



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:42 PM UTC

PDB ID : 1PPK / pdb_00001ppk
Title : CRYSTALLOGRAPHIC ANALYSIS OF TRANSITION STATE MIMICS
BOUND TO PENICILLOPEPSIN: PHOSPHOROUS-CONTAINING PEP-
TIDE ANALOGUES
Authors : Strynadka, N.C.J.; James, M.N.G.
Deposited on : 1994-01-20
Resolution : 1.80 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

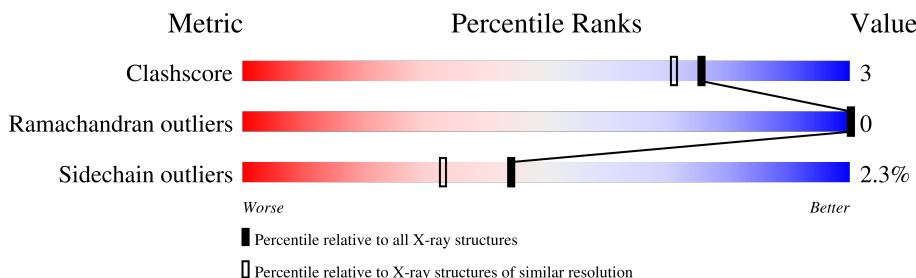
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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.

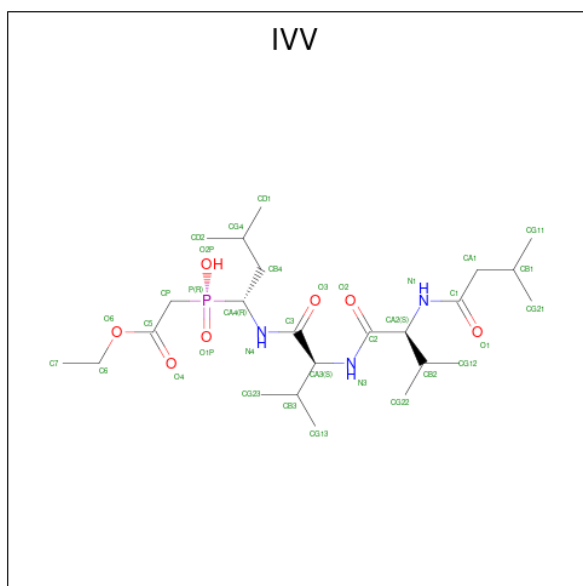
Mol	Chain	Length	Quality of chain
1	E	323	57% 40% .

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.

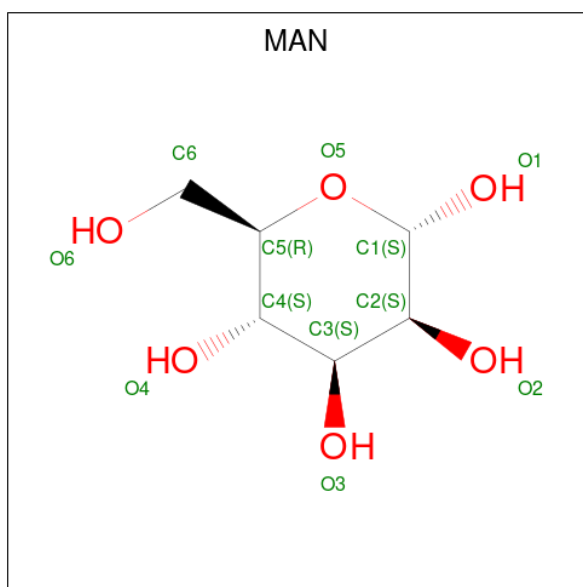
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	323	Total	C	N	O	S	0	0	0
			2366	1479	377	508	2			

- Molecule 2 is N-(3-methylbutanoyl)-L-valyl-N-{(1R)-1-[(R)-(2-ethoxy-2-oxoethyl)(hydroxy)phosphoryl]-3-methylbutyl}-L-valinamide (CCD ID: IVV) (formula: $C_{24}H_{46}N_3O_7P$).



