



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:27 AM UTC

PDB ID : 1FMO / pdb_00001fmo
Title : CRYSTAL STRUCTURE OF A POLYHISTIDINE-TAGGED RECOMBINANT CATALYTIC SUBUNIT OF CAMP-DEPENDENT PROTEIN KINASE COMPLEXED WITH THE PEPTIDE INHIBITOR PKI(5-24) AND ADENOSINE
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Deposited on : 1997-07-08
Resolution : 2.20 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)
Xtrriage (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

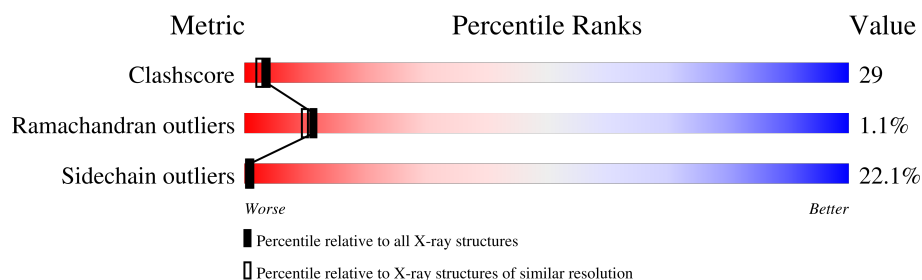
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	350	
2	I	20	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3058 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 CAMP-DEPENDENT PROTEIN KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	E	338	2792	1808	467	507	2	8	0	0	0

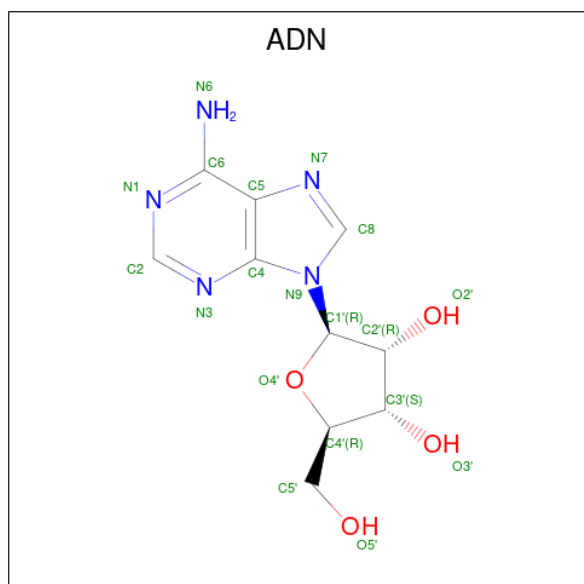
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	197	TPO	THR	modified residue	UNP P05132
E	338	SEP	SER	modified residue	UNP P05132

- Molecule 2 is a protein called HEAT STABLE RABBIT SKELETAL MUSCLE INHIBITOR PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	20	157	94	32	31	0	0	0

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is water.

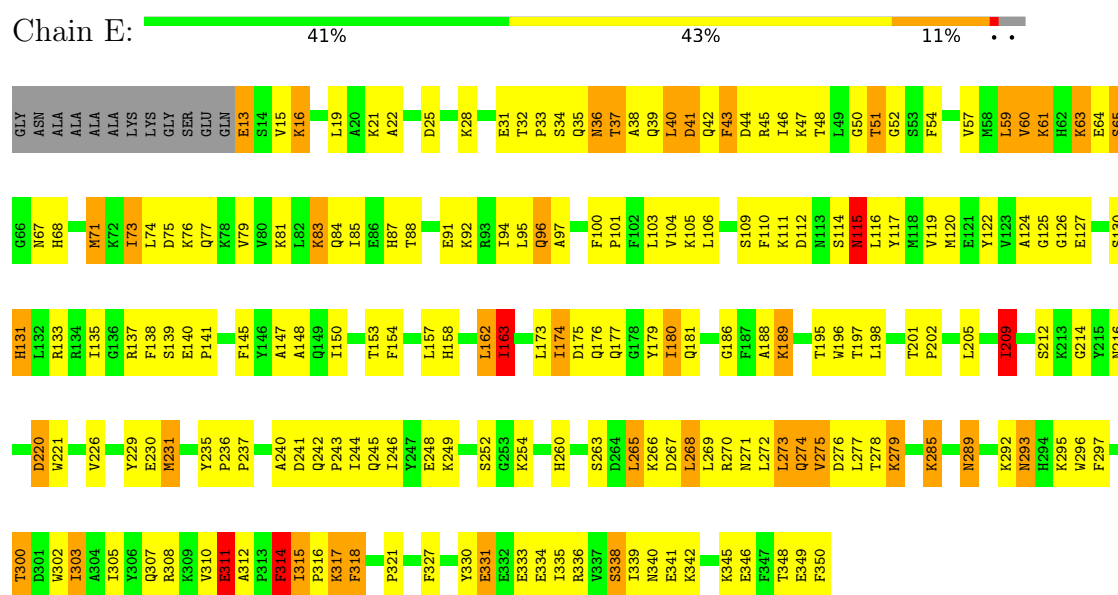
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	83	Total	O	0	0
			83	83		
4	I	7	Total	O	0	0
			7	7		

