Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2024 – 04:48 pm BST

PDB ID	:	9EOY
Title	:	Structure of Thr354Asn, Glu355Gln, Thr412Asn, Ile414Met, Ile464His, and Phe467Met mutant human CaMKII alpha hub bound to PIPA
Authors	:	Narayanan, D.; Larsen, A.S.G.; Solbak, S.M.O.; Wellendorph, P.; Gee, C.L.; Kastrup, J.S.
Deposited on	:	2024-03-15
Resolution	:	2.10 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:

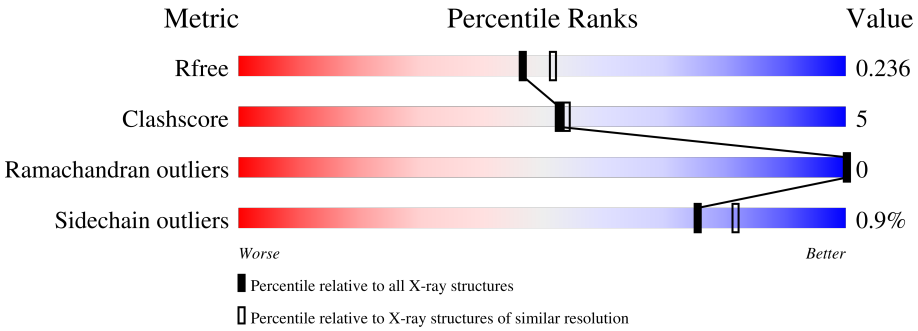
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)

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	135	87% 11% •
1	B	135	84% 13% ••
1	C	135	79% 17% ••
1	D	135	77% 20% ••
1	E	135	84% 13% ••
1	F	135	88% 10% •

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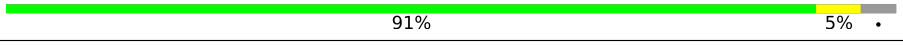
Mol	Chain	Length	Quality of chain
1	G	135	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7710 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	1	0
			1077	675	196	198	8			
1	B	133	Total	C	N	O	S	0	2	0
			1096	687	205	196	8			
1	C	132	Total	C	N	O	S	0	0	0
			1071	671	196	196	8			
1	D	132	Total	C	N	O	S	0	0	0
			1071	671	196	196	8			
1	E	133	Total	C	N	O	S	0	1	0
			1083	679	199	196	9			
1	F	132	Total	C	N	O	S	0	0	0
			1071	671	196	196	8			
1	G	130	Total	C	N	O	S	0	1	0
			1062	667	194	192	9			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	GLY	-	expression tag	UNP Q9UQM7
A	342	PRO	-	expression tag	UNP Q9UQM7
A	343	HIS	-	expression tag	UNP Q9UQM7
A	344	MET	-	expression tag	UNP Q9UQM7
A	354	ASN	THR	engineered mutation	UNP Q9UQM7
A	355	GLN	GLU	engineered mutation	UNP Q9UQM7
A	412	ASN	THR	engineered mutation	UNP Q9UQM7
A	414	MET	ILE	engineered mutation	UNP Q9UQM7
A	464	HIS	ILE	engineered mutation	UNP Q9UQM7
A	467	MET	PHE	engineered mutation	UNP Q9UQM7
B	341	GLY	-	expression tag	UNP Q9UQM7
B	342	PRO	-	expression tag	UNP Q9UQM7
B	343	HIS	-	expression tag	UNP Q9UQM7
B	344	MET	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	354	ASN	THR	engineered mutation	UNP Q9UQM7
B	355	GLN	GLU	engineered mutation	UNP Q9UQM7
B	412	ASN	THR	engineered mutation	UNP Q9UQM7
B	414	MET	ILE	engineered mutation	UNP Q9UQM7
B	464	HIS	ILE	engineered mutation	UNP Q9UQM7
B	467	MET	PHE	engineered mutation	UNP Q9UQM7
C	341	GLY	-	expression tag	UNP Q9UQM7
C	342	PRO	-	expression tag	UNP Q9UQM7
C	343	HIS	-	expression tag	UNP Q9UQM7
C	344	MET	-	expression tag	UNP Q9UQM7
C	354	ASN	THR	engineered mutation	UNP Q9UQM7
C	355	GLN	GLU	engineered mutation	UNP Q9UQM7
C	412	ASN	THR	engineered mutation	UNP Q9UQM7
C	414	MET	ILE	engineered mutation	UNP Q9UQM7
C	464	HIS	ILE	engineered mutation	UNP Q9UQM7
C	467	MET	PHE	engineered mutation	UNP Q9UQM7
D	341	GLY	-	expression tag	UNP Q9UQM7
D	342	PRO	-	expression tag	UNP Q9UQM7
D	343	HIS	-	expression tag	UNP Q9UQM7
D	344	MET	-	expression tag	UNP Q9UQM7
D	354	ASN	THR	engineered mutation	UNP Q9UQM7
D	355	GLN	GLU	engineered mutation	UNP Q9UQM7
D	412	ASN	THR	engineered mutation	UNP Q9UQM7
D	414	MET	ILE	engineered mutation	UNP Q9UQM7
D	464	HIS	ILE	engineered mutation	UNP Q9UQM7
D	467	MET	PHE	engineered mutation	UNP Q9UQM7
E	341	GLY	-	expression tag	UNP Q9UQM7
E	342	PRO	-	expression tag	UNP Q9UQM7
E	343	HIS	-	expression tag	UNP Q9UQM7
E	344	MET	-	expression tag	UNP Q9UQM7
E	354	ASN	THR	engineered mutation	UNP Q9UQM7
E	355	GLN	GLU	engineered mutation	UNP Q9UQM7
E	412	ASN	THR	engineered mutation	UNP Q9UQM7
E	414	MET	ILE	engineered mutation	UNP Q9UQM7
E	464	HIS	ILE	engineered mutation	UNP Q9UQM7
E	467	MET	PHE	engineered mutation	UNP Q9UQM7
F	341	GLY	-	expression tag	UNP Q9UQM7
F	342	PRO	-	expression tag	UNP Q9UQM7
F	343	HIS	-	expression tag	UNP Q9UQM7
F	344	MET	-	expression tag	UNP Q9UQM7
F	354	ASN	THR	engineered mutation	UNP Q9UQM7
F	355	GLN	GLU	engineered mutation	UNP Q9UQM7

