



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:55 PM UTC

PDB ID : 6Z83 / pdb_00006z83
Title : CK2 alpha bound to chemical probe SGC-CK2-1
Authors : Kraemer, A.; Wells, C.; Drewry, D.H.; Pickett, J.E.; Axtman, A.D.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2020-06-02
Resolution : 2.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

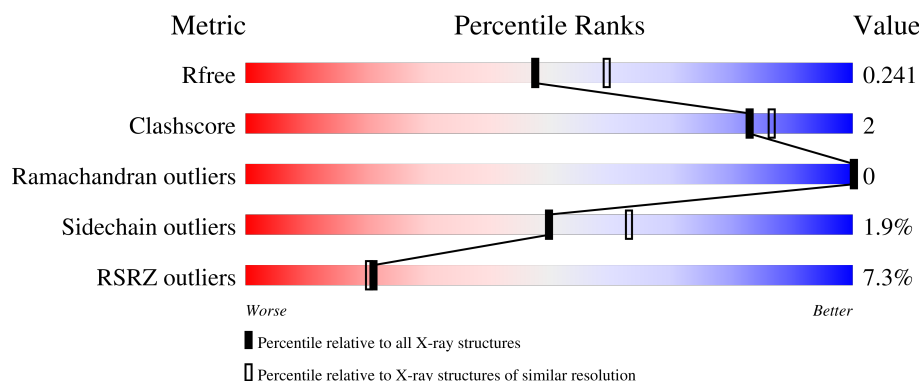
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	AAA	359	8% 84% 7% 9%
1	BBB	359	5% 84% 7% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5881 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	AAA	327	Total	C	N	O	S	0	0	0
			2715	1746	471	487	11			
1	BBB	330	Total	C	N	O	S	0	0	0
			2726	1757	466	492	11			

There are 44 discrepancies between the modelled and reference sequences:

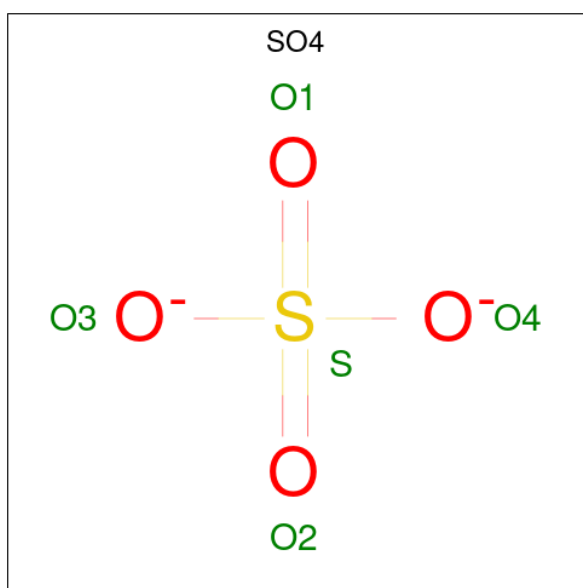
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-21	MET	-	initiating methionine	UNP P68400
AAA	-20	HIS	-	expression tag	UNP P68400
AAA	-19	HIS	-	expression tag	UNP P68400
AAA	-18	HIS	-	expression tag	UNP P68400
AAA	-17	HIS	-	expression tag	UNP P68400
AAA	-16	HIS	-	expression tag	UNP P68400
AAA	-15	HIS	-	expression tag	UNP P68400
AAA	-14	SER	-	expression tag	UNP P68400
AAA	-13	SER	-	expression tag	UNP P68400
AAA	-12	GLY	-	expression tag	UNP P68400
AAA	-11	VAL	-	expression tag	UNP P68400
AAA	-10	ASP	-	expression tag	UNP P68400
AAA	-9	LEU	-	expression tag	UNP P68400
AAA	-8	GLY	-	expression tag	UNP P68400
AAA	-7	THR	-	expression tag	UNP P68400
AAA	-6	GLU	-	expression tag	UNP P68400
AAA	-5	ASN	-	expression tag	UNP P68400
AAA	-4	LEU	-	expression tag	UNP P68400
AAA	-3	TYR	-	expression tag	UNP P68400
AAA	-2	PHE	-	expression tag	UNP P68400
AAA	-1	GLN	-	expression tag	UNP P68400
AAA	0	SER	-	expression tag	UNP P68400
BBB	-21	MET	-	initiating methionine	UNP P68400
BBB	-20	HIS	-	expression tag	UNP P68400
BBB	-19	HIS	-	expression tag	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-18	HIS	-	expression tag	UNP P68400
BBB	-17	HIS	-	expression tag	UNP P68400
BBB	-16	HIS	-	expression tag	UNP P68400
BBB	-15	HIS	-	expression tag	UNP P68400
BBB	-14	SER	-	expression tag	UNP P68400
BBB	-13	SER	-	expression tag	UNP P68400
BBB	-12	GLY	-	expression tag	UNP P68400
BBB	-11	VAL	-	expression tag	UNP P68400
BBB	-10	ASP	-	expression tag	UNP P68400
BBB	-9	LEU	-	expression tag	UNP P68400
BBB	-8	GLY	-	expression tag	UNP P68400
BBB	-7	THR	-	expression tag	UNP P68400
BBB	-6	GLU	-	expression tag	UNP P68400
BBB	-5	ASN	-	expression tag	UNP P68400
BBB	-4	LEU	-	expression tag	UNP P68400
BBB	-3	TYR	-	expression tag	UNP P68400
BBB	-2	PHE	-	expression tag	UNP P68400
BBB	-1	GLN	-	expression tag	UNP P68400
BBB	0	SER	-	expression tag	UNP P68400

