



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:22 AM UTC

PDB ID : 9EPX / pdb_00009epx
Title : Crystal structure of human Casein Kinase II subunit alpha (CK2a1) in complex with allosteric ligand FGC3331
Authors : Kraemer, A.; Greco, F.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2024-03-20
Resolution : 2.60 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

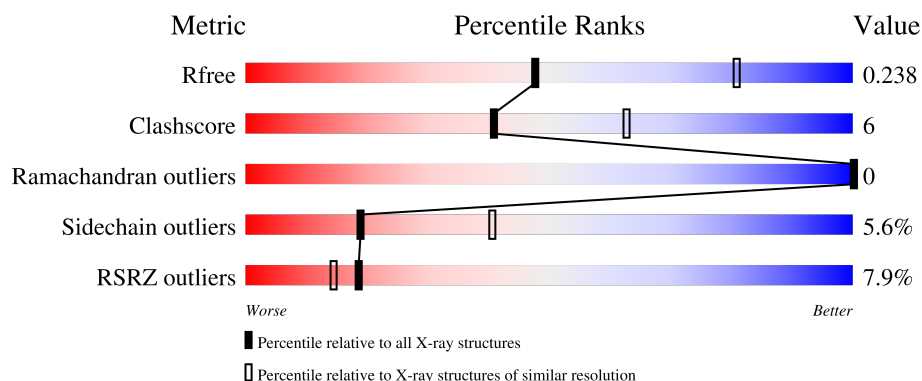
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	7% 84% 12% ..
1	B	338	9% 77% 19% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5643 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.

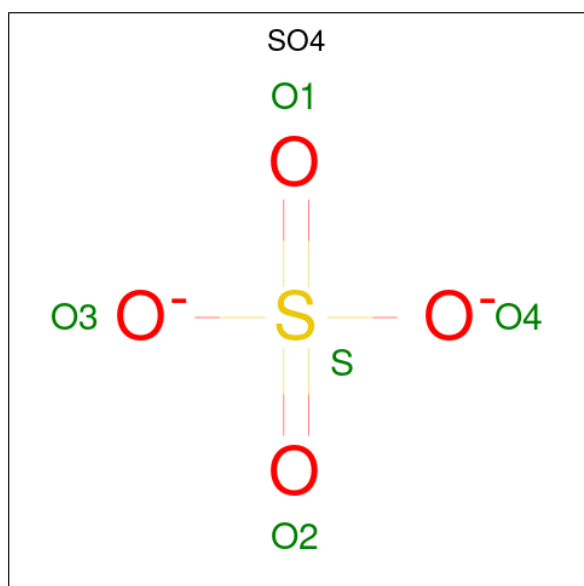
- Molecule 1 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2697	1737	469	480	11			
1	B	329	Total	C	N	O	S	0	0	0
			2721	1744	475	491	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P68400
B	0	SER	-	expression tag	UNP P68400

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O S	0	0
			5	4 1		

Continued on next page...

Continued from previous page...

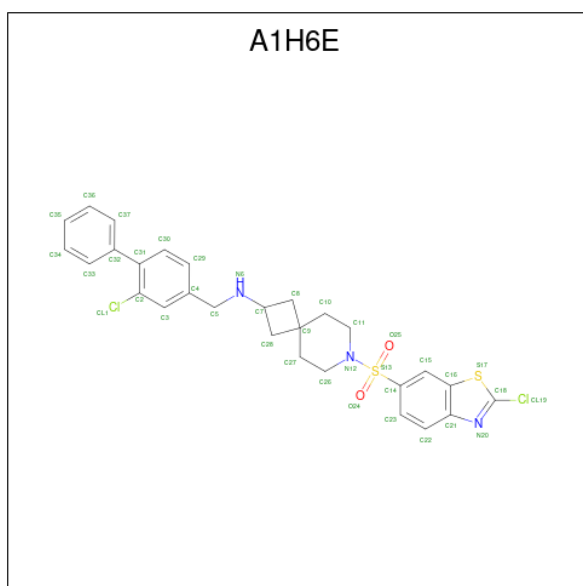
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is 7-[(2-chloranyl-1,3-benzothiazol-6-yl)sulfonyl]- {N}-[(3-chloranyl-4-phenyl-phe nyl)methyl]-7-azaspiro[3.5]nonan-2-amine (CCD ID: A1H6E) (formula: $C_{28}H_{27}Cl_2N_3O_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			37	28	2	3	2	2		
4	B	1	Total	C	Cl	N	O	S	0	0
			37	28	2	3	2	2		

