



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 05:07 AM EDT

PDB ID : 1EED
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

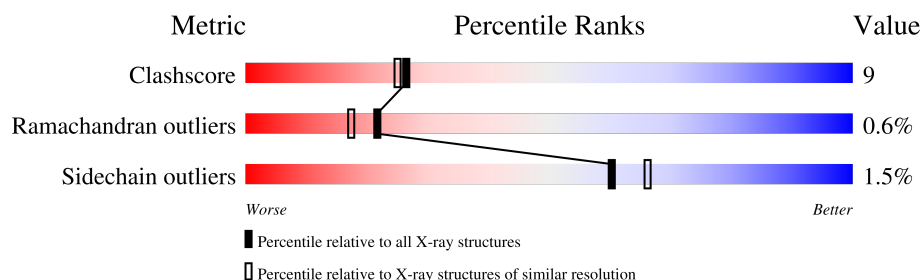
1 Overall quality at a glance

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	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (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	

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](#)

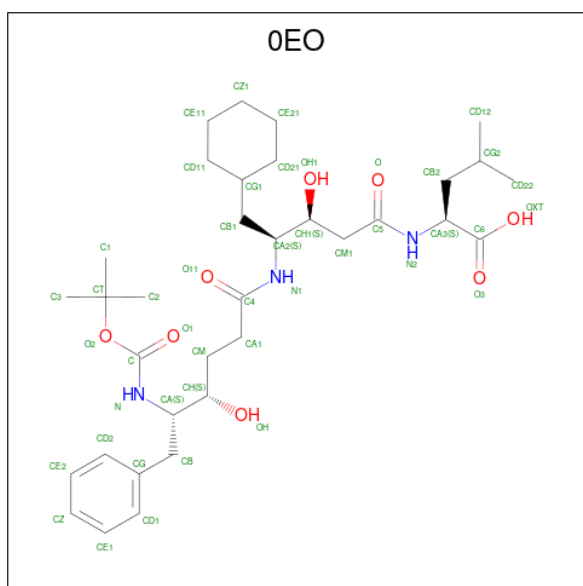
There are 3 unique types of molecules in this entry. The entry contains 2712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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 (three-letter code: 0EO) (formula: C₃₄H₅₅N₃O₈).

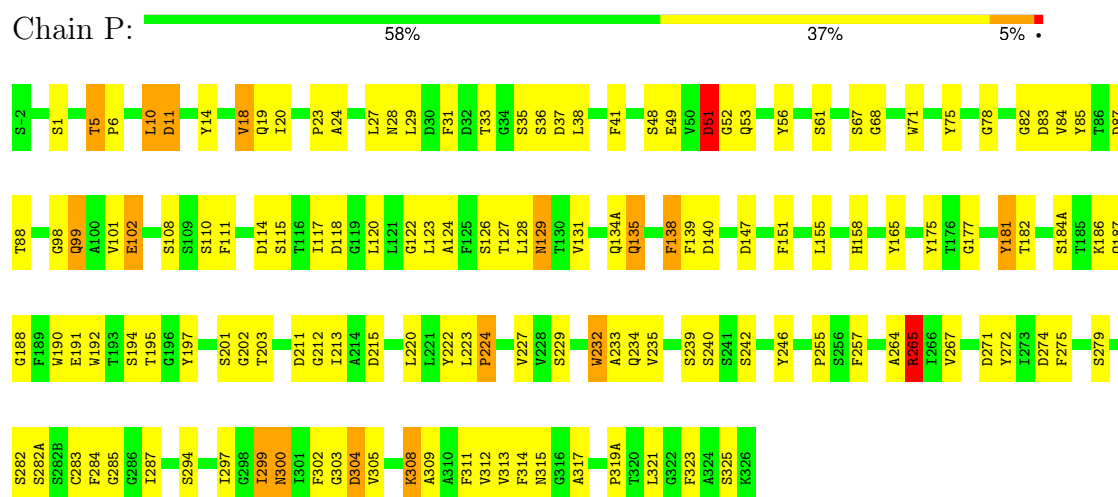


3 Residue-property plots

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 [i](#)

