



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:59 PM UTC

PDB ID : 2CPK / pdb_00002cpk
Title : CRYSTAL STRUCTURE OF THE CATALYTIC SUBUNIT OF CYCLIC ADENOSINE MONOPHOSPHATE-DEPENDENT PROTEIN KINASE
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Deposited on : 1992-10-21
Resolution : 2.70 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
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

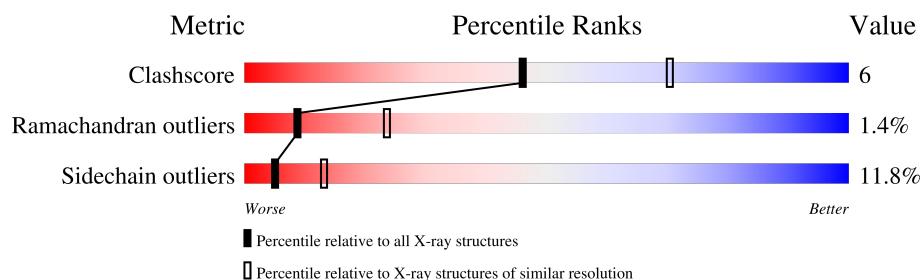
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	350	
2	I	20	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2822 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, CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	336	Total	C	N	O	P	S	0	0	0
			2665	1732	439	483	3	8			

- Molecule 2 is a protein called PEPTIDE INHIBITOR 20-MER.

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

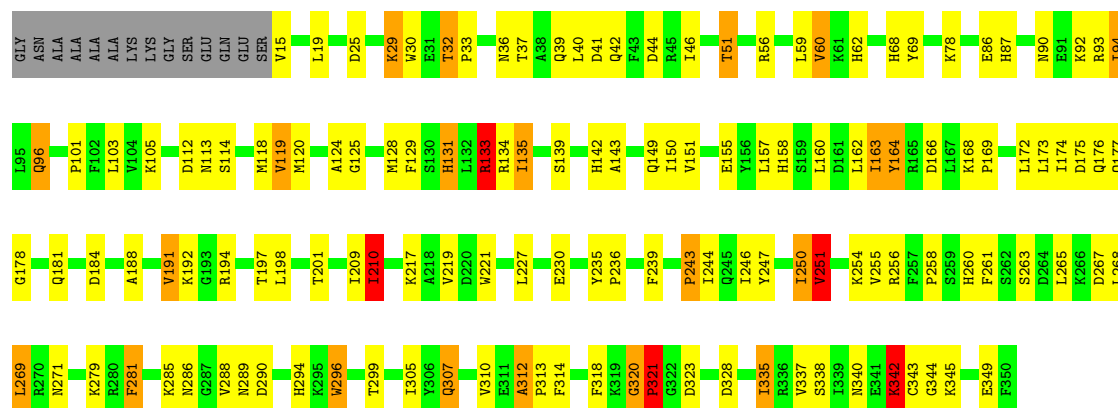
3 Residue-property plots

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.

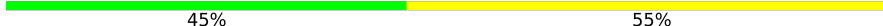
Note EDS was not executed.

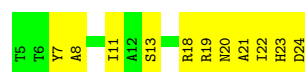
• Molecule 1: cAMP-DEPENDENT PROTEIN KINASE, CATALYTIC SUBUNIT

Chain E: 



• Molecule 2: PEPTIDE INHIBITOR 20-MER

Chain I: 



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	73.62Å 76.52Å 80.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2822	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: SEP, 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	1.34	18/2702 (0.7%)	2.13	103/3662 (2.8%)
2	I	1.34	1/159 (0.6%)	2.31	13/212 (6.1%)
All	All	1.34	19/2861 (0.7%)	2.14	116/3874 (3.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	256	ARG	NE-CZ	7.79	1.41	1.33
1	E	335	ILE	CA-CB	7.47	1.63	1.54
1	E	87	HIS	CD2-NE2	-7.14	1.29	1.37
1	E	68	HIS	CD2-NE2	-6.98	1.30	1.37
1	E	62	HIS	CD2-NE2	-6.91	1.30	1.37
1	E	260	HIS	CD2-NE2	-6.89	1.30	1.37
1	E	158	HIS	CD2-NE2	-6.48	1.30	1.37
1	E	210	ILE	CA-CB	6.39	1.62	1.54
1	E	294	HIS	CD2-NE2	-6.13	1.31	1.37
2	I	23	HIS	CD2-NE2	-5.71	1.31	1.37
1	E	256	ARG	CZ-NH2	5.56	1.40	1.33
1	E	236	PRO	CA-CB	-5.52	1.49	1.54
1	E	194	ARG	CZ-NH2	5.50	1.40	1.33
1	E	158	HIS	CG-ND1	-5.50	1.32	1.38
1	E	131	HIS	CD2-NE2	-5.48	1.31	1.37
1	E	281	PHE	CA-CB	-5.46	1.44	1.53
1	E	194	ARG	NE-CZ	5.39	1.39	1.33
1	E	142	HIS	CD2-NE2	-5.03	1.32	1.37
1	E	221	TRP	NE1-CE2	-5.00	1.31	1.37