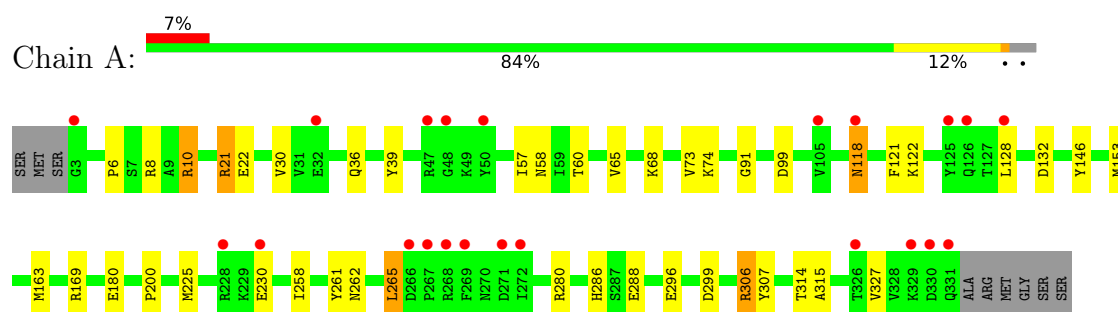
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total 31	O 31	0	0
5	B	36	Total 36	O 36	0	0

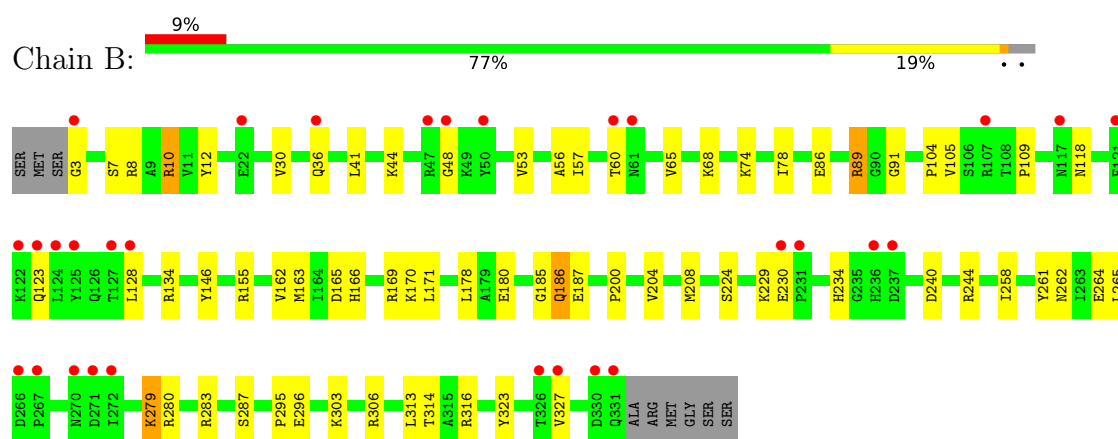
3 Residue-property plots [i](#)

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 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.

