



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 06:07 PM EDT

PDB ID : 5SFG  
Title : Crystal Structure of human phosphodiesterase 10 in complex with N-[(3R)-1-(5-chloropyridin-2-yl)pyrrolidin-3-yl]-6-cyclopropyl-3-(pyrimidin-5-ylamino)pyridine-2-carboxamide  
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Deposited on : 2022-01-21  
Resolution : 2.31 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.31.2  
buster-report : 1.1.7 (2018)  
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) : 2.31.2

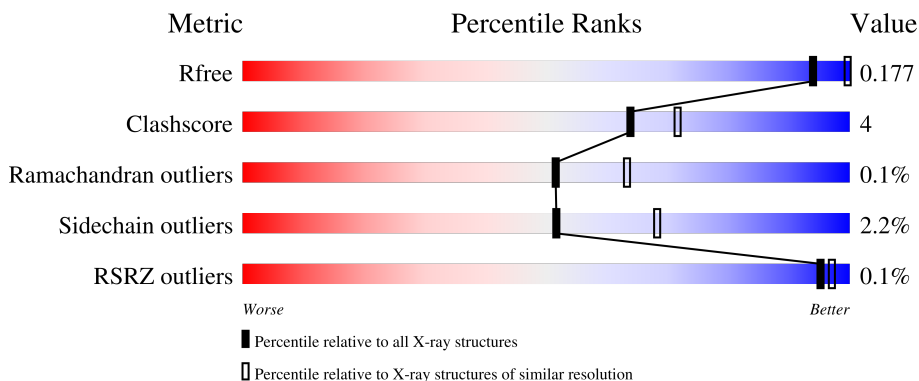
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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))
$R_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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  $\geq 3$ , 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	343	 81% 10% • 9%
1	B	343	 84% 8% • 8%
1	C	343	 82% 9% 9%
1	D	343	 78% 12% 10%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10904 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 and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2541	1624	432	461	24	0	0	0
1	B	315	2551	1630	434	463	24	0	0	0
1	C	313	2541	1624	432	461	24	0	0	0
1	D	310	2519	1612	429	454	24	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	SER	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	SER	-	expression tag	UNP Q9Y233
C	447	GLY	-	expression tag	UNP Q9Y233
C	448	SER	-	expression tag	UNP Q9Y233
D	447	GLY	-	expression tag	UNP Q9Y233
D	448	SER	-	expression tag	UNP Q9Y233

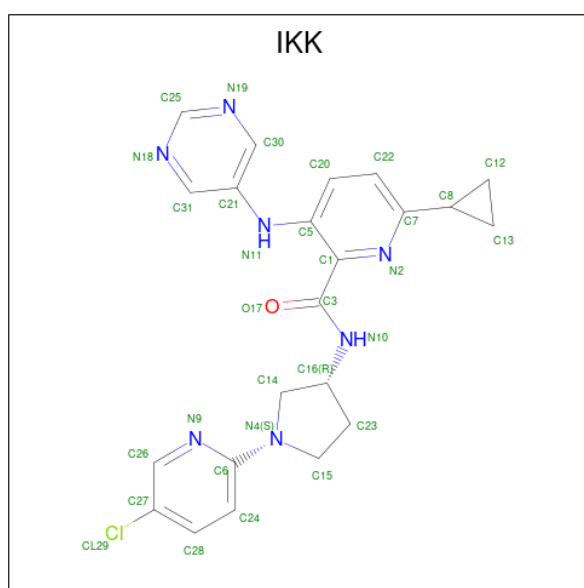
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is N-[(3R)-1-(5-chloropyridin-2-yl)pyrrolidin-3-yl]-6-cyclopropyl-3-[(pyrimidin-5-yl)amino]pyridine-2-carboxamide (three-letter code: IKK) (formula: C<sub>22</sub>H<sub>22</sub>ClN<sub>7</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 31 22 1 7 1	0	0
4	B	1	Total C Cl N O 31 22 1 7 1	0	0
4	C	1	Total C Cl N O 31 22 1 7 1	0	0
4	D	1	Total C Cl N O 31 22 1 7 1	0	0


- Molecule 5 is water.

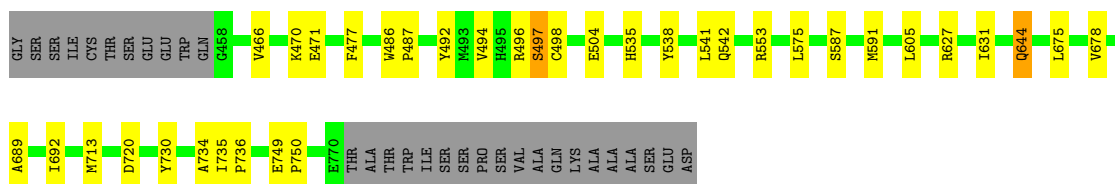
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	161	Total 161	O 161	0	0
5	B	174	Total 174	O 174	0	0
5	C	175	Total 175	O 175	0	0
5	D	110	Total 110	O 110	0	0

### 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: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain A: 




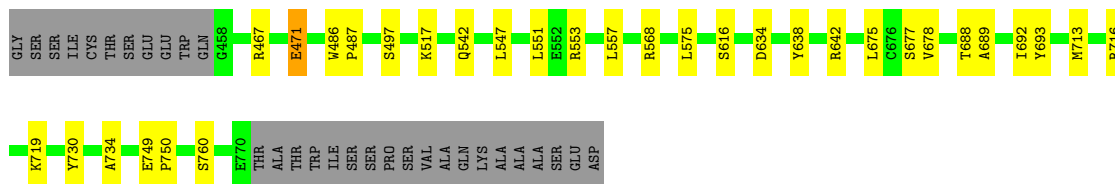
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain B: 




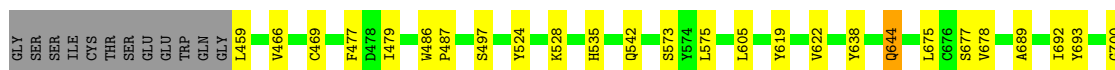
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain C: 



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain D: 



Q709	P710	I711	M712	M713	M714	D715	R716	K719	L727	Y730	N731	A734	I735	P736	T740	Q743	P746	I766	R767	G768	GLU	GLU	THR	ALA	ALA	THR	THR	TRP	TRP	ILF	SER	SER	SER	PRO	SER	VAL	VAL	ALA	ALA	GLN	GLN	LYS	ALA	ALA	ALA	ALA	ALA	SER	SER	GLU	ASP
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.15Å 136.15Å 235.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.79 – 2.31 43.79 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.79-2.31) 95.9 (43.79-2.31)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.160 , 0.195 0.149 , 0.177	Depositor DCC
$R_{free}$ test set	3514 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 16.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.360 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.624 for H, K, L 0.376 for K, H, -L	Depositor
Outliers	0 of 70628 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IKK, MG, CME, ZN

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	0.64	0/2592	0.69	0/3507
1	B	0.63	0/2602	0.69	0/3521
1	C	0.63	0/2592	0.70	0/3507
1	D	0.64	0/2570	0.69	0/3478
All	All	0.63	0/10356	0.69	0/14013

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2541	0	2511	20	0
1	B	2551	0	2515	16	0
1	C	2541	0	2511	19	0
1	D	2519	0	2496	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	0	5	0
4	B	31	0	0	2	0
4	C	31	0	0	6	0
4	D	31	0	0	5	0
5	A	161	0	0	0	0
5	B	174	0	0	3	0
5	C	175	0	0	4	0
5	D	110	0	0	1	0
All	All	10904	0	10033	85	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 4.

All (85) 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:C:689:ALA:O	1:C:692:ILE:HG22	1.77	0.84
4:D:803:IKK:C31	4:D:803:IKK:C20	2.57	0.80
4:B:803:IKK:C31	4:B:803:IKK:C20	2.61	0.77
1:C:713:MET:HB2	4:C:803:IKK:C24	2.16	0.76
1:B:568:ARG:O	5:B:901:HOH:O	2.09	0.70
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.74	0.70
1:D:644:GLN:HE21	1:D:644:GLN:HA	1.60	0.65
1:A:713:MET:HG3	4:A:803:IKK:C6	2.26	0.65
4:C:803:IKK:C20	4:C:803:IKK:C31	2.73	0.65
1:A:497:SER:HA	1:A:542:GLN:NE2	2.14	0.62
4:A:803:IKK:C31	4:A:803:IKK:C20	2.78	0.62
1:D:713:MET:HA	4:D:803:IKK:C26	2.30	0.61
1:D:677:SER:OG	4:D:803:IKK:N18	2.35	0.59
1:D:689:ALA:O	1:D:692:ILE:HG22	2.02	0.59
1:A:466:VAL:CG1	1:A:470:LYS:HE3	2.33	0.58
1:C:716:ARG:O	1:C:719:LYS:HG3	2.03	0.58
1:C:713:MET:HB2	4:C:803:IKK:C6	2.35	0.56
1:A:575:LEU:HD11	1:A:591:MET:SD	2.46	0.56
1:D:693:TYR:OH	4:D:803:IKK:N9	2.37	0.56
1:A:541:LEU:HD22	1:A:553:ARG:HG2	1.87	0.55
1:C:542:GLN:NE2	5:C:903:HOH:O	2.39	0.55
1:A:675:LEU:O	1:A:678:VAL:HG22	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:GLU:N	1:A:750:PRO:CD	2.70	0.55
1:B:724:GLN:NE2	5:B:904:HOH:O	2.40	0.54
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.43	0.53
4:B:803:IKK:O17	4:B:803:IKK:N11	2.40	0.53
1:C:497:SER:OG	1:C:557:LEU:HD11	2.09	0.52
4:C:803:IKK:O17	4:C:803:IKK:N11	2.42	0.52
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.45	0.51
1:D:700:GLY:HA3	1:D:714:MET:O	2.10	0.51
1:D:524:TYR:CD2	1:D:692:ILE:HD13	2.45	0.51
1:B:467:ARG:O	1:B:471:GLU:HB2	2.10	0.51
1:B:700:GLY:HA3	1:B:714:MET:O	2.10	0.51
1:D:716:ARG:O	1:D:719:LYS:HG3	2.11	0.50
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.93	0.49
1:B:510:ARG:NH1	1:B:607:GLY:O	2.42	0.49
1:A:627:ARG:O	1:A:631:ILE:HG12	2.13	0.49
1:D:675:LEU:O	1:D:678:VAL:HG22	2.12	0.49
1:C:749:GLU:HB3	1:C:750:PRO:HD3	1.94	0.49
1:D:469:CYS:SG	5:D:997:HOH:O	2.57	0.49
1:A:713:MET:HG3	4:A:803:IKK:N9	2.28	0.48
1:D:727:LEU:HD23	1:D:731:ASN:ND2	2.29	0.48
1:C:713:MET:HB2	4:C:803:IKK:C28	2.43	0.48
1:C:730:TYR:HA	1:C:734:ALA:HB3	1.96	0.47
1:B:642:ARG:NH2	5:B:913:HOH:O	2.47	0.47
1:C:634:ASP:OD2	5:C:901:HOH:O	2.21	0.47
1:D:713:MET:HA	4:D:803:IKK:C27	2.45	0.46
1:C:553:ARG:NH1	5:C:919:HOH:O	2.49	0.46
1:A:466:VAL:HG13	1:A:470:LYS:HE3	1.97	0.46
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.97	0.46
1:D:740:THR:HA	1:D:743:GLN:HE21	1.80	0.46
1:D:766:ILE:HG22	1:D:766:ILE:O	2.15	0.45
1:B:638:TYR:OH	1:B:642:ARG:HD3	2.16	0.45
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.16	0.45
1:B:467:ARG:HA	1:B:470:LYS:HE3	1.99	0.45
1:D:486:TRP:N	1:D:487:PRO:CD	2.80	0.45
1:B:493:MET:O	1:B:497:SER:HB2	2.18	0.44
1:C:675:LEU:O	1:C:678:VAL:HG22	2.17	0.44
1:A:713:MET:HA	4:A:803:IKK:C26	2.48	0.44
1:B:767:ARG:NH2	1:B:769:GLU:OE1	2.51	0.43
1:C:486:TRP:N	1:C:487:PRO:CD	2.82	0.43
1:B:509:CME:O	1:B:513:MET:HG2	2.18	0.43
1:D:711:ILE:HD11	1:D:713:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.94	0.43
1:D:497:SER:HA	1:D:542:GLN:NE2	2.34	0.43
1:B:727:LEU:HD22	1:B:731:ASN:ND2	2.34	0.43
1:C:677:SER:OG	1:C:688:THR:HG21	2.18	0.43
1:C:693:TYR:OH	4:C:803:IKK:N9	2.52	0.43
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.00	0.42
1:D:479:ILE:HD11	1:D:528:LYS:HG3	2.01	0.42
1:D:619:TYR:O	1:D:622:VAL:HG12	2.19	0.42
1:A:689:ALA:O	1:A:692:ILE:HG22	2.19	0.42
1:D:735:ILE:HB	1:D:736:PRO:HD3	2.00	0.42
1:B:749:GLU:N	1:B:750:PRO:CD	2.83	0.41
1:A:494:VAL:O	1:A:498:CYS:HB3	2.21	0.41
1:C:568:ARG:NH1	5:C:925:HOH:O	2.53	0.41
1:D:766:ILE:O	1:D:766:ILE:CG2	2.69	0.41
1:A:535:HIS:O	1:A:538:TYR:HB3	2.20	0.41
1:C:467:ARG:O	1:C:471:GLU:HB2	2.20	0.41
1:B:689:ALA:O	1:B:692:ILE:HG22	2.21	0.41
1:A:644:GLN:CA	1:A:644:GLN:HE21	2.33	0.41
1:A:486:TRP:N	1:A:487:PRO:CD	2.84	0.40
4:A:803:IKK:N11	4:A:803:IKK:O17	2.53	0.40
1:B:562:CYS:HB3	1:B:565:LEU:HD12	2.04	0.40
1:D:477:PHE:HB3	1:D:535:HIS:CE1	2.57	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	310/343 (90%)	298 (96%)	12 (4%)	0	100	100
1	B	312/343 (91%)	304 (97%)	8 (3%)	0	100	100
1	C	310/343 (90%)	304 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	307/343 (90%)	298 (97%)	8 (3%)	1 (0%)	41	50
All	All	1239/1372 (90%)	1204 (97%)	34 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	466	VAL

### 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	281/305 (92%)	274 (98%)	7 (2%)	47	64
1	B	281/305 (92%)	276 (98%)	5 (2%)	59	74
1	C	281/305 (92%)	275 (98%)	6 (2%)	53	70
1	D	279/305 (92%)	272 (98%)	7 (2%)	47	64
All	All	1122/1220 (92%)	1097 (98%)	25 (2%)	52	68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	GLU
1	A	497	SER
1	A	504	GLU
1	A	587	SER
1	A	605	LEU
1	A	644	GLN
1	A	720	ASP
1	B	459	LEU
1	B	471	GLU
1	B	605	LEU
1	B	650	GLN
1	B	727	LEU
1	C	471	GLU

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Mol	Chain	Res	Type
1	C	517	LYS
1	C	547	LEU
1	C	575	LEU
1	C	616	SER
1	C	760	SER
1	D	459	LEU
1	D	573	SER
1	D	575	LEU
1	D	605	LEU
1	D	638	TYR
1	D	644	GLN
1	D	709	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	542	GLN
1	A	604	GLN
1	A	644	GLN
1	A	743	GLN
1	B	542	GLN
1	B	576	GLN
1	B	604	GLN
1	B	724	GLN
1	B	731	ASN
1	B	743	GLN
1	C	542	GLN
1	C	604	GLN
1	C	743	GLN
1	D	542	GLN
1	D	604	GLN
1	D	621	GLN
1	D	644	GLN
1	D	731	ASN
1	D	743	GLN
1	D	761	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	CME	D	509	1	8,9,10	0.49	0	5,9,11	0.20	0
1	CME	A	509	1	8,9,10	0.60	0	5,9,11	0.44	0
1	CME	B	509	1	8,9,10	0.46	0	5,9,11	0.29	0
1	CME	C	509	1	8,9,10	0.49	0	5,9,11	0.52	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
1	CME	D	509	1	-	2/5/8/10	-
1	CME	A	509	1	-	2/5/8/10	-
1	CME	B	509	1	-	1/5/8/10	-
1	CME	C	509	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	509	CME	CE-SD-SG-CB
1	A	509	CME	SD-CE-CZ-OH

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Mol	Chain	Res	Type	Atoms
1	C	509	CME	SD-CE-CZ-OH
1	B	509	CME	SD-CE-CZ-OH
1	A	509	CME	CZ-CE-SD-SG
1	D	509	CME	CZ-CE-SD-SG
1	D	509	CME	SD-CE-CZ-OH

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	509	CME	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	IKK	D	803	-	35,35,35	0.87	1 (2%)	43,49,49	1.88	13 (30%)
4	IKK	B	803	-	35,35,35	0.98	3 (8%)	43,49,49	1.93	10 (23%)
4	IKK	C	803	-	35,35,35	0.92	2 (5%)	43,49,49	1.77	9 (20%)
4	IKK	A	803	-	35,35,35	0.95	1 (2%)	43,49,49	1.95	11 (25%)

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	IKK	D	803	-	-	2/20/31/31	0/5/5/5
4	IKK	B	803	-	-	2/20/31/31	0/5/5/5
4	IKK	C	803	-	-	3/20/31/31	0/5/5/5
4	IKK	A	803	-	-	0/20/31/31	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	IKK	C1-C3	-2.47	1.46	1.50
4	A	803	IKK	C14-N4	2.36	1.49	1.46
4	B	803	IKK	C14-N4	2.28	1.49	1.46
4	D	803	IKK	C14-N4	2.28	1.49	1.46
4	C	803	IKK	C7-N2	-2.16	1.32	1.34
4	B	803	IKK	C23-C16	2.02	1.57	1.52
4	B	803	IKK	C1-C3	-2.01	1.47	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	IKK	C3-C1-N2	6.12	121.70	115.99
4	A	803	IKK	C15-N4-C6	-5.34	117.07	123.60
4	B	803	IKK	C31-N18-C25	5.04	122.25	115.80
4	D	803	IKK	C3-C1-N2	4.94	120.61	115.99
4	A	803	IKK	C30-N19-C25	4.73	121.86	115.80
4	C	803	IKK	C12-C8-C7	-4.56	114.98	120.33
4	C	803	IKK	C31-N18-C25	4.53	121.60	115.80
4	D	803	IKK	C31-N18-C25	4.46	121.50	115.80
4	A	803	IKK	C31-N18-C25	4.33	121.35	115.80
4	A	803	IKK	C3-C1-N2	4.27	119.98	115.99
4	C	803	IKK	C30-N19-C25	3.56	120.36	115.80
4	C	803	IKK	C15-N4-C6	-3.43	119.40	123.60
4	C	803	IKK	C3-C1-N2	3.41	119.18	115.99
4	B	803	IKK	C12-C8-C7	-3.38	116.36	120.33
4	B	803	IKK	C30-N19-C25	3.29	120.02	115.80
4	D	803	IKK	C14-C16-N10	3.23	119.60	112.69
4	D	803	IKK	O17-C3-N10	-3.20	116.56	122.45
4	D	803	IKK	C30-N19-C25	3.19	119.88	115.80
4	A	803	IKK	N19-C25-N18	-3.07	120.61	126.61
4	A	803	IKK	C12-C8-C7	-2.90	116.92	120.33
4	D	803	IKK	C15-N4-C6	-2.88	120.07	123.60
4	D	803	IKK	C16-N10-C3	-2.78	118.70	122.55
4	B	803	IKK	N19-C25-N18	-2.73	121.26	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	IKK	N19-C25-N18	-2.69	121.34	126.61
4	C	803	IKK	C24-C6-N4	-2.64	116.97	121.70
4	B	803	IKK	C8-C7-N2	2.52	122.18	117.17
4	B	803	IKK	C24-C28-C27	-2.49	116.61	119.24
4	A	803	IKK	C26-N9-C6	2.46	121.80	117.30
4	D	803	IKK	C26-N9-C6	2.43	121.74	117.30
4	D	803	IKK	C21-C31-N18	-2.42	118.34	123.13
4	C	803	IKK	C21-C31-N18	-2.35	118.48	123.13
4	A	803	IKK	C28-C27-CL29	2.34	123.01	119.35
4	D	803	IKK	N19-C25-N18	-2.26	122.19	126.61
4	A	803	IKK	C23-C15-N4	-2.24	100.72	103.35
4	D	803	IKK	N9-C6-N4	2.20	120.09	116.79
4	B	803	IKK	C21-C31-N18	-2.16	118.86	123.13
4	D	803	IKK	C24-C6-N4	-2.16	117.83	121.70
4	D	803	IKK	C8-C7-N2	2.15	121.43	117.17
4	C	803	IKK	N9-C6-N4	2.13	119.98	116.79
4	A	803	IKK	C15-N4-C14	2.08	116.94	111.55
4	B	803	IKK	C15-N4-C6	-2.08	121.06	123.60
4	B	803	IKK	C14-N4-C6	-2.07	121.06	123.60
4	A	803	IKK	C8-C7-N2	2.02	121.18	117.17

There are no chirality outliers.

All (7) torsion outliers are listed below:

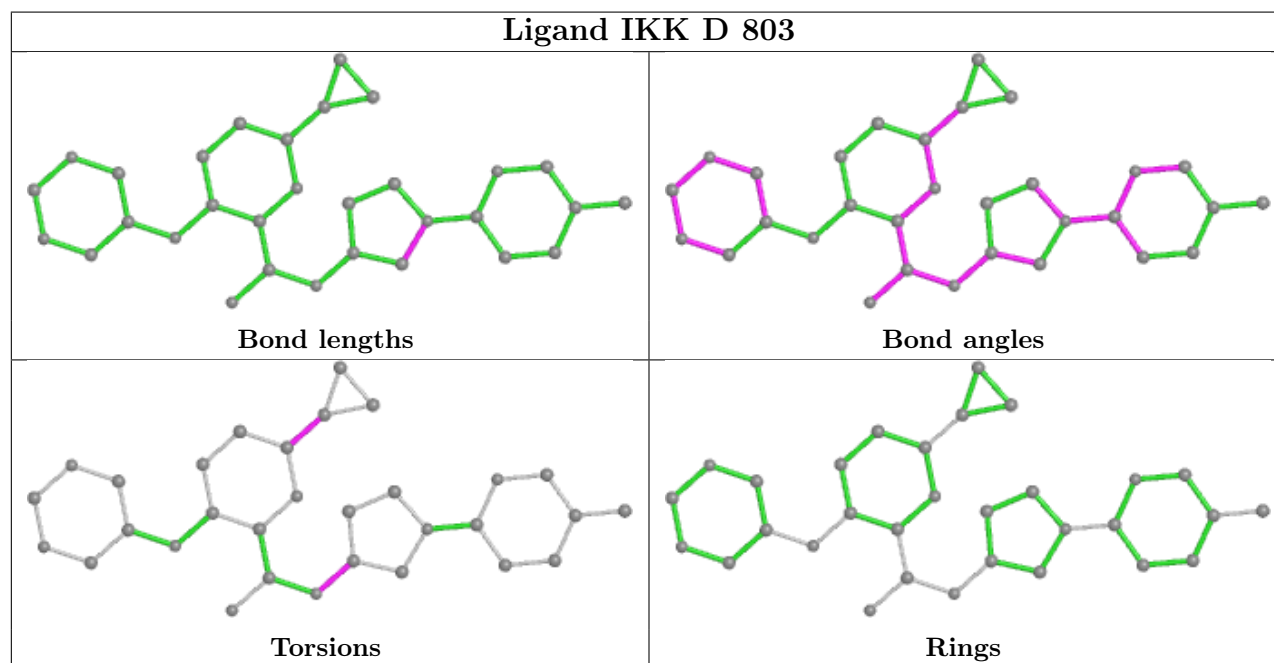
Mol	Chain	Res	Type	Atoms
4	C	803	IKK	N2-C7-C8-C12
4	D	803	IKK	N2-C7-C8-C13
4	B	803	IKK	C22-C7-C8-C12
4	C	803	IKK	N2-C7-C8-C13
4	B	803	IKK	C22-C7-C8-C13
4	C	803	IKK	C14-C16-N10-C3
4	D	803	IKK	C14-C16-N10-C3

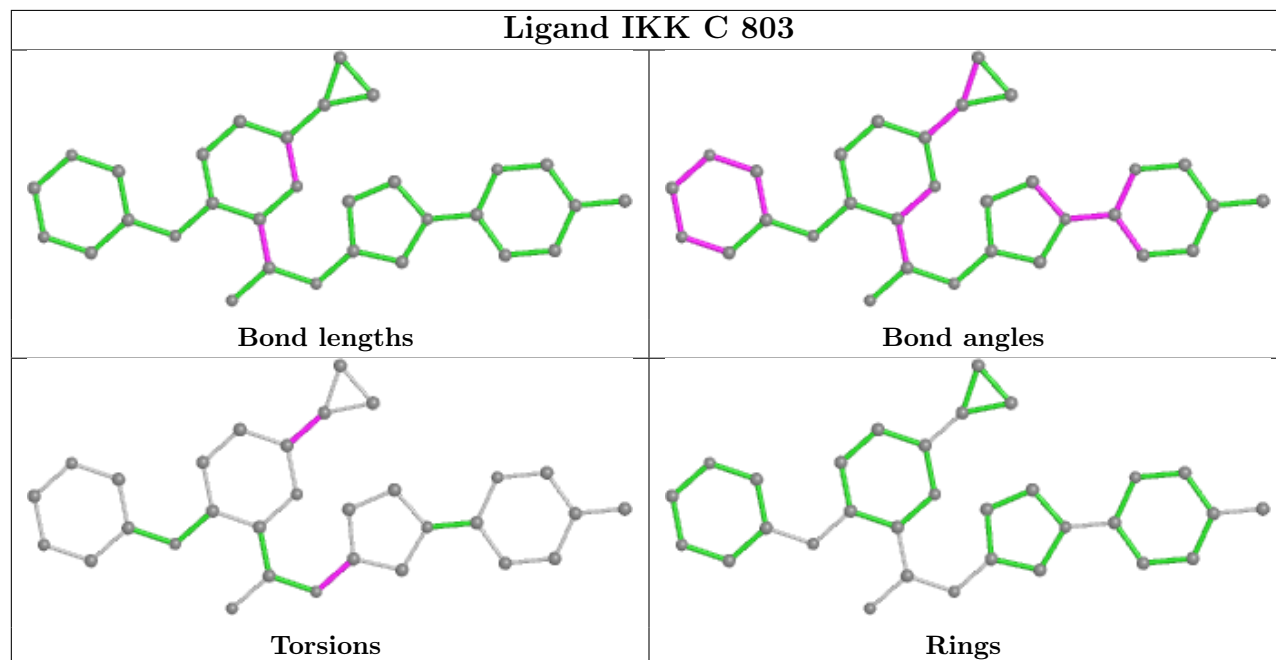
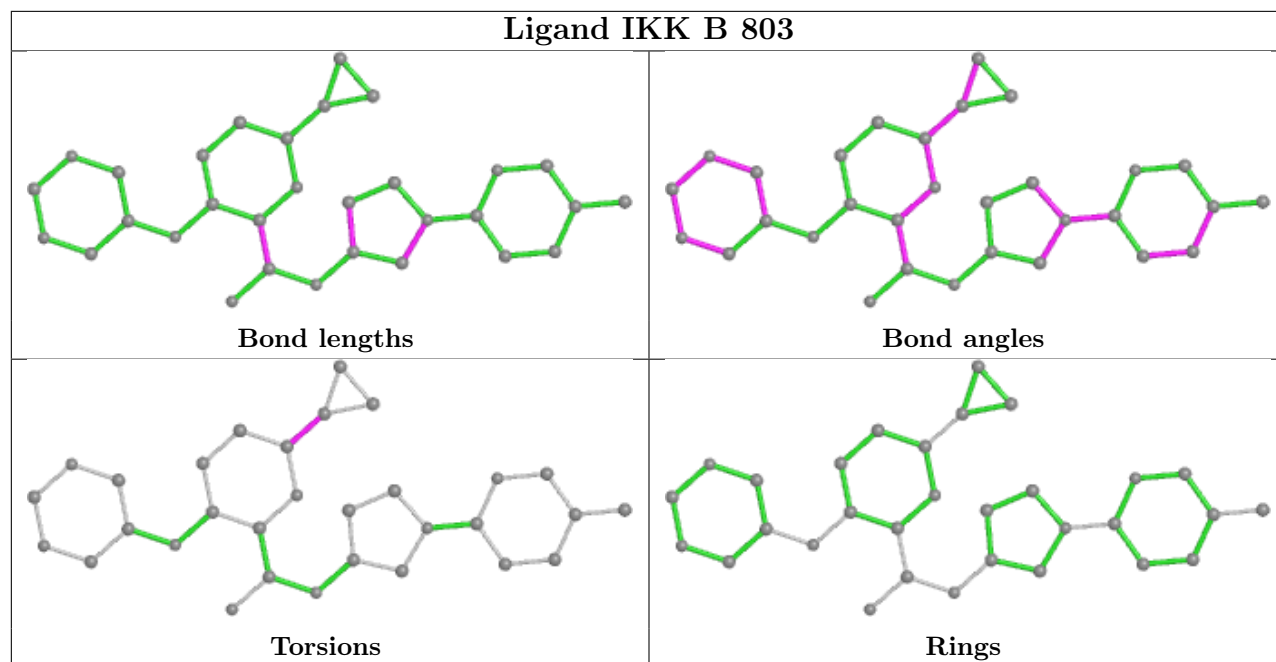
There are no ring outliers.

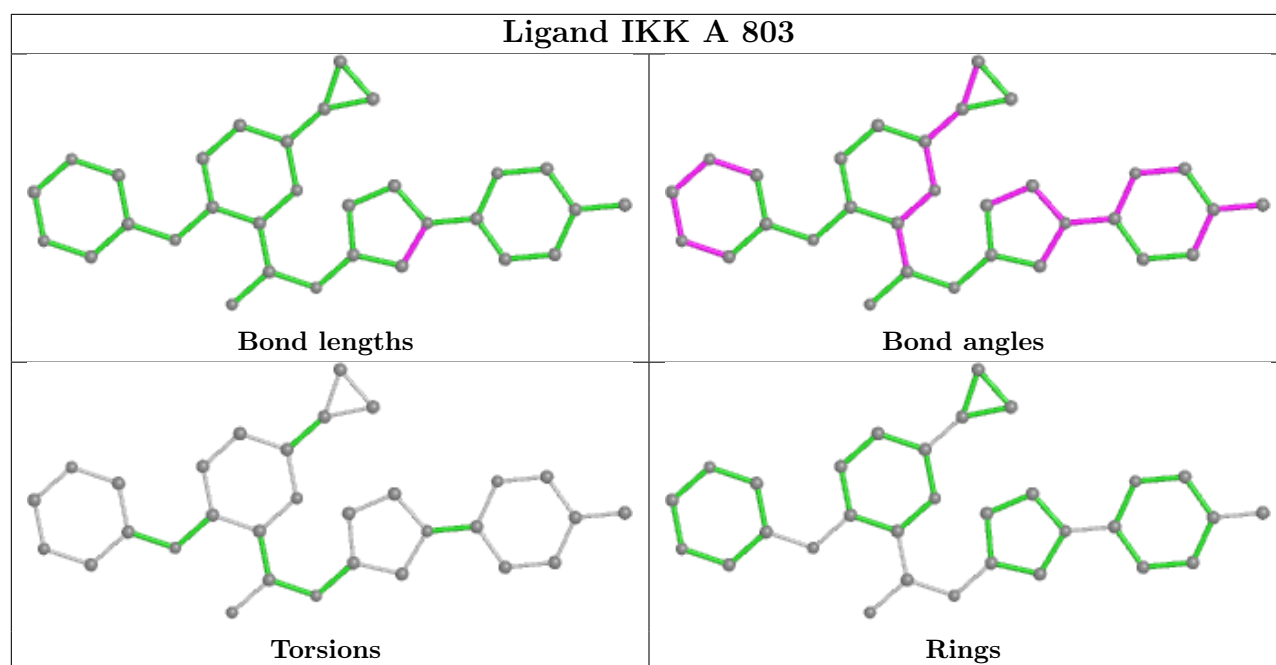
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	803	IKK	5	0
4	B	803	IKK	2	0
4	C	803	IKK	6	0
4	A	803	IKK	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	312/343 (90%)	-0.64	0 <b>100</b>   <b>100</b>	27, 37, 55, 75	0
1	B	314/343 (91%)	-0.68	1 (0%) <b>94</b>   <b>96</b>	26, 35, 52, 79	0
1	C	312/343 (90%)	-0.68	0 <b>100</b>   <b>100</b>	26, 36, 52, 73	0
1	D	309/343 (90%)	-0.65	0 <b>100</b>   <b>100</b>	31, 41, 53, 67	0
All	All	1247/1372 (90%)	-0.66	1 (0%) <b>95</b>   <b>97</b>	26, 38, 54, 79	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	457	GLN	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CME	B	509	10/11	0.94	0.11	36,42,53,56	0
1	CME	A	509	10/11	0.96	0.11	39,46,51,54	0
1	CME	C	509	10/11	0.96	0.10	37,42,58,58	0
1	CME	D	509	10/11	0.96	0.12	40,45,73,76	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

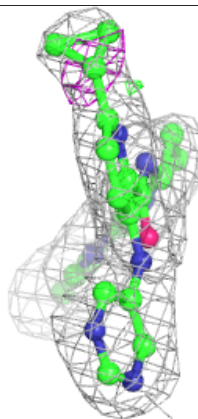
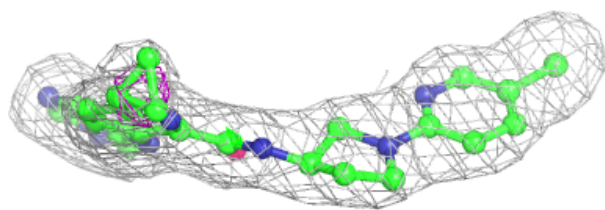