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	112	ASP	CA-CB-CG	11.62	124.22	112.60
1	E	289	ASN	CA-CB-CG	-10.08	102.52	112.60
1	E	113	ASN	OD1-CG-ND2	-9.48	113.12	122.60
1	E	328	ASP	CA-CB-CG	9.26	121.86	112.60
1	E	164	TYR	CA-C-O	-8.66	111.32	120.58
1	E	335	ILE	N-CA-C	-8.65	97.47	108.89
1	E	254	LYS	N-CA-C	-8.59	94.52	108.52
1	E	310	VAL	N-CA-C	-8.58	97.71	109.55
1	E	290	ASP	CA-CB-CG	8.21	120.81	112.60
1	E	113	ASN	CB-CG-ND2	8.05	128.47	116.40
1	E	194	ARG	N-CA-C	7.83	122.12	110.52
1	E	142	HIS	CA-CB-CG	7.80	121.61	113.80
1	E	251	VAL	N-CA-CB	-7.79	99.95	110.54
2	I	23	HIS	O-C-N	7.77	132.74	122.33
1	E	164	TYR	O-C-N	-7.74	113.65	122.93
1	E	236	PRO	O-C-N	-7.59	117.58	121.15
1	E	320	GLY	CA-C-N	7.54	129.27	119.84
1	E	320	GLY	C-N-CA	7.54	129.27	119.84
1	E	103	LEU	CA-C-O	-7.52	112.01	120.66
1	E	62	HIS	CB-CG-CD2	-7.20	121.84	131.20
1	E	143	ALA	N-CA-C	-7.20	103.37	111.07
1	E	219	VAL	N-CA-C	-7.18	103.47	110.72
1	E	192	LYS	N-CA-C	-7.10	97.67	108.96
1	E	86	GLU	O-C-N	-7.09	113.55	122.27
1	E	344	GLY	N-CA-C	7.09	121.22	112.64
1	E	93	ARG	CA-C-O	-6.94	113.06	120.42
1	E	124	ALA	N-CA-C	6.92	120.98	112.54
1	E	314	PHE	N-CA-C	-6.89	98.61	109.50
1	E	312	ALA	CA-C-N	6.87	127.15	119.32
1	E	312	ALA	C-N-CA	6.87	127.15	119.32
1	E	191	VAL	CB-CA-C	-6.84	99.47	110.28
1	E	133	ARG	NE-CZ-NH1	6.55	128.06	121.50
1	E	221	TRP	CG-CD2-CE3	6.52	140.42	133.90
2	I	21	ALA	O-C-N	6.46	130.26	122.96
1	E	68	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	E	175	ASP	CA-CB-CG	6.40	119.00	112.60
1	E	78	LYS	N-CA-C	-6.37	104.42	111.36
1	E	101	PRO	N-CA-C	6.35	122.22	113.65
1	E	294	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	E	305	ILE	O-C-N	6.30	128.45	121.90
1	E	173	LEU	CA-C-O	-6.29	113.88	121.05
1	E	149	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	E	342	LYS	O-C-N	-6.26	114.26	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	19	ARG	O-C-N	-6.26	115.71	123.04
2	I	23	HIS	CA-C-N	6.19	132.84	121.70
2	I	23	HIS	C-N-CA	6.19	132.84	121.70
1	E	188	ALA	N-CA-C	-6.17	101.80	110.50
1	E	260	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	E	51	THR	N-CA-CB	-6.06	101.80	111.43
1	E	92	LYS	CA-CB-CG	-6.02	102.06	114.10
1	E	44	ASP	CA-CB-CG	-6.02	106.58	112.60
1	E	235	TYR	O-C-N	-5.97	117.17	121.83
1	E	60	VAL	N-CA-CB	-5.93	101.38	112.36
1	E	286	ASN	CA-CB-CG	5.91	118.51	112.60
1	E	39	GLN	N-CA-C	-5.90	100.53	109.85
1	E	343	CYS	N-CA-C	5.89	118.75	109.39
1	E	256	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	E	235	TYR	CA-C-N	5.87	123.89	119.66
