



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:16 PM UTC

PDB ID : 1PPL / pdb_00001ppl
Title : CRYSTALLOGRAPHIC ANALYSIS OF TRANSITION-STATE MIMICS
BOUND TO PENICILLOPEPSIN: PHOSPHORUS-CONTAINING PEP-
TIDE ANALOGUES
Authors : Fraser, M.E.; James, M.N.G.
Deposited on : 1992-06-01
Resolution : 1.70 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

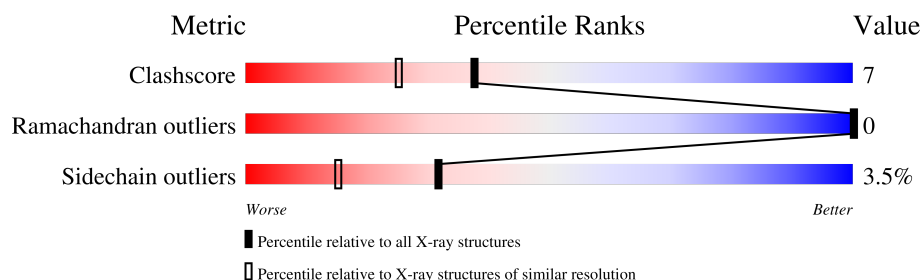
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	323	57% 38% .

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
4	XYS	E	330	X	-	-	-
5	SO4	E	331	-	-	X	-

2 Entry composition [i](#)

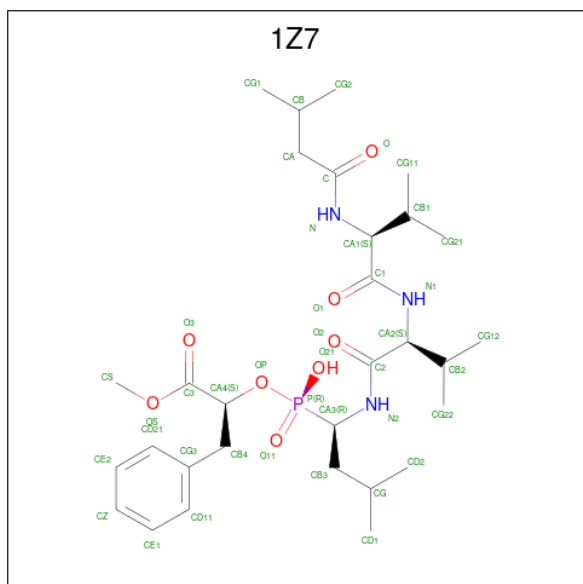
There are 6 unique types of molecules in this entry. The entry contains 2713 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PENICILLOPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	323	2370	1480	378	510	2	0	2	0

- Molecule 2 is N-(3-methylbutanoyl)-L-valyl-N-{(1S)-1-[(R)-[(1R)-1-benzyl-2-methoxy-2-oxoethoxy](hydroxy)phosphoryl]-3-methylbutyl}-L- valinamide (CCD ID: 1Z7) (formula: C₃₀H₅₀N₃O₈P).



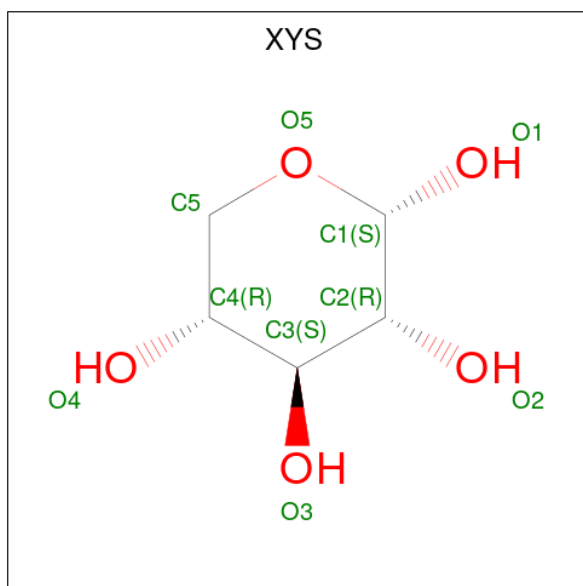
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	42	30	3	8	1	0	0

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is alpha-D-xylopyranose (CCD ID: YYS) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			9	5	4		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	276	Total	O	0	0
			276	276		

