



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:13 PM UTC

PDB ID : 1EED / pdb_00001eed
Title : X-ray crystallographic analysis of inhibition of endothiapepsin by cyclohexyl renin inhibitors
Authors : Blundell, T.L.; Frazao, C.; Cooper, J.B.
Deposited on : 1992-06-15
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

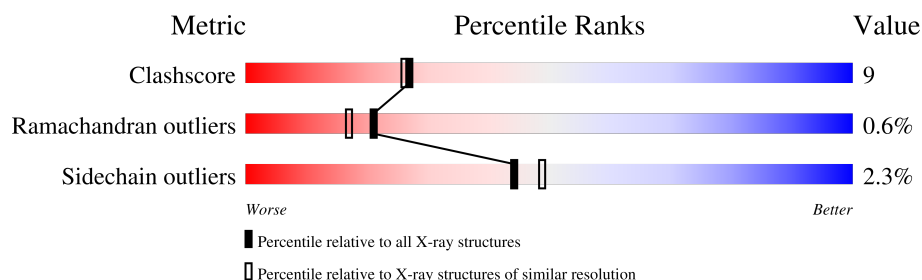
1 Overall quality at a glance

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	P	330	 33% 58% 9%

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
2	0EO	P	327	-	-	X	-

2 Entry composition [i](#)

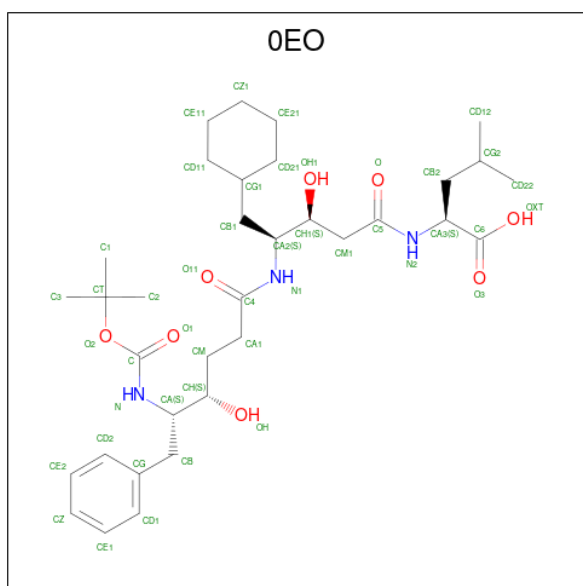
There are 3 unique types of molecules in this entry. The entry contains 2712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	P	330	Total	C	N	O	S	0	0	0
			2389	1514	366	507	2			

- Molecule 2 is (2S)-2-[[[(3S,4S)-5-cyclohexyl-4-[[[(4S,5S)-5-[(2-methylpropan-2-yl)oxycarbonyl amino]-4-oxidanyl-6-phenyl-hexanoyl]amino]-3-oxidanyl-pentanoyl]amino]-4-methyl-pentan oic acid (CCD ID: 0EO) (formula: C₃₄H₅₅N₃O₈).

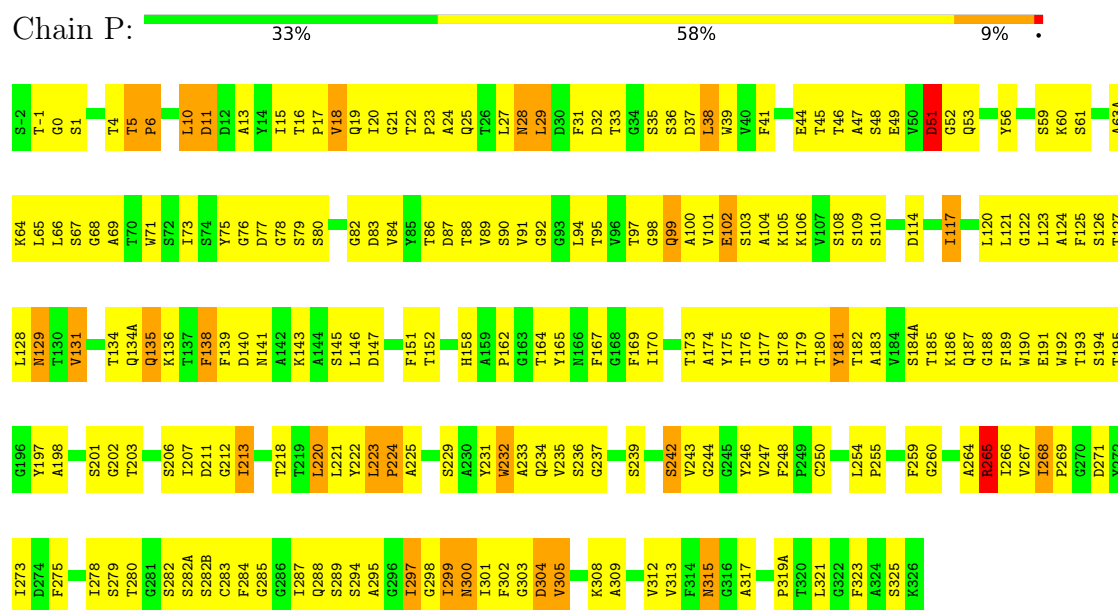


3 Residue-property plots

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: ENDOTHAPEPSIN



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	43.10Å 75.70Å 42.90Å 90.00° 96.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2712	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: 0EO

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	P	3.06	259/2445 (10.6%)	2.72	214/3345 (6.4%)