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



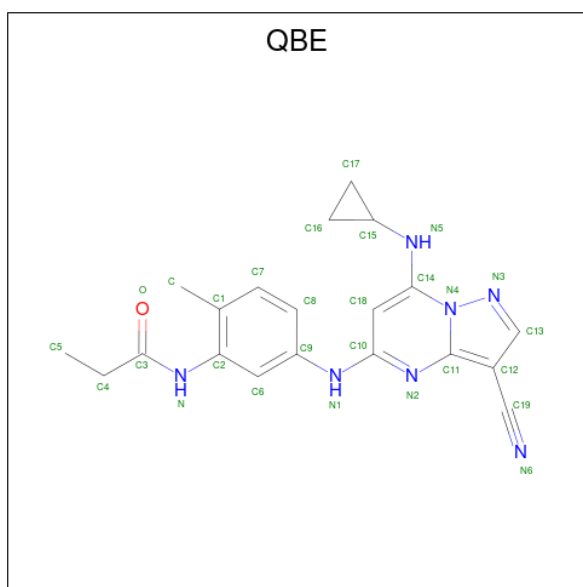
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	AAA	1	Total	O	S	0	0
			5	4	1		

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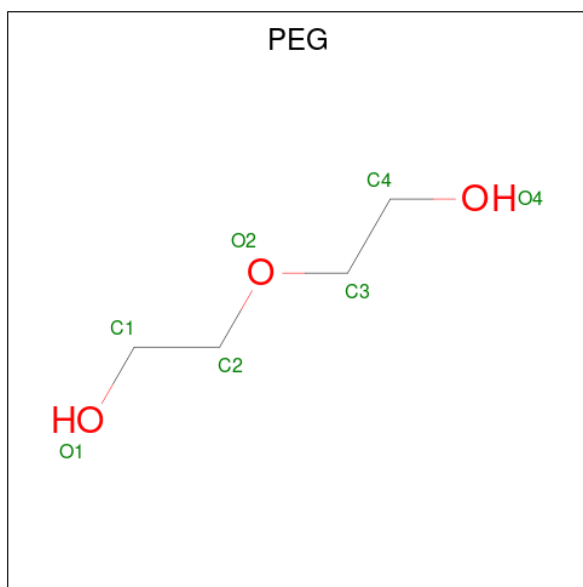
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5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

- Molecule 3 is {N}-[5-[[3-cyano-7-(cyclopropylamino)-3 {H}-pyrazolo[1,5-a]pyrimidin-5-yl]amino]-2-methyl-phenyl]propanamide (CCD ID: QBE) (formula: C₂₀H₂₁N₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			28	20	7	1		
3	BBB	1	Total	C	N	O	0	0
			28	20	7	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			7	4	3		
4	AAA	1	Total	C	O	0	0
			7	4	3		
4	BBB	1	Total	C	O	0	0
			7	4	3		
4	BBB	1	Total	C	O	0	0
			7	4	3		
4	BBB	1	Total	C	O	0	0
			7	4	3		
4	BBB	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	125	Total	O	0	0
			125	125		