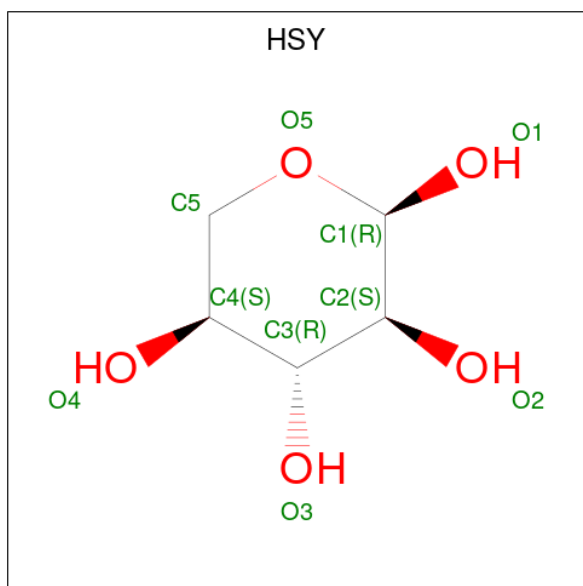
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			35	24	3	7	1		

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $\text{C}_6\text{H}_{12}\text{O}_6$).



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

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



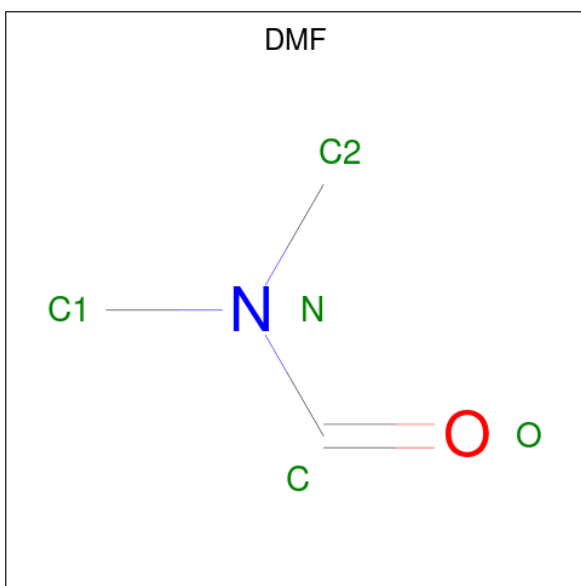
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			9	5	4		

- 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 DIMETHYLFORMAMIDE (CCD ID: DMF) (formula: C_3H_7NO).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	275	Total 275	O 275	0	0

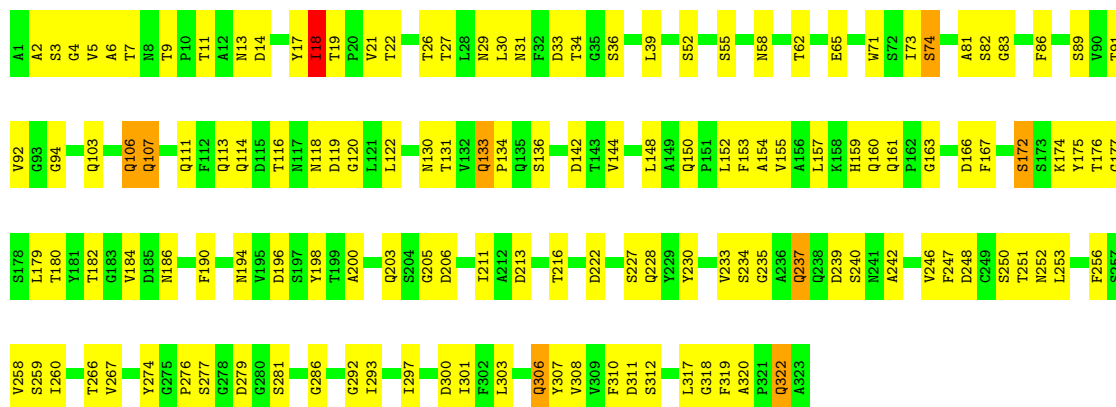
3 Residue-property plots

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	97.48Å 46.55Å 66.42Å 90.00° 116.14° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.132 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2706	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: DMF, SO4, HSY, IVV, MAN