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	P	0	1

All (259) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	129	ASN	N-CA	15.43	1.65	1.46
1	P	158	HIS	ND1-CE1	15.39	1.48	1.32
1	P	212	GLY	C-O	-14.39	1.08	1.23
1	P	192	TRP	CA-C	11.33	1.66	1.52
1	P	19	GLN	N-CA	11.31	1.60	1.46
1	P	101	VAL	CA-CB	11.04	1.68	1.53
1	P	18	VAL	CA-C	10.86	1.65	1.52
1	P	300	ASN	CA-C	10.81	1.67	1.52
1	P	138	PHE	N-CA	10.67	1.59	1.46
1	P	158	HIS	CD2-NE2	10.43	1.49	1.37
1	P	87	ASP	N-CA	10.43	1.58	1.46
1	P	194	SER	CA-C	10.36	1.66	1.52
1	P	223	LEU	N-CA	10.23	1.55	1.45
1	P	82	GLY	N-CA	10.05	1.59	1.45
1	P	265	ARG	CD-NE	9.96	1.60	1.46
1	P	28	ASN	CA-C	9.91	1.65	1.52
1	P	202	GLY	N-CA	9.73	1.57	1.45
1	P	303	GLY	N-CA	9.67	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	41	PHE	N-CA	9.59	1.57	1.46
1	P	190	TRP	CA-C	9.42	1.64	1.53
1	P	212	GLY	CA-C	9.29	1.62	1.51
1	P	233	ALA	N-CA	9.28	1.58	1.46
1	P	302	PHE	CA-C	9.23	1.65	1.52
1	P	5	THR	CA-C	-9.03	1.44	1.52
1	P	102	GLU	CA-CB	9.01	1.65	1.53
1	P	10	LEU	N-CA	8.78	1.57	1.46
1	P	182	THR	C-O	8.73	1.34	1.23
1	P	5	THR	CA-CB	8.69	1.70	1.54
1	P	24	ALA	N-CA	8.66	1.57	1.46
1	P	222	TYR	CA-C	8.61	1.63	1.52
1	P	255	PRO	CA-CB	8.56	1.65	1.53
1	P	218	THR	N-CA	8.41	1.56	1.46
1	P	195	THR	N-CA	8.40	1.57	1.46
1	P	182	THR	N-CA	8.33	1.56	1.45
1	P	271	ASP	N-CA	8.32	1.57	1.46
1	P	287	ILE	N-CA	8.29	1.57	1.46
1	P	35	SER	N-CA	8.21	1.55	1.46
1	P	61	SER	CA-CB	8.13	1.65	1.53
1	P	84	VAL	CA-CB	8.04	1.66	1.54
1	P	27	LEU	C-O	-8.03	1.13	1.23
1	P	128	LEU	C-N	-8.01	1.22	1.33
1	P	21	GLY	N-CA	7.98	1.53	1.45
1	P	15	ILE	N-CA	7.93	1.55	1.46
1	P	305	VAL	CA-C	-7.90	1.42	1.52
1	P	98	GLY	N-CA	7.79	1.56	1.45
1	P	165	TYR	N-CA	7.78	1.55	1.46
1	P	188	GLY	N-CA	7.72	1.56	1.45
1	P	1	SER	N-CA	7.72	1.55	1.46
1	P	99	GLN	N-CA	7.70	1.55	1.46
1	P	29	LEU	N-CA	7.66	1.54	1.45
1	P	91	VAL	N-CA	7.65	1.56	1.46
1	P	236	SER	CA-C	-7.63	1.42	1.52
1	P	35	SER	CB-OG	7.62	1.57	1.42
1	P	27	LEU	CA-C	7.58	1.61	1.52
1	P	202	GLY	C-N	7.57	1.43	1.33
1	P	127	THR	CA-CB	7.56	1.66	1.53
1	P	304	ASP	CA-CB	7.55	1.65	1.53
1	P	32	ASP	N-CA	7.55	1.55	1.46
1	P	289	SER	N-CA	7.53	1.55	1.46
1	P	221	LEU	CA-C	7.51	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	135	GLN	CD-OE1	7.46	1.37	1.23
1	P	16	THR	CA-C	7.43	1.58	1.52
1	P	170	ILE	CA-CB	7.41	1.63	1.54
1	P	300	ASN	CG-ND2	-7.37	1.17	1.33
1	P	110	SER	CA-CB	7.35	1.65	1.53
1	P	152	THR	CA-C	-7.35	1.44	1.52
1	P	259	PHE	CA-C	-7.34	1.43	1.52
1	P	89	VAL	N-CA	7.33	1.55	1.46
1	P	198	ALA	CA-C	-7.32	1.43	1.52
1	P	147	ASP	CA-C	7.30	1.62	1.52
1	P	179	ILE	CA-C	7.29	1.61	1.52
1	P	294	SER	N-CA	7.25	1.55	1.46
1	P	69	ALA	CA-C	-7.22	1.43	1.52
1	P	297	ILE	N-CA	7.21	1.55	1.46
1	P	101	VAL	CA-C	-7.19	1.43	1.52
1	P	31	PHE	CA-C	7.17	1.62	1.52
1	P	37	ASP	C-O	-7.15	1.14	1.24
1	P	79	SER	N-CA	7.15	1.54	1.45
1	P	106	LYS	N-CA	7.06	1.54	1.45
1	P	80	SER	CA-C	7.04	1.61	1.52
1	P	122	GLY	N-CA	6.96	1.56	1.45
1	P	177	GLY	N-CA	6.96	1.56	1.45
1	P	49	GLU	N-CA	6.96	1.55	1.46
1	P	254	LEU	CA-C	-6.94	1.44	1.53