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: CAMP-DEPENDENT PROTEIN KINASE



• Molecule 2: HEAT STABLE RABBIT SKELETAL MUSCLE INHIBITOR PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.08Å 78.44Å 80.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	85.0 (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	TNT 5E, X-PLOR 3.1	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3058	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: SEP, ADN, TPO

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	1.18	2/2840 (0.1%)	1.53	27/3824 (0.7%)
2	I	1.29	1/159 (0.6%)	1.59	3/212 (1.4%)
All	All	1.19	3/2999 (0.1%)	1.53	30/4036 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	311	GLU	CD-OE2	5.44	1.35	1.25
1	E	349	GLU	CD-OE1	5.25	1.35	1.25
2	I	7	TYR	CA-C	-5.08	1.46	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	293	ASN	CA-CB-CG	7.53	120.13	112.60
1	E	221	TRP	N-CA-CB	7.01	120.54	110.16
2	I	19	ARG	N-CA-C	6.95	119.60	108.41
1	E	236	PRO	O-C-N	6.76	124.33	121.15
1	E	54	PHE	CA-CB-CG	-6.72	107.08	113.80
1	E	209	ILE	CB-CA-C	-6.66	103.03	112.22
1	E	317	LYS	N-CA-CB	6.61	120.96	110.65
1	E	163	ILE	CB-CA-C	6.51	119.83	110.33
1	E	28	LYS	N-CA-C	6.02	117.64	111.14
1	E	220	ASP	N-CA-C	-6.01	104.85	111.82
2	I	16	THR	N-CA-C	-6.00	106.12	113.50
1	E	41	ASP	CA-CB-CG	5.75	118.35	112.60
1	E	300	THR	N-CA-C	5.71	118.03	108.96
1	E	235	TYR	CA-C-N	5.67	123.75	119.66
1	E	235	TYR	C-N-CA	5.67	123.75	119.66
1	E	236	PRO	N-CA-CB	5.64	106.16	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	ASN	N-CA-C	5.55	117.84	109.41
1	E	94	ILE	CB-CA-C	-5.48	104.86	112.04
1	E	235	TYR	O-C-N	5.41	125.17	121.71
1	E	314	PHE	CA-CB-CG	5.41	119.20	113.80
1	E	114	SER	N-CA-C	5.27	119.77	112.45
2	I	11	ILE	N-CA-C	5.26	117.62	111.05
1	E	154	PHE	CA-CB-CG	-5.22	108.58	113.80
1	E	57	VAL	N-CA-CB	5.21	118.41	111.64
1	E	139	SER	N-CA-C	-5.16	102.64	110.28
1	E	316	PRO	CA-C-N	-5.15	115.74	123.00
1	E	316	PRO	C-N-CA	-5.15	115.74	123.00
1	E	321	PRO	N-CA-CB	5.08	107.36	103.30
1	E	43	PHE	N-CA-C	5.06	117.74	109.59
1	E	131	HIS	CA-CB-CG	-5.04	108.76	113.80

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	2792	0	2774	167	0
2	I	157	0	146	7	0
3	E	19	0	13	2	0
4	E	83	0	0	5	0
4	I	7	0	0	2	0
All	All	3058	0	2933	172	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 29.