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	1.75	29/2420 (1.2%)	2.35	146/3304 (4.4%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	GLY	N-CA	10.45	1.55	1.45
1	E	7	THR	CA-CB	7.29	1.63	1.53
1	E	122	LEU	C-O	7.27	1.32	1.24
1	E	246	VAL	CA-C	7.22	1.61	1.52
1	E	267	VAL	CA-C	6.73	1.58	1.53
1	E	247	PHE	N-CA	6.57	1.53	1.46
1	E	190	PHE	N-CA	6.56	1.53	1.45
1	E	36	SER	N-CA	6.53	1.54	1.45
1	E	320	ALA	N-CA	6.47	1.52	1.46
1	E	120	GLY	N-CA	6.28	1.52	1.44
1	E	176	THR	CA-CB	6.21	1.63	1.53
1	E	161	GLN	CA-C	6.21	1.59	1.52
1	E	136	SER	N-CA	6.16	1.54	1.45
1	E	65	GLU	C-O	6.14	1.31	1.23
1	E	82	SER	N-CA	5.97	1.53	1.45
1	E	157	LEU	CA-C	5.95	1.60	1.52
1	E	86	PHE	C-O	5.87	1.31	1.23
1	E	152	LEU	N-CA	5.86	1.53	1.46
1	E	26	THR	CA-CB	5.82	1.61	1.53
1	E	307	TYR	N-CA	5.79	1.53	1.46
1	E	62	THR	CA-CB	5.53	1.63	1.54
1	E	216	THR	CA-C	5.27	1.58	1.52
1	E	153	PHE	CA-C	5.23	1.59	1.52
1	E	131	THR	C-N	-5.18	1.27	1.33
1	E	211	ILE	C-O	5.12	1.29	1.24
1	E	27	THR	CA-CB	5.11	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	266	THR	CA-CB	5.08	1.61	1.53
1	E	310	PHE	N-CA	5.03	1.52	1.46
1	E	318	GLY	N-CA	5.01	1.52	1.46