• Molecule 1: Casein kinase II subunit alpha



• Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.16Å 128.16Å 124.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.31 – 2.60 45.31 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.31-2.60) 100.0 (45.31-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.214 , 0.246 (Not available) , 0.238	Depositor DCC
R_{free} test set	1664 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5643	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3316e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SO4, EDO, A1H6E

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	0.60	0/2771	1.07	3/3760 (0.1%)
1	B	0.62	0/2794	1.07	3/3787 (0.1%)
All	All	0.61	0/5565	1.07	6/7547 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	GLU	CB-CG-CD	6.42	123.52	112.60
1	B	230	GLU	N-CA-CB	6.26	116.34	110.39
1	B	234	HIS	CA-CB-CG	6.20	120.00	113.80
1	A	230	GLU	CB-CG-CD	5.37	121.72	112.60
1	A	99	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	165	ASP	CA-CB-CG	5.02	117.62	112.60

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	A	2697	0	2590	37	0
1	B	2721	0	2617	39	0
2	A	30	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	50	0	0	2	0
3	A	4	0	6	0	0
4	A	37	0	0	1	0
4	B	37	0	0	1	0
5	A	31	0	0	1	0
5	B	36	0	0	1	0
All	All	5643	0	5213	70	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 (70) 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:21:ARG:HH11	1:A:21:ARG:HG3	1.21	1.05
1:A:58:ASN:OD1	1:A:60:THR:HB	1.76	0.86
1:B:185:GLY:HA2	1:B:208:MET:HE3	1.58	0.85
1:A:280:ARG:HD3	1:B:306:ARG:NH2	1.94	0.83
1:A:21:ARG:HG3	1:A:21:ARG:NH1	1.85	0.82
1:A:314:THR:HG23	5:A:525:HOH:O	1.79	0.81
1:A:128:LEU:HD11	1:A:225:MET:HE1	1.64	0.79
1:A:280:ARG:CD	1:B:306:ARG:NH2	2.45	0.79
1:A:280:ARG:CD	1:B:306:ARG:HH21	1.97	0.76
1:A:128:LEU:CD1	1:A:225:MET:HE1	2.19	0.73
1:A:73:VAL:HG12	1:A:74:LYS:N	2.04	0.72
1:A:128:LEU:CD1	1:A:225:MET:CE	2.68	0.72
1:A:306:ARG:NH1	1:B:280:ARG:HD3	2.05	0.71
1:B:155:ARG:NH2	1:B:180:GLU:HB2	2.07	0.68
1:A:280:ARG:NE	1:B:306:ARG:HH21	1.92	0.68
1:A:280:ARG:HD3	1:B:306:ARG:HH21	1.57	0.68
1:B:155:ARG:HH21	1:B:180:GLU:HB2	1.61	0.64
1:A:128:LEU:HD11	1:A:225:MET:CE	2.29	0.63
1:B:36:GLN:HG3	1:B:104:PRO:HD3	1.83	0.59
1:A:73:VAL:CG1	1:A:74:LYS:N	2.66	0.58
1:B:240:ASP:O	1:B:244:ARG:HG2	2.04	0.57
1:A:132:ASP:OD1	1:A:169:ARG:NH2	2.39	0.56
1:B:118:ASN:OD1	1:B:163:MET:HE3	2.06	0.55
