



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:38 PM GMT

PDB ID : 1JLU
Title : Crystal Structure of the Catalytic Subunit of cAMP-dependent Protein Kinase
Complexed with a Phosphorylated Substrate Peptide and Detergent
Authors : Madhusudan; Trafny, E.A.; Xuong, N.-H.; Adams, J.A.; Ten Eyck, L.F.; Taylor, S.S.; Sowadski, J.M.
Deposited on : 2001-07-16
Resolution : 2.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

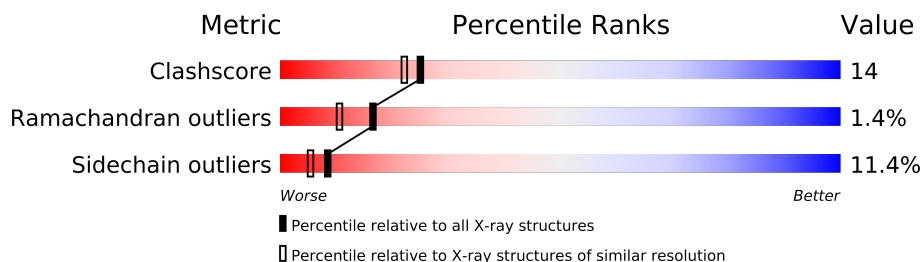
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	350	
2	S	20	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2962 atoms, of which 0 are hydrogen and 0 are deuterium.

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 AMP-DEPENDENT PROTEIN KINASE, ALPHA-CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	339	Total	C	N	O	P	S	0	0	0
			2679	1742	446	481	2	8			

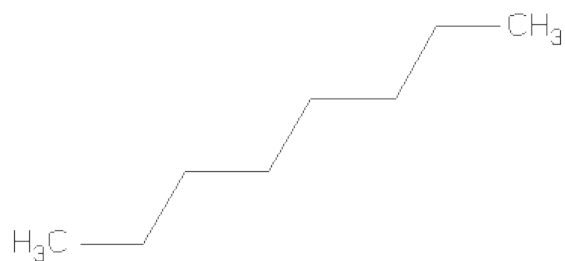
- Molecule 2 is a protein called CAMP-DEPENDENT PROTEIN KINASE INHIBITOR, MUSCLE/BRAIN FORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	20	Total	C	N	O	P	0	0	0
			159	93	31	34	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	376	ALA	ASN	ENGINEERED MUTATION	UNP P27776
S	377	SEP	ALA	ENGINEERED MUTATION	UNP P27776

- Molecule 3 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 8 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	102	Total O 102 102	0	0
4	S	14	Total O 14 14	0	0

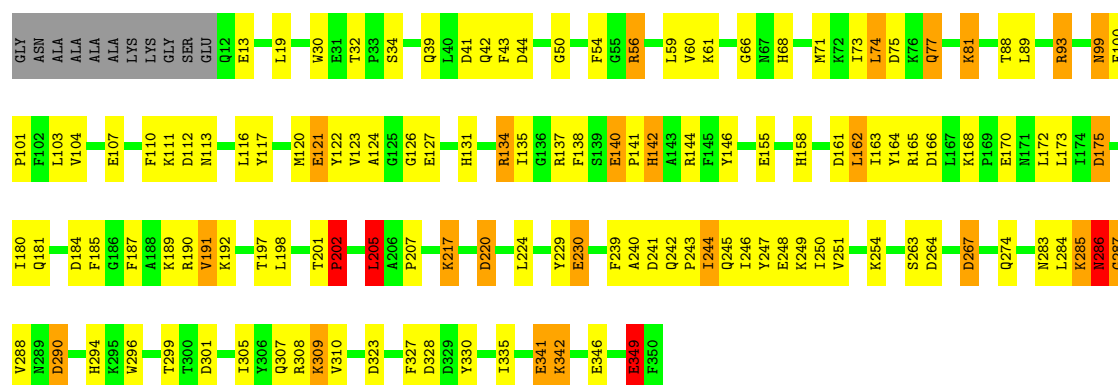
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: AMP-DEPENDENT PROTEIN KINASE, ALPHA-CATALYTIC SUBUNIT

Chain E: 



• Molecule 2: CAMP-DEPENDENT PROTEIN KINASE INHIBITOR, MUSCLE/BRAIN FORM

Chain S: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.87Å 75.58Å 80.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2962	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: TPO, OCT, SEP

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	0.95	12/2726 (0.4%)	1.40	40/3691 (1.1%)
2	S	0.92	0/150	1.80	6/198 (3.0%)
All	All	0.95	12/2876 (0.4%)	1.42	46/3889 (1.2%)

