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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 09:07 AM EDT

PDB ID	:	6BYS
Title	:	Structures of the PKA RI alpha holoenzyme with the FLHCC driver J-PKAc alpha or native PRKAc alpha
Authors	:	Cao, B.; Lu, T.W.; Martinez Fiesco, J.A.; Tomasini, M.; Fan, L.; Simon, S.M.; Taylor, S.S.; Zhang, P.
Deposited on	:	2017-12-21
Resolution	:	4.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

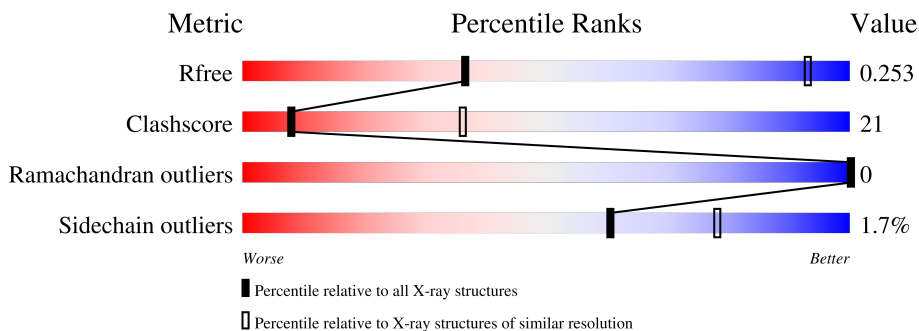|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 4.75 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		21
Ramachandran outliers		0
Sidechain outliers		1.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (5.70-3.80)
Clashscore	141614	1163 (5.70-3.80)
Ramachandran outliers	138981	1098 (5.70-3.80)
Sidechain outliers	138945	1078 (5.70-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	350	60% 35% • •
1	C	350	58% 36% • •
1	E	350	60% 34% • •
1	G	350	61% 33% • •
2	B	379	44% 31% • 24%
2	D	379	46% 28% • 24%
2	F	379	45% 30% • 24%

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Mol	Chain	Length	Quality of chain
2	H	379	

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
1	SEP	C	338	-	-	X	-
1	SEP	G	338	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20336 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 subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			
1	C	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			
1	E	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			
1	G	338	Total	C	N	O	P	S	0	0	0
			2798	1811	468	508	3	8			

- Molecule 2 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			
2	D	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			
2	F	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			
2	H	288	Total	C	N	O	S	0	0	0
			2286	1444	397	437	8			

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.

- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain A:

- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain C:

- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain E:

F100 P101 F102 L103 V104 K105 L106 E107 F108 K111 D112 M118 V119 Y122 V123 E127 M128 F129 F138 S139 H142 A143 R144 T153 F154 L157 D161 R165 K168 R169 E170 N171 I174 D175 Q176 Y179 V182 T183 D184 F185 G186 F187 R190 V191