1:A:21:ARG:HH11	1:A:21:ARG:CG	2.04	0.55
1:B:10:ARG:NH1	1:B:314:THR:HG23	2.23	0.53
1:B:41:LEU:HD23	1:B:56:ALA:HB2	1.90	0.53
1:B:3:GLY:N	5:B:503:HOH:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:TYR:O	1:A:262:ASN:C	2.53	0.51
1:A:73:VAL:HG12	1:A:74:LYS:H	1.76	0.49
4:A:408:A1H6E:CL1	4:A:408:A1H6E:C37	2.99	0.48
1:A:286:HIS:ND1	1:A:288:GLU:OE1	2.47	0.47
1:B:279:LYS:HD3	1:B:283:ARG:CZ	2.44	0.47
1:B:53:VAL:HG22	1:B:68:LYS:HG2	1.96	0.47
1:A:73:VAL:CG1	1:A:74:LYS:H	2.26	0.47
1:B:8:ARG:NH2	1:B:208:MET:HE1	2.30	0.47
1:B:12:TYR:OH	1:B:316:ARG:NH1	2.48	0.46
1:B:166:HIS:CD2	1:B:169:ARG:HH11	2.34	0.46
1:A:118:ASN:OD1	1:A:163:MET:HE3	2.15	0.46
1:B:7:SER:O	1:B:208:MET:HE2	2.16	0.46
1:B:303:LYS:HB3	1:B:313:LEU:HG	1.97	0.46
1:B:155:ARG:HD3	1:B:178:LEU:O	2.16	0.45
1:B:224:SER:HB2	1:B:229:LYS:O	2.16	0.45
1:A:91:GLY:HA3	1:A:146:TYR:CE2	2.53	0.44
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.81	0.44
1:A:299:ASP:HB2	1:B:295:PRO:HB3	2.00	0.43
1:B:86:GLU:HG2	1:B:89:ARG:NH2	2.33	0.43
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.82	0.43
1:B:78:ILE:HD13	1:B:109:PRO:HG2	2.01	0.43
1:B:162:VAL:O	4:B:411:A1H6E:N6	2.52	0.43
1:A:21:ARG:HG3	1:A:22:GLU:N	2.34	0.42
1:B:186:GLN:HG3	1:B:187:GLU:N	2.33	0.42
1:B:200:PRO:O	1:B:204:VAL:HG22	2.18	0.42
1:A:121:PHE:O	1:A:122:LYS:C	2.63	0.42
1:A:21:ARG:NH1	1:A:22:GLU:HA	2.35	0.42
1:A:265:LEU:HD12	1:A:265:LEU:HA	1.76	0.42
1:B:91:GLY:HA3	1:B:146:TYR:CE2	2.55	0.42
1:B:8:ARG:NH2	1:B:208:MET:CE	2.82	0.42
1:B:229:LYS:HE3	2:B:407:SO4:O3	2.19	0.42
1:B:261:TYR:O	1:B:262:ASN:C	2.63	0.42
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.55	0.42
1:A:200:PRO:HG2	1:A:307:TYR:HA	2.01	0.42
1:B:7:SER:H	1:B:208:MET:HE2	1.85	0.42
1:B:171:LEU:HD23	1:B:171:LEU:C	2.45	0.42
1:A:10:ARG:H	1:A:10:ARG:HG3	1.58	0.41
1:A:6:PRO:HB3	1:A:8:ARG:HH22	1.85	0.41
1:A:21:ARG:HH12	1:A:22:GLU:HA	1.85	0.41
1:A:39:TYR:HA	1:A:57:ILE:O	2.21	0.40
1:A:314:THR:HG22	1:A:315:ALA:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HH11	1:A:22:GLU:N	2.19	0.40
1:B:48:GLY:O	2:B:408:SO4:O4	2.39	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	A	327/338 (97%)	304 (93%)	23 (7%)	0	100	100
1	B	327/338 (97%)	312 (95%)	15 (5%)	0	100	100
All	All	654/676 (97%)	616 (94%)	38 (6%)	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	283/310 (91%)	270 (95%)	13 (5%)	24	49
1	B	289/310 (93%)	270 (93%)	19 (7%)	15	34
All	All	572/620 (92%)	540 (94%)	32 (6%)	19	40