All (172) 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:45:ARG:HD3	1:E:335:ILE:HD11	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:ALA:HB1	1:E:245:GLN:HE21	1.35	0.90
1:E:65:SER:HB2	1:E:67:ASN:ND2	1.88	0.87
1:E:45:ARG:CD	1:E:335:ILE:HD11	2.12	0.80
1:E:243:PRO:HA	1:E:246:ILE:HD12	1.66	0.78
1:E:265:LEU:HD12	1:E:265:LEU:O	1.84	0.78
1:E:131:HIS:O	1:E:135:ILE:HD13	1.86	0.76
1:E:310:VAL:HG22	1:E:311:GLU:H	1.50	0.75
1:E:314:PHE:C	1:E:315:ILE:HD13	2.12	0.74
1:E:312:ALA:CB	1:E:315:ILE:HD11	2.18	0.73
1:E:65:SER:HB2	1:E:67:ASN:HD22	1.52	0.73
1:E:145:PHE:HE1	1:E:310:VAL:HG13	1.55	0.72
1:E:73:ILE:HG23	1:E:117:TYR:CD2	2.24	0.72
1:E:314:PHE:O	1:E:315:ILE:HD13	1.90	0.71
1:E:274:GLN:HE21	1:E:274:GLN:HA	1.53	0.71
1:E:266:LYS:O	1:E:270:ARG:HG3	1.90	0.71
1:E:216:ASN:HB2	4:E:384:HOH:O	1.92	0.70
1:E:33:PRO:HB3	1:E:96:GLN:OE1	1.91	0.69
1:E:100:PHE:CG	1:E:101:PRO:HD2	2.28	0.69
1:E:303:ILE:O	1:E:307:GLN:HG3	1.93	0.67
1:E:277:LEU:HD12	1:E:277:LEU:N	2.09	0.67
1:E:43:PHE:CD2	1:E:60:VAL:HG11	2.30	0.66
1:E:92:LYS:NZ	1:E:350:PHE:OXT	2.27	0.66
2:I:23:HIS:H	2:I:23:HIS:CD2	2.15	0.65
1:E:100:PHE:CD2	1:E:101:PRO:HD2	2.31	0.65
1:E:244:ILE:H	1:E:244:ILE:HD12	1.61	0.64
1:E:311:GLU:HG2	1:E:311:GLU:O	1.96	0.64
1:E:240:ALA:HB1	1:E:245:GLN:NE2	2.11	0.64
1:E:163:ILE:O	1:E:188:ALA:HA	1.98	0.63
1:E:212:SER:HA	4:E:385:HOH:O	1.98	0.63
1:E:60:VAL:O	1:E:68:HIS:HA	1.98	0.63
1:E:312:ALA:HB1	1:E:315:ILE:HD11	1.80	0.62
1:E:244:ILE:H	1:E:244:ILE:CD1	2.12	0.62
1:E:176:GLN:HA	1:E:318:PHE:CZ	2.35	0.62
1:E:19:LEU:O	1:E:22:ALA:HB3	2.00	0.61
1:E:285:LYS:HZ3	1:E:285:LYS:N	1.98	0.61
1:E:46:ILE:HD12	1:E:59:LEU:HD13	1.83	0.61
1:E:331:GLU:H	1:E:331:GLU:CD	2.07	0.61
1:E:189:LYS:NZ	1:E:195:THR:OG1	2.29	0.61
1:E:312:ALA:HB3	1:E:315:ILE:HD11	1.82	0.60
1:E:76:LYS:NZ	1:E:112:ASP:O	2.29	0.60
1:E:179:TYR:OH	1:E:310:VAL:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:VAL:HG12	1:E:105:LYS:N	2.17	0.59
1:E:274:GLN:NE2	1:E:275:VAL:N	2.51	0.59
1:E:126:GLY:HA2	1:E:327:PHE:CZ	2.37	0.59
1:E:244:ILE:HD12	1:E:244:ILE:N	2.17	0.58
1:E:274:GLN:HE21	1:E:274:GLN:CA	2.16	0.58
1:E:310:VAL:HG22	1:E:311:GLU:N	2.17	0.58
1:E:76:LYS:HE2	1:E:342:LYS:O	2.04	0.58
1:E:265:LEU:HD22	1:E:296:TRP:CZ2	2.39	0.58
1:E:179:TYR:HB2	1:E:308:ARG:NH1	2.18	0.57
2:I:23:HIS:H	2:I:23:HIS:HD2	1.51	0.57
1:E:145:PHE:HE1	1:E:310:VAL:CG1	2.16	0.57
1:E:43:PHE:HD2	1:E:60:VAL:CG1	2.18	0.57
1:E:64:GLU:HG3	1:E:65:SER:N	2.19	0.57
1:E:31:GLU:C	1:E:33:PRO:HD3	2.29	0.57
1:E:147:ALA:O	1:E:150:ILE:N	2.36	0.56
2:I:5:THR:O	2:I:8:ALA:HB3	2.06	0.56