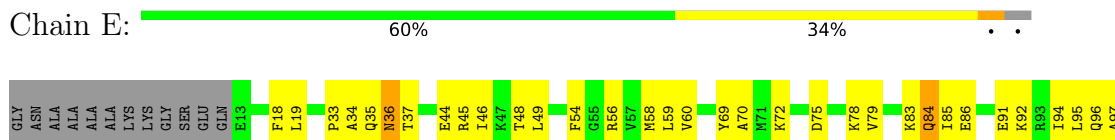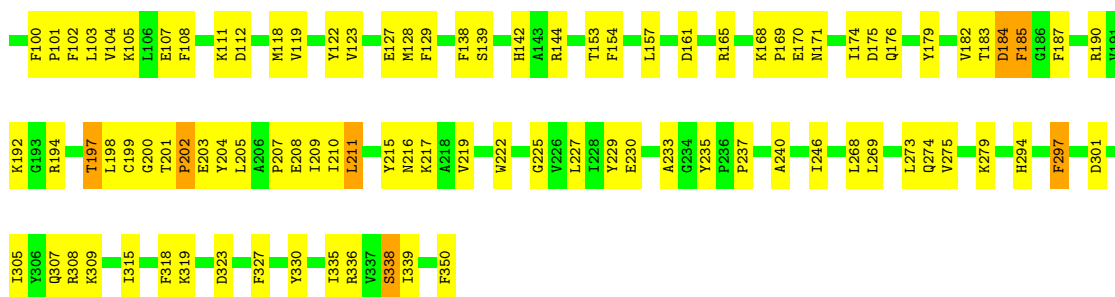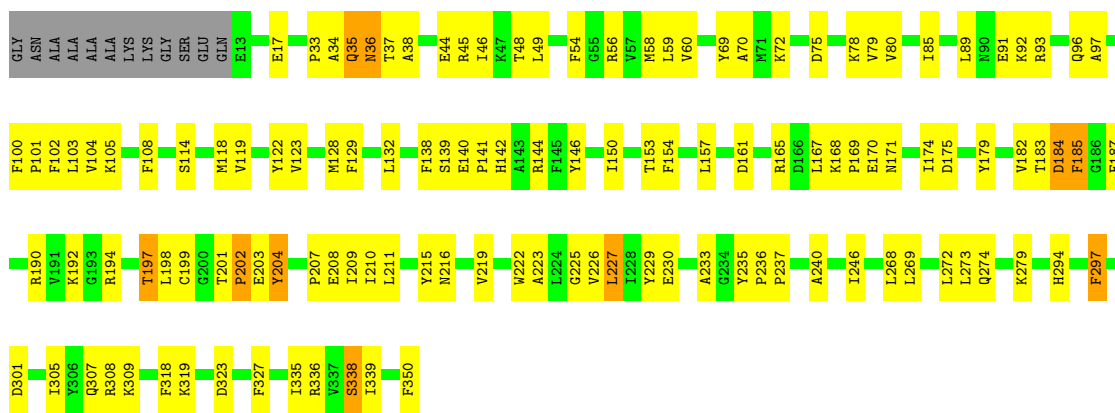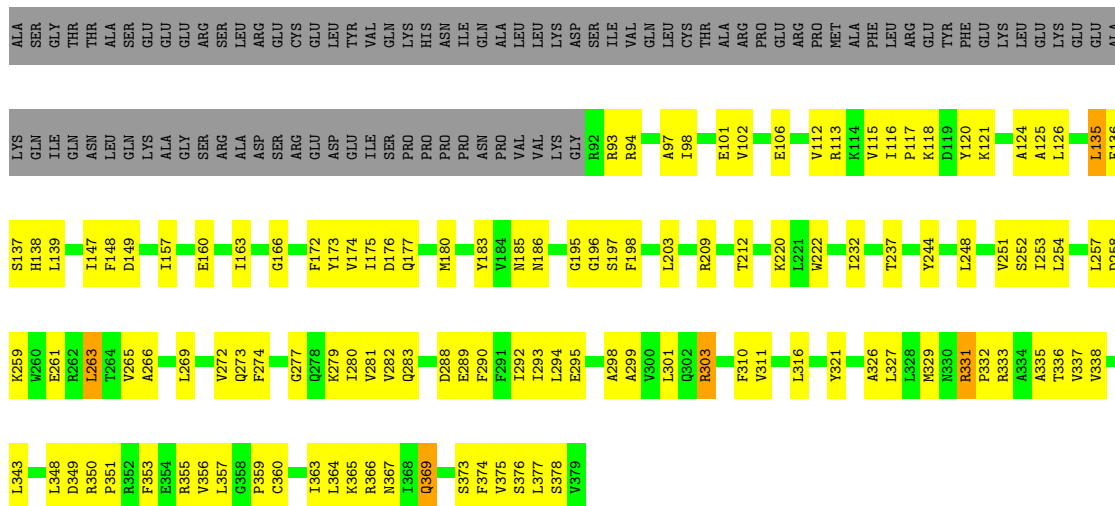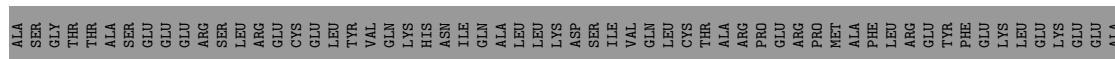K192 G193 R194 T197 L198 C199 G200 T201 P202 E203 Y204 L205 A206 P207 E208 I209 I210 L211 Y215 N216 K217 A218 V219 W222 G225 V226 L227 I228 Y229 E230 A233 G234 Y235 P236 P237 A240 I246 L268 L269 L273 Q274 V275 K279 H294 F297 D301