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

Mol	Chain	Res	Type
1	A	10	ARG
1	A	21	ARG
1	A	30	VAL
1	A	36	GLN
1	A	65	VAL
1	A	68	LYS
1	A	118	ASN
1	A	153	MET
1	A	258	ILE
1	A	265	LEU
1	A	296	GLU
1	A	306	ARG
1	A	327	VAL
1	B	10	ARG
1	B	30	VAL
1	B	44	LYS
1	B	57	ILE
1	B	60	THR
1	B	65	VAL
1	B	74	LYS
1	B	89	ARG
1	B	105	VAL
1	B	123	GLN
1	B	170	LYS
1	B	186	GLN
1	B	258	ILE
1	B	264	GLU
1	B	265	LEU
1	B	279	LYS
1	B	287	SER
1	B	296	GLU
1	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	62	ASN
1	A	186	GLN
1	A	238	ASN
1	A	262	ASN
1	A	270	ASN
1	A	291	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	123	GLN
1	B	207	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 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	$\# Z > 2$
2	SO4	B	409	-	4,4,4	0.25	0	6,6,6	0.30	0
2	SO4	B	407	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.15	0
2	SO4	B	404	-	4,4,4	0.27	0	6,6,6	0.29	0
3	EDO	A	407	-	3,3,3	0.16	0	2,2,2	0.10	0
2	SO4	A	403	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	A	406	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	B	410	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	B	405	-	4,4,4	0.27	0	6,6,6	0.19	0
2	SO4	B	401	-	4,4,4	0.35	0	6,6,6	0.33	0
2	SO4	A	405	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	B	402	-	4,4,4	0.27	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.24	0
4	A1H6E	B	411	-	41,42,42	0.57	1 (2%)	55,63,63	0.48	0
2	SO4	A	404	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	B	406	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	B	408	-	4,4,4	0.32	0	6,6,6	0.20	0
2	SO4	B	403	-	4,4,4	0.30	0	6,6,6	0.14	0
4	A1H6E	A	408	-	41,42,42	0.53	1 (2%)	55,63,63	0.48	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	A1H6E	B	411	-	-	0/19/43/43	0/6/6/6
3	EDO	A	407	-	-	1/1/1/1	-
4	A1H6E	A	408	-	-	0/19/43/43	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	411	A1H6E	C28-C7	-2.72	1.51	1.54
4	A	408	A1H6E	C28-C7	-2.54	1.51	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