1	P	282	SER	N-CA	6.91	1.54	1.45
1	P	232	TRP	NE1-CE2	-6.91	1.29	1.37
1	P	38	LEU	N-CA	6.90	1.55	1.46
1	P	243	VAL	CA-CB	6.89	1.63	1.54
1	P	73	ILE	N-CA	6.88	1.54	1.46
1	P	178	SER	N-CA	6.87	1.54	1.45
1	P	301	ILE	N-CA	6.86	1.55	1.46
1	P	145	SER	N-CA	6.84	1.55	1.46
1	P	167	PHE	CA-C	-6.84	1.44	1.52
1	P	212	GLY	N-CA	6.81	1.51	1.45
1	P	300	ASN	CB-CG	6.81	1.69	1.52
1	P	282	SER	CB-OG	6.76	1.55	1.42
1	P	22	THR	CA-C	6.73	1.61	1.52
1	P	131	VAL	N-CA	6.72	1.54	1.46
1	P	86	THR	CA-C	6.71	1.61	1.52
1	P	33	THR	CB-OG1	6.69	1.54	1.43
1	P	234	GLN	CD-OE1	6.69	1.36	1.23
1	P	267	VAL	CA-CB	6.69	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	53	GLN	CD-OE1	6.68	1.36	1.23
1	P	259	PHE	C-O	6.67	1.32	1.23
1	P	123	LEU	CA-C	6.66	1.61	1.52
1	P	127	THR	CA-C	-6.65	1.43	1.52
1	P	273	ILE	CA-C	-6.65	1.44	1.52
1	P	121	LEU	CA-C	6.62	1.60	1.52
1	P	134(A)	GLN	CA-CB	6.61	1.64	1.53
1	P	128	LEU	CA-C	6.60	1.62	1.52
1	P	275	PHE	N-CA	-6.56	1.38	1.46
1	P	198	ALA	N-CA	6.50	1.54	1.45
1	P	295	ALA	N-CA	6.50	1.54	1.46
1	P	203	THR	CA-CB	6.46	1.63	1.53
1	P	59	SER	N-CA	6.44	1.54	1.46
1	P	126	SER	CA-CB	6.43	1.64	1.53
1	P	109	SER	N-CA	-6.41	1.38	1.46
1	P	139	PHE	CA-CB	6.39	1.63	1.53
1	P	167	PHE	N-CA	6.36	1.53	1.46
1	P	176	THR	C-N	-6.36	1.25	1.33
1	P	187	GLN	CD-OE1	6.36	1.35	1.23
1	P	223	LEU	C-N	6.35	1.41	1.33
1	P	297	ILE	CA-CB	6.32	1.62	1.54
1	P	135	GLN	N-CA	6.32	1.53	1.45
1	P	-1	THR	N-CA	6.29	1.54	1.45
1	P	224	PRO	CA-CB	6.26	1.62	1.53
1	P	325	SER	CA-C	6.24	1.61	1.53
1	P	266	ILE	CA-CB	-6.18	1.47	1.54
1	P	36	SER	CA-C	6.18	1.60	1.52
1	P	90	SER	CA-C	6.18	1.60	1.52
1	P	80	SER	C-O	-6.16	1.16	1.23
1	P	108	SER	CA-CB	6.12	1.63	1.53
1	P	46	THR	CA-CB	6.12	1.63	1.53
1	P	78	GLY	N-CA	6.12	1.54	1.44
1	P	185	THR	N-CA	6.11	1.53	1.46
1	P	278	ILE	N-CA	6.10	1.54	1.46
1	P	229	SER	C-O	6.08	1.31	1.24
1	P	134(A)	GLN	CD-OE1	6.06	1.35	1.23
1	P	179	ILE	C-O	-6.05	1.16	1.24
1	P	39	TRP	N-CA	-6.05	1.38	1.45
1	P	213	ILE	N-CA	6.02	1.53	1.46
1	P	75	TYR	CA-C	6.01	1.61	1.53
1	P	260	GLY	CA-C	6.00	1.58	1.52
1	P	294	SER	CB-OG	5.99	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	97	THR	CB-OG1	-5.99	1.34	1.43
1	P	87	ASP	CG-OD2	-5.97	1.14	1.25
1	P	191	GLU	CA-CB	5.97	1.62	1.53
1	P	164	THR	C-O	5.95	1.30	1.23
1	P	201	SER	N-CA	5.95	1.52	1.46
1	P	229	SER	CA-CB	5.93	1.63	1.53
1	P	175	TYR	N-CA	5.92	1.53	1.45
1	P	280	THR	N-CA	5.90	1.53	1.46
1	P	282(B)	SER	C-N	-5.88	1.25	1.33
1	P	190	TRP	NE1-CE2	-5.86	1.31	1.37
1	P	0	GLY	C-N	-5.85	1.25	1.33
1	P	73	ILE	CA-CB	-5.82	1.46	1.54
1	P	24	ALA	CA-C	-5.80	1.44	1.52
1	P	181	TYR	C-N	-5.80	1.25	1.33
1	P	266	ILE	N-CA	5.79	1.53	1.46
1	P	68	GLY	N-CA	5.79	1.55	1.44
1	P	218	THR	C-O	-5.79	1.16	1.24
1	P	19	GLN	CD-OE1	5.79	1.34	1.23
1	P	139	PHE	CA-C	-5.77	1.45	1.52
1	P	250	CYS	CA-CB	5.75	1.63	1.53
1	P	29	LEU	CA-C	5.72	1.59	1.52
1	P	207	ILE	C-O	-5.71	1.18	1.24
1	P	126	SER	N-CA	5.70	1.53	1.46
1	P	300	ASN	C-N	-5.70	1.26	1.33
1	P	76	GLY	N-CA	5.70	1.53	1.45
1	P	53	GLN	CA-CB	5.70	1.62	1.53
1	P	66	LEU	N-CA	5.70	1.53	1.46
1	P	141	ASN	C-N	-5.70	1.26	1.33