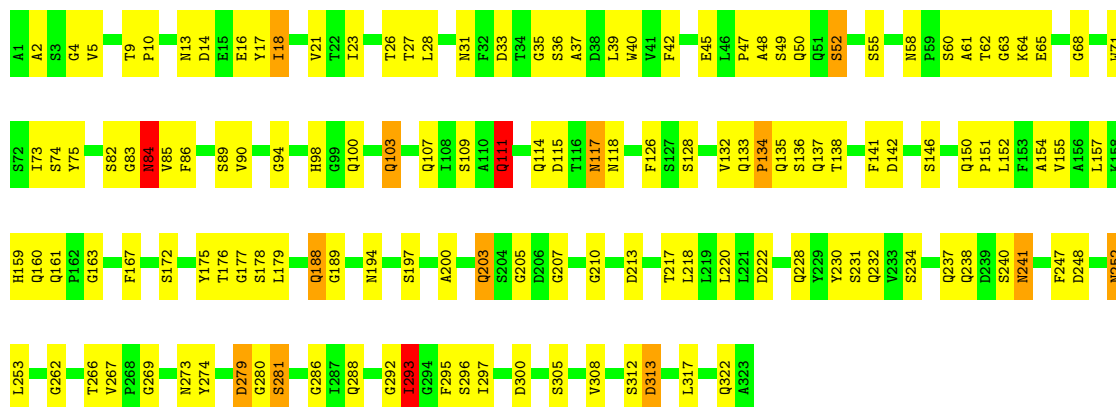
3 Residue-property plots

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: PENICILLOPEPSIN

Chain E: 



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	97.50Å 46.46Å 65.93Å 90.00° 115.20° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2713	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 1Z7, MAN, YYS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	E	1.79	36/2435 (1.5%)	2.39	148/3325 (4.5%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	SER	N-CA	7.49	1.55	1.45
1	E	266	THR	C-N	-6.84	1.27	1.33
1	E	71	TRP	N-CA	6.59	1.54	1.45
1	E	210	GLY	N-CA	6.58	1.52	1.45
1	E	136	SER	N-CA	6.49	1.54	1.45
1	E	267	VAL	CA-C	6.37	1.58	1.53
1	E	85	VAL	CA-C	-6.36	1.44	1.52
1	E	167	PHE	N-CA	6.33	1.53	1.46
1	E	161	GLN	CA-C	6.29	1.59	1.52
1	E	205	GLY	N-CA	6.04	1.51	1.45
1	E	18	ILE	C-O	5.93	1.30	1.24
1	E	138	THR	CA-CB	5.91	1.62	1.53
1	E	159	HIS	CA-CB	5.91	1.60	1.53
1	E	317	LEU	CA-C	5.81	1.59	1.52
1	E	63	GLY	C-N	-5.80	1.25	1.33
1	E	266	THR	CA-CB	5.57	1.61	1.53
1	E	82	SER	C-O	5.50	1.30	1.23
1	E	136	SER	CA-C	-5.47	1.45	1.53
1	E	220	LEU	C-N	-5.47	1.25	1.33
1	E	222	ASP	C-O	5.41	1.30	1.23
1	E	142	ASP	C-O	5.27	1.30	1.24
1	E	65	GLU	C-O	5.20	1.30	1.23
1	E	200	ALA	N-CA	5.17	1.53	1.46
1	E	288	GLN	N-CA	5.16	1.52	1.45
1	E	100	GLN	C-O	5.15	1.30	1.23
1	E	128	SER	C-O	5.15	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	296	SER	N-CA	5.14	1.51	1.45
1	E	159	HIS	CG-CD2	5.13	1.41	1.35
1	E	218	LEU	N-CA	5.13	1.51	1.45
1	E	9	THR	CB-OG1	5.12	1.51	1.43
1	E	163	GLY	CA-C	5.12	1.59	1.51
1	E	248	ASP	C-N	-5.10	1.27	1.34
1	E	274	TYR	N-CA	5.09	1.52	1.46
1	E	73	ILE	N-CA	5.08	1.51	1.46
1	E	132	VAL	CA-CB	-5.03	1.48	1.54
1	E	197	SER	C-O	5.00	1.29	1.23