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	237	GLN	OE1-CD-NE2	-11.32	111.28	122.60
1	E	237	GLN	CB-CG-CD	11.02	131.34	112.60
1	E	150	GLN	OE1-CD-NE2	9.23	131.83	122.60
1	E	160	GLN	CG-CD-NE2	9.20	130.19	116.40
1	E	52	SER	O-C-N	8.88	133.85	122.93
1	E	317	LEU	O-C-N	8.77	133.74	123.30
1	E	83	GLY	O-C-N	8.50	130.85	123.80
1	E	13	ASN	OD1-CG-ND2	8.37	130.97	122.60
1	E	155	VAL	O-C-N	8.29	132.25	123.05
1	E	111	GLN	OE1-CD-NE2	8.00	130.60	122.60
1	E	317	LEU	CA-C-O	-7.91	111.82	120.36
1	E	150	GLN	O-C-N	7.91	130.24	121.94
1	E	7	THR	CA-CB-OG1	-7.87	97.80	109.60
1	E	300	ASP	CA-C-O	-7.86	112.15	120.63
1	E	172	SER	CA-CB-OG	-7.79	95.52	111.10
1	E	167	PHE	CA-CB-CG	-7.66	106.14	113.80
1	E	150	GLN	CA-C-O	-7.49	111.94	120.03
1	E	118	ASN	O-C-N	7.37	132.74	123.15
1	E	317	LEU	CA-C-N	-7.31	115.71	122.80
1	E	317	LEU	C-N-CA	-7.31	115.71	122.80
1	E	89	SER	CA-CB-OG	-7.31	96.48	111.10
1	E	300	ASP	O-C-N	7.18	129.74	122.12
1	E	308	VAL	O-C-N	7.16	130.99	123.26
1	E	267	VAL	O-C-N	7.14	127.03	121.46
1	E	55	SER	N-CA-C	-7.12	97.63	109.46
1	E	182	THR	O-C-N	7.12	131.53	123.27
1	E	92	VAL	O-C-N	7.12	129.94	123.03
1	E	256	PHE	CA-C-O	-7.11	112.43	120.32
1	E	18	ILE	CB-CA-C	7.01	121.61	110.82
1	E	154	ALA	O-C-N	6.97	131.61	123.17
1	E	246	VAL	O-C-N	6.95	130.75	123.04
1	E	17	TYR	CA-C-O	-6.88	112.93	120.36
1	E	276	PRO	O-C-N	6.87	131.23	122.85
1	E	301	ILE	O-C-N	6.85	128.51	121.87
1	E	81	ALA	O-C-N	6.72	130.61	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	134	PRO	N-CD-CG	-6.70	95.77	103.80
1	E	58	ASN	O-C-N	6.69	128.58	121.02
1	E	6	ALA	CA-C-O	-6.69	113.62	120.71
1	E	13	ASN	CA-C-O	-6.68	112.63	119.78
1	E	198	TYR	O-C-N	6.67	131.24	123.17
1	E	14	ASP	CA-CB-CG	6.65	119.25	112.60
1	E	297	ILE	O-C-N	6.60	131.53	122.88
1	E	216	THR	CA-CB-OG1	-6.58	99.73	109.60
1	E	19	THR	O-C-N	6.57	128.84	121.94
1	E	89	SER	O-C-N	6.55	130.69	123.22
1	E	94	GLY	CA-C-O	-6.53	111.69	119.00
1	E	276	PRO	CA-C-O	-6.53	114.20	121.32
1	E	182	THR	CA-C-O	-6.43	113.60	121.06
1	E	213	ASP	N-CA-CB	-6.30	100.06	110.95
1	E	161	GLN	O-C-N	6.28	126.24	121.85
1	E	312	SER	CA-C-O	-6.25	111.70	119.38
1	E	182	THR	CA-CB-OG1	-6.24	100.23	109.60
1	E	130	ASN	CA-CB-CG	-6.24	106.36	112.60
1	E	307	TYR	N-CA-C	-6.23	99.04	109.07
1	E	159	HIS	CA-CB-CG	-6.11	107.69	113.80
1	E	248	ASP	CA-C-O	-6.10	113.96	120.92
1	E	114	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	E	116	THR	O-C-N	6.08	130.23	122.39
1	E	5	VAL	O-C-N	6.07	129.75	123.20
1	E	119	ASP	O-C-N	6.04	130.07	122.22
1	E	22	THR	CA-CB-OG1	-6.02	100.57	109.60
1	E	206	ASP	CB-CA-C	6.01	121.72	109.76
1	E	253	LEU	CA-C-O	-5.99	115.21	120.60
1	E	74	SER	CB-CA-C	5.96	121.16	109.35
1	E	26	THR	CA-CB-OG1	-5.91	100.73	109.60
1	E	306	GLN	CA-C-N	-5.90	114.86	123.00
1	E	306	GLN	C-N-CA	-5.90	114.86	123.00
1	E	154	ALA	CA-C-N	-5.89	114.23	122.71
1	E	154	ALA	C-N-CA	-5.89	114.23	122.71
1	E	9	THR	CA-CB-CG2	-5.88	100.50	110.50
1	E	186	ASN	O-C-N	5.86	129.56	122.35
1	E	308	VAL	CA-C-O	-5.86	114.24	120.39
1	E	89	SER	CA-C-O	-5.84	113.94	120.54