1	P	284	PHE	N-CA	-5.69	1.39	1.46
1	P	183	ALA	N-CA	5.68	1.53	1.45
1	P	138	PHE	C-N	5.65	1.41	1.33
1	P	1	SER	CA-C	-5.63	1.45	1.52
1	P	170	ILE	C-O	5.63	1.30	1.24
1	P	288	GLN	CA-C	5.62	1.59	1.52
1	P	17	PRO	CA-CB	5.62	1.61	1.53
1	P	254	LEU	C-N	5.61	1.40	1.33
1	P	235	VAL	N-CA	5.59	1.54	1.46
1	P	36	SER	CB-OG	5.59	1.53	1.42
1	P	313	VAL	CA-C	-5.57	1.45	1.52
1	P	23	PRO	C-N	-5.54	1.25	1.33
1	P	6	PRO	C-O	5.53	1.30	1.23
1	P	211	ASP	CA-C	5.52	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	19	GLN	CA-C	5.51	1.59	1.52
1	P	165	TYR	C-O	5.51	1.30	1.24
1	P	203	THR	N-CA	-5.51	1.38	1.45
1	P	302	PHE	C-N	-5.50	1.24	1.33
1	P	11	ASP	CA-CB	5.50	1.61	1.53
1	P	135	GLN	C-O	-5.49	1.17	1.23
1	P	44	GLU	CA-C	-5.48	1.45	1.52
1	P	19	GLN	C-O	-5.48	1.17	1.24
1	P	129	ASN	CG-OD1	5.48	1.33	1.23
1	P	4	THR	C-O	-5.47	1.17	1.24
1	P	41	PHE	CA-CB	-5.47	1.44	1.53
1	P	235	VAL	CA-CB	5.47	1.61	1.53
1	P	124	ALA	N-CA	5.45	1.53	1.46
1	P	222	TYR	CE1-CZ	5.45	1.51	1.38
1	P	180	THR	C-N	5.43	1.41	1.33
1	P	248	PHE	N-CA	5.38	1.51	1.46
1	P	169	PHE	CA-C	5.37	1.59	1.52
1	P	104	ALA	CA-CB	5.36	1.60	1.53
1	P	145	SER	CA-C	-5.36	1.45	1.52
1	P	88	THR	C-O	-5.36	1.17	1.24
1	P	129	ASN	CG-ND2	-5.36	1.22	1.33
1	P	102	GLU	C-O	-5.35	1.17	1.24
1	P	231	TYR	N-CA	5.33	1.52	1.46
1	P	325	SER	C-N	-5.33	1.25	1.33
1	P	31	PHE	CD1-CE1	5.33	1.54	1.38
1	P	231	TYR	CA-CB	5.32	1.61	1.53
1	P	174	ALA	C-N	-5.31	1.26	1.33
1	P	191	GLU	C-N	5.30	1.40	1.33
1	P	284	PHE	C-N	5.29	1.41	1.33
1	P	193	THR	N-CA	5.28	1.52	1.46
1	P	269	PRO	CA-C	-5.27	1.45	1.52
1	P	94	LEU	CA-CB	5.27	1.61	1.53
1	P	282(A)	SER	CA-CB	5.27	1.62	1.53
1	P	237	GLY	C-N	-5.26	1.26	1.33
1	P	146	LEU	CA-CB	5.25	1.62	1.53
1	P	82	GLY	CA-C	-5.25	1.44	1.51
1	P	184(A)	SER	CA-CB	5.24	1.60	1.53
1	P	129	ASN	CB-CG	5.23	1.65	1.52
1	P	87	ASP	CB-CG	5.23	1.65	1.52
1	P	59	SER	C-O	5.23	1.30	1.24
1	P	60	LYS	C-N	5.22	1.40	1.33
1	P	288	GLN	CD-OE1	5.22	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	117	ILE	CA-C	5.22	1.59	1.52
1	P	63(A)	ALA	CA-C	-5.20	1.46	1.52
1	P	17	PRO	N-CA	5.19	1.53	1.47
1	P	60	LYS	C-O	-5.18	1.17	1.24
1	P	134	THR	CA-C	-5.18	1.46	1.52
1	P	280	THR	CA-CB	5.16	1.62	1.53
1	P	284	PHE	CA-C	-5.14	1.46	1.52
1	P	56	TYR	CA-CB	-5.14	1.45	1.53
1	P	301	ILE	C-O	-5.14	1.18	1.24
1	P	223	LEU	CA-CB	-5.14	1.47	1.53
1	P	247	VAL	N-CA	5.12	1.51	1.46
1	P	37	ASP	CA-C	5.12	1.58	1.52
1	P	48	SER	N-CA	5.12	1.52	1.46
1	P	110	SER	CB-OG	-5.12	1.31	1.42
1	P	266	ILE	CA-C	-5.11	1.46	1.52
1	P	268	ILE	CA-C	-5.11	1.47	1.52
1	P	182	THR	CA-C	-5.10	1.46	1.52
1	P	201	SER	CA-CB	5.10	1.60	1.53
1	P	239	SER	CA-CB	5.10	1.60	1.53
1	P	63(A)	ALA	CA-CB	5.09	1.61	1.53
1	P	143	LYS	CA-CB	5.08	1.61	1.53
1	P	220	LEU	C-O	-5.07	1.16	1.23
1	P	45	THR	CA-C	-5.06	1.46	1.52
1	P	28	ASN	CB-CG	5.05	1.64	1.52
1	P	189	PHE	C-O	5.04	1.30	1.23
1	P	279	SER	N-CA	5.03	1.52	1.45
1	P	275	PHE	CA-C	5.03	1.59	1.52
1	P	179	ILE	CB-CG1	5.03	1.63	1.53
1	P	236	SER	C-N	5.03	1.39	1.33
1	P	99	GLN	CA-C	-5.01	1.46	1.52
1	P	147	ASP	C-N	-5.00	1.27	1.33