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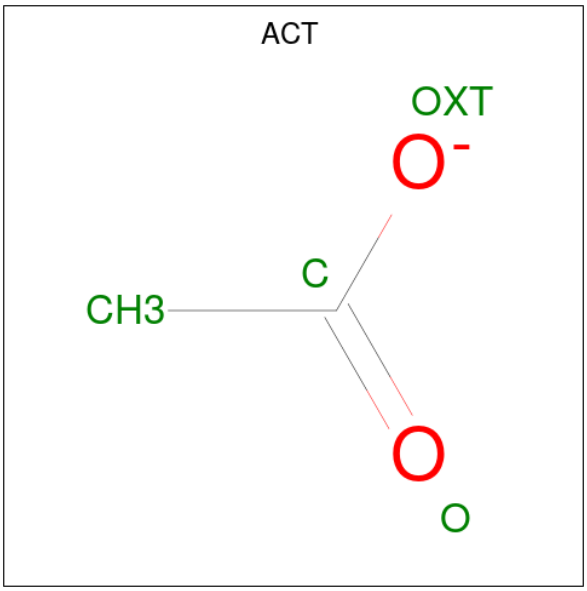
Chain	Residue	Modelled	Actual	Comment	Reference
F	412	ASN	THR	engineered mutation	UNP Q9UQM7
F	414	MET	ILE	engineered mutation	UNP Q9UQM7
F	464	HIS	ILE	engineered mutation	UNP Q9UQM7
F	467	MET	PHE	engineered mutation	UNP Q9UQM7
G	341	GLY	-	expression tag	UNP Q9UQM7
G	342	PRO	-	expression tag	UNP Q9UQM7
G	343	HIS	-	expression tag	UNP Q9UQM7
G	344	MET	-	expression tag	UNP Q9UQM7
G	354	ASN	THR	engineered mutation	UNP Q9UQM7
G	355	GLN	GLU	engineered mutation	UNP Q9UQM7
G	412	ASN	THR	engineered mutation	UNP Q9UQM7
G	414	MET	ILE	engineered mutation	UNP Q9UQM7
G	464	HIS	ILE	engineered mutation	UNP Q9UQM7
G	467	MET	PHE	engineered mutation	UNP Q9UQM7

