:84:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.72	0.48
1:A:305:ASN:ND2	3:A:650:HOH:O	2.46	0.47
1:A:68:LEU:HD22	1:A:106:ASN:HB3	1.96	0.47
1:A:271:LEU:O	1:A:277:LYS:HA	2.14	0.47
1:A:241:ASP:CG	1:A:303:ILE:HD11	2.38	0.47
1:A:267:GLU:O	1:A:279:PRO:HA	2.14	0.47
1:A:268:ASP:HB3	1:A:277:LYS:CB	2.44	0.47
1:A:116:GLN:O	1:A:138:ALA:HA	2.15	0.47
1:A:78:LEU:HB3	1:A:82:ALA:HB3	1.98	0.46
1:A:120:GLU:O	1:A:123:LYS:HD2	2.16	0.46
1:A:133:ASP:HB3	1:A:136:GLU:HB2	1.97	0.45
1:A:178:ASP:HB2	3:A:622:HOH:O	2.16	0.45
1:A:215:ASP:O	1:A:218:PRO:HD2	2.17	0.45
1:A:268:ASP:HB3	1:A:277:LYS:HB3	1.98	0.45
1:A:181:ARG:HD3	3:A:658:HOH:O	2.17	0.45
1:A:196:LYS:NZ	1:A:196:LYS:HB3	2.32	0.45
1:A:141:CYS:SG	1:A:216:ALA:CB	3.06	0.44
1:A:199:THR:HG22	1:A:200:ALA:O	2.18	0.44
1:A:295:GLN:HG3	3:A:600:HOH:O	2.17	0.44
1:A:11:PHE:O	1:A:101:GLY:HA3	2.18	0.44
1:A:115:LYS:HG2	1:A:121:LEU:HB3	1.99	0.44
1:A:131:PRO:HD2	3:A:591:HOH:O	2.17	0.44
1:A:194:THR:O	1:A:195:THR:C	2.61	0.44
1:A:23:PRO:HB2	3:A:671:HOH:O	2.18	0.43
1:A:194:THR:O	1:A:194:THR:HG22	2.18	0.43
1:A:210:ALA:CB	1:A:266:LEU:HD22	2.46	0.43
1:A:167:GLU:OE2	1:A:171:ARG:NE	2.46	0.43
1:A:299:LYS:HA	1:A:299:LYS:HD3	1.92	0.43
1:A:76:GLN:O	1:A:85:LEU:N	2.41	0.42
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.68	0.42
1:A:189:LEU:O	1:A:253:THR:HB	2.19	0.42
1:A:267:GLU:HB2	3:A:546:HOH:O	2.20	0.42
1:A:294:LYS:HD2	1:A:295:GLN:NE2	2.35	0.42
1:A:287:LYS:HD2	1:A:291:ILE:HD11	2.02	0.41
1:A:18:ASN:O	1:A:19:PHE:C	2.63	0.41
1:A:144:PHE:CE1	1:A:150:GLY:HA3	2.56	0.41
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.88	0.41
1:A:264:GLY:O	1:A:280:TRP:HB2	2.21	0.41
1:A:127:LEU:HG	1:A:281:TYR:CG	2.56	0.41
1:A:197:CYS:O	1:A:208:PRO:HD2	2.21	0.41
1:A:252:ASN:O	1:A:261:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:O	1:A:289:ARG:N	2.41	0.40
1:A:154:LEU:O	1:A:158:PHE:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PHE:N	3:A:664:HOH:O[2_654]	2.07	0.13

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	A	300/306 (98%)	271 (90%)	27 (9%)	2 (1%)	18	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLY
1	A	202	PRO

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	A	239/241 (99%)	197 (82%)	42 (18%)	2 2

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	38	LYS
1	A	41	TYR
1	A	42	PRO
1	A	54	ILE
1	A	63	SER
1	A	68	LEU
1	A	75	LYS
1	A	78	LEU
1	A	108	LEU
1	A	121	LEU
1	A	123	LYS
1	A	127	LEU
1	A	132	VAL
1	A	137	PRO
1	A	140	LYS
1	A	141	CYS
1	A	147	THR
1	A	155	ASP
1	A	158	PHE
1	A	159	GLU
1	A	168	LEU
1	A	171	ARG
1	A	189	LEU
1	A	192	GLU
1	A	196	LYS
1	A	205	THR
1	A	207	LEU
1	A	211	ASP
1	A	215	ASP
1	A	217	LEU
1	A	222	GLN
1	A	225	LYS
1	A	226	ARG
1	A	249	THR
1	A	266	LEU
1	A	271	LEU
1	A	273	LEU

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Mol	Chain	Res	Type
1	A	286	ASP
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	76	GLN
1	A	94	GLN
1	A	228	ASN
1	A	270	GLN
1	A	295	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	DEP	A	400	1	4,7,7	1.85	2 (50%)	2,7,7	1.74	1 (50%)

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	DEP	A	400	1	-	0/2/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	DEP	O2-C3	2.39	1.50	1.44
2	A	400	DEP	C4-C3	2.07	1.62	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	DEP	O2-C3-C4	2.26	126.25	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	DEP	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.