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	51	ASP	CA-CB-CG	23.57	136.17	112.60
1	P	201	SER	CA-C-N	-10.94	110.52	122.55
1	P	201	SER	C-N-CA	-10.94	110.52	122.55
1	P	283	CYS	CA-C-N	10.87	137.48	121.72
1	P	283	CYS	C-N-CA	10.87	137.48	121.72
1	P	24	ALA	CA-C-O	10.33	132.58	120.70
1	P	300	ASN	CA-CB-CG	-10.17	102.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1	SER	O-C-N	-9.78	111.41	123.44
1	P	138	PHE	O-C-N	-9.67	111.87	122.12
1	P	28	ASN	CA-CB-CG	-9.58	103.02	112.60
1	P	67	SER	CA-C-N	-9.10	109.02	123.31
1	P	67	SER	C-N-CA	-9.10	109.02	123.31
1	P	275	PHE	CA-CB-CG	-8.95	104.85	113.80
1	P	140	ASP	CA-CB-CG	-8.89	103.70	112.60
1	P	83	ASP	CA-C-O	-8.73	111.37	121.49
1	P	124	ALA	O-C-N	-8.69	111.03	122.59
1	P	13	ALA	CA-C-O	-8.24	112.46	121.28
1	P	255	PRO	CA-N-CD	8.19	123.47	112.00
1	P	138	PHE	CA-CB-CG	-8.16	105.64	113.80
1	P	24	ALA	O-C-N	-8.14	112.18	123.01
1	P	288	GLN	OE1-CD-NE2	-8.10	114.50	122.60
1	P	123	LEU	O-C-N	8.09	133.34	122.26
1	P	309	ALA	O-C-N	-8.02	111.39	122.46
1	P	300	ASN	OD1-CG-ND2	7.81	130.41	122.60
1	P	192	TRP	CA-C-O	-7.79	113.13	121.38
1	P	127	THR	O-C-N	-7.79	112.27	122.39
1	P	229	SER	CA-C-N	7.78	130.71	120.28
1	P	229	SER	C-N-CA	7.78	130.71	120.28
1	P	224	PRO	N-CA-CB	-7.74	95.25	103.38
1	P	20	ILE	CA-C-N	-7.72	109.61	122.43
1	P	20	ILE	C-N-CA	-7.72	109.61	122.43
1	P	102	GLU	CA-CB-CG	-7.70	98.69	114.10
1	P	192	TRP	O-C-N	7.65	131.29	123.26
1	P	235	VAL	N-CA-CB	-7.54	102.40	111.90
1	P	125	PHE	CA-CB-CG	-7.52	106.28	113.80
1	P	223	LEU	CA-C-O	7.47	127.37	120.50
1	P	77	ASP	CA-C-N	-7.41	112.04	122.86
1	P	77	ASP	C-N-CA	-7.41	112.04	122.86
1	P	151	PHE	CA-CB-CG	7.37	121.17	113.80
1	P	25	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	P	36	SER	CA-C-O	-7.31	111.90	120.53
1	P	223	LEU	O-C-N	-7.31	117.03	121.71
1	P	315	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	P	138	PHE	N-CA-CB	-7.26	99.45	110.12
1	P	127	THR	CA-C-O	7.17	128.16	119.49
1	P	323	PHE	CG-CD1-CE1	-7.14	108.55	120.70
1	P	235	VAL	CA-C-O	7.13	128.32	120.48
1	P	255	PRO	CB-CA-C	-7.12	101.63	110.95
1	P	224	PRO	CA-N-CD	7.10	121.95	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	202	GLY	O-C-N	-7.09	115.94	122.96
1	P	304	ASP	CA-CB-CG	-7.06	105.54	112.60
1	P	66	LEU	CA-C-O	7.05	127.88	120.54
1	P	265	ARG	CA-CB-CG	-7.04	100.01	114.10
1	P	138	PHE	CA-C-O	6.94	127.91	120.55
1	P	53	GLN	OE1-CD-NE2	-6.94	115.66	122.60
1	P	31	PHE	CD1-CG-CD2	6.90	128.95	118.60
1	P	191	GLU	CA-CB-CG	-6.87	100.35	114.10
1	P	16	THR	CA-C-N	-6.87	112.89	119.76
1	P	16	THR	C-N-CA	-6.87	112.89	119.76
1	P	298	GLY	CA-C-N	-6.81	112.42	122.23
1	P	298	GLY	C-N-CA	-6.81	112.42	122.23
1	P	233	ALA	N-CA-C	-6.78	104.27	112.54
1	P	84	VAL	N-CA-C	6.78	118.48	108.45
1	P	191	GLU	CA-C-O	6.76	128.31	120.80
1	P	273	ILE	CA-C-O	6.75	126.98	119.42
1	P	323	PHE	CZ-CE2-CD2	-6.70	107.93	120.00
1	P	129	ASN	CA-CB-CG	-6.66	105.94	112.60
1	P	309	ALA	CA-C-O	6.64	127.68	119.05
1	P	206	SER	CA-C-N	-6.64	114.23	123.13
1	P	206	SER	C-N-CA	-6.64	114.23	123.13
1	P	211	ASP	CA-CB-CG	-6.63	105.97	112.60
1	P	27	LEU	CA-C-N	-6.62	113.71	123.11
1	P	27	LEU	C-N-CA	-6.62	113.71	123.11
1	P	297	ILE	N-CA-CB	-6.62	100.53	111.98
1	P	255	PRO	N-CA-CB	-6.60	96.45	103.38
1	P	280	THR	CA-C-N	-6.59	112.84	122.46
1	P	280	THR	C-N-CA	-6.59	112.84	122.46
1	P	313	VAL	CA-CB-CG2	6.51	121.47	110.40
1	P	242	SER	CA-C-N	-6.51	112.39	121.77
1	P	242	SER	C-N-CA	-6.51	112.39	121.77
1	P	108	SER	CA-C-N	6.50	130.56	120.82
1	P	108	SER	C-N-CA	6.50	130.56	120.82
1	P	165	TYR	CB-CG-CD2	6.49	130.53	120.80
1	P	223	LEU	CA-C-N	-6.48	113.62	120.03
1	P	223	LEU	C-N-CA	-6.48	113.62	120.03
1	P	123	LEU	CA-C-O	-6.47	112.27	119.78
1	P	225	ALA	CA-C-N	-6.44	109.87	121.14
1	P	225	ALA	C-N-CA	-6.44	109.87	121.14
1	P	323	PHE	CG-CD2-CE2	6.43	131.63	120.70
1	P	275	PHE	N-CA-CB	6.43	119.52	110.07
1	P	49	GLU	CA-C-N	-6.40	114.86	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	49	GLU	C-N-CA	-6.40	114.86	122.93
1	P	191	GLU	CB-CG-CD	-6.38	101.75	112.60
1	P	302	PHE	CE1-CZ-CE2	6.36	131.44	120.00
1	P	49	GLU	CA-CB-CG	-6.35	101.41	114.10
1	P	158	HIS	CB-CG-CD2	-6.31	122.99	131.20
1	P	18	VAL	O-C-N	6.31	129.85	123.10
1	P	41	PHE	CZ-CE2-CD2	-6.28	108.70	120.00
1	P	302	PHE	CA-CB-CG	-6.26	107.54	113.80
1	P	1	SER	CA-C-O	6.22	128.60	120.21
1	P	88	THR	CA-C-N	-6.19	113.80	122.71
1	P	88	THR	C-N-CA	-6.19	113.80	122.71
1	P	11	ASP	CB-CA-C	-6.18	102.96	111.73
1	P	134(A)	GLN	OE1-CD-NE2	6.17	128.78	122.60
1	P	18	VAL	CA-CB-CG1	6.17	120.88	110.40
1	P	300	ASN	O-C-N	6.16	129.96	123.06
1	P	304	ASP	CB-CA-C	-6.15	98.86	110.67
1	P	129	ASN	CA-C-O	6.12	127.92	121.19
1	P	101	VAL	N-CA-CB	-6.11	104.20	111.90