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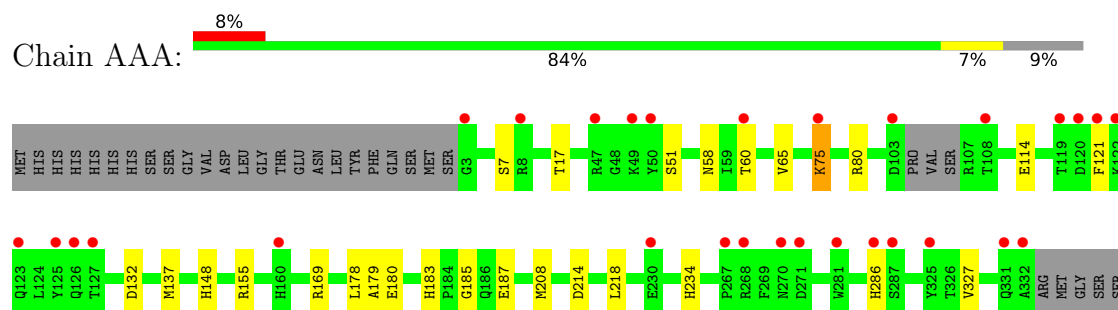
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	BBB	150	Total	O	0	0
			150	150		

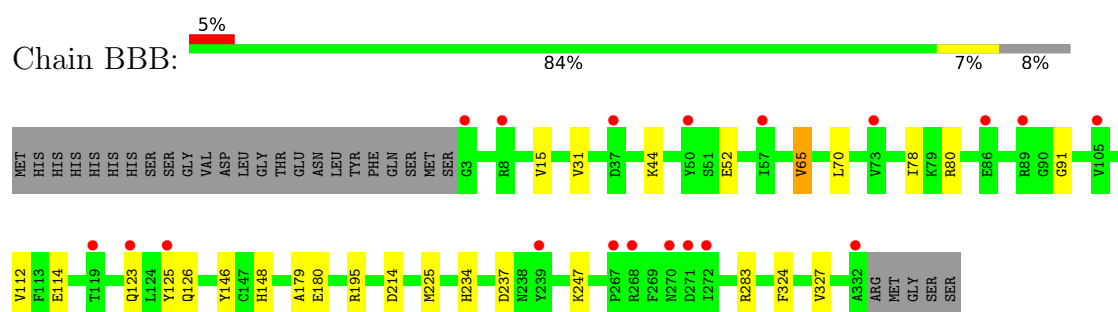
3 Residue-property plots [i](#)

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	126.96Å 126.96Å 124.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.89 – 2.17 44.89 – 2.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.89-2.17) 100.0 (44.89-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.214 , 0.245 0.220 , 0.241	Depositor DCC
R_{free} test set	2767 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5881	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 27.04 % 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 2.3619e-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: QBE, PEG, SO4

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	AAA	0.91	2/2788 (0.1%)	1.04	4/3777 (0.1%)
1	BBB	0.88	0/2801	1.02	1/3799 (0.0%)
All	All	0.89	2/5589 (0.0%)	1.03	5/7576 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	187	GLU	C-O	5.92	1.31	1.24
1	AAA	327	VAL	C-O	5.36	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	234	HIS	CA-C-O	-5.70	114.88	122.51
1	AAA	234	HIS	CA-C-O	-5.39	116.04	122.13
1	AAA	51	SER	CA-C-N	5.29	130.45	122.99
1	AAA	51	SER	C-N-CA	5.29	130.45	122.99
1	AAA	17	THR	N-CA-C	-5.28	105.70	111.82

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	AAA	2715	0	2613	12	0
1	BBB	2726	0	2618	14	0
2	AAA	25	0	0	1	0
2	BBB	35	0	0	0	0
3	AAA	28	0	0	0	0
3	BBB	28	0	0	0	0
4	AAA	14	0	20	0	0
4	BBB	35	0	50	1	0
5	AAA	125	0	0	3	0
5	BBB	150	0	0	1	0
All	All	5881	0	5301	26	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 2.