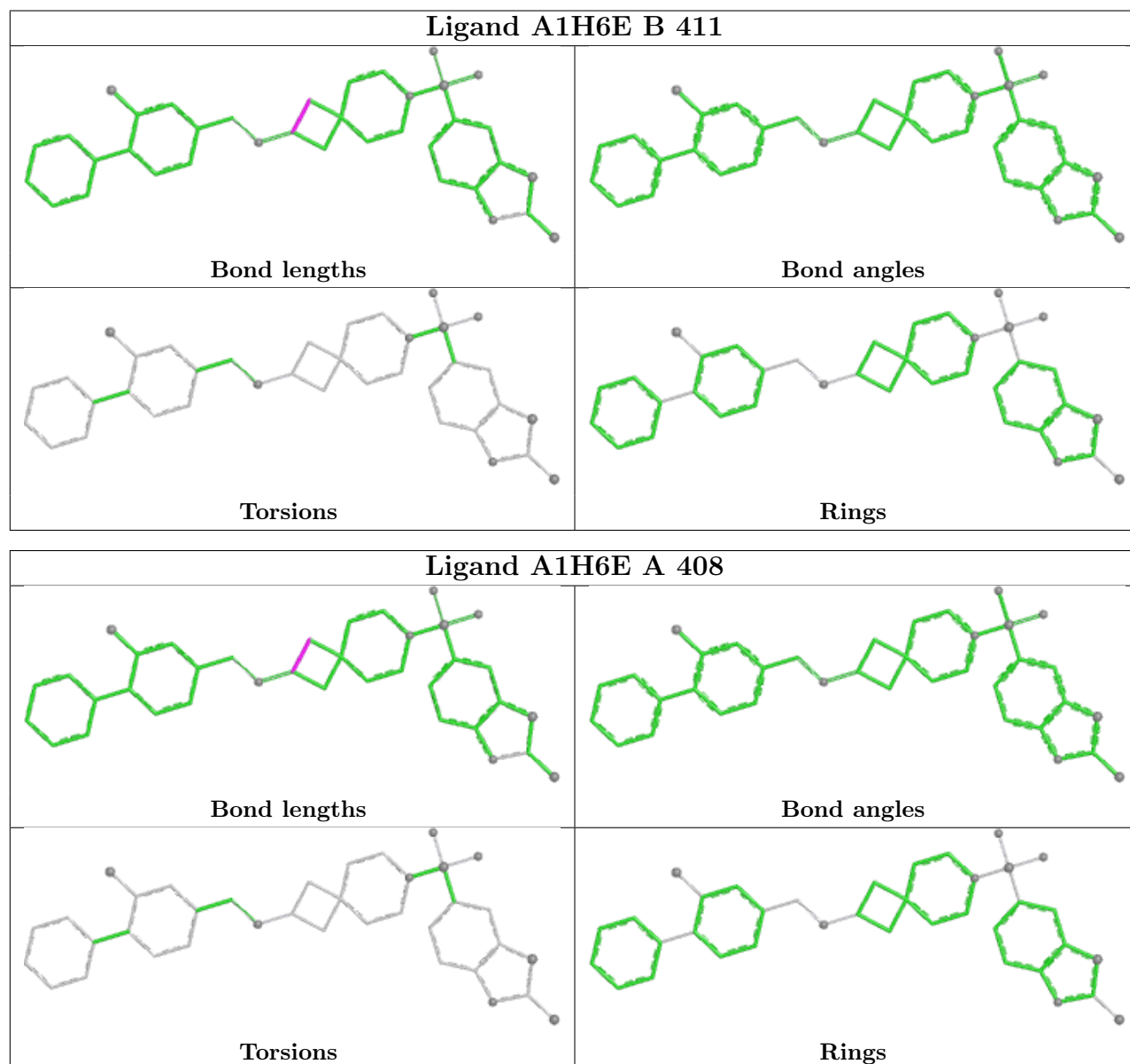
Mol	Chain	Res	Type	Atoms
3	A	407	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	407	SO4	1	0
4	B	411	A1H6E	1	0
2	B	408	SO4	1	0
4	A	408	A1H6E	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 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/338 (97%)	0.21	22 (6%) 24 19	29, 48, 77, 108	0
1	B	329/338 (97%)	0.38	30 (9%) 15 11	30, 49, 86, 115	0
All	All	658/676 (97%)	0.30	52 (7%) 18 14	29, 49, 84, 115	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	GLU	6.2
1	B	330	ASP	6.1
1	A	105	VAL	5.4
1	B	125	TYR	5.1
1	A	266	ASP	4.8
1	A	330	ASP	4.5
1	B	271	ASP	4.3
1	B	272	ILE	4.1
1	A	272	ILE	4.1
1	B	47	ARG	3.9
1	B	121	PHE	3.6
1	B	236	HIS	3.3
1	B	267	PRO	3.3
1	A	267	PRO	3.2
1	B	122	LYS	3.1
1	A	268	ARG	3.1
1	B	107	ARG	3.1
1	B	266	ASP	3.0
1	B	127	THR	3.0
1	B	231	PRO	2.9
1	B	50	TYR	2.9
1	A	32	GLU	2.8
1	A	271	ASP	2.8
1	A	329	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	331	GLN	2.7
1	B	3	GLY	2.7
1	A	326	THR	2.6
1	A	331	GLN	2.6
1	A	126	GLN	2.6
1	B	22	GLU	2.5
1	A	48	GLY	2.5
1	B	327	VAL	2.5
1	B	128	LEU	2.5
1	A	128	LEU	2.4
1	A	118	ASN	2.4
1	B	124	LEU	2.3
1	A	3	GLY	2.3
1	B	237	ASP	2.3
1	B	60	THR	2.3
1	B	326	THR	2.3
1	B	117	ASN	2.2
1	B	36	GLN	2.2
1	B	48	GLY	2.2
1	A	269	PHE	2.2
1	B	61	ASN	2.2
1	A	125	TYR	2.1
1	B	270	ASN	2.1
1	B	123	GLN	2.0
1	A	50	TYR	2.0
1	A	47	ARG	2.0
1	A	230	GLU	2.0
1	A	228	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