1:E:73:ILE:HG23	1:E:117:TYR:CE2	2.40	0.56
1:E:269:LEU:O	1:E:273:LEU:HB2	2.06	0.55
1:E:44:ASP:OD2	1:E:63:LYS:NZ	2.39	0.55
1:E:277:LEU:C	1:E:279:LYS:H	2.15	0.55
1:E:145:PHE:CE1	1:E:310:VAL:HG13	2.39	0.55
1:E:242:GLN:HB2	1:E:245:GLN:OE1	2.08	0.54
1:E:340:ASN:O	1:E:342:LYS:HG2	2.07	0.54
1:E:265:LEU:HD12	1:E:265:LEU:C	2.28	0.54
1:E:13:GLU:HB3	1:E:16:LYS:HG2	1.90	0.53
1:E:85:ILE:HG13	4:E:431:HOH:O	2.09	0.53
1:E:109:SER:O	1:E:110:PHE:HB3	2.08	0.53
1:E:179:TYR:HB2	1:E:308:ARG:HH12	1.73	0.52
1:E:39:GLN:O	1:E:42:GLN:HG3	2.08	0.52
1:E:285:LYS:HZ3	1:E:285:LYS:H	1.56	0.52
1:E:42:GLN:O	1:E:63:LYS:HG3	2.10	0.52
1:E:87:HIS:HA	4:E:358:HOH:O	2.08	0.52
1:E:43:PHE:HD2	1:E:60:VAL:HG11	1.71	0.51
1:E:125:GLY:HA3	1:E:174:ILE:O	2.11	0.51
1:E:158:HIS:HE1	1:E:220:ASP:OD2	1.93	0.51
1:E:289:ASN:O	1:E:293:ASN:HB2	2.10	0.51
1:E:346:GLU:OE1	1:E:346:GLU:N	2.37	0.51
1:E:267:ASP:O	1:E:271:ASN:OD1	2.29	0.50
1:E:138:PHE:HD2	1:E:231:MET:HG3	1.75	0.50
1:E:122:TYR:CE2	1:E:124:ALA:HB2	2.47	0.50
1:E:138:PHE:CD2	1:E:231:MET:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:GLU:OE1	2:I:19:ARG:NH1	2.42	0.50
1:E:292:LYS:HA	1:E:302:TRP:CZ2	2.47	0.49
1:E:45:ARG:HD3	1:E:335:ILE:CD1	2.31	0.49
1:E:230:GLU:OE1	2:I:19:ARG:NH2	2.44	0.49
1:E:180:ILE:CG2	1:E:181:GLN:N	2.76	0.49
1:E:173:LEU:HD11	3:E:351:ADN:C5	2.42	0.49
1:E:175:ASP:OD2	1:E:308:ARG:NH2	2.45	0.49
1:E:61:LYS:HG3	1:E:68:HIS:CE1	2.48	0.49
1:E:140:GLU:HB2	1:E:141:PRO:HD3	1.96	0.48
1:E:307:GLN:O	1:E:308:ARG:HB2	2.12	0.48
1:E:226:VAL:HG23	1:E:273:LEU:HD11	1.95	0.48
1:E:229:TYR:CE2	1:E:237:PRO:HB3	2.48	0.48
1:E:285:LYS:H	1:E:285:LYS:NZ	2.11	0.48
1:E:338:SEP:C	1:E:340:ASN:H	2.26	0.48
1:E:338:SEP:O2P	1:E:338:SEP:HA	2.12	0.48
1:E:138:PHE:HD2	1:E:231:MET:CG	2.27	0.48
1:E:96:GLN:NE2	1:E:97:ALA:HB2	2.29	0.48
1:E:274:GLN:NE2	1:E:274:GLN:CA	2.77	0.47
1:E:245:GLN:O	1:E:249:LYS:HG3	2.14	0.47
1:E:91:GLU:O	1:E:95:LEU:HB2	2.15	0.47
1:E:157:LEU:HA	1:E:157:LEU:HD23	1.58	0.47
1:E:198:LEU:HD12	1:E:209:ILE:HG22	1.97	0.47
1:E:46:ILE:HD12	1:E:59:LEU:CD1	2.44	0.47
1:E:196:TRP:CD1	1:E:214:GLY:HA2	2.50	0.47
1:E:310:VAL:CG2	1:E:311:GLU:H	2.23	0.46
1:E:140:GLU:N	1:E:141:PRO:CD	2.78	0.46
1:E:285:LYS:H	1:E:285:LYS:HE2	1.79	0.46
1:E:103:LEU:HD21	1:E:153:THR:CG2	2.46	0.46
1:E:249:LYS:O	1:E:252:SER:HB2	2.16	0.46
1:E:226:VAL:CG2	1:E:273:LEU:HD11	2.45	0.46
1:E:105:LYS:HB3	1:E:105:LYS:HE2	1.82	0.46
1:E:40:LEU:HA	1:E:40:LEU:HD23	1.57	0.46
1:E:274:GLN:NE2	1:E:275:VAL:H	2.12	0.46
1:E:277:LEU:N	1:E:277:LEU:CD1	2.78	0.46
1:E:330:TYR:HA	1:E:331:GLU:OE2	2.15	0.46
1:E:248:GLU:O	1:E:252:SER:OG	2.29	0.46