All (26) 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:BBB:80:ARG:HD3	1:BBB:179:ALA:O	1.89	0.72
1:BBB:125:TYR:CZ	1:BBB:225:MET:HE2	2.31	0.66
1:AAA:185:GLY:HA2	1:AAA:208:MET:HE3	1.77	0.66
1:AAA:80:ARG:HD3	1:AAA:179:ALA:O	1.96	0.64
1:AAA:148:HIS:HE1	1:AAA:214:ASP:OD2	1.89	0.55
1:BBB:44:LYS:HE3	1:BBB:52:GLU:HG3	1.90	0.54
1:AAA:183:HIS:HE1	5:AAA:519:HOH:O	1.91	0.54
1:AAA:7:SER:O	1:AAA:208:MET:HE2	2.08	0.53
1:AAA:75:LYS:HE2	2:AAA:401:SO4:O4	2.09	0.52
1:AAA:155:ARG:HD3	1:AAA:178:LEU:O	2.09	0.52
1:BBB:195:ARG:HD2	1:BBB:237:ASP:C	2.34	0.52
1:AAA:132:ASP:OD1	1:AAA:169:ARG:NH2	2.44	0.49
1:BBB:65:VAL:CG1	1:BBB:112:VAL:HG13	2.43	0.49
1:BBB:324:PHE:O	1:BBB:327:VAL:HG22	2.15	0.47
1:BBB:65:VAL:HG13	1:BBB:112:VAL:HG13	1.97	0.46
1:AAA:58:ASN:OD1	1:AAA:60:THR:HB	2.17	0.45
1:BBB:247:LYS:HD3	4:BBB:409:PEG:C1	2.46	0.45
1:BBB:70:LEU:HD13	1:BBB:78:ILE:HG12	1.99	0.44
1:BBB:123:GLN:O	1:BBB:126:GLN:HG2	2.18	0.43
1:AAA:155:ARG:NH1	5:AAA:504:HOH:O	2.49	0.43
1:BBB:195:ARG:HD3	5:BBB:517:HOH:O	2.18	0.43
1:BBB:148:HIS:HE1	1:BBB:214:ASP:OD2	2.02	0.43
1:AAA:286:HIS:HB2	5:AAA:613:HOH:O	2.19	0.42
1:BBB:125:TYR:CE2	1:BBB:225:MET:HE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:137:MET:HE1	1:AAA:218:LEU:HG	2.03	0.40
1:BBB:91:GLY:HA3	1:BBB:146:TYR:CE2	2.56	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	AAA	323/359 (90%)	314 (97%)	9 (3%)	0	100	100
1	BBB	328/359 (91%)	322 (98%)	6 (2%)	0	100	100
All	All	651/718 (91%)	636 (98%)	15 (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	AAA	287/329 (87%)	282 (98%)	5 (2%)	53	66
1	BBB	288/329 (88%)	282 (98%)	6 (2%)	47	59
All	All	575/658 (87%)	564 (98%)	11 (2%)	50	63

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	65	VAL
1	AAA	75	LYS
1	AAA	114	GLU
1	AAA	121	PHE
1	AAA	180	GLU
1	BBB	15	VAL
1	BBB	31	VAL
1	BBB	65	VAL
1	BBB	114	GLU
1	BBB	180	GLU
1	BBB	283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