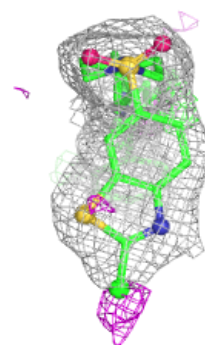
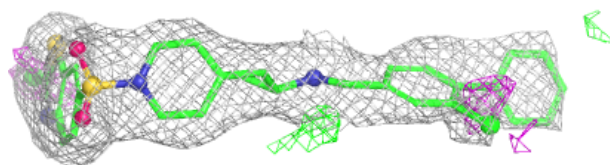
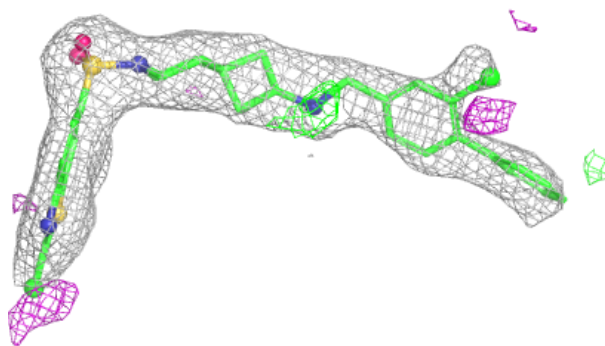
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	405	5/5	0.57	0.15	113,122,123,124	0
2	SO4	B	403	5/5	0.73	0.12	92,106,109,110	0
2	SO4	B	404	5/5	0.74	0.17	68,71,99,100	0
2	SO4	A	405	5/5	0.77	0.16	74,76,86,105	0
2	SO4	B	409	5/5	0.77	0.14	66,78,94,95	0
2	SO4	A	404	5/5	0.79	0.12	89,97,102,108	0
2	SO4	B	407	5/5	0.85	0.14	93,103,110,126	0
3	EDO	A	407	4/4	0.85	0.18	62,68,68,72	0
2	SO4	B	410	5/5	0.87	0.11	60,79,83,83	0
2	SO4	B	406	5/5	0.88	0.17	69,95,100,107	0
4	A1H6E	B	411	37/37	0.89	0.17	42,53,89,112	0
2	SO4	B	402	5/5	0.90	0.08	63,65,79,83	0
2	SO4	A	402	5/5	0.91	0.10	61,70,71,81	0
4	A1H6E	A	408	37/37	0.91	0.14	39,50,82,91	0
2	SO4	B	408	5/5	0.91	0.13	70,77,81,86	0
2	SO4	A	406	5/5	0.94	0.09	47,50,59,62	0
2	SO4	B	401	5/5	0.94	0.12	49,58,61,63	0
2	SO4	A	403	5/5	0.96	0.11	47,56,62,75	0
2	SO4	A	401	5/5	0.98	0.10	44,48,57,59	0

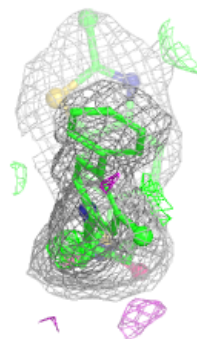
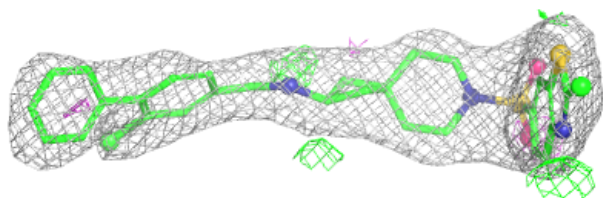
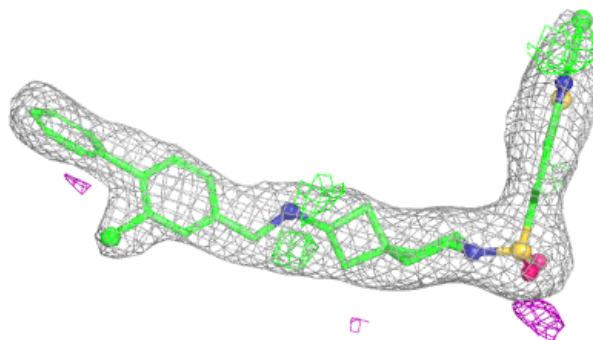
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H6E B 411:

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

**Electron density around A1H6E A 408:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.