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	313	ASP	CA-CB-CG	-14.86	97.74	112.60
1	E	279	ASP	CA-CB-CG	10.66	123.26	112.60
1	E	292	GLY	CA-C-O	-9.66	107.02	119.58
1	E	84	ASN	OD1-CG-ND2	-9.28	113.32	122.60
1	E	300	ASP	O-C-N	9.19	131.86	122.12
1	E	117	ASN	OD1-CG-ND2	9.01	131.61	122.60
1	E	118	ASN	OD1-CG-ND2	-8.88	113.72	122.60
1	E	161	GLN	O-C-N	8.86	128.12	121.65
1	E	136	SER	O-C-N	-8.62	112.96	122.79
1	E	267	VAL	O-C-N	8.36	126.64	121.37
1	E	247	PHE	CA-C-O	8.32	130.19	121.38
1	E	234	SER	O-C-N	8.18	133.09	122.95
1	E	177	GLY	CA-C-O	-8.13	111.59	121.67
1	E	58	ASN	CB-CA-C	8.06	118.55	110.33
1	E	135	GLN	OE1-CD-NE2	-7.97	114.63	122.60
1	E	50	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	E	266	THR	O-C-N	7.78	132.47	123.29
1	E	52	SER	CA-C-O	-7.68	112.17	120.92
1	E	262	GLY	CA-C-O	7.61	127.18	119.27
1	E	177	GLY	O-C-N	7.60	131.06	122.62
1	E	252	ASN	OD1-CG-ND2	7.59	130.19	122.60
1	E	74	SER	CA-C-O	-7.57	112.18	120.36
1	E	89	SER	O-C-N	7.38	131.64	123.22
1	E	167	PHE	CA-CB-CG	-7.36	106.44	113.80
1	E	13	ASN	OD1-CG-ND2	7.27	129.87	122.60
1	E	126	PHE	O-C-N	7.22	131.38	122.86
1	E	17	TYR	CA-C-O	-7.13	112.66	120.36
1	E	55	SER	N-CA-C	-7.08	97.69	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	137	GLN	OE1-CD-NE2	7.08	129.68	122.60
1	E	16	GLU	CG-CD-OE2	-7.07	102.14	118.40
1	E	58	ASN	OD1-CG-ND2	7.04	129.64	122.60
1	E	279	ASP	CB-CG-OD2	6.99	134.49	118.40
1	E	281	SER	N-CA-CB	-6.92	101.19	111.43
1	E	61	ALA	CA-C-O	-6.88	113.12	120.42
1	E	16	GLU	CG-CD-OE1	6.84	134.14	118.40
1	E	52	SER	O-C-N	6.83	131.42	122.95
1	E	300	ASP	CA-C-O	-6.83	113.31	120.55
1	E	155	VAL	O-C-N	6.83	130.63	123.05
1	E	26	THR	CA-CB-OG1	-6.81	99.39	109.60
1	E	269	GLY	CA-C-O	-6.75	113.11	120.40
1	E	85	VAL	N-CA-C	6.68	118.42	108.46
1	E	111	GLN	CB-CG-CD	6.67	123.94	112.60
1	E	48	ALA	CA-C-O	-6.62	113.48	120.63
1	E	89	SER	CA-C-N	-6.58	113.64	122.98
1	E	89	SER	C-N-CA	-6.58	113.64	122.98
1	E	83	GLY	O-C-N	6.50	129.19	123.80
1	E	292	GLY	O-C-N	6.50	130.26	122.34
1	E	141	PHE	CA-C-O	-6.48	114.02	120.82
1	E	114	GLN	CG-CD-NE2	-6.46	106.72	116.40
1	E	240	SER	CA-C-O	-6.43	112.84	120.10
1	E	23	ILE	O-C-N	6.38	129.96	123.20
1	E	52	SER	CA-CB-OG	-6.36	98.37	111.10
1	E	313	ASP	OD1-CG-OD2	6.26	137.92	122.90
1	E	135	GLN	O-C-N	6.25	130.73	123.30
1	E	213	ASP	N-CA-CB	-6.13	100.87	110.87
1	E	305	SER	CA-C-O	-6.11	112.20	119.35
1	E	176	THR	CA-C-O	6.11	127.58	120.80
1	E	313	ASP	CB-CG-OD2	-6.11	104.36	118.40
1	E	322	GLN	OE1-CD-NE2	6.07	128.67	122.60
1	E	115	ASP	N-CA-CB	-6.06	101.32	110.35
1	E	157	LEU	O-C-N	6.05	130.27	123.19
1	E	188	GLN	OE1-CD-NE2	5.98	128.58	122.60
1	E	293	ILE	CA-CB-CG2	5.97	120.65	110.50
1	E	238	GLN	OE1-CD-NE2	5.92	128.52	122.60
1	E	58	ASN	O-C-N	5.91	127.09	120.83
1	E	35	GLY	O-C-N	5.91	129.74	122.29
1	E	103	GLN	OE1-CD-NE2	5.90	128.50	122.60
1	E	150	GLN	CA-C-O	-5.88	113.12	120.23
1	E	160	GLN	O-C-N	-5.87	114.72	122.40
1	E	86	PHE	CA-C-O	-5.84	114.60	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	217	THR	CA-C-O	-5.84	114.23	120.42
1	E	74	SER	CA-CB-OG	-5.84	99.42	111.10
1	E	137	GLN	CG-CD-NE2	-5.83	107.65	116.40