1	E	235	TYR	C-N-CA	5.87	123.89	119.66
1	E	168	LYS	CA-C-N	5.81	127.11	119.84
1	E	168	LYS	C-N-CA	5.81	127.11	119.84
1	E	239	PHE	CA-CB-CG	5.80	119.60	113.80
1	E	119	VAL	N-CA-C	-5.79	100.14	108.48
1	E	46	ILE	O-C-N	-5.75	114.00	121.99
1	E	210	ILE	CB-CG1-CD1	-5.74	101.75	113.80
1	E	96	GLN	CG-CD-NE2	5.73	124.99	116.40
1	E	32	THR	CA-C-N	5.70	125.65	119.78
1	E	32	THR	C-N-CA	5.70	125.65	119.78
1	E	86	GLU	CB-CG-CD	5.68	122.26	112.60
1	E	312	ALA	N-CA-C	5.68	117.85	109.50
2	I	11	ILE	N-CA-C	5.64	119.94	112.04
1	E	131	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	E	227	LEU	CA-C-O	-5.63	115.09	121.00
2	I	20	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	E	163	ILE	CB-CA-C	5.59	117.97	110.42
2	I	18	ARG	N-CA-C	-5.59	101.37	109.59
1	E	176	GLN	OE1-CD-NE2	-5.57	117.03	122.60
2	I	8	ALA	CB-CA-C	-5.54	102.18	110.88
1	E	68	HIS	CE1-NE2-CD2	5.53	114.53	109.00
2	I	13	SER	N-CA-C	-5.52	101.55	110.32
1	E	118	MET	CG-SD-CE	-5.52	88.76	100.90
1	E	133	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	E	68	HIS	CG-CD2-NE2	-5.49	101.71	107.20
1	E	307	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	E	221	TRP	CB-CG-CD1	-5.41	118.78	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	236	PRO	CA-C-O	-5.39	116.47	120.73
1	E	271	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	E	279	LYS	N-CA-CB	-5.38	102.70	110.56
1	E	296	TRP	CG-CD2-CE3	5.36	139.26	133.90
1	E	51	THR	OG1-CB-CG2	5.36	120.01	109.30
1	E	135	ILE	N-CA-C	-5.33	104.43	111.09
1	E	163	ILE	CB-CG1-CD1	-5.31	102.65	113.80
1	E	318	PHE	N-CA-C	-5.31	100.59	109.24
1	E	30	TRP	CG-CD2-CE3	5.30	139.20	133.90
1	E	181	GLN	CG-CD-NE2	5.28	124.31	116.40
1	E	201	THR	N-CA-C	-5.26	100.98	109.40
1	E	239	PHE	O-C-N	-5.26	117.39	123.33
1	E	134	ARG	N-CA-C	5.25	116.81	111.14
1	E	78	LYS	CA-CB-CG	5.24	124.58	114.10
1	E	321	PRO	N-CA-C	5.24	123.26	112.47
2	I	7	TYR	O-C-N	5.23	127.66	122.12
1	E	267	ASP	CA-CB-CG	5.22	117.82	112.60
1	E	236	PRO	N-CA-CB	-5.21	100.51	103.22
1	E	131	HIS	CB-CG-ND1	5.20	130.51	122.70
1	E	285	LYS	O-C-N	-5.17	116.71	122.09
1	E	250	ILE	CA-C-O	5.14	127.20	120.78
1	E	177	GLN	O-C-N	-5.14	115.76	122.59
1	E	60	VAL	CB-CA-C	5.13	118.97	110.30
2	I	24	ASP	CA-CB-CG	5.13	117.73	112.60
1	E	114	SER	N-CA-C	5.10	120.50	113.97
1	E	305	ILE	N-CA-CB	-5.08	104.07	110.57
1	E	163	ILE	N-CA-CB	-5.07	104.92	111.82
1	E	166	ASP	N-CA-C	5.06	118.88	109.56
1	E	94	ILE	CB-CA-C	-5.03	105.35	112.14
2	I	23	HIS	CA-C-O	5.02	125.72	119.79
1	E	158	HIS	CB-CG-CD2	-5.02	124.67	131.20