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0

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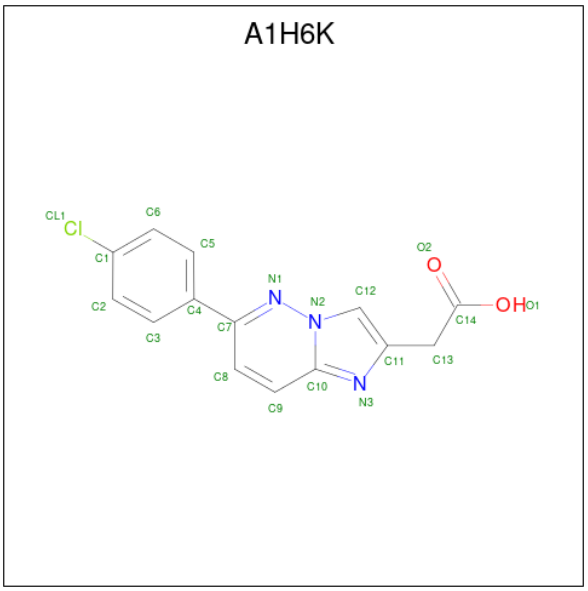
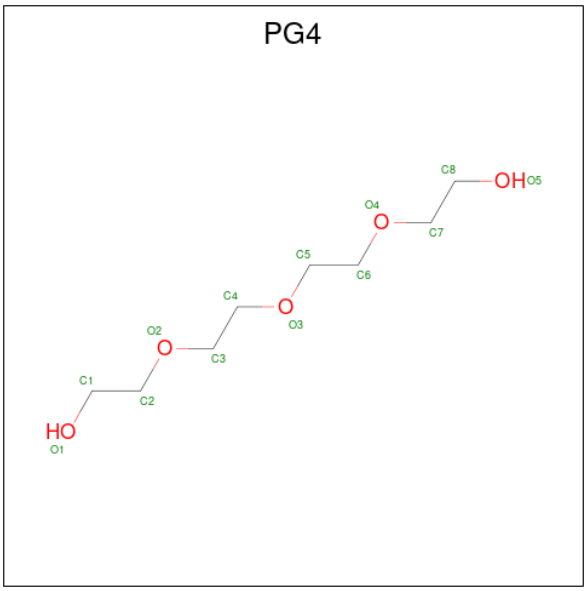
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0

- Molecule 3 is 2-[6-(4-chlorophenyl)imidazo[1,2-b]pyridazin-2-yl]ethanoic acid (three-letter code: A1H6K) (formula: $C_{14}H_{10}ClN_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C Cl N O 20 14 1 3 2	0	0
3	D	1	Total C Cl N O 20 14 1 3 2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 13 8 5	0	0

- Molecule 5 is water.

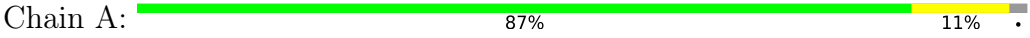
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total O 14 14	0	0
5	B	13	Total O 13 13	0	0
5	C	8	Total O 8 8	0	0
5	D	11	Total O 11 11	0	0
5	E	17	Total O 17 17	0	0
5	F	17	Total O 17 17	0	0
5	G	22	Total O 22 22	0	0

3 Residue-property plots (i)

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: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain A:



• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

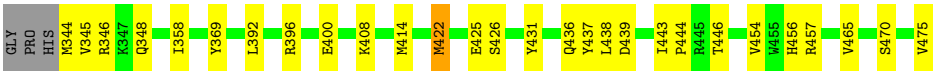
Chain B:

• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain C:

• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain D:

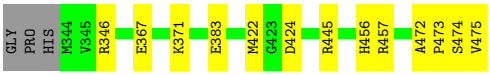


• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain E:

• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain F:



• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	103.05Å 182.92Å 107.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.48 – 2.10 46.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.48-2.10) 100.0 (46.48-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.224 , 0.251 0.223 , 0.236	Depositor DCC
R_{free} test set	3049 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.016 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7710	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: A1H6K, PG4, ACT

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	0.25	0/1108	0.52	0/1497
1	B	0.27	0/1132	0.56	0/1528
1	C	0.26	0/1099	0.57	0/1484
1	D	0.25	0/1099	0.50	0/1484
1	E	0.24	0/1116	0.50	0/1508
1	F	0.25	0/1099	0.51	0/1484
1	G	0.25	0/1093	0.52	0/1476
All	All	0.25	0/7746	0.53	0/10461

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	A	0	1
1	B	0	1
1	C	0	2
1	F	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	445	ARG	Sidechain
1	B	445	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	433	ARG	Sidechain
1	C	445	ARG	Sidechain
1	F	445	ARG	Sidechain

5.2 Too-close contacts (i)

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	1077	0	1033	11	0
1	B	1096	0	1059	13	0
1	C	1071	0	1027	18	0
1	D	1071	0	1027	19	0
1	E	1083	0	1038	12	0
1	F	1071	0	1027	7	0
1	G	1062	0	1022	4	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	E	4	0	3	1	0
2	F	4	0	3	0	0
2	G	4	0	3	0	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
4	C	13	0	18	2	0
5	A	14	0	0	0	0
5	B	13	0	0	0	0
5	C	8	0	0	0	0
5	D	11	0	0	0	0
5	E	17	0	0	0	0
5	F	17	0	0	0	0
5	G	22	0	0	0	0
All	All	7710	0	7269	73	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 5.