1	P	183	ALA	CA-C-O	6.10	128.21	121.56
1	P	139	PHE	N-CA-C	6.07	117.89	111.28
1	P	18	VAL	CB-CA-C	-6.02	101.23	110.50
1	P	284	PHE	CA-C-N	-5.95	114.59	120.60
1	P	284	PHE	C-N-CA	-5.95	114.59	120.60
1	P	47	ALA	CA-C-N	-5.94	110.07	121.94
1	P	47	ALA	C-N-CA	-5.94	110.07	121.94
1	P	192	TRP	CZ3-CH2-CZ2	-5.93	113.80	121.50
1	P	236	SER	O-C-N	-5.93	114.98	122.27
1	P	244	GLY	O-C-N	-5.92	115.90	122.47
1	P	162	PRO	O-C-N	-5.91	115.79	123.00
1	P	17	PRO	N-CA-CB	-5.88	97.87	103.34
1	P	275	PHE	CD1-CG-CD2	5.81	127.32	118.60
1	P	284	PHE	CA-CB-CG	5.81	119.61	113.80
1	P	243	VAL	N-CA-CB	-5.79	103.27	112.07
1	P	35	SER	CA-C-N	-5.77	112.00	122.50
1	P	35	SER	C-N-CA	-5.77	112.00	122.50
1	P	95	THR	CA-CB-OG1	-5.75	100.97	109.60
1	P	126	SER	CA-CB-OG	-5.75	99.60	111.10
1	P	135	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	P	220	LEU	CA-C-O	5.75	129.49	121.73
1	P	65	LEU	CA-C-N	-5.74	115.38	122.84
1	P	65	LEU	C-N-CA	-5.74	115.38	122.84
1	P	104	ALA	N-CA-C	5.73	118.01	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	139	PHE	CA-C-O	5.71	126.61	120.55
1	P	180	THR	CA-C-O	5.70	126.59	120.38
1	P	282	SER	CA-C-O	-5.69	115.10	121.81
1	P	201	SER	N-CA-C	-5.65	106.18	112.57
1	P	99	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	P	90	SER	CA-C-N	-5.63	114.99	122.98
1	P	90	SER	C-N-CA	-5.63	114.99	122.98
1	P	173	THR	CA-C-O	5.62	126.30	119.11
1	P	158	HIS	CA-CB-CG	-5.60	108.20	113.80
1	P	124	ALA	CA-C-O	5.58	128.50	120.51
1	P	265	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	P	235	VAL	CA-CB-CG1	-5.53	100.99	110.40
1	P	147	ASP	CA-CB-CG	-5.50	107.09	112.60
1	P	201	SER	CB-CA-C	-5.50	102.54	111.06
1	P	23	PRO	CA-N-CD	5.49	119.19	111.50
1	P	88	THR	CA-CB-OG1	-5.49	101.37	109.60
1	P	103	SER	O-C-N	-5.45	117.01	123.22
1	P	92	GLY	CA-C-N	-5.44	113.97	122.51
1	P	92	GLY	C-N-CA	-5.44	113.97	122.51
1	P	236	SER	CA-C-O	5.44	126.23	119.97
1	P	90	SER	O-C-N	5.44	129.90	123.27
1	P	165	TYR	CB-CG-CD1	-5.43	112.66	120.80
1	P	31	PHE	CG-CD1-CE1	-5.42	111.50	120.70
1	P	212	GLY	O-C-N	5.41	129.02	123.29
1	P	28	ASN	O-C-N	5.40	129.94	123.13
1	P	192	TRP	CA-C-N	-5.40	115.39	123.00
1	P	192	TRP	C-N-CA	-5.40	115.39	123.00
1	P	190	TRP	CA-CB-CG	-5.39	103.36	113.60
1	P	297	ILE	CB-CA-C	-5.38	102.99	110.95
1	P	315	ASN	CB-CG-ND2	5.37	124.46	116.40
1	P	110	SER	CB-CA-C	-5.36	100.37	110.67
1	P	129	ASN	O-C-N	-5.36	116.27	122.87
1	P	99	GLN	CG-CD-OE1	-5.36	110.08	120.80
1	P	267	VAL	CA-CB-CG1	-5.36	101.28	110.40
1	P	147	ASP	N-CA-C	-5.36	106.00	112.54
1	P	18	VAL	CA-C-N	-5.30	115.63	123.05
1	P	18	VAL	C-N-CA	-5.30	115.63	123.05
1	P	190	TRP	CG-CD1-NE1	-5.30	103.31	110.20
1	P	211	ASP	CA-C-N	-5.29	112.04	121.93
1	P	211	ASP	C-N-CA	-5.29	112.04	121.93
1	P	280	THR	O-C-N	-5.28	116.37	122.87
1	P	184(A)	SER	CA-C-N	-5.27	114.29	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	184(A)	SER	C-N-CA	-5.27	114.29	122.67
1	P	236	SER	CA-C-N	-5.27	113.34	122.83
1	P	236	SER	C-N-CA	-5.27	113.34	122.83
1	P	183	ALA	O-C-N	-5.25	116.67	122.86
1	P	28	ASN	CB-CA-C	-5.25	102.24	110.79
1	P	173	THR	O-C-N	-5.25	114.77	122.43
1	P	271	ASP	N-CA-C	-5.24	106.15	112.54
1	P	86	THR	CA-C-O	-5.23	114.99	120.80
1	P	202	GLY	CA-C-O	5.22	127.40	121.92
1	P	231	TYR	CA-CB-CG	-5.21	104.52	113.90
1	P	51	ASP	OD1-CG-OD2	5.18	135.33	122.90
1	P	32	ASP	CA-CB-CG	-5.17	107.43	112.60
1	P	127	THR	CA-CB-OG1	-5.16	101.85	109.60
1	P	91	VAL	N-CA-CB	-5.16	104.80	111.82
1	P	66	LEU	O-C-N	-5.15	116.92	123.05
1	P	197	TYR	CG-CD1-CE1	-5.15	113.48	121.20
1	P	312	VAL	CA-CB-CG2	5.14	119.14	110.40
1	P	69	ALA	O-C-N	-5.12	117.22	123.16
1	P	165	TYR	CG-CD2-CE2	5.12	128.88	121.20
1	P	212	GLY	CA-C-N	-5.12	114.07	122.67
1	P	212	GLY	C-N-CA	-5.12	114.07	122.67
1	P	246	TYR	CG-CD1-CE1	-5.11	113.54	121.20
1	P	179	ILE	CB-CA-C	-5.10	104.23	111.21
1	P	100	ALA	CA-C-O	5.09	126.56	120.70
1	P	302	PHE	O-C-N	5.09	129.44	122.41
1	P	136	LYS	CA-CB-CG	-5.08	103.94	114.10
1	P	190	TRP	CB-CA-C	-5.07	103.72	111.83
1	P	176	THR	CA-C-N	5.07	129.95	120.07
1	P	176	THR	C-N-CA	5.07	129.95	120.07
1	P	56	TYR	CA-C-O	5.06	126.46	120.69
1	P	284	PHE	N-CA-C	5.06	116.99	109.25
1	P	73	ILE	CA-C-N	-5.05	114.73	122.62
1	P	73	ILE	C-N-CA	-5.05	114.73	122.62
1	P	152	THR	CB-CA-C	5.03	118.44	109.38
1	P	127	THR	N-CA-C	5.03	118.52	112.38
1	P	105	LYS	CA-CB-CG	-5.01	104.07	114.10
1	P	194	SER	N-CA-C	-5.01	103.06	110.48
1	P	221	LEU	CA-C-N	-5.01	116.03	123.05
1	P	221	LEU	C-N-CA	-5.01	116.03	123.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	265	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2389	0	2280	24	0
2	P	45	0	54	22	0
3	P	278	0	0	1	1
All	All	2712	0	2334	44	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 9.