1:E:274:GLN:HE21	1:E:275:VAL:N	2.14	0.45
1:E:285:LYS:H	1:E:285:LYS:CE	2.29	0.45
1:E:201:THR:HG23	1:E:202:PRO:HD2	1.97	0.45
1:E:96:GLN:O	1:E:96:GLN:HG2	2.16	0.45
1:E:74:LEU:O	1:E:115:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:LEU:HD12	1:E:277:LEU:H	1.79	0.45
1:E:71:MET:HE3	1:E:119:VAL:HG22	1.98	0.45
1:E:140:GLU:N	1:E:141:PRO:HD2	2.32	0.45
1:E:331:GLU:CD	1:E:331:GLU:N	2.75	0.45
2:I:15:ARG:HA	4:I:363:HOH:O	2.16	0.45
1:E:73:ILE:CG2	1:E:117:TYR:CE2	2.99	0.45
1:E:276:ASP:CG	1:E:279:LYS:HZ2	2.25	0.45
1:E:240:ALA:CB	1:E:245:GLN:HB2	2.47	0.44
1:E:312:ALA:HB1	1:E:315:ILE:CD1	2.44	0.44
1:E:131:HIS:N	1:E:131:HIS:CD2	2.83	0.44
1:E:37:THR:O	1:E:38:ALA:HB2	2.17	0.44
1:E:106:LEU:HD12	1:E:119:VAL:O	2.18	0.44
1:E:48:THR:HB	1:E:330:TYR:HB2	2.01	0.43
1:E:50:GLY:HA2	1:E:330:TYR:CZ	2.54	0.43
1:E:100:PHE:CG	1:E:101:PRO:CD	2.99	0.43
1:E:265:LEU:HD12	1:E:269:LEU:HG	2.01	0.43
1:E:268:LEU:HD11	1:E:297:PHE:HE2	1.84	0.43
1:E:331:GLU:OE2	1:E:331:GLU:N	2.51	0.43
1:E:241:ASP:H	1:E:245:GLN:HE22	1.65	0.43
1:E:79:VAL:HG13	1:E:84:GLN:HB2	2.01	0.43
1:E:314:PHE:C	1:E:314:PHE:CD1	2.97	0.43
1:E:59:LEU:HD22	1:E:60:VAL:N	2.34	0.42
2:I:16:THR:N	4:I:363:HOH:O	2.51	0.42
1:E:13:GLU:C	1:E:15:VAL:N	2.77	0.42
1:E:104:VAL:CG1	1:E:105:LYS:N	2.82	0.42
1:E:285:LYS:HE2	1:E:285:LYS:HB2	1.56	0.42
1:E:34:SER:O	1:E:92:LYS:HE3	2.19	0.42
1:E:157:LEU:O	1:E:162:LEU:HB2	2.19	0.42
1:E:31:GLU:O	1:E:33:PRO:HD3	2.19	0.42
1:E:59:LEU:HD22	1:E:60:VAL:H	1.85	0.42
1:E:277:LEU:C	1:E:279:LYS:N	2.78	0.42
1:E:50:GLY:HA2	1:E:330:TYR:CE1	2.54	0.42
1:E:265:LEU:O	1:E:269:LEU:HG	2.20	0.41
1:E:85:ILE:HD13	1:E:346:GLU:HB3	2.02	0.41
1:E:88:THR:HG21	1:E:116:LEU:CD1	2.50	0.41
1:E:133:ARG:NH2	1:E:230:GLU:OE2	2.51	0.41
1:E:180:ILE:HG22	1:E:181:GLN:N	2.36	0.41
1:E:51:THR:HG23	1:E:52:GLY:N	2.35	0.41
1:E:175:ASP:OD2	1:E:308:ARG:NH1	2.54	0.41
1:E:268:LEU:HD11	1:E:297:PHE:CE2	2.56	0.41
1:E:135:ILE:CD1	1:E:135:ILE:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:LYS:HA	4:E:431:HOH:O	2.21	0.40
1:E:274:GLN:HE21	1:E:275:VAL:H	1.68	0.40
1:E:127:GLU:OE2	3:E:351:ADN:O2'	2.34	0.40
1:E:65:SER:CB	1:E:67:ASN:HD22	2.29	0.40
1:E:303:ILE:C	1:E:307:GLN:HE21	2.29	0.40
1:E:310:VAL:CG2	1:E:311:GLU:N	2.84	0.40
1:E:276:ASP:OD1	1:E:278:THR:OG1	2.27	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	334/350 (95%)	291 (87%)	39 (12%)	4 (1%)	10	8
2	I	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
All	All	352/370 (95%)	307 (87%)	41 (12%)	4 (1%)	11	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	36	ASN
1	E	148	ALA
1	E	289	ASN
1	E	186	GLY