All (73) 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:A:405:ARG:HH11	1:A:405:ARG:HG3	1.53	0.73
1:F:346:ARG:HH22	1:F:457:ARG:HH22	1.36	0.71
1:E:342:PRO:HG2	1:E:346:ARG:HH11	1.57	0.69
1:B:402:LEU:HD11	1:D:444:PRO:HD2	1.76	0.68
1:E:422:MET:HG2	1:F:456:HIS:HB2	1.76	0.68
1:C:391:GLY:O	1:C:395:HIS:ND1	2.27	0.67
1:B:391:GLY:O	1:B:395:HIS:ND1	2.28	0.66
1:A:456:HIS:HB2	1:B:422:MET:HG2	1.76	0.66
1:B:397:PHE:HE2	1:D:444:PRO:HB3	1.63	0.62
1:C:456:HIS:HB2	1:D:422:MET:HG2	1.80	0.62
1:A:403:TRP:HZ2	1:A:475:VAL:HG13	1.66	0.61
1:A:422:MET:HG2	1:B:456:HIS:HB2	1.82	0.60
1:A:344:MET:HB2	1:A:347:LYS:HG3	1.85	0.58
1:A:382:PRO:HB2	1:A:473:PRO:HA	1.86	0.57
1:A:408:LYS:HD3	1:A:438:LEU:HB2	1.84	0.57
1:D:436:GLN:HG2	1:D:446:THR:HG22	1.87	0.57
1:B:351:ILE:HG13	1:B:419:ILE:HD11	1.86	0.57
1:F:383:GLU:OE2	1:F:474:SER:HB3	2.05	0.57
1:D:408:LYS:HE3	1:D:438:LEU:H	1.71	0.56
1:C:346:ARG:NH2	1:C:423:GLY:O	2.38	0.55
1:D:369:TYR:HE1	1:D:392:LEU:HD12	1.71	0.55
1:C:364:GLY:HA3	4:C:503:PG4:H72	1.88	0.54
1:E:351:ILE:HG13	1:E:419:ILE:HD11	1.87	0.54
1:D:396:ARG:NE	1:D:400:GLU:OE1	2.41	0.54
1:C:422:MET:HG2	1:D:456:HIS:HB2	1.90	0.53
1:A:383:GLU:OE2	1:A:475:VAL:HG12	2.08	0.53
1:C:351:ILE:HG13	1:C:419:ILE:HD11	1.89	0.53
1:F:424:ASP:O	1:F:457:ARG:NH2	2.42	0.52
1:C:377:MET:HG3	1:C:391:GLY:HA3	1.92	0.52
1:B:444:PRO:C	1:B:445:ARG:HD2	2.31	0.51
1:A:362:SER:OG	1:A:412:ASN:ND2	2.43	0.51
1:E:443:ILE:HD11	1:E:445:ARG:HH21	1.76	0.50
1:D:344:MET:HG2	1:D:346:ARG:HB3	1.94	0.50
1:G:346:ARG:HH11	1:G:462:TRP:HZ2	1.60	0.49
1:C:443:ILE:HD11	1:C:445:ARG:NH2	2.27	0.48
1:E:420:HIS:HB2	1:E:428[B]:CYS:SG	2.54	0.48
1:E:350:ILE:HA	1:E:353:VAL:HG12	1.96	0.47
1:E:346:ARG:NH2	1:E:424:ASP:OD1	2.49	0.46
1:G:414[A]:MET:HG2	1:G:417:PRO:HG3	1.98	0.46
1:B:375:PRO:HA	1:B:392:LEU:HD12	1.98	0.46
1:D:439:ASP:OD1	1:D:443:ILE:HG12	2.16	0.46
1:D:437:TYR:CD2	1:D:475:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:TYR:O	1:D:444:PRO:HA	2.17	0.45
1:B:373:CYS:HB2	1:B:392:LEU:HD21	1.99	0.45
1:F:475:VAL:HG13	1:G:444:PRO:HG2	1.98	0.45
1:D:425:GLU:HA	1:D:457:ARG:HB2	1.99	0.44
1:E:378:THR:OG1	1:E:466:HIS:ND1	2.45	0.44
1:C:422:MET:HB3	1:D:426:SER:OG	2.18	0.43
1:C:470:SER:HB3	1:D:470:SER:HB3	1.99	0.43
1:D:454:VAL:O	1:D:465:VAL:HG12	2.18	0.43
1:E:443:ILE:CD1	1:E:445:ARG:HH21	2.31	0.43
1:B:349:GLU:HA	1:B:352:LYS:NZ	2.34	0.42
1:G:346:ARG:HH12	1:G:424:ASP:C	2.22	0.42
1:E:369:TYR:OH	2:E:501:ACT:OXT	2.34	0.42
1:C:443:ILE:HA	1:C:444:PRO:HD3	1.86	0.42
1:D:345:VAL:HA	1:D:348:GLN:HB2	2.01	0.42
1:E:401:ASN:HA	1:E:405:ARG:HH22	1.84	0.42
1:A:382:PRO:CB	1:A:473:PRO:HA	2.50	0.42
1:C:353:VAL:O	1:C:372:MET:HE1	2.19	0.42
1:D:414:MET:HG3	1:D:431:TYR:CD2	2.55	0.42
1:F:472:ALA:HA	1:F:473:PRO:HD3	1.88	0.42
1:C:350:ILE:HA	1:C:353:VAL:HG12	2.01	0.41
1:E:375:PRO:HA	1:E:392:LEU:HD12	2.02	0.41
1:D:358:ILE:HD11	1:D:431:TYR:OH	2.21	0.41
1:C:402:LEU:HB2	4:C:503:PG4:H51	2.02	0.41
1:F:367:GLU:O	1:F:371:LYS:HG3	2.21	0.41
1:A:422:MET:HG2	1:B:456:HIS:CB	2.50	0.41
1:C:451:GLU:OE2	1:C:469:ARG:HD3	2.21	0.41
1:C:464:HIS:CE1	1:C:467:MET:HB3	2.56	0.41
1:B:344:MET:O	1:B:348:GLN:HG2	2.20	0.41
1:C:415:LEU:HD23	1:C:415:LEU:HA	1.89	0.41
1:C:422:MET:HB2	1:C:426:SER:OG	2.21	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	A	131/135 (97%)	128 (98%)	3 (2%)	0	100	100
1	B	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	C	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
1	D	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
1	E	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
1	F	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
1	G	129/135 (96%)	126 (98%)	3 (2%)	0	100	100
All	All	915/945 (97%)	892 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	116/117 (99%)	116 (100%)	0	100	100
1	B	118/117 (101%)	116 (98%)	2 (2%)	56	63
1	C	115/117 (98%)	114 (99%)	1 (1%)	75	82
1	D	115/117 (98%)	114 (99%)	1 (1%)	75	82
1	E	117/117 (100%)	116 (99%)	1 (1%)	75	82
1	F	115/117 (98%)	114 (99%)	1 (1%)	75	82
1	G	114/117 (97%)	113 (99%)	1 (1%)	75	82
All	All	810/819 (99%)	803 (99%)	7 (1%)	75	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	422	MET
1	B	443	ILE