1	E	262	GLY	N-CA-C	5.83	122.02	115.08
1	E	154	ALA	CA-C-N	-5.81	114.34	122.71
1	E	154	ALA	C-N-CA	-5.81	114.34	122.71
1	E	90	VAL	O-C-N	5.80	129.21	123.18
1	E	297	ILE	O-C-N	5.80	129.19	122.99
1	E	83	GLY	CA-C-O	-5.79	116.46	121.04
1	E	230	TYR	O-C-N	5.79	130.19	122.43
1	E	266	THR	CA-C-O	-5.79	114.07	120.38
1	E	107	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	E	141	PHE	O-C-N	5.78	128.02	122.07
1	E	21	VAL	O-C-N	5.77	129.30	123.07
1	E	2	ALA	CA-C-O	5.75	128.06	121.28
1	E	281	SER	CA-CB-OG	-5.71	99.68	111.10
1	E	21	VAL	CA-C-N	-5.68	115.22	122.77
1	E	21	VAL	C-N-CA	-5.68	115.22	122.77
1	E	241	ASN	CA-CB-CG	5.67	118.27	112.60
1	E	200	ALA	CA-C-O	-5.65	114.26	120.70
1	E	71	TRP	N-CA-C	-5.64	100.50	109.07
1	E	75	TYR	CA-C-N	5.63	127.17	120.14
1	E	75	TYR	C-N-CA	5.63	127.17	120.14
1	E	58	ASN	CB-CG-OD1	-5.62	109.57	120.80
1	E	146	SER	CA-C-O	-5.61	112.48	119.38
1	E	237	GLN	OE1-CD-NE2	5.61	128.21	122.60
1	E	4	GLY	O-C-N	5.60	128.96	123.76
1	E	109	SER	CA-CB-OG	-5.57	99.95	111.10
1	E	178	SER	CA-CB-OG	-5.56	99.99	111.10
1	E	42	PHE	N-CA-C	-5.54	102.20	110.23
1	E	94	GLY	CA-C-O	-5.54	112.38	119.13
1	E	5	VAL	CA-C-O	-5.53	114.59	120.39
1	E	232	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	E	280	GLY	O-C-N	5.50	129.85	122.70
1	E	280	GLY	N-CA-C	-5.49	100.17	113.18
1	E	98	HIS	CA-CB-CG	-5.48	108.32	113.80
1	E	84	ASN	CB-CG-ND2	5.46	124.59	116.40
1	E	31	ASN	N-CA-CB	-5.46	101.36	110.37
1	E	60	SER	CA-CB-OG	-5.44	100.23	111.10
1	E	85	VAL	N-CA-CB	-5.43	102.53	111.44
1	E	63	GLY	CA-C-O	-5.43	115.48	121.94
1	E	189	GLY	CA-C-O	-5.42	112.99	119.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	308	VAL	O-C-N	5.41	129.10	123.26
1	E	252	ASN	CA-C-O	-5.39	114.81	120.58
1	E	231	SER	N-CA-C	-5.37	105.98	112.54
1	E	252	ASN	CA-CB-CG	-5.37	107.23	112.60
1	E	252	ASN	O-C-N	5.37	129.37	122.93
1	E	207	GLY	CA-C-O	5.36	130.45	122.62
1	E	230	TYR	CA-C-O	-5.36	112.79	119.38
1	E	62	THR	CA-CB-OG1	-5.30	101.65	109.60
1	E	238	GLN	CA-CB-CG	-5.30	103.50	114.10
1	E	68	GLY	CA-C-N	-5.30	113.64	122.64
1	E	68	GLY	C-N-CA	-5.30	113.64	122.64
1	E	10	PRO	N-CA-CB	5.29	108.28	103.15
1	E	234	SER	CA-C-O	-5.28	114.90	120.92
1	E	286	GLY	CA-C-O	-5.26	113.24	119.45
1	E	49	SER	CA-C-O	-5.25	112.92	119.38
1	E	280	GLY	CA-C-N	-5.23	114.42	123.25
1	E	280	GLY	C-N-CA	-5.23	114.42	123.25
1	E	137	GLN	CA-C-O	-5.22	115.10	121.78
1	E	14	ASP	CA-CB-CG	5.21	117.81	112.60
1	E	65	GLU	CA-C-N	5.20	130.47	122.77
1	E	65	GLU	C-N-CA	5.20	130.47	122.77
1	E	317	LEU	CA-C-N	-5.17	117.79	122.80
1	E	317	LEU	C-N-CA	-5.17	117.79	122.80
1	E	33	ASP	CA-CB-CG	-5.13	107.47	112.60
1	E	4	GLY	CA-C-N	-5.12	116.44	123.14
1	E	4	GLY	C-N-CA	-5.12	116.44	123.14
1	E	273	ASN	CA-CB-CG	-5.10	107.50	112.60
1	E	279	ASP	OD1-CG-OD2	-5.10	110.66	122.90
1	E	37	ALA	CA-C-O	-5.05	114.00	119.95
1	E	203	GLN	CA-C-O	-5.02	115.27	120.70
1	E	194	ASN	O-C-N	5.02	129.58	123.21
1	E	313	ASP	N-CA-CB	-5.01	101.97	109.88
1	E	253	LEU	CA-C-O	-5.00	116.10	120.60
1	E	68	GLY	O-C-N	5.00	128.74	122.39
1	E	194	ASN	CA-C-N	-5.00	115.18	122.68
1	E	194	ASN	C-N-CA	-5.00	115.18	122.68