5.1 Standard geometry [i](#)

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	2.32	92/2445 (3.8%)	2.35	119/3345 (3.6%)

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 (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	35	SER	CB-OG	11.64	1.57	1.42
1	P	282	SER	CB-OG	10.32	1.55	1.42
1	P	222	TYR	CE1-CZ	9.83	1.51	1.38
1	P	212	GLY	C-O	-9.59	1.08	1.23
1	P	129	ASN	N-CA	9.34	1.65	1.46
1	P	82	GLY	N-CA	9.27	1.59	1.46
1	P	294	SER	CB-OG	9.13	1.54	1.42
1	P	165	TYR	CE2-CZ	8.73	1.50	1.38
1	P	36	SER	CB-OG	8.52	1.53	1.42
1	P	110	SER	CA-CB	8.36	1.65	1.52
1	P	265	ARG	CD-NE	8.08	1.60	1.46
1	P	61	SER	CA-CB	8.06	1.65	1.52
1	P	191	GLU	CB-CG	7.97	1.67	1.52
1	P	110	SER	CB-OG	-7.95	1.31	1.42
1	P	300	ASN	CB-CG	7.83	1.69	1.51
1	P	126	SER	CA-CB	7.76	1.64	1.52
1	P	31	PHE	CD1-CE1	7.69	1.54	1.39
1	P	202	GLY	N-CA	7.39	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	314	PHE	CE2-CZ	7.12	1.50	1.37
1	P	122	GLY	N-CA	7.12	1.56	1.46
1	P	188	GLY	N-CA	7.08	1.56	1.46
1	P	108	SER	CA-CB	6.99	1.63	1.52
1	P	325	SER	CB-OG	6.94	1.51	1.42
1	P	75	TYR	CE1-CZ	6.84	1.47	1.38
1	P	19	GLN	N-CA	6.83	1.60	1.46
1	P	139	PHE	CG-CD2	6.83	1.49	1.38
1	P	229	SER	CA-CB	6.79	1.63	1.52
1	P	177	GLY	N-CA	6.78	1.56	1.46
1	P	98	GLY	N-CA	6.78	1.56	1.46
1	P	303	GLY	N-CA	6.69	1.56	1.46
1	P	212	GLY	CA-C	6.63	1.62	1.51
1	P	48	SER	CB-OG	6.60	1.50	1.42
1	P	246	TYR	CD1-CE1	6.60	1.49	1.39
1	P	282(A)	SER	CA-CB	6.57	1.62	1.52
1	P	138	PHE	N-CA	6.46	1.59	1.46
1	P	1	SER	CB-OG	6.43	1.50	1.42
1	P	240	SER	CB-OG	6.42	1.50	1.42
1	P	101	VAL	CA-CB	6.40	1.68	1.54
1	P	5	THR	CA-CB	6.39	1.70	1.53
1	P	87	ASP	CB-CG	6.37	1.65	1.51
1	P	311	PHE	CG-CD1	6.36	1.48	1.38
1	P	135	GLN	CD-OE1	6.26	1.37	1.24
1	P	68	GLY	N-CA	6.14	1.55	1.46