I305 Y306 Q307 R308 K309 I315 F318 K319 D323 F327 Y330 I335 R336 V337 S338 I339 F350

• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain G:

61% 33% • •

GLY ASN ALA ALA ALA LYS GLY SER GLU GLN E13 E17 P33 A34 Q35 N36 T37 A38 E44 R45 I46 K47 T48 L49 F54 G55 R56 V57 M58 L59 V60 Y69 A70 M71 K72 D75 K78 V79 V80 I85 L89 N90 E91 K92 R93 Q96 A97

F100 P101 F102 L103 V104 K105 F108 S114 M118 V119 Y122 V123 M128 F129 L132 F138 S139 E140 P141 H142 A143 R144 F145 Y146 I150 T153 F154 L157 D161 R165 D166 L167 K168 P169 E170 N171 I174 D175 Y179 V182 T183 D184 F185 G186 F187

R190 V191 K192 G193 R194 T197 L198 C199 G200 T201 P202 E203 Y204 P207 E208 I209 I210 L211 Y215 N216 V219 W222 A223 L224 G225 V226 L227 I228 Y229 E230 A233 G234 Y235 P236 P237 A240 I246 L268 L269 L272 L273 Q274 K279 H294 F297

D301 I305 Y306 Q307 R308 K309 F318 K319 D323 F327 I335 R336 V337 S338 I339 F350

• Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain B:

44% 31% • 24%

ALA SER GLY THR ALA SER GLU GLU ARG SER LEU ARG GLU CYS GLU LEU TYR VAL GLN LYS HIS ASN ILE GLN ALA LEU LEU LYS ASP SER ILE VAL GLN LEU CYS THR ALA ARG PRO GLU ARG PRO MET ALA PHE LEU ARG GLU TYR PHE GLU LYS LEU GLU LYS GLU GLU ALA

LYS GLN ILE GLN ASN LEU GLN LYS ALA GLY SER ARG ALA ASP SER ARG GLU ASP ILE SER PRO PRO PRO ASN PRO VAL VAL LYS GLY R92 R93 R94 A97 I98 E101 V102 E106 V112 R113 K114 V115 I116 P117 K118 D119 Y120 K121 A124 A125 L126 L135 F136

S137 H138 L139 I147 F148 D149 I157 E160 I163 G166 F172 Y173 V174 I175 D176 Q177 M180 Y183 V184 N185 N186 G195 S197 F198 L203 R209 T212 K220 L221 W222 I232 T237 Y244 L248 V251 S252 I253 L254 L257 D258

K259 W260 E261 R262 L263 T264 V265 A266 L269 V272 Q273 F274 G277 Q278 K279 I280 V281 V282 Q283 D288 E289 F290 F291 I292 I293 L294 E295 A298 A299 V300 L301 Q302 R303 F310 V311 L316 Y321 A326 L327 L328 M329 N330 R331 P332 R333 A334 A335 T336 V337 V338

L343 L348 D349 R350 P351 R352 F353 E354 R355 V356 L357 G358 P359 C360 I363 L364 K365 R366 N367 I368 Q369 S373 F374 V375 S376 L377 S378 V379

• Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain D:

46% 28% • 24%

ALA SER GLY THR ALA SER GLU GLU ARG SER LEU ARG GLU CYS GLU LEU TYR VAL GLN LYS HIS ASN ILE GLN ALA LEU LEU LYS ASP SER ILE VAL GLN LEU CYS THR ALA ARG PRO GLU ARG PRO MET ALA PHE LEU ARG GLU TYR PHE GLU LYS LEU GLU LYS GLU GLU ALA