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	2665	0	2532	32	0
2	I	157	0	146	0	0
All	All	2822	0	2678	32	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 6.

All (32) 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:155:GLU:HG3	1:E:288:VAL:HG11	1.60	0.84
1:E:243:PRO:HA	1:E:246:ILE:HD12	1.67	0.76
1:E:198:LEU:HD23	1:E:209:ILE:HG22	1.75	0.69
1:E:210:ILE:HD13	1:E:247:TYR:HB3	1.72	0.68
1:E:125:GLY:HA3	1:E:174:ILE:O	2.04	0.57
1:E:131:HIS:HB3	1:E:135:ILE:HD12	1.89	0.54
1:E:105:LYS:O	1:E:120:MET:HB2	2.11	0.50
1:E:258:PRO:HG2	1:E:261:PHE:CE1	2.48	0.49
1:E:244:ILE:H	1:E:244:ILE:HD12	1.78	0.48
1:E:33:PRO:HA	1:E:96:GLN:OE1	2.14	0.48
1:E:69:TYR:HB3	1:E:119:VAL:HG12	1.96	0.47
1:E:25:ASP:O	1:E:29:LYS:HG2	2.14	0.47
1:E:191:VAL:HG23	1:E:191:VAL:O	2.15	0.47
1:E:210:ILE:HD11	1:E:251:VAL:HG21	1.97	0.46
1:E:342:LYS:HD3	1:E:342:LYS:HA	1.71	0.46
1:E:128:MET:HE3	1:E:172:LEU:HB2	1.99	0.44
1:E:163:ILE:HD13	1:E:163:ILE:HG21	1.61	0.44
1:E:56:ARG:HG2	1:E:56:ARG:NH1	2.33	0.43
1:E:56:ARG:HG2	1:E:56:ARG:HH11	1.83	0.43
1:E:243:PRO:O	1:E:246:ILE:HB	2.19	0.42
1:E:265:LEU:HG	1:E:269:LEU:HD22	2.02	0.42
1:E:90:ASN:O	1:E:94:ILE:HD12	2.19	0.42
1:E:340:ASN:HB2	1:E:342:LYS:NZ	2.35	0.42
1:E:320:GLY:O	1:E:323:ASP:HB2	2.20	0.42
1:E:29:LYS:HG2	1:E:29:LYS:H	1.69	0.41
1:E:157:LEU:HD13	1:E:164:TYR:HB2	2.02	0.41
1:E:150:ILE:HD11	1:E:172:LEU:HD22	2.01	0.41
1:E:150:ILE:O	1:E:151:VAL:C	2.64	0.41
1:E:129:PHE:CE1	1:E:133:ARG:NH1	2.89	0.40
1:E:312:ALA:HA	1:E:313:PRO:HD3	1.92	0.40
1:E:133:ARG:NH2	1:E:230:GLU:OE2	2.55	0.40
1:E:178:GLY:HA3	1:E:312:ALA:HB1	2.02	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	331/350 (95%)	312 (94%)	14 (4%)	5 (2%)	8	22
2	I	18/20 (90%)	18 (100%)	0	0	100	100
All	All	349/370 (94%)	330 (95%)	14 (4%)	5 (1%)	9	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	184	ASP
1	E	217	LYS
1	E	321	PRO
1	E	41	ASP
1	E	342	LYS

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	264/302 (87%)	232 (88%)	32 (12%)	5	12
2	I	15/15 (100%)	14 (93%)	1 (7%)	15	36
All	All	279/317 (88%)	246 (88%)	33 (12%)	5	13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	15	VAL
1	E	19	LEU
1	E	29	LYS
1	E	32	THR
1	E	36	ASN
1	E	37	THR
1	E	40	LEU
1	E	42	GLN
1	E	51	THR
1	E	59	LEU
1	E	60	VAL
1	E	133	ARG
1	E	160	LEU
1	E	162	LEU
1	E	169	PRO
1	E	210	ILE
1	E	243	PRO
1	E	250	ILE
1	E	251	VAL
1	E	255	VAL
1	E	263	SER
1	E	268	LEU
1	E	269	LEU
1	E	281	PHE
1	E	296	TRP
1	E	299	THR
1	E	307	GLN
1	E	321	PRO
1	E	335	ILE
1	E	337	VAL
1	E	345	LYS
1	E	349	GLU
2	I	22	ILE

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

Mol	Chain	Res	Type
1	E	62	HIS
1	E	115	ASN
1	E	158	HIS
1	E	181	GLN
1	E	242	GLN
1	E	245	GLN

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Mol	Chain	Res	Type
2	I	20	ASN
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 ⓘ

3 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	SEP	E	139	1	8,9,10	0.95	0	7,12,14	2.64	3 (42%)
1	TPO	E	197	1	8,10,11	1.70	2 (25%)	10,14,16	1.61	2 (20%)
1	SEP	E	338	1	8,9,10	0.87	0	7,12,14	3.30	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	SEP	E	139	1	-	1/6/8/10	-
1	TPO	E	197	1	-	1/9/11/13	-
1	SEP	E	338	1	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	197	TPO	P-OG1	-3.30	1.53	1.59
1	E	197	TPO	P-O2P	-2.30	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	338	SEP	OG-CB-CA	7.65	115.59	108.14
1	E	139	SEP	OG-CB-CA	5.46	113.46	108.14
1	E	197	TPO	O-C-CA	-3.10	116.79	124.77
1	E	338	SEP	O3P-P-OG	-2.82	99.30	106.67
1	E	139	SEP	O2P-P-OG	-2.68	99.67	106.67
1	E	139	SEP	O3P-P-O2P	2.25	116.25	107.80
1	E	197	TPO	OG1-P-O1P	-2.18	101.56	109.33
1	E	338	SEP	O3P-P-O2P	2.12	115.77	107.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	139	SEP	C-CA-CB-OG
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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.