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	E	1	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	13	GLU	CD-OE2	8.52	1.35	1.25
1	E	127	GLU	CD-OE2	6.92	1.33	1.25
1	E	140	GLU	CD-OE2	6.35	1.32	1.25
1	E	107	GLU	CD-OE2	5.91	1.32	1.25
1	E	230	GLU	CD-OE2	5.86	1.32	1.25
1	E	121	GLU	CD-OE2	5.84	1.32	1.25
1	E	346	GLU	CD-OE2	5.48	1.31	1.25
1	E	248	GLU	CD-OE2	5.46	1.31	1.25
1	E	155	GLU	CD-OE2	5.43	1.31	1.25
1	E	341	GLU	CD-OE2	5.28	1.31	1.25
1	E	155	GLU	CD-OE1	-5.07	1.20	1.25
1	E	349	GLU	CD-OE2	5.02	1.31	1.25

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	375	ARG	NE-CZ-NH1	9.58	125.09	120.30
2	S	375	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	E	220	ASP	CB-CG-OD1	9.15	126.53	118.30
1	E	290	ASP	CB-CG-OD2	-8.92	110.28	118.30
1	E	184	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	E	112	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	E	93	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	E	93	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	E	184	ASP	CB-CG-OD1	7.91	125.42	118.30
1	E	308	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	E	229	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	E	220	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	E	44	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	E	290	ASP	CB-CG-OD1	7.24	124.82	118.30
1	E	41	ASP	CB-CG-OD2	-7.22	111.80	118.30
2	S	374	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	E	112	ASP	CB-CG-OD1	7.05	124.64	118.30
1	E	267	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	E	161	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	E	137	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	E	241	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	E	187	PHE	CB-CG-CD1	-6.37	116.34	120.80
1	E	175	ASP	CB-CG-OD1	6.29	123.96	118.30
1	E	241	ASP	CB-CG-OD1	6.22	123.89	118.30
2	S	380	ASP	CB-CG-OD1	6.07	123.77	118.30
1	E	75	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	E	175	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	E	166	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	E	192	LYS	N-CA-C	-5.90	95.06	111.00
1	E	267	ASP	CB-CG-OD1	5.87	123.58	118.30
1	E	41	ASP	CB-CG-OD1	5.86	123.58	118.30
1	E	166	ASP	CB-CG-OD1	5.83	123.55	118.30
1	E	137	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	286	ASN	CB-CA-C	-5.70	99.00	110.40
1	E	134	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	E	202	PRO	N-CA-CB	5.53	109.94	103.30
1	E	229	TYR	CB-CG-CD1	5.42	124.25	121.00
2	S	380	ASP	CB-CG-OD2	-5.36	113.47	118.30
2	S	374	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	E	56	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	E	264	ASP	CB-CG-OD1	5.26	123.04	118.30
1	E	134	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	E	205	LEU	CB-CA-C	-5.17	100.38	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	328	ASP	CB-CG-OD1	5.12	122.91	118.30
1	E	323	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	E	301	ASP	CB-CG-OD1	5.02	122.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	77	GLN	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2679	0	2567	74	0
2	S	159	0	144	5	0
3	E	8	0	18	0	0
4	E	102	0	0	7	0
4	S	14	0	0	0	0
All	All	2962	0	2729	77	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (77) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:294:HIS:HD2	1:E:296:TRP:H	1.13	0.96
1:E:131:HIS:HD2	1:E:134:ARG:HH22	1.10	0.93
1:E:122:TYR:CE2	1:E:124:ALA:HB2	2.10	0.87