1	E	206	ASP	CB-CG-OD1	5.79	131.73	118.40
1	E	2	ALA	N-CA-C	-5.79	100.75	109.95
1	E	184	VAL	O-C-N	5.76	129.01	123.14
1	E	311	ASP	N-CA-CB	-5.74	101.53	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	ILE	O-C-N	5.73	129.13	123.00
1	E	200	ALA	O-C-N	5.71	130.44	123.01
1	E	252	ASN	CA-C-O	-5.71	114.47	120.58
1	E	259	SER	CA-CB-OG	-5.71	99.69	111.10
1	E	106	GLN	N-CA-C	-5.69	106.88	113.88
1	E	320	ALA	N-CA-C	-5.67	103.12	108.22
1	E	131	THR	CA-C-O	-5.65	112.44	119.28
1	E	247	PHE	CA-CB-CG	-5.65	108.15	113.80
1	E	33	ASP	N-CA-CB	-5.63	102.28	110.84
1	E	142	ASP	CB-CG-OD1	5.63	131.35	118.40
1	E	267	VAL	N-CA-C	-5.60	101.50	107.77
1	E	286	GLY	N-CA-C	-5.59	107.99	115.32
1	E	4	GLY	O-C-N	5.58	128.95	123.76
1	E	177	GLY	O-C-N	5.58	128.27	122.86
1	E	194	ASN	O-C-N	5.55	130.26	123.21
1	E	258	VAL	CA-C-O	-5.53	114.87	121.28
1	E	227	SER	CA-CB-OG	-5.52	100.05	111.10
1	E	237	GLN	O-C-N	5.52	129.68	123.27
1	E	150	GLN	CA-CB-CG	-5.52	103.06	114.10
1	E	319	PHE	O-C-N	5.51	129.99	123.27
1	E	196	ASP	OD1-CG-OD2	5.50	136.10	122.90
1	E	180	THR	CA-C-O	-5.47	114.45	120.36
1	E	157	LEU	O-C-N	5.46	129.58	123.19
1	E	248	ASP	O-C-N	5.46	129.72	122.95
1	E	3	SER	CA-CB-OG	-5.44	100.23	111.10
1	E	281	SER	N-CA-C	5.43	119.22	112.59
1	E	113	GLN	CG-CD-NE2	5.43	124.55	116.40
1	E	322	GLN	CA-C-O	-5.41	115.11	121.16
1	E	89	SER	CA-C-N	-5.40	115.48	122.99
1	E	89	SER	C-N-CA	-5.40	115.48	122.99
1	E	174	LYS	CG-CD-CE	5.40	123.71	111.30
1	E	292	GLY	CA-C-O	-5.38	112.44	119.44
1	E	230	TYR	O-C-N	5.38	129.64	122.43
1	E	21	VAL	CA-C-N	-5.38	115.30	122.72
1	E	21	VAL	C-N-CA	-5.38	115.30	122.72
1	E	306	GLN	O-C-N	5.37	130.14	123.15
1	E	297	ILE	CA-C-O	-5.36	114.39	120.66
1	E	163	GLY	CA-C-N	-5.36	115.08	122.69
1	E	163	GLY	C-N-CA	-5.36	115.08	122.69
1	E	234	SER	O-C-N	5.33	129.56	122.95
1	E	106	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	E	5	VAL	CA-C-O	-5.30	114.74	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	222	ASP	CA-CB-CG	-5.30	107.30	112.60
1	E	274	TYR	CA-C-O	5.28	126.02	120.42
1	E	11	THR	N-CA-C	-5.28	101.68	109.86
1	E	62	THR	CA-CB-OG1	-5.26	101.72	109.60
1	E	153	PHE	N-CA-C	-5.24	101.33	109.24
1	E	91	THR	O-C-N	5.22	129.51	123.30
1	E	206	ASP	OD1-CG-OD2	-5.21	110.39	122.90
1	E	166	ASP	CA-C-N	-5.18	115.84	123.00
1	E	166	ASP	C-N-CA	-5.18	115.84	123.00
1	E	247	PHE	CA-C-O	5.18	126.87	121.38
1	E	148	LEU	N-CA-CB	-5.15	102.99	110.36
1	E	26	THR	CA-C-O	-5.13	114.84	120.43
1	E	34	THR	CA-CB-OG1	-5.08	101.98	109.60
1	E	240	SER	CA-C-O	-5.08	114.36	120.10
1	E	259	SER	CA-C-O	-5.07	114.74	120.32
1	E	256	PHE	CA-C-N	-5.07	114.63	122.59
1	E	256	PHE	C-N-CA	-5.07	114.63	122.59
1	E	293	ILE	CA-C-O	-5.07	112.89	119.53
1	E	260	ILE	CA-C-O	-5.06	114.92	120.48
1	E	30	LEU	CA-C-O	-5.06	115.44	121.56
1	E	303	LEU	N-CA-C	5.05	117.52	111.71
1	E	281	SER	N-CA-CB	-5.05	102.85	110.92
1	E	144	VAL	O-C-N	5.04	127.24	122.20
1	E	196	ASP	CA-CB-CG	-5.03	107.57	112.60
1	E	250	SER	CA-CB-OG	-5.02	101.05	111.10
1	E	319	PHE	CA-C-N	-5.01	114.24	122.26
1	E	319	PHE	C-N-CA	-5.01	114.24	122.26