LYS GLN ILE GLN ASN LEU GLN LYS ALA GLY SER ARG ALA ASP SER ARG GLU ASP ILE SER PRO PRO PRO ASN PRO VAL VAL LYS GLY R92 R93 R94 R95 G96 A97 I98 E101 V102 K114 K118 D119 Y120 K121 L126 N133 V134 L135 F136 S137 H138 N142

I147 F148 D149 E160 I163 G166 D167 F172 Y173 V174 I175 D176 Q177 M180 Y183 V184 N185 N186 S197 F198 G199 E200 L203 I204 P208 R209 A210 A211 T212 V213 K214 K220 L221 W222 I232 T237 Y244 L248 S252 I253 L254 L257 D258 K259

W260 E261 V265 A266 L269 V272 Q273 F274 G277 Q278 K279 I280 V281 V282 Q283 D288 E289 F290 F291 I292 I293 L294 E295 A298 A299 V300 L301 Q302 R303 F310 L316 A326 L327 L328 M329 N330 R331 P332 R333 A334 A335 T336 V337 V338 L343 L348 D349 R350

F353 V356 L357 G358 P359 C360 I363 L364 K365 R366 N367 I368 Q369 S373 F374 V375 S376 L377 S378 V379

• Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain F: 45% 30% • 24%

ALA SER GLY THR ALA SER GLU GLU GLU ARG SER LEU ARG GLU CYS GLU LEU TYR VAL GLN HIS ASN ILE ALA LEU LEU LYS ASP SER ILE VAL GLN LEU CYS THR ALA ARG PRO GLU ARG PRO MET ALA PHE LEU ARG GLU TYR PHE GLU LYS LEU GLU LYS GLU GLU ALA

LYS GLN ILE GLN ASN LEU GLN LYS ALA GLY SER ARG ALA ASP SER ARG GLU ASP ILE SER PRO PRO PRO ASN PRO VAL VAL LYS GLY R92 R93 R94 R95 G96 A97 I98 S99 A100 E101 V102 V112 R113 K114 V115 I116 P117 K118 K121 L126 L135 F136 S137 H138 L139

D140 D141 N142 E143 R144 S145 D146 I147 F148 D149 V154 S155 F156 E160 I163 G166 F172 Y173 V174 I175 D176 Q177 M180 Y183 G196 S197 F198 L203 R209 T212 V213 K214 K220 L221 W222 I232 R239 Y244 L248 S252 I253 L254

L257 D258 K259 W260 E261 R262 L263 T264 V265 A266 L269 V272 Q273 F274 G277 Q278 K279 I280 V281 V282 Q283 G284 E285 D288 E289 F290 F291 I292 I293 L294 E295 A298 A299 V300 L301 Q302 R303 F310 L316 A326 L327 L328 M329 N330 R331 P332 R333 A334 A335 T336 V337 V338

L343 K344 C345 L348 D349 R350 P351 R352 F353 E354 R355 V356 L357 G358 P359 C360 I363 L364 K365 R366 Q369 S373 F374 V375 S376 L377 S378 V379

• Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain H: 49% 26% • 24%

ALA SER GLY THR ALA SER GLU GLU GLU ARG SER LEU ARG GLU CYS GLU LEU TYR VAL GLN HIS ASN ILE ALA LEU LEU LYS ASP SER ILE VAL GLN LEU CYS THR ALA ARG PRO GLU ARG PRO MET ALA PHE LEU ARG GLU TYR PHE GLU LYS LEU GLU LYS GLU GLU ALA

LYS GLN ILE GLN ASN LEU GLN LYS ALA GLY SER ARG ALA ASP SER ARG GLU ASP ILE SER PRO PRO PRO ASN PRO VAL VAL LYS GLY R92 R93 R94 R95 I98 E101 V102 K118 D119 Y120 K121 T122 M123 A124 A125 L126 A127 K128 L135 F136 S137 H138 L139 I147

F148 D149 I163 G166 F172 Y173 V174 I175 D176 Q177 M180 Y183 G195 G196 S197 F198 L203 R209 T212 K220 L221 W222 I232 Y244 L248 V251 S252 I253 L254 L257 D258 K259 W260 E261 R262 L263 T264 V265 A266 L269 V272 Q273 F274