All (44) 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:P:51:ASP:OD1	1:P:52:GLY:N	1.81	1.11
2:P:327:0EO:CD12	2:P:327:0EO:HD11	0.97	1.10
2:P:327:0EO:HD24	2:P:327:0EO:CD22	0.97	1.09
2:P:327:0EO:CD12	2:P:327:0EO:HD15	0.97	1.09
2:P:327:0EO:CD12	2:P:327:0EO:HD14	0.97	1.07
2:P:327:0EO:CD22	2:P:327:0EO:HD21	0.97	1.06
2:P:327:0EO:CD22	2:P:327:0EO:HD25	0.97	1.02
2:P:327:0EO:HD15	2:P:327:0EO:CG2	1.99	0.92
2:P:327:0EO:HD11	2:P:327:0EO:CG2	1.99	0.92
2:P:327:0EO:HD14	2:P:327:0EO:CG2	1.99	0.91
2:P:327:0EO:HD25	2:P:327:0EO:CG2	2.05	0.87
2:P:327:0EO:HD24	2:P:327:0EO:CG2	2.05	0.86
2:P:327:0EO:HD24	2:P:327:0EO:HD21	1.58	0.86
2:P:327:0EO:HD24	2:P:327:0EO:HD25	1.58	0.85
2:P:327:0EO:HD21	2:P:327:0EO:CG2	2.05	0.85
2:P:327:0EO:HD11	2:P:327:0EO:HD14	1.58	0.85
1:P:120:LEU:HD21	2:P:327:0EO:HD23	1.57	0.85
2:P:327:0EO:HD11	2:P:327:0EO:HD15	1.58	0.84
2:P:327:0EO:HD15	2:P:327:0EO:HD14	1.58	0.84
2:P:327:0EO:HD21	2:P:327:0EO:HD25	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:VAL:HG21	1:P:29:LEU:HD12	1.81	0.63
1:P:129:ASN:ND2	1:P:135:GLN:H	1.97	0.63
1:P:220:LEU:HD11	2:P:327:0EO:H13	1.81	0.62
1:P:114:ASP:OD2	1:P:117:ILE:HD12	2.03	0.59
1:P:299:ILE:HD12	3:P:405:HOH:O	2.07	0.54
1:P:213:ILE:HG23	1:P:299:ILE:HD11	1.91	0.53
1:P:99:GLN:NE2	1:P:138:PHE:HA	2.24	0.53
1:P:264:ALA:C	1:P:265:ARG:HG2	2.34	0.52
1:P:38:LEU:C	1:P:38:LEU:HD23	2.36	0.51
1:P:129:ASN:ND2	1:P:131:VAL:H	2.10	0.49
1:P:304:ASP:O	1:P:308:LYS:HG2	2.15	0.46
1:P:315:ASN:O	1:P:319(A):PRO:HA	2.17	0.45
1:P:299:ILE:HG13	1:P:300:ASN:N	2.32	0.44
2:P:327:0EO:HD1	2:P:327:0EO:N	2.32	0.44
1:P:297:ILE:HG22	1:P:299:ILE:H	1.83	0.43
1:P:71:TRP:CE2	1:P:102:GLU:HB3	2.53	0.43
1:P:5:THR:CG2	1:P:6:PRO:HD2	2.49	0.42
2:P:327:0EO:O1	2:P:327:0EO:H23	2.18	0.42
1:P:181:TYR:HA	1:P:321:LEU:O	2.20	0.42
1:P:10:LEU:O	1:P:11:ASP:HB2	2.19	0.42
1:P:223:LEU:HB3	1:P:224:PRO:CD	2.50	0.42
1:P:186:LYS:HE3	1:P:186:LYS:HB2	1.66	0.41
1:P:232:TRP:CZ2	1:P:285:GLY:HA3	2.55	0.41
1:P:223:LEU:HB3	1:P:224:PRO:HD2	2.01	0.41