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	2366	0	2181	13	0
2	E	35	0	45	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	11	0	10	0	0
4	E	9	0	7	0	0
5	E	5	0	0	1	0
6	E	5	0	7	1	0
7	E	275	0	0	2	0
All	All	2706	0	2250	14	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 3.

All (14) 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:E:235:GLY:HA2	7:E:616:HOH:O	1.93	0.68
1:E:179:LEU:N	5:E:326:SO4:O2	2.31	0.60
1:E:106:GLN:C	1:E:107:GLN:HG2	2.25	0.60
2:E:700:IVV:C5	6:E:327:DMF:H23	2.35	0.57
1:E:233:VAL:HG13	1:E:251:THR:HG21	1.89	0.54
1:E:306:GLN:C	1:E:322:GLN:HG3	2.37	0.50
1:E:133:GLN:NE2	7:E:589:HOH:O	2.46	0.47
1:E:239:ASP:OD1	1:E:279:ASP:OD2	2.33	0.46
1:E:71:TRP:CE2	1:E:103:GLN:HB3	2.52	0.45
1:E:203:GLN:OE1	1:E:228:GLN:HG3	2.17	0.45
1:E:18:ILE:HG13	1:E:29:ASN:HB3	2.01	0.42
1:E:172:SER:HA	1:E:175:TYR:CE1	2.55	0.42
1:E:31:ASN:HD22	1:E:31:ASN:C	2.28	0.42
1:E:242:ALA:HB1	1:E:277:SER:HB2	2.03	0.41

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	321/323 (99%)	318 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	259/259 (100%)	253 (98%)	6 (2%)	44	33

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

Mol	Chain	Res	Type
1	E	18	ILE
1	E	39	LEU
1	E	74	SER
1	E	107	GLN
1	E	133	GLN
1	E	237	GLN

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

Mol	Chain	Res	Type
1	E	31	ASN
1	E	107	GLN
1	E	133	GLN
1	E	135	GLN
1	E	161	GLN
1	E	188	GLN
1	E	306	GLN
1	E	316	GLN

5.3.3 RNA ⓘ

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](#)

5 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$
2	IVV	E	700	-	31,34,34	1.45	4 (12%)	37,47,47	1.57	9 (24%)
6	DMF	E	327	-	4,4,4	0.45	0	4,4,4	0.59	0
4	HSY	E	325	1	9,9,10	0.88	0	10,12,14	4.02	5 (50%)
5	SO4	E	326	-	4,4,4	0.66	0	6,6,6	0.29	0
3	MAN	E	324	1	11,11,12	1.12	1 (9%)	15,15,17	1.37	1 (6%)

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
4	HSY	E	325	1	-	-	0/1/1/1
2	IVV	E	700	-	-	6/46/50/50	-
3	MAN	E	324	1	-	0/2/19/22	0/1/1/1
6	DMF	E	327	-	-	2/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	IVV	CB4-CA4	4.83	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	700	IVV	O6-C5	3.14	1.42	1.33
3	E	324	MAN	O2-C2	2.73	1.49	1.43
2	E	700	IVV	CA2-N1	2.63	1.51	1.45
2	E	700	IVV	O2-C2	2.44	1.28	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	325	HSY	C5-O5-C1	10.67	128.64	111.42
4	E	325	HSY	C5-C4-C3	3.68	115.00	109.64
4	E	325	HSY	O4-C4-C5	3.52	117.28	109.22
3	E	324	MAN	O2-C2-C1	-3.15	102.02	109.22
2	E	700	IVV	O1-C1-CA1	-3.13	116.95	121.54
2	E	700	IVV	O6-C5-O4	-2.92	116.33	123.63
4	E	325	HSY	O4-C4-C3	-2.75	104.46	110.15
2	E	700	IVV	CA2-N1-C1	-2.73	116.42	121.80
2	E	700	IVV	CG21-CB1-CA1	-2.59	101.08	111.16
4	E	325	HSY	O2-C2-C1	2.59	115.15	109.22
2	E	700	IVV	CB2-CA2-N1	-2.52	105.36	111.44
2	E	700	IVV	CA1-C1-N1	2.43	119.57	116.25
2	E	700	IVV	O3-C3-N4	2.38	127.22	122.96
2	E	700	IVV	O2-C2-N3	2.25	126.98	122.96
2	E	700	IVV	C3-CA3-N3	-2.17	104.41	110.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