21 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	$\# Z > 2$
4	PEG	BBB	412	-	6,6,6	0.18	0	5,5,5	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	AAA	408	-	6,6,6	0.16	0	5,5,5	0.08	0
2	SO4	BBB	407	-	4,4,4	0.38	0	6,6,6	0.08	0
4	PEG	BBB	409	-	6,6,6	0.12	0	5,5,5	0.12	0
3	QBE	AAA	406	-	29,31,31	0.19	0	42,44,44	0.69	1 (2%)
2	SO4	BBB	403	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	AAA	403	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	AAA	405	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	AAA	402	-	4,4,4	0.32	0	6,6,6	0.10	0
4	PEG	BBB	411	-	6,6,6	0.14	0	5,5,5	0.06	0
3	QBE	BBB	408	-	29,31,31	0.24	0	42,44,44	0.66	1 (2%)
2	SO4	BBB	402	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	BBB	405	-	4,4,4	0.32	0	6,6,6	0.08	0
4	PEG	BBB	410	-	6,6,6	0.16	0	5,5,5	0.11	0
2	SO4	BBB	406	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	AAA	404	-	4,4,4	0.33	0	6,6,6	0.09	0
4	PEG	BBB	413	-	6,6,6	0.13	0	5,5,5	0.12	0
4	PEG	AAA	407	-	6,6,6	0.13	0	5,5,5	0.06	0
2	SO4	BBB	401	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	AAA	401	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	BBB	404	-	4,4,4	0.32	0	6,6,6	0.07	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	PEG	BBB	412	-	-	3/4/4/4	-
4	PEG	AAA	407	-	-	2/4/4/4	-
4	PEG	AAA	408	-	-	2/4/4/4	-
4	PEG	BBB	410	-	-	1/4/4/4	-
4	PEG	BBB	409	-	-	3/4/4/4	-
3	QBE	AAA	406	-	-	2/13/18/18	0/4/4/4
4	PEG	BBB	411	-	-	3/4/4/4	-
4	PEG	BBB	413	-	-	3/4/4/4	-
3	QBE	BBB	408	-	-	2/13/18/18	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	406	QBE	C9-N1-C10	2.14	132.33	128.08
3	BBB	408	QBE	C9-N1-C10	2.12	132.29	128.08

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	406	QBE	O-C3-N-C2
3	BBB	408	QBE	O-C3-N-C2
3	AAA	406	QBE	C4-C3-N-C2
3	BBB	408	QBE	C4-C3-N-C2
4	BBB	411	PEG	O2-C3-C4-O4
4	BBB	412	PEG	O1-C1-C2-O2
4	AAA	408	PEG	O1-C1-C2-O2
4	BBB	411	PEG	O1-C1-C2-O2
4	BBB	410	PEG	O1-C1-C2-O2
4	BBB	412	PEG	O2-C3-C4-O4
4	BBB	413	PEG	O1-C1-C2-O2
4	BBB	413	PEG	O2-C3-C4-O4
4	AAA	407	PEG	O1-C1-C2-O2
4	BBB	409	PEG	C4-C3-O2-C2
4	BBB	409	PEG	O2-C3-C4-O4
4	BBB	409	PEG	O1-C1-C2-O2
4	AAA	407	PEG	O2-C3-C4-O4
4	AAA	408	PEG	C4-C3-O2-C2
4	BBB	412	PEG	C1-C2-O2-C3
4	BBB	411	PEG	C1-C2-O2-C3
4	BBB	413	PEG	C1-C2-O2-C3