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	297/303 (98%)	231 (78%)	66 (22%)	1	1
2	I	15/15 (100%)	12 (80%)	3 (20%)	1	1
All	All	312/318 (98%)	243 (78%)	69 (22%)	1	1

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	13	GLU
1	E	16	LYS
1	E	21	LYS
1	E	25	ASP
1	E	32	THR
1	E	35	GLN
1	E	36	ASN
1	E	37	THR
1	E	40	LEU
1	E	41	ASP
1	E	47	LYS
1	E	51	THR
1	E	59	LEU
1	E	60	VAL
1	E	61	LYS
1	E	63	LYS
1	E	65	SER
1	E	71	MET
1	E	73	ILE
1	E	75	ASP
1	E	77	GLN
1	E	81	LYS
1	E	83	LYS
1	E	96	GLN
1	E	111	LYS
1	E	115	ASN
1	E	120	MET
1	E	130	SER
1	E	137	ARG
1	E	162	LEU
1	E	163	ILE
1	E	174	ILE
1	E	177	GLN

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Mol	Chain	Res	Type
1	E	180	ILE
1	E	189	LYS
1	E	205	LEU
1	E	209	ILE
1	E	231	MET
1	E	254	LYS
1	E	260	HIS
1	E	263	SER
1	E	265	LEU
1	E	268	LEU
1	E	272	LEU
1	E	273	LEU
1	E	274	GLN
1	E	275	VAL
1	E	279	LYS
1	E	285	LYS
1	E	295	LYS
1	E	300	THR
1	E	303	ILE
1	E	305	ILE
1	E	311	GLU
1	E	314	PHE
1	E	315	ILE
1	E	317	LYS
1	E	318	PHE
1	E	331	GLU
1	E	333	GLU
1	E	334	GLU
1	E	336	ARG
1	E	339	ILE
1	E	341	GLU
1	E	345	LYS
1	E	348	THR
2	I	15	ARG
2	I	22	ILE
2	I	23	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	62	HIS
1	E	67	ASN