1:E:131:HIS:CD2	1:E:134:ARG:HH22	1.97	0.82
1:E:217:LYS:NZ	1:E:283:ASN:HD22	1.78	0.82
1:E:217:LYS:HZ1	1:E:283:ASN:HD22	1.25	0.81
4:E:407:HOH:O	2:S:374:ARG:HD2	1.82	0.79
1:E:30:TRP:CZ3	1:E:93:ARG:HG2	2.26	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:135:ILE:HD12	1:E:138:PHE:HE2	1.57	0.68
1:E:168:LYS:HG3	1:E:170:GLU:HB2	1.75	0.67
1:E:59:LEU:HD11	1:E:68:HIS:HB3	1.77	0.66
1:E:189:LYS:HG2	1:E:191:VAL:HG22	1.77	0.66
1:E:131:HIS:HD2	1:E:134:ARG:NH2	1.90	0.64
1:E:307:GLN:OE1	1:E:309:LYS:HE3	1.97	0.64
1:E:285:LYS:O	1:E:285:LYS:HG3	1.97	0.63
1:E:77:GLN:O	1:E:81:LYS:HG3	1.98	0.62
1:E:144:ARG:HD2	4:E:490:HOH:O	2.00	0.61
1:E:294:HIS:CD2	1:E:296:TRP:H	2.05	0.59
1:E:242:GLN:N	1:E:245:GLN:OE1	2.31	0.59
1:E:170:GLU:OE2	2:S:375:ARG:HD2	2.02	0.58
1:E:100:PHE:CG	1:E:101:PRO:HD2	2.39	0.58
1:E:71:MET:CE	1:E:73:ILE:HD11	2.34	0.56
1:E:43:PHE:HB3	1:E:60:VAL:HG13	1.87	0.56
1:E:99:ASN:C	1:E:99:ASN:HD22	2.08	0.56
1:E:126:GLY:HA2	1:E:327:PHE:CZ	2.41	0.56
1:E:71:MET:HE3	1:E:73:ILE:HD11	1.87	0.55
1:E:142:HIS:CE1	1:E:146:TYR:CE2	2.95	0.55
1:E:103:LEU:HD22	1:E:185:PHE:HZ	1.73	0.54
1:E:205:LEU:HD12	4:E:492:HOH:O	2.08	0.53
1:E:113:ASN:ND2	1:E:341:GLU:HB3	2.24	0.53
1:E:240:ALA:CB	1:E:245:GLN:HB2	2.39	0.53
1:E:110:PHE:CE2	1:E:117:TYR:CD2	2.98	0.51
1:E:158:HIS:HE1	1:E:220:ASP:OD2	1.94	0.51
1:E:123:VAL:CG1	1:E:175:ASP:HA	2.41	0.50
1:E:30:TRP:CE3	1:E:93:ARG:HG2	2.47	0.50
1:E:165:ARG:HH12	1:E:197:TPO:P	2.33	0.50
2:S:363:TYR:O	2:S:367:ILE:HG12	2.11	0.50
1:E:140:GLU:N	1:E:141:PRO:HD2	2.26	0.50
1:E:189:LYS:HE3	4:E:496:HOH:O	2.11	0.49
1:E:61:LYS:HE2	1:E:66:GLY:HA2	1.94	0.49
1:E:89:LEU:HD22	1:E:349:GLU:HG2	1.94	0.49
1:E:180:ILE:CG2	1:E:181:GLN:N	2.76	0.48
1:E:140:GLU:HB2	1:E:141:PRO:HD3	1.95	0.48
1:E:217:LYS:NZ	1:E:283:ASN:ND2	2.54	0.48
1:E:39:GLN:HB2	1:E:42:GLN:HG3	1.96	0.47
1:E:88:THR:HG21	1:E:116:LEU:CD1	2.45	0.47
1:E:247:TYR:O	1:E:251:VAL:HG22	2.15	0.47
1:E:239:PHE:O	1:E:249:LYS:HE2	2.15	0.47
1:E:284:LEU:HB2	1:E:290:ASP:OD1	2.15	0.47
1:E:305:ILE:HD13	1:E:310:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:201:THR:O	1:E:202:PRO:C	2.54	0.46
2:S:372:THR:HG22	2:S:372:THR:O	2.15	0.46
1:E:142:HIS:HE1	1:E:146:TYR:CE2	2.34	0.45
1:E:164:TYR:O	1:E:165:ARG:HB2	2.15	0.45
1:E:121:GLU:HB2	4:E:398:HOH:O	2.16	0.45
1:E:140:GLU:N	1:E:141:PRO:CD	2.80	0.45
1:E:244:ILE:HA	1:E:244:ILE:HD12	1.73	0.44
1:E:56:ARG:HH22	1:E:335:ILE:HA	1.81	0.44
1:E:285:LYS:O	1:E:286:ASN:ND2	2.51	0.44
1:E:131:HIS:O	1:E:135:ILE:HG13	2.18	0.43
1:E:103:LEU:HD22	1:E:185:PHE:CZ	2.54	0.43
1:E:104:VAL:O	1:E:104:VAL:HG13	2.18	0.43
1:E:50:GLY:HA2	1:E:330:TYR:CZ	2.53	0.43
1:E:162:LEU:HD12	1:E:190:ARG:HA	2.01	0.42
1:E:50:GLY:HA2	1:E:330:TYR:CE2	2.54	0.42
1:E:305:ILE:HD13	1:E:305:ILE:HA	1.78	0.42
1:E:342:LYS:HE3	4:E:470:HOH:O	2.20	0.41
1:E:246:ILE:O	1:E:250:ILE:HG13	2.19	0.41
1:E:263:SER:N	4:E:426:HOH:O	2.49	0.41
1:E:74:LEU:HD12	1:E:74:LEU:HA	1.82	0.41
1:E:230:GLU:CD	2:S:375:ARG:HH22	2.24	0.41
1:E:305:ILE:HD13	1:E:310:VAL:HG21	2.02	0.41
1:E:267:ASP:OD2	1:E:294:HIS:HE1	2.04	0.41
1:E:100:PHE:CG	1:E:101:PRO:CD	3.04	0.41
1:E:286:ASN:O	1:E:287:GLY:C	2.60	0.40
1:E:168:LYS:HE3	1:E:201:THR:OG1	2.22	0.40
1:E:100:PHE:CD1	1:E:101:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	335/350 (96%)	318 (95%)	12 (4%)	5 (2%)	15 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
All	All	352/370 (95%)	334 (95%)	13 (4%)	5 (1%)	16	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	286	ASN
1	E	202	PRO
1	E	288	VAL
1	E	243	PRO
1	E	287	GLY