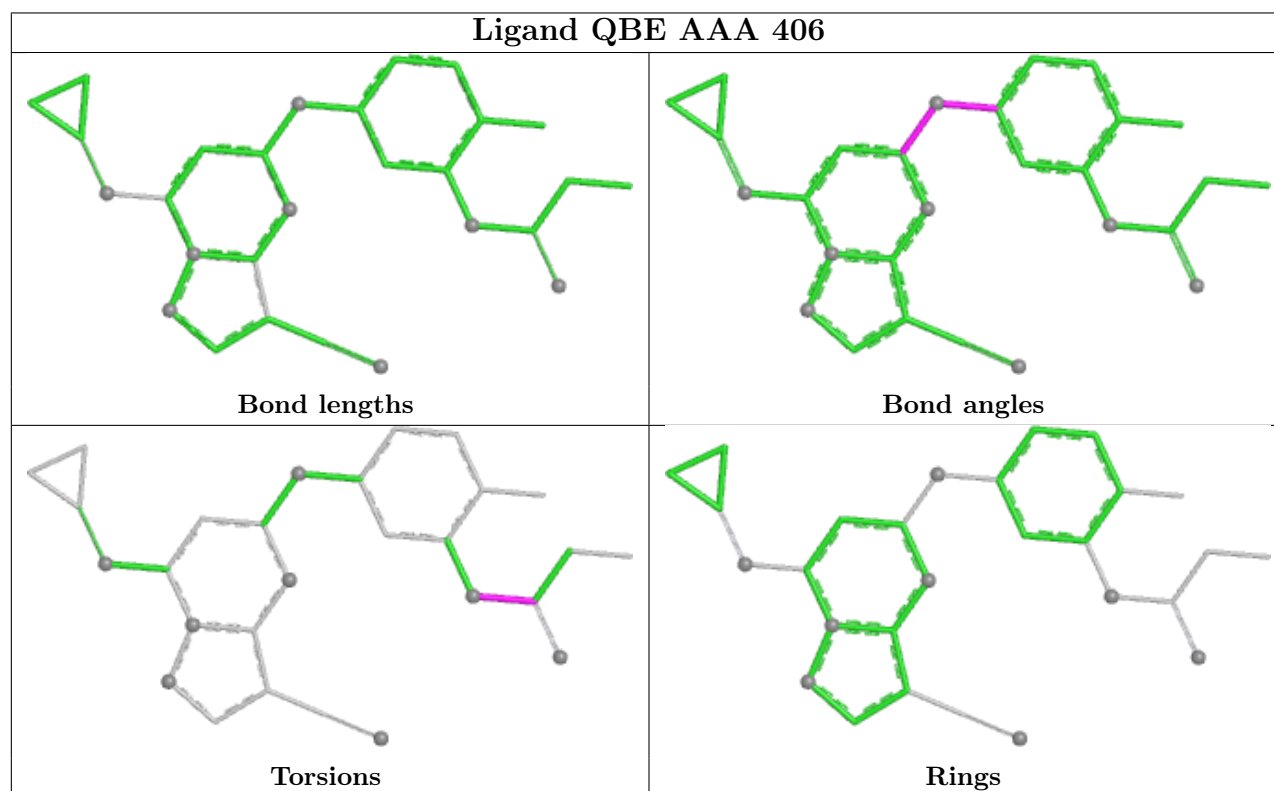
There are no ring outliers.