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	E	2370	0	2182	25	0
2	E	42	0	49	8	0
3	E	11	0	10	0	0
4	E	9	0	8	0	0
5	E	5	0	0	2	0
6	E	276	0	0	6	0
All	All	2713	0	2249	33	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 7.

All (33) 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)
2:E:324:1Z7:CD21	2:E:324:1Z7:HD2	0.97	1.15
2:E:324:1Z7:HD1	2:E:324:1Z7:CD11	0.97	1.06
1:E:241:ASN:HB2	1:E:279:ASP:OD1	1.53	1.06
2:E:324:1Z7:CG3	2:E:324:1Z7:CE2	2.41	0.97
2:E:324:1Z7:CG3	2:E:324:1Z7:CE1	2.40	0.93
2:E:324:1Z7:HD2	2:E:324:1Z7:CE2	2.04	0.86
2:E:324:1Z7:HD1	2:E:324:1Z7:CG3	2.06	0.86
2:E:324:1Z7:HD1	2:E:324:1Z7:CE1	2.07	0.84
2:E:324:1Z7:HD2	2:E:324:1Z7:CG3	2.06	0.84
1:E:281:SER:O	6:E:506:HOH:O	2.10	0.69
1:E:293:ILE:HD12	1:E:295:PHE:H	1.64	0.63
1:E:188:GLN:OE1	6:E:487:HOH:O	2.16	0.63
1:E:179:LEU:N	5:E:331:SO4:O2	2.30	0.62
1:E:293:ILE:HD11	1:E:295:PHE:O	2.01	0.59
1:E:84:ASN:HD22	1:E:84:ASN:H	1.58	0.51
1:E:172:SER:HA	1:E:175:TYR:CE1	2.48	0.48
1:E:111:GLN:HB2	6:E:496:HOH:O	2.14	0.48
1:E:117:ASN:ND2	6:E:513:HOH:O	2.48	0.47
1:E:203:GLN:NE2	1:E:228:GLN:HG3	2.31	0.46
1:E:133[B]:GLN:NE2	6:E:469:HOH:O	1.99	0.45
1:E:175:TYR:OH	5:E:331:SO4:O4	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:PRO:HB2	1:E:312:SER:OG	2.18	0.44
1:E:40:TRP:HA	1:E:103:GLN:O	2.18	0.43
1:E:293:ILE:CD1	1:E:295:PHE:O	2.66	0.43
1:E:64:LYS:HD3	1:E:64:LYS:HA	1.78	0.43
1:E:252:ASN:ND2	6:E:570:HOH:O	2.52	0.42
1:E:133[B]:GLN:HE21	1:E:134:PRO:HA	1.85	0.42
1:E:252:ASN:HD22	1:E:252:ASN:HA	1.67	0.42
1:E:45:GLU:OE2	1:E:84:ASN:ND2	2.46	0.41
1:E:27:THR:C	1:E:28:LEU:HD12	2.45	0.41
1:E:152:LEU:HD12	1:E:152:LEU:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	323/323 (100%)	320 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	261/259 (101%)	252 (97%)	9 (3%)	32	16