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Mol	Chain	Res	Type
1	E	68	HIS
1	E	77	GLN
1	E	131	HIS
1	E	158	HIS
1	E	242	GLN
1	E	245	GLN
1	E	271	ASN
1	E	274	GLN
1	E	283	ASN
1	E	307	GLN
2	I	23	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	E	197	1	8,10,11	1.33	1 (12%)	10,14,16	1.30	2 (20%)
1	SEP	E	338	1	8,9,10	1.02	0	7,12,14	2.03	3 (42%)

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
1	TPO	E	197	1	-	1/9/11/13	-
1	SEP	E	338	1	-	2/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	197	TPO	P-O2P	-2.30	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	338	SEP	OG-CB-CA	3.42	111.47	108.14
1	E	338	SEP	O3P-P-O1P	3.22	123.38	110.83
1	E	197	TPO	P-OG1-CB	-2.58	116.32	123.33
1	E	338	SEP	O2P-P-O1P	-2.33	101.75	110.83
1	E	197	TPO	O2P-P-O1P	2.25	119.60	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	197	TPO	O-C-CA-CB
1	E	338	SEP	N-CA-CB-OG
1	E	338	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	338	SEP	2	0

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	$\# Z > 2$
3	ADN	E	351	-	21,21,21	0.38	0	31,31,31	0.54	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	ADN	E	351	-	-	1/6/22/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

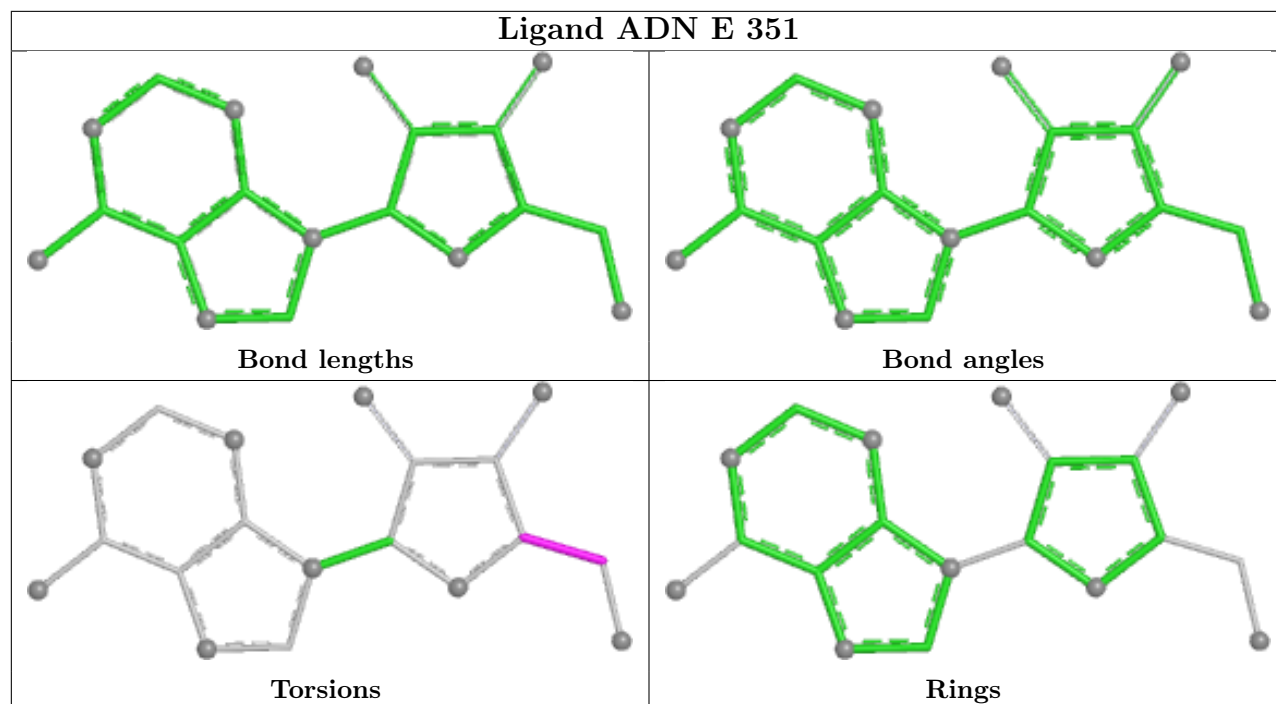
Mol	Chain	Res	Type	Atoms
3	E	351	ADN	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	351	ADN	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.