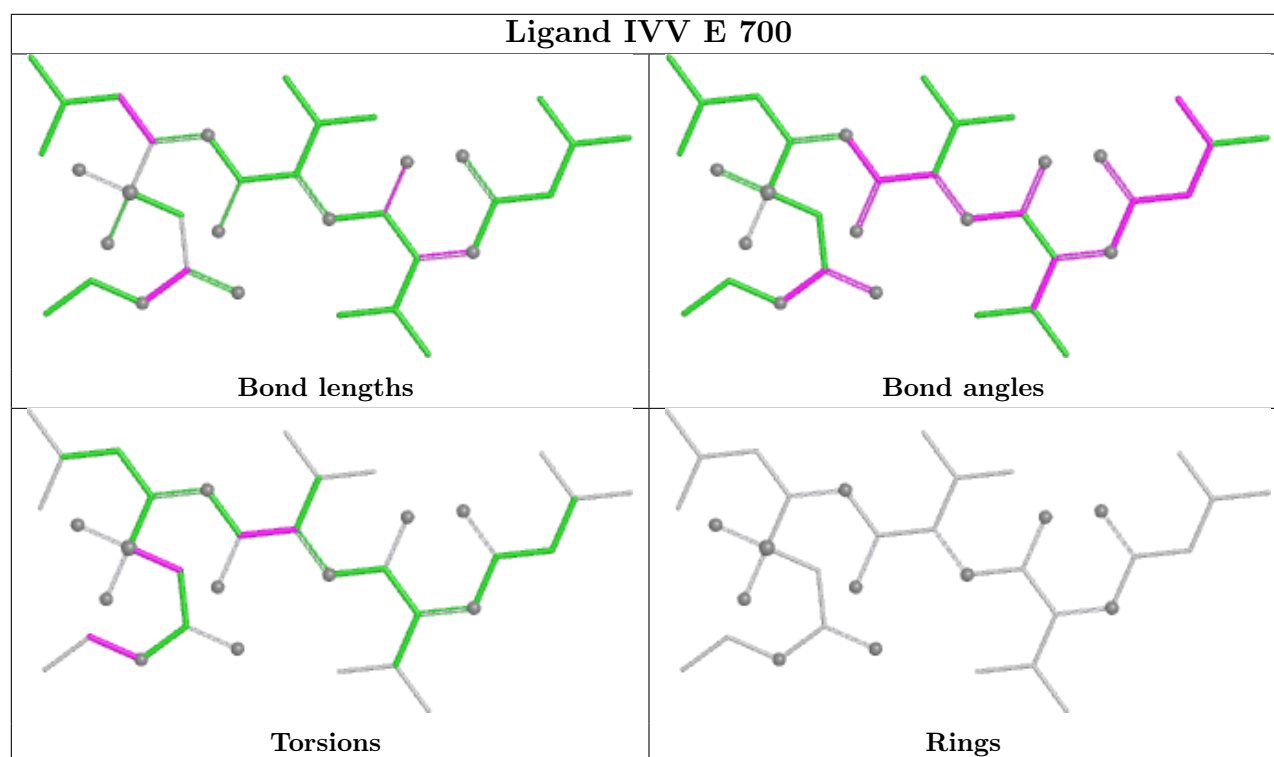
Mol	Chain	Res	Type	Atoms
6	E	327	DMF	O-C-N-C2
6	E	327	DMF	O-C-N-C1
2	E	700	IVV	O3-C3-CA3-N3
2	E	700	IVV	N4-C3-CA3-N3
2	E	700	IVV	C7-C6-O6-C5
2	E	700	IVV	N4-C3-CA3-CB3
2	E	700	IVV	O3-C3-CA3-CB3
2	E	700	IVV	C5-CP-P-O2P

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	700	IVV	1	0
6	E	327	DMF	1	0
5	E	326	SO4	1	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 ⓘ

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.