G277 Q278 K279 I280 V281 V282 Q283 D288 E289 F290 F291 I292 I293 L294 E295 A298 A299 V300 L301 Q302 R303 F310 L316 Y321 A326 L327 L328 M329 N330 R331 P332 R333 A334 A335 T336 V337 V338 L343 L348 D349 R350 F353 V356 L357 G358 P359 C360 I363

L364 K365 R366 Q369 F374 V375 S378 V379

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.50Å 186.16Å 186.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.16 – 4.75 48.54 – 4.75	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.16-4.75) 88.4 (48.54-4.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 4.86Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.212 , 0.255 0.214 , 0.253	Depositor DCC
R_{free} test set	1995 reflections (8.18%)	wwPDB-VP
Wilson B-factor (Å^2)	187.0	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 213.7	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,l,k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20336	wwPDB-VP
Average B, all atoms (Å^2)	269.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 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	A	0.57	0/2837	0.86	7/3819 (0.2%)
1	C	0.56	1/2837 (0.0%)	0.85	10/3819 (0.3%)
1	E	0.56	0/2837	0.85	10/3819 (0.3%)
1	G	0.53	0/2837	0.83	7/3819 (0.2%)
2	B	0.58	0/2326	0.77	2/3136 (0.1%)
2	D	0.57	0/2326	0.78	0/3136
2	F	0.57	0/2326	0.78	0/3136
2	H	0.61	2/2326 (0.1%)	0.91	6/3136 (0.2%)
All	All	0.57	3/20652 (0.0%)	0.83	42/27820 (0.2%)

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	C	0	1
2	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	84	GLN	CD-OE1	-7.89	1.06	1.24
2	H	120	TYR	CG-CD1	-7.40	1.29	1.39
2	H	120	TYR	CE1-CZ	-6.15	1.30	1.38

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	120	TYR	CB-CG-CD2	-20.04	108.97	121.00
2	H	120	TYR	CD1-CG-CD2	-12.38	104.28	117.90
1	A	35	GLN	CB-CA-C	-11.08	88.25	110.40
1	C	35	GLN	CB-CA-C	-10.55	89.31	110.40
2	H	120	TYR	CB-CG-CD1	10.43	127.26	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	84	GLN	Sidechain
2	H	120	TYR	Sidechain

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	A	2798	0	2773	104	0
1	C	2798	0	2774	127	0
1	E	2798	0	2774	112	0
1	G	2798	0	2774	120	0
2	B	2286	0	2274	134	0
2	D	2286	0	2274	119	0
2	F	2286	0	2274	131	0
2	H	2286	0	2274	106	0
All	All	20336	0	20191	867	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 21.

The worst 5 of 867 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:G:204:TYR:OH	1:G:227:LEU:CB	1.90	1.20
2:B:195:GLY:HA3	2:H:120:TYR:CE2	1.79	1.18
1:G:204:TYR:OH	1:G:227:LEU:HB2	0.99	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:GLU:OE1	2:D:94:ARG:NH2	1.80	1.13
2:B:195:GLY:HA3	2:H:120:TYR:HE2	1.00	1.08

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	A	333/350 (95%)	280 (84%)	53 (16%)	0	100	100
1	C	333/350 (95%)	277 (83%)	56 (17%)	0	100	100
1	E	333/350 (95%)	277 (83%)	56 (17%)	0	100	100
1	G	333/350 (95%)	275 (83%)	58 (17%)	0	100	100
2	B	286/379 (76%)	246 (86%)	40 (14%)	0	100	100
2	D	286/379 (76%)	247 (86%)	39 (14%)	0	100	100
2	F	286/379 (76%)	247 (86%)	39 (14%)	0	100	100
2	H	286/379 (76%)	245 (86%)	41 (14%)	0	100	100
All	All	2476/2916 (85%)	2094 (85%)	382 (15%)	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	A	296/302 (98%)	292 (99%)	4 (1%)	67	81
1	C	296/302 (98%)	293 (99%)	3 (1%)	76	86
1	E	296/302 (98%)	291 (98%)	5 (2%)	60	78
1	G	296/302 (98%)	291 (98%)	5 (2%)	60	78
2	B	244/324 (75%)	240 (98%)	4 (2%)	62	79
2	D	244/324 (75%)	239 (98%)	5 (2%)	55	73
2	F	244/324 (75%)	239 (98%)	5 (2%)	55	73
2	H	244/324 (75%)	238 (98%)	6 (2%)	47	68
All	All	2160/2504 (86%)	2123 (98%)	37 (2%)	60	78