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Mol	Chain	Res	Type
1	C	422	MET
1	D	422	MET
1	E	422	MET
1	F	422	MET
1	G	422	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	395	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)

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)

9 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	$\#\|Z\| > 2$
3	A1H6K	D	501	-	18,22,22	1.43	4 (22%)	20,31,31	1.72	4 (20%)
2	ACT	C	501	-	3,3,3	1.27	0	3,3,3	1.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ACT	A	501	-	3,3,3	1.28	0	3,3,3	1.38	0
4	PG4	C	503	-	12,12,12	0.14	0	11,11,11	0.14	0
2	ACT	G	501	-	3,3,3	1.28	0	3,3,3	1.54	0
2	ACT	E	501	-	3,3,3	1.27	0	3,3,3	1.39	0
2	ACT	F	501	-	3,3,3	1.28	0	3,3,3	1.53	0
3	A1H6K	C	502	-	18,22,22	1.50	3 (16%)	20,31,31	0.74	0
2	ACT	B	501	-	3,3,3	1.25	0	3,3,3	1.38	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
4	PG4	C	503	-	-	5/10/10/10	-
3	A1H6K	D	501	-	-	1/6/8/8	0/3/3/3
3	A1H6K	C	502	-	-	0/6/8/8	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	A1H6K	C10-N3	3.54	1.36	1.33
3	C	502	A1H6K	C10-N3	3.50	1.36	1.33
3	C	502	A1H6K	C7-N1	2.94	1.36	1.33
3	C	502	A1H6K	C12-C11	2.55	1.40	1.36
3	D	501	A1H6K	C12-C11	2.34	1.39	1.36
3	D	501	A1H6K	C7-N1	2.33	1.36	1.33
3	D	501	A1H6K	C9-C8	2.14	1.41	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	A1H6K	C4-C7-N1	-5.08	110.46	115.67
3	D	501	A1H6K	C5-C4-C7	-3.33	116.03	121.28
3	D	501	A1H6K	C8-C7-C4	2.46	126.72	121.93
3	D	501	A1H6K	C3-C4-C7	2.35	125.00	121.28

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503	PG4	C6-C5-O3-C4
4	C	503	PG4	C1-C2-O2-C3
4	C	503	PG4	O3-C5-C6-O4
4	C	503	PG4	C5-C6-O4-C7
4	C	503	PG4	C4-C3-O2-C2
3	D	501	A1H6K	C11-C13-C14-O2