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	ILE
1	E	39	LEU
1	E	47	PRO
1	E	52	SER
1	E	84	ASN
1	E	111	GLN
1	E	134	PRO
1	E	293	ILE
1	E	313	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	13	ASN
1	E	50	GLN
1	E	58	ASN
1	E	107	GLN
1	E	117	ASN
1	E	160	GLN
1	E	194	ASN
1	E	203	GLN
1	E	228	GLN
1	E	237	GLN
1	E	252	ASN
1	E	306	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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	329	1	11,11,12	0.85	0	15,15,17	1.71	5 (33%)
4	XYS	E	330	1	9,9,10	1.26	1 (11%)	10,12,14	3.67	6 (60%)
2	1Z7	E	324	-	41,42,42	1.79	11 (26%)	49,58,58	1.94	15 (30%)
5	SO4	E	331	-	4,4,4	0.84	0	6,6,6	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	329	1	-	0/2/19/22	0/1/1/1
4	XYS	E	330	1	4/4/3/4	-	0/1/1/1
2	1Z7	E	324	-	-	3/57/57/57	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	324	1Z7	P-O21	-4.47	1.46	1.56
2	E	324	1Z7	P-OP	-4.44	1.50	1.57
2	E	324	1Z7	CA2-N1	3.61	1.53	1.45
2	E	324	1Z7	OS-C3	3.06	1.40	1.33
2	E	324	1Z7	CB3-CA3	3.01	1.56	1.53
2	E	324	1Z7	P-CA3	-2.96	1.80	1.84
2	E	324	1Z7	O-C	2.83	1.28	1.23
2	E	324	1Z7	CA4-C3	2.46	1.55	1.51
4	E	330	XYS	O2-C2	-2.44	1.38	1.43
2	E	324	1Z7	O1-C1	2.35	1.27	1.23
2	E	324	1Z7	CB4-CA4	2.13	1.55	1.53
2	E	324	1Z7	CA2-C2	2.01	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	330	XYS	C5-O5-C1	8.58	125.27	111.42
2	E	324	1Z7	CA-C-N	6.57	125.23	116.25
4	E	330	XYS	O4-C4-C3	-5.04	99.70	110.15
2	E	324	1Z7	O11-P-CA3	-3.66	109.19	114.19
2	E	324	1Z7	O-C-CA	-3.56	116.33	121.54
2	E	324	1Z7	C2-CA2-N1	-3.26	101.47	110.32
4	E	330	XYS	O3-C3-C2	3.07	116.32	110.05
2	E	324	1Z7	OP-P-O11	-3.05	109.13	115.13
4	E	330	XYS	O2-C2-C3	3.05	116.46	110.15
3	E	329	MAN	C6-C5-C4	3.04	120.48	113.02
2	E	324	1Z7	O2-C2-N2	2.77	127.92	122.96
2	E	324	1Z7	CG-CB3-CA3	2.74	120.38	114.81
2	E	324	1Z7	CA2-N1-C1	-2.73	115.14	121.90
2	E	324	1Z7	O-C-N	-2.67	118.44	122.95
2	E	324	1Z7	OS-C3-CA4	2.51	116.17	110.78
2	E	324	1Z7	CB1-CA1-N	-2.50	105.40	111.44
3	E	329	MAN	C3-C4-C5	-2.42	105.85	110.23
4	E	330	XYS	O4-C4-C5	2.41	114.74	109.22
2	E	324	1Z7	CG1-CB-CA	-2.33	102.11	111.16
2	E	324	1Z7	CG3-CB4-CA4	2.33	117.17	113.20
4	E	330	XYS	C1-C2-C3	-2.31	106.28	109.64
2	E	324	1Z7	CD2-CG-CD1	2.28	120.71	110.53
2	E	324	1Z7	O1-C1-N1	2.23	126.95	122.96
3	E	329	MAN	O4-C4-C3	-2.23	105.12	110.38
3	E	329	MAN	C1-C2-C3	-2.08	106.61	109.64
3	E	329	MAN	O3-C3-C2	-2.02	105.92	110.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	330	XYS	C4
4	E	330	XYS	C1
4	E	330	XYS	C3
4	E	330	XYS	C2