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	185	PHE
2	H	331	ARG
1	G	204	TYR
2	H	120	TYR
2	D	137	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	138	HIS
1	E	84	GLN
1	E	87	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	G	338	1	8,9,10	1.54	1 (12%)	8,12,14	1.87	2 (25%)
1	TPO	A	197	1	8,10,11	1.58	2 (25%)	10,14,16	2.33	2 (20%)
1	SEP	A	139	1	8,9,10	1.65	1 (12%)	8,12,14	1.82	1 (12%)
1	SEP	C	139	1	8,9,10	1.67	1 (12%)	8,12,14	1.84	1 (12%)
1	TPO	E	197	1	8,10,11	1.65	2 (25%)	10,14,16	2.46	2 (20%)
1	TPO	G	197	1	8,10,11	1.62	1 (12%)	10,14,16	2.35	2 (20%)
1	SEP	E	338	1	8,9,10	1.53	1 (12%)	8,12,14	1.79	2 (25%)
1	SEP	C	338	1	8,9,10	1.49	1 (12%)	8,12,14	1.79	3 (37%)
1	SEP	E	139	1	8,9,10	1.74	1 (12%)	8,12,14	2.23	1 (12%)
1	SEP	G	139	1	8,9,10	1.61	1 (12%)	8,12,14	1.94	2 (25%)
1	SEP	A	338	1	8,9,10	1.93	1 (12%)	8,12,14	1.69	2 (25%)
1	TPO	C	197	1	8,10,11	1.69	1 (12%)	10,14,16	2.35	2 (20%)

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	G	338	1	-	4/5/8/10	-
1	TPO	A	197	1	-	1/9/11/13	-
1	SEP	A	139	1	-	2/5/8/10	-
1	SEP	C	139	1	-	1/5/8/10	-
1	TPO	E	197	1	-	1/9/11/13	-
1	TPO	G	197	1	-	1/9/11/13	-
1	SEP	E	338	1	-	4/5/8/10	-
1	SEP	C	338	1	-	5/5/8/10	-
1	SEP	E	139	1	-	1/5/8/10	-
1	SEP	G	139	1	-	3/5/8/10	-
1	SEP	A	338	1	-	4/5/8/10	-
1	TPO	C	197	1	-	1/9/11/13	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	P-O1P	4.77	1.65	1.50
1	E	139	SEP	P-O1P	3.64	1.62	1.50
1	C	139	SEP	P-O1P	3.62	1.62	1.50
1	G	338	SEP	P-O1P	3.57	1.62	1.50
1	C	197	TPO	P-O1P	3.48	1.61	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	197	TPO	P-OG1-CB	-6.92	102.30	123.21
1	G	197	TPO	P-OG1-CB	-6.60	103.28	123.21
1	C	197	TPO	P-OG1-CB	-6.43	103.78	123.21
1	A	197	TPO	P-OG1-CB	-6.41	103.84	123.21
1	E	139	SEP	OG-CB-CA	5.64	113.63	108.14

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	139	SEP	N-CA-CB-OG
1	A	338	SEP	CB-OG-P-O2P
1	A	338	SEP	CB-OG-P-O3P
1	C	139	SEP	N-CA-CB-OG
1	C	338	SEP	CB-OG-P-O2P

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	338	SEP	4	0
1	A	197	TPO	1	0
1	E	197	TPO	1	0
1	G	197	TPO	2	0
1	E	338	SEP	3	0
1	C	338	SEP	4	0
1	A	338	SEP	2	0
1	C	197	TPO	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.