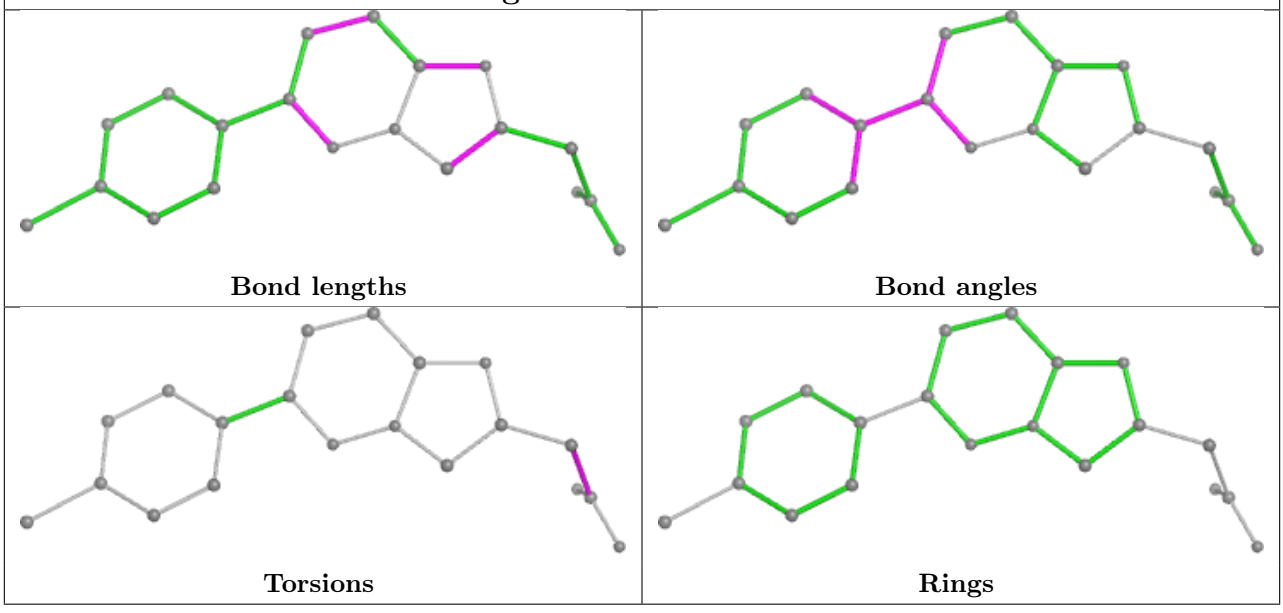
There are no ring outliers.

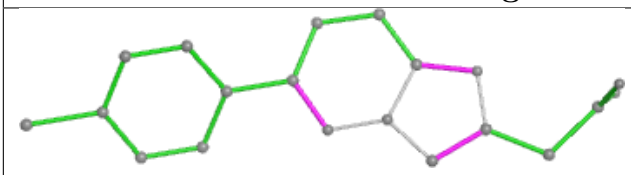
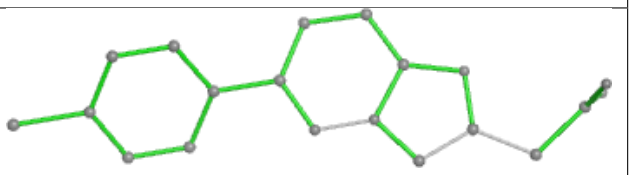
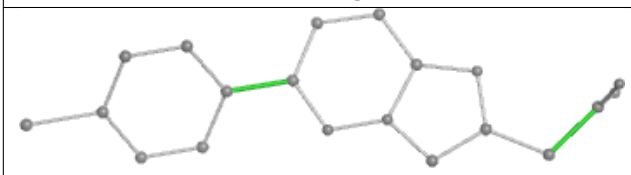
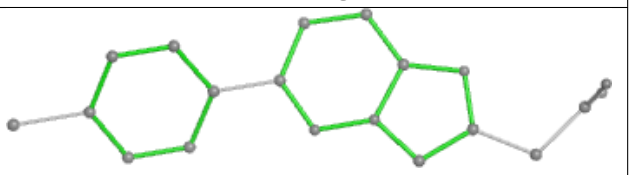
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	PG4	2	0
2	E	501	ACT	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 then 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.

Ligand A1H6K D 501



Ligand A1H6K C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

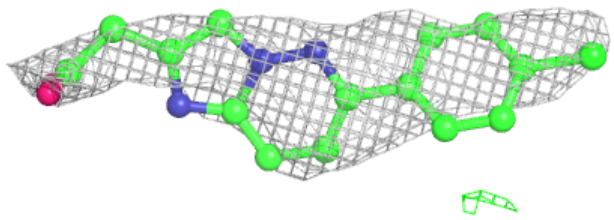
6.4 Ligands

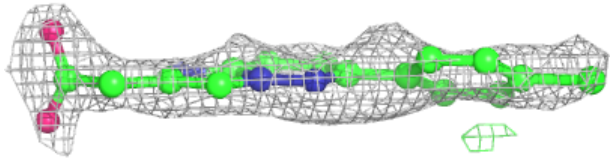
Unable to reproduce the depositors R factor - this section is therefore empty.