All (3) torsion outliers are listed below:

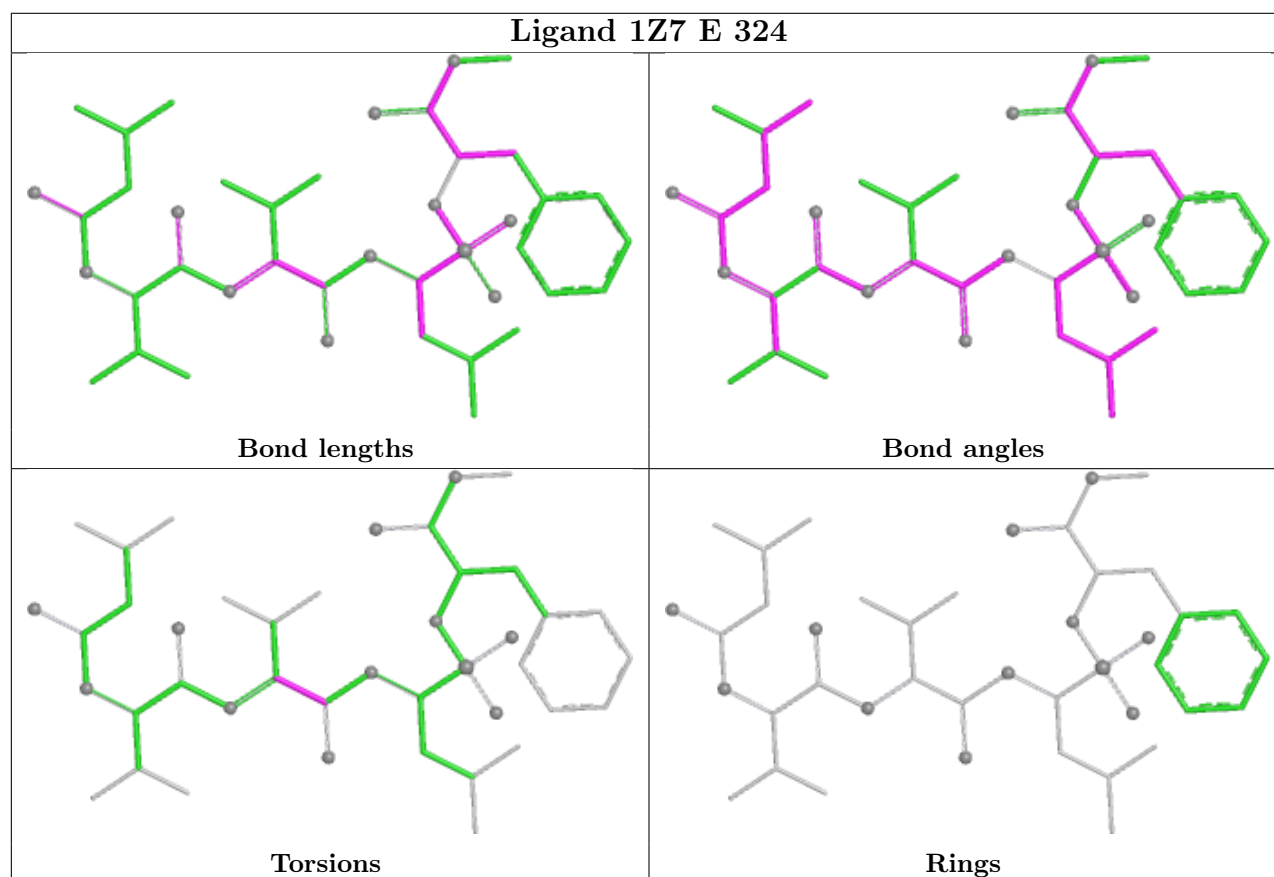
Mol	Chain	Res	Type	Atoms
2	E	324	1Z7	N2-C2-CA2-N1
2	E	324	1Z7	O2-C2-CA2-N1
2	E	324	1Z7	N2-C2-CA2-CB2

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	324	1Z7	8	0
5	E	331	SO4	2	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.