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	267/303 (88%)	238 (89%)	29 (11%)	9	6
2	S	14/14 (100%)	11 (79%)	3 (21%)	1	0
All	All	281/317 (89%)	249 (89%)	32 (11%)	8	5

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	19	LEU
1	E	32	THR
1	E	34	SER
1	E	54	PHE
1	E	74	LEU
1	E	77	GLN
1	E	81	LYS
1	E	99	ASN
1	E	111	LYS
1	E	120	MET
1	E	142	HIS
1	E	162	LEU
1	E	163	ILE

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Mol	Chain	Res	Type
1	E	172	LEU
1	E	173	LEU
1	E	191	VAL
1	E	198	LEU
1	E	205	LEU
1	E	207	PRO
1	E	217	LYS
1	E	224	LEU
1	E	244	ILE
1	E	254	LYS
1	E	274	GLN
1	E	285	LYS
1	E	299	THR
1	E	309	LYS
1	E	342	LYS
1	E	349	GLU
2	S	375	ARG
2	S	379	HIS
2	S	380	ASP

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

Mol	Chain	Res	Type
1	E	36	ASN
1	E	62	HIS
1	E	67	ASN
1	E	99	ASN
1	E	113	ASN
1	E	131	HIS
1	E	142	HIS
1	E	158	HIS
1	E	177	GLN
1	E	283	ASN
1	E	294	HIS
2	S	379	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	TPO	E	197	1	10,10,11	4.57	2 (20%)	12,14,16	2.57	5 (41%)
1	SEP	E	338	1	9,9,10	6.73	3 (33%)	10,12,14	2.19	2 (20%)
2	SEP	S	377	2	9,9,10	6.17	2 (22%)	10,12,14	2.33	3 (30%)

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	-	0/9/11/13	0/0/0/0
1	SEP	E	338	1	-	0/6/8/10	0/0/0/0
2	SEP	S	377	2	-	0/6/8/10	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	338	SEP	O-C	19.77	1.25	1.11
2	S	377	SEP	O-C	18.17	1.23	1.11
1	E	197	TPO	O-C	14.04	1.21	1.11
1	E	338	SEP	CA-C	3.12	1.54	1.48
2	S	377	SEP	CA-C	2.38	1.52	1.48
1	E	338	SEP	P-O3P	-2.12	1.47	1.54
1	E	197	TPO	P-O3P	-2.05	1.47	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	377	SEP	C-CA-N	-6.31	107.53	113.83
1	E	197	TPO	O2P-P-O1P	6.08	130.31	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	338	SEP	O2P-P-O1P	-4.73	94.99	110.44
1	E	197	TPO	CB-CA-N	3.50	114.48	109.60
1	E	338	SEP	O3P-P-O1P	3.34	121.36	110.44
1	E	197	TPO	O3P-P-O1P	-3.22	99.90	110.44
1	E	197	TPO	OG1-CB-CA	3.15	112.82	107.55
2	S	377	SEP	O3P-P-O1P	2.21	117.68	110.44
2	S	377	SEP	O2P-P-O1P	-2.21	103.22	110.44
1	E	197	TPO	CG2-CB-CA	-2.15	108.78	113.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	OCT	E	381	-	7,7,7	0.56	0	6,6,6	0.15	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	OCT	E	381	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.