1	P	129	ASN	CB-CG	6.12	1.65	1.51
1	P	323	PHE	CG-CD2	-6.11	1.29	1.38
1	P	283	CYS	CB-SG	6.10	1.92	1.82
1	P	233	ALA	N-CA	6.10	1.58	1.46
1	P	182	THR	C-O	6.04	1.34	1.23
1	P	255	PRO	CA-CB	6.04	1.65	1.53
1	P	300	ASN	CG-ND2	-6.03	1.17	1.32
1	P	232	TRP	CD1-NE1	5.96	1.48	1.38
1	P	28	ASN	CB-CG	5.92	1.64	1.51
1	P	232	TRP	NE1-CE2	-5.92	1.29	1.37
1	P	87	ASP	N-CA	5.91	1.58	1.46
1	P	41	PHE	N-CA	5.75	1.57	1.46
1	P	78	GLY	N-CA	5.70	1.54	1.46
1	P	10	LEU	N-CA	5.62	1.57	1.46
1	P	84	VAL	CA-CB	5.62	1.66	1.54
1	P	33	THR	CB-OG1	5.61	1.54	1.43
1	P	234	GLN	CD-OE1	5.59	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	53	GLN	CD-OE1	5.59	1.36	1.24
1	P	24	ALA	N-CA	5.53	1.57	1.46
1	P	300	ASN	CA-C	5.47	1.67	1.52
1	P	165	TYR	CE1-CZ	-5.46	1.31	1.38
1	P	271	ASP	N-CA	5.46	1.57	1.46
1	P	115	SER	CB-OG	5.41	1.49	1.42
1	P	304	ASP	CA-CB	5.40	1.65	1.53
1	P	195	THR	N-CA	5.39	1.57	1.46
1	P	287	ILE	N-CA	5.36	1.57	1.46
1	P	235	VAL	CB-CG1	5.36	1.64	1.52
1	P	41	PHE	CE2-CZ	5.33	1.47	1.37
1	P	165	TYR	CG-CD1	5.33	1.46	1.39
1	P	279	SER	CA-CB	5.31	1.60	1.52
1	P	187	GLN	CD-OE1	5.31	1.35	1.24
1	P	184(A)	SER	CA-CB	5.30	1.60	1.52
1	P	267	VAL	CB-CG1	5.30	1.64	1.52
1	P	158	HIS	ND1-CE1	5.28	1.48	1.34
1	P	138	PHE	CE2-CZ	5.25	1.47	1.37
1	P	190	TRP	CD1-NE1	5.25	1.46	1.38
1	P	102	GLU	CA-CB	5.22	1.65	1.53
1	P	232	TRP	CZ3-CH2	5.21	1.48	1.40
1	P	127	THR	CA-CB	5.19	1.66	1.53
1	P	194	SER	CA-C	5.18	1.66	1.52
1	P	239	SER	CA-CB	5.14	1.60	1.52
1	P	182	THR	N-CA	5.13	1.56	1.46
1	P	192	TRP	CA-C	5.11	1.66	1.52
1	P	265	ARG	CZ-NH2	5.09	1.39	1.33
1	P	27	LEU	C-O	-5.08	1.13	1.23
1	P	134(A)	GLN	CD-OE1	5.05	1.35	1.24
1	P	190	TRP	NE1-CE2	-5.04	1.31	1.37
1	P	14	TYR	CB-CG	5.01	1.59	1.51
1	P	302	PHE	CD1-CE1	5.01	1.49	1.39