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)
3:P:406:HOH:O	3:P:586:HOH:O[2_555]	2.15	0.05

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	P	328/330 (99%)	323 (98%)	3 (1%)	2 (1%)	21	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	317	ALA
1	P	305	VAL

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	P	263/263 (100%)	257 (98%)	6 (2%)	44	49

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

Mol	Chain	Res	Type
1	P	28	ASN
1	P	51	ASP
1	P	64	LYS
1	P	242	SER
1	P	268	ILE
1	P	299	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	28	ASN
1	P	99	GLN
1	P	129	ASN
1	P	141	ASN
1	P	166	ASN
1	P	187	GLN

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Mol	Chain	Res	Type
1	P	300	ASN
1	P	315	ASN

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 ⓘ

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	0EO	P	327	-	46,46,46	1.45	4 (8%)	58,62,62	1.26	7 (12%)

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	0EO	P	327	-	-	9/50/58/58	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	327	0EO	O2-C	6.52	1.47	1.34
2	P	327	0EO	CD21-CG1	-3.57	1.42	1.52
2	P	327	0EO	O1-C	3.16	1.27	1.21
2	P	327	0EO	CA-N	2.70	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	327	0EO	CB-CA-CH	-4.32	104.63	111.66
2	P	327	0EO	CB1-CA2-CH1	-3.06	107.93	112.55
2	P	327	0EO	O2-C-O1	-3.01	120.29	125.64
2	P	327	0EO	OXT-C6-O3	-2.96	117.37	124.08
2	P	327	0EO	CA1-CM-CH	-2.57	109.54	114.81
2	P	327	0EO	OXT-C6-CA3	2.41	121.68	113.51
2	P	327	0EO	O2-C-N	2.40	113.95	110.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	327	0EO	N-CA-CH-CM
2	P	327	0EO	CB-CA-CH-CM
2	P	327	0EO	N-CA-CH-OH
2	P	327	0EO	CB-CA-CH-OH
2	P	327	0EO	C4-CA1-CM-CH
2	P	327	0EO	CA-CB-CG-CD1
2	P	327	0EO	CA-CB-CG-CD2
2	P	327	0EO	OXT-C6-CA3-N2
2	P	327	0EO	O3-C6-CA3-N2

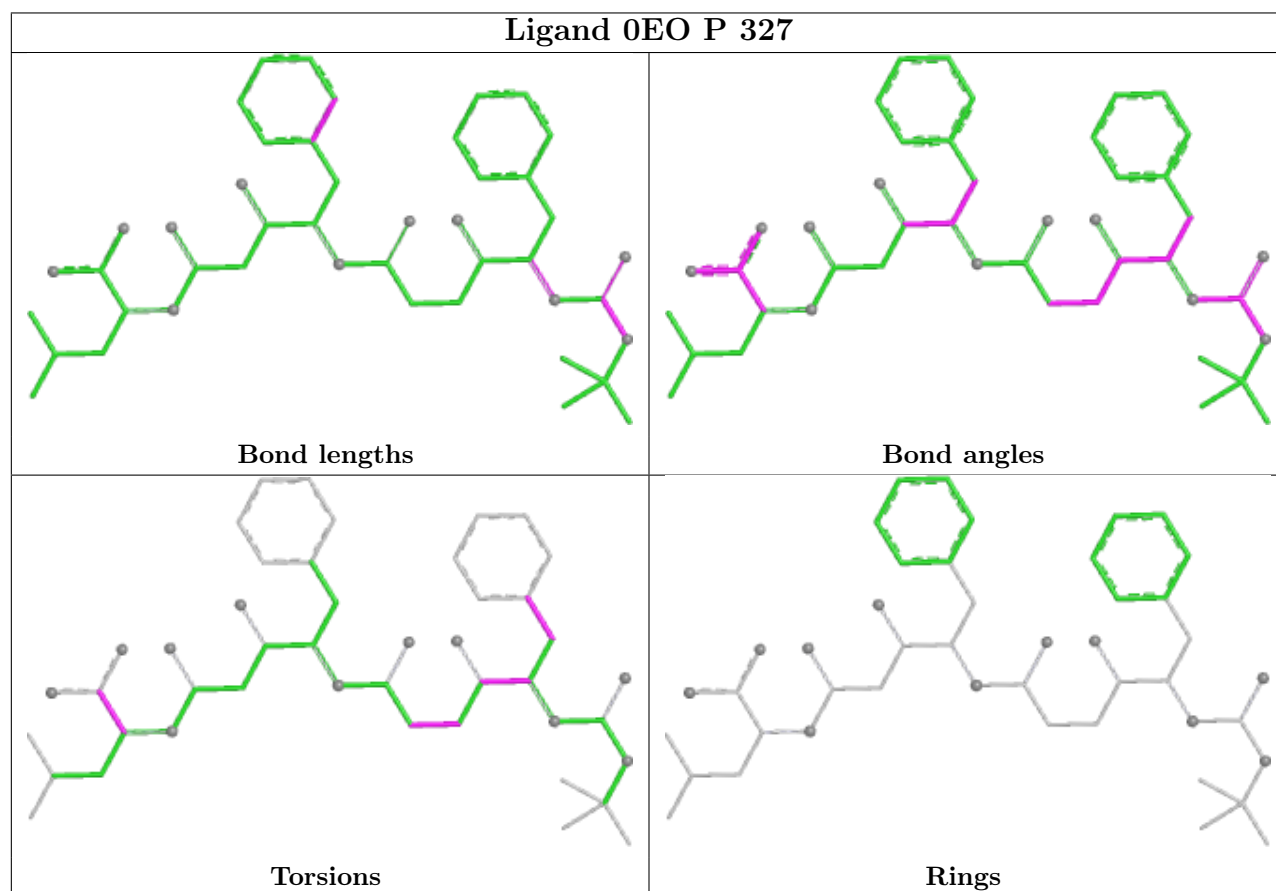
There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	327	0EO	22	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.