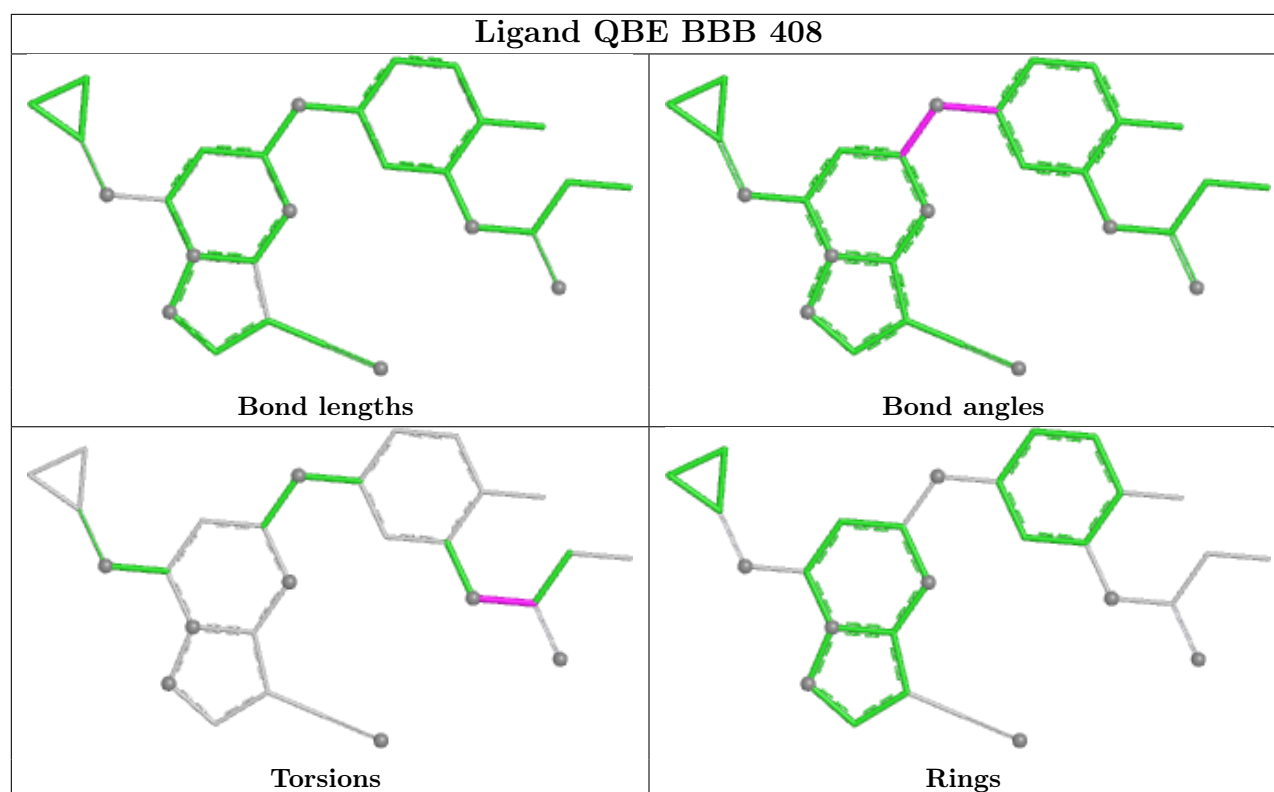
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	409	PEG	1	0
2	AAA	401	SO4	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	AAA	327/359 (91%)	0.60	29 (8%) 15 14	26, 38, 64, 87	0
1	BBB	330/359 (91%)	0.44	19 (5%) 29 28	24, 36, 56, 78	0
All	All	657/718 (91%)	0.52	48 (7%) 21 20	24, 37, 61, 87	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	121	PHE	6.6
1	AAA	332	ALA	6.4
1	AAA	120	ASP	5.7
1	BBB	332	ALA	5.3
1	BBB	270	ASN	4.7
1	AAA	50	TYR	4.6
1	AAA	125	TYR	4.5
1	AAA	60	THR	4.2
1	AAA	126	GLN	4.2
1	AAA	268	ARG	4.0
1	BBB	50	TYR	3.9
1	BBB	268	ARG	3.7
1	AAA	103	ASP	3.6
1	BBB	267	PRO	3.5
1	BBB	3	GLY	3.2
1	BBB	272	ILE	3.1
1	AAA	123	GLN	3.1
1	AAA	270	ASN	3.0
1	AAA	3	GLY	2.8
1	AAA	47	ARG	2.8
1	BBB	271	ASP	2.7
1	AAA	122	LYS	2.7
1	AAA	267	PRO	2.7
1	AAA	271	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	125	TYR	2.6
1	AAA	75	LYS	2.6
1	AAA	119	THR	2.5
1	AAA	286	HIS	2.4
1	BBB	105	VAL	2.4
1	AAA	49	LYS	2.4
1	AAA	127	THR	2.4
1	AAA	230	GLU	2.3
1	AAA	281	TRP	2.2
1	BBB	123	GLN	2.2
1	AAA	287	SER	2.2
1	BBB	73	VAL	2.2
1	BBB	37	ASP	2.2
1	BBB	86	GLU	2.2
1	BBB	239	TYR	2.2
1	AAA	8	ARG	2.2
1	BBB	8	ARG	2.1
1	AAA	108	THR	2.1
1	AAA	331	GLN	2.1
1	BBB	89	ARG	2.1
1	AAA	325	TYR	2.0
1	BBB	57	ILE	2.0
1	AAA	160	HIS	2.0
1	BBB	119	THR	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](#)