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	165	TYR	CB-CG-CD2	15.89	130.53	121.00
1	P	165	TYR	CB-CG-CD1	-13.91	112.66	121.00
1	P	265	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	P	31	PHE	CB-CG-CD1	-11.98	112.42	120.80
1	P	75	TYR	CB-CG-CD2	-11.62	114.03	121.00
1	P	323	PHE	CG-CD1-CE1	-11.13	108.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	51	ASP	CA-CB-CG	10.35	136.17	113.40
1	P	323	PHE	CZ-CE2-CD2	-10.14	107.93	120.10
1	P	323	PHE	CG-CD2-CE2	9.85	131.63	120.80
1	P	197	TYR	CG-CD1-CE1	-9.77	113.48	121.30
1	P	246	TYR	CG-CD1-CE1	-9.70	113.54	121.30
1	P	41	PHE	CZ-CE2-CD2	-9.50	108.70	120.10
1	P	165	TYR	CG-CD2-CE2	9.47	128.88	121.30
1	P	191	GLU	OE1-CD-OE2	-9.31	112.13	123.30
1	P	56	TYR	CB-CG-CD2	-9.25	115.45	121.00
1	P	165	TYR	CD1-CE1-CZ	9.12	128.01	119.80
1	P	246	TYR	CB-CG-CD2	-9.11	115.54	121.00
1	P	111	PHE	CB-CG-CD2	-9.04	114.47	120.80
1	P	139	PHE	CB-CG-CD1	9.02	127.11	120.80
1	P	51	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	P	85	TYR	CG-CD2-CE2	-8.69	114.35	121.30
1	P	31	PHE	CG-CD1-CE1	-8.46	111.50	120.80
1	P	255	PRO	CA-N-CD	8.40	123.47	111.70
1	P	140	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	P	274	ASP	CB-CG-OD1	8.37	125.83	118.30
1	P	165	TYR	CZ-CE2-CD2	-8.34	112.30	119.80
1	P	31	PHE	CD1-CG-CD2	8.19	128.95	118.30
1	P	140	ASP	CB-CG-OD1	8.19	125.67	118.30
1	P	75	TYR	CG-CD2-CE2	-8.01	114.89	121.30
1	P	175	TYR	CB-CG-CD1	-7.83	116.30	121.00
1	P	190	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	P	284	PHE	CB-CG-CD1	-7.42	115.60	120.80
1	P	88	THR	CA-CB-CG2	-7.33	102.14	112.40
1	P	275	PHE	CG-CD2-CE2	-7.33	112.73	120.80
1	P	165	TYR	CG-CD1-CE1	-7.32	115.44	121.30
1	P	224	PRO	CA-N-CD	7.32	121.95	111.70
1	P	124	ALA	O-C-N	-7.29	111.03	122.70
1	P	203	THR	CA-CB-CG2	-7.28	102.21	112.40
1	P	257	PHE	CD1-CE1-CZ	-7.24	111.42	120.10
1	P	41	PHE	CG-CD2-CE2	7.23	128.76	120.80
1	P	5	THR	CA-CB-CG2	-7.10	102.46	112.40
1	P	41	PHE	CG-CD1-CE1	-7.08	113.01	120.80
1	P	309	ALA	O-C-N	-7.07	111.39	122.70
1	P	1	SER	O-C-N	-7.06	111.41	122.70
1	P	313	VAL	CA-CB-CG2	7.05	121.47	110.90
1	P	302	PHE	CD1-CE1-CZ	-7.02	111.67	120.10
1	P	275	PHE	CD1-CG-CD2	6.94	127.32	118.30
1	P	211	ASP	CB-CG-OD2	-6.88	112.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	308	LYS	CD-CE-NZ	6.87	127.50	111.70
1	P	181	TYR	CB-CG-CD1	-6.81	116.91	121.00
1	P	190	TRP	CG-CD1-NE1	-6.79	103.31	110.10
1	P	75	TYR	CD1-CG-CD2	6.78	125.36	117.90
1	P	138	PHE	O-C-N	-6.77	111.87	122.70
1	P	14	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	P	102	GLU	CA-CB-CG	-6.68	98.69	113.40
1	P	224	PRO	N-CA-CB	-6.68	95.25	102.60
1	P	18	VAL	CA-CB-CG1	6.66	120.88	110.90
1	P	123	LEU	O-C-N	6.65	133.34	122.70
1	P	235	VAL	CA-CB-CG1	-6.61	100.99	110.90