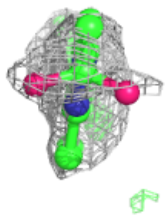
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1H6K C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

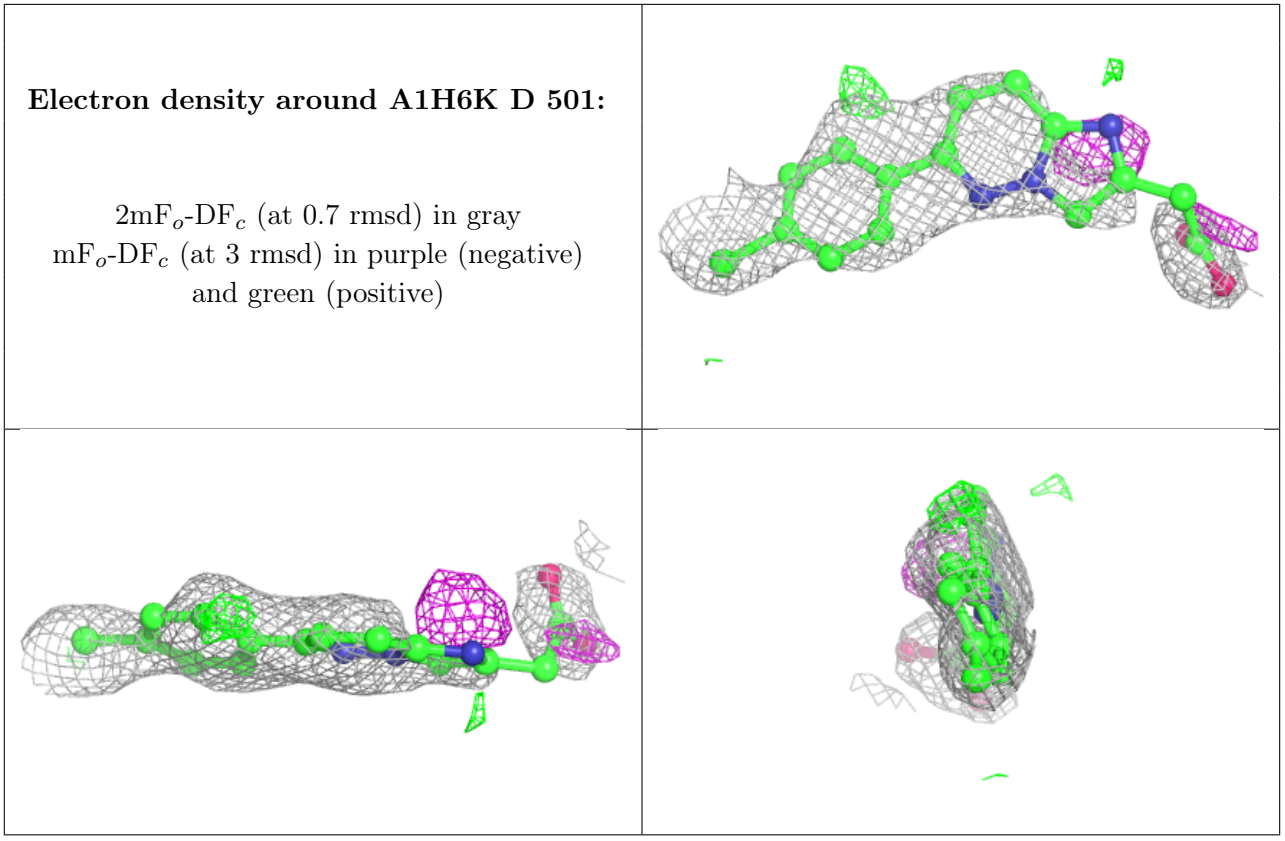






Electron density around A1H6K D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

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