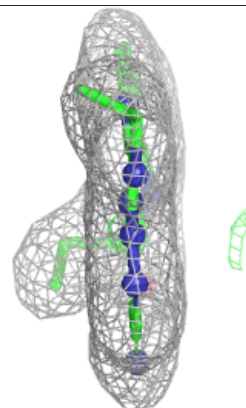
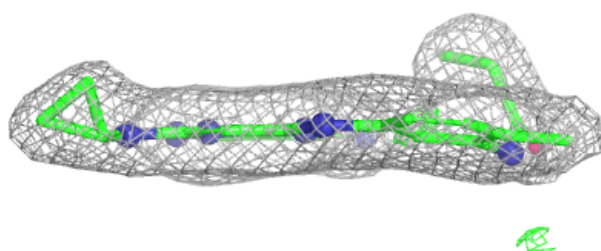
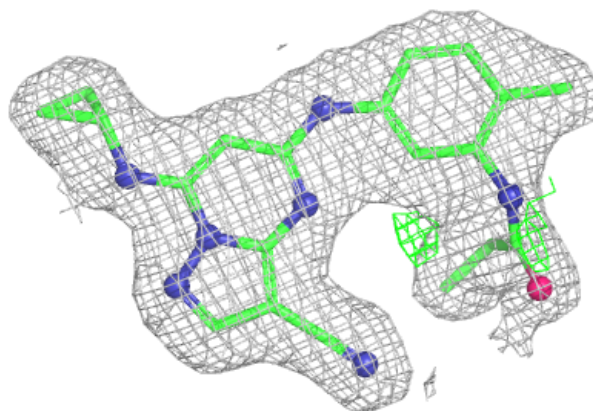
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	BBB	410	7/7	0.62	0.39	88,90,92,95	0
2	SO4	BBB	402	5/5	0.64	0.17	152,154,156,156	0
2	SO4	BBB	401	5/5	0.68	0.15	98,98,100,101	0
2	SO4	BBB	406	5/5	0.71	0.14	91,92,93,94	0
2	SO4	BBB	405	5/5	0.74	0.14	79,79,83,83	0
4	PEG	BBB	411	7/7	0.76	0.24	67,69,73,75	0
4	PEG	BBB	412	7/7	0.78	0.23	59,68,72,73	0
4	PEG	BBB	409	7/7	0.80	0.26	61,62,65,65	0
2	SO4	AAA	404	5/5	0.81	0.14	87,88,89,90	0
4	PEG	AAA	407	7/7	0.82	0.27	72,73,74,74	0
4	PEG	BBB	413	7/7	0.82	0.20	56,59,64,64	0
2	SO4	BBB	404	5/5	0.83	0.12	64,69,70,71	0
2	SO4	BBB	403	5/5	0.88	0.11	62,63,65,66	0
4	PEG	AAA	408	7/7	0.89	0.15	60,61,62,62	0
3	QBE	AAA	406	28/28	0.93	0.10	32,39,42,42	0
2	SO4	AAA	403	5/5	0.93	0.07	64,64,66,69	0
2	SO4	AAA	401	5/5	0.94	0.12	54,54,55,57	0
2	SO4	AAA	402	5/5	0.95	0.12	50,53,54,55	0
3	QBE	BBB	408	28/28	0.96	0.06	28,30,36,36	0
2	SO4	BBB	407	5/5	0.96	0.09	51,51,53,54	0
2	SO4	AAA	405	5/5	0.97	0.07	42,43,44,45	0

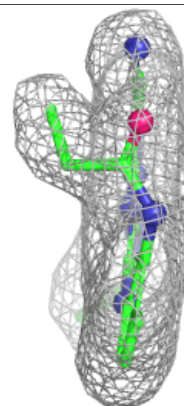
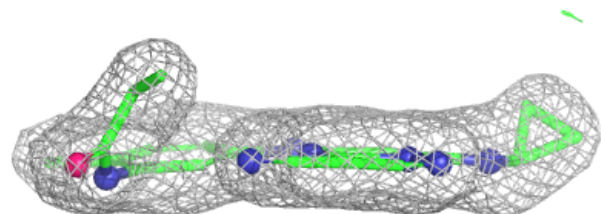
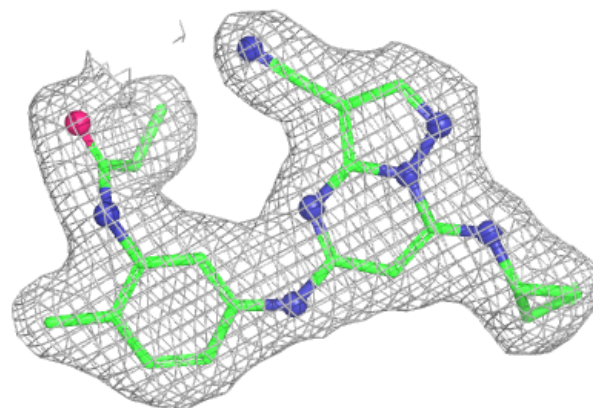
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QBE AAA 406:

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

**Electron density around QBE BBB 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.