1	P	311	PHE	CG-CD2-CE2	6.58	128.04	120.80
1	P	24	ALA	O-C-N	-6.58	112.18	122.70
1	P	323	PHE	CD1-CE1-CZ	6.56	127.97	120.10
1	P	314	PHE	CG-CD2-CE2	6.55	128.01	120.80
1	P	127	THR	O-C-N	-6.52	112.27	122.70
1	P	192	TRP	CZ3-CH2-CZ2	-6.50	113.80	121.60
1	P	222	TYR	CD1-CE1-CZ	-6.46	113.98	119.80
1	P	275	PHE	CB-CG-CD1	-6.45	116.29	120.80
1	P	111	PHE	CG-CD2-CE2	-6.42	113.74	120.80
1	P	267	VAL	CA-CB-CG1	-6.41	101.28	110.90
1	P	302	PHE	CE1-CZ-CE2	6.36	131.44	120.00
1	P	51	ASP	OD1-CG-OD2	6.33	135.33	123.30
1	P	67	SER	C-N-CA	-6.32	109.02	122.30
1	P	211	ASP	CB-CG-OD1	6.32	123.99	118.30
1	P	283	CYS	C-N-CA	6.31	137.48	121.70
1	P	85	TYR	CB-CG-CD2	-6.31	117.21	121.00
1	P	275	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	P	222	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	P	138	PHE	N-CA-CB	-6.19	99.45	110.60
1	P	311	PHE	CB-CG-CD2	6.19	125.14	120.80
1	P	246	TYR	CD1-CG-CD2	6.18	124.70	117.90
1	P	275	PHE	CD1-CE1-CZ	-6.17	112.69	120.10
1	P	118	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	P	265	ARG	CA-CB-CG	-6.08	100.01	113.40
1	P	20	ILE	C-N-CA	-6.04	109.61	122.30
1	P	83	ASP	CB-CG-OD2	6.03	123.73	118.30
1	P	139	PHE	CB-CG-CD2	-5.98	116.61	120.80
1	P	24	ALA	CA-C-O	5.94	132.58	120.10
1	P	191	GLU	CA-CB-CG	-5.93	100.35	113.40
1	P	272	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	P	192	TRP	CE3-CZ3-CH2	5.81	127.60	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	311	PHE	CZ-CE2-CD2	-5.80	113.14	120.10
1	P	11	ASP	CB-CG-OD2	5.79	123.51	118.30
1	P	304	ASP	CB-CA-C	-5.77	98.86	110.40
1	P	99	GLN	CG-CD-OE1	-5.76	110.08	121.60
1	P	311	PHE	CB-CG-CD1	-5.76	116.77	120.80
1	P	128	LEU	CB-CG-CD1	-5.75	101.23	111.00
1	P	151	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	P	127	THR	CA-CB-CG2	-5.68	104.45	112.40
1	P	201	SER	C-N-CA	-5.61	110.52	122.30
1	P	255	PRO	N-CA-CB	-5.59	96.45	102.60
1	P	312	VAL	CA-CB-CG2	5.49	119.14	110.90
1	P	41	PHE	CD1-CE1-CZ	5.46	126.65	120.10
1	P	49	GLU	CA-CB-CG	-5.45	101.41	113.40
1	P	190	TRP	CA-CB-CG	-5.44	103.36	113.70
1	P	192	TRP	O-C-N	5.37	131.29	122.70
1	P	184(A)	SER	N-CA-CB	-5.36	102.46	110.50
1	P	85	TYR	CZ-CE2-CD2	5.36	124.62	119.80
1	P	274	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	P	18	VAL	CB-CA-C	-5.35	101.23	111.40
1	P	23	PRO	CA-N-CD	5.35	119.19	111.70
1	P	232	TRP	CE3-CZ3-CH2	-5.25	115.42	121.20
1	P	147	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	P	215	ASP	CB-CG-OD2	5.14	122.93	118.30
1	P	110	SER	CB-CA-C	-5.12	100.37	110.10
1	P	48	SER	N-CA-CB	-5.06	102.92	110.50
1	P	155	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	P	181	TYR	CG-CD2-CE2	-5.06	117.25	121.30
1	P	227	VAL	CA-CB-CG2	5.05	118.48	110.90
1	P	246	TYR	CZ-CE2-CD2	-5.02	115.28	119.80

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
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:129:ASN:ND2	1:P:131:VAL:H	2.10	0.49
1:P:264:ALA:C	1:P:265:ARG:HG2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:38:LEU:C	1:P:38:LEU:HD23	2.36	0.46
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 [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	P	328/330 (99%)	323 (98%)	3 (1%)	2 (1%)	22 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	317	ALA

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Mol	Chain	Res	Type
1	P	305	VAL

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	P	263/263 (100%)	259 (98%)	4 (2%)	60	66

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	37	ASP
1	P	51	ASP
1	P	242	SER
1	P	299	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	19	GLN
1	P	28	ASN
1	P	99	GLN
1	P	129	ASN
1	P	134(A)	GLN
1	P	135	GLN
1	P	141	ASN
1	P	166	ASN
1	P	187	GLN
1	P	300	ASN

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	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:

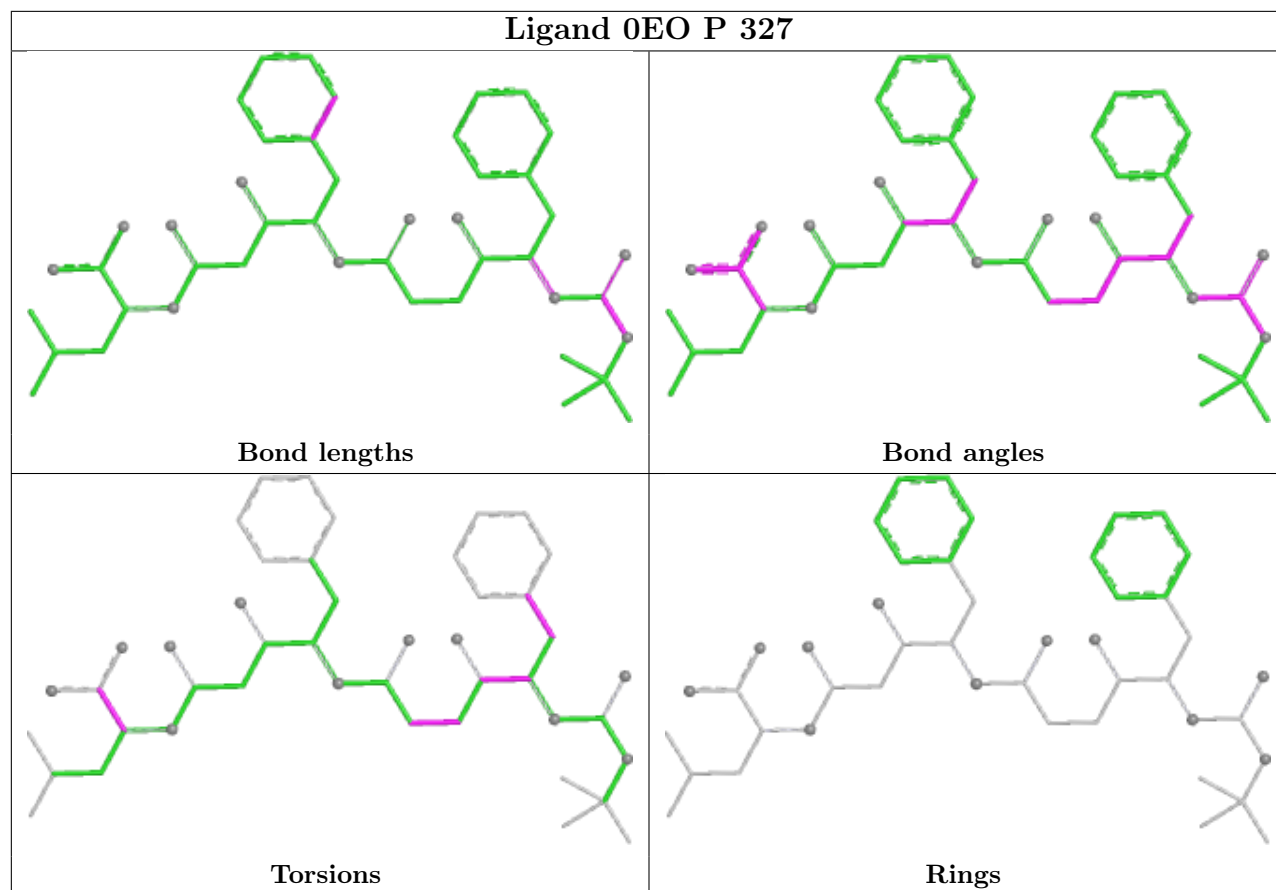
Mol	Chain	Res	Type	Atoms
2	P	327	0EO	N-CA-CH-CM
2	P	327	0EO	CB-CA-CH-CM
2	P	327	0EO	N-CA-CH-OH
2	P	327	0EO	CB-CA-CH-OH
2	P	327	0EO	C4-CA1-CM-CH
2	P	327	0EO	CA-CB-CG-CD1
2	P	327	0EO	CA-CB-CG-CD2
2	P	327	0EO	OXT-C6-CA3-N2
2	P	327	0EO	O3-C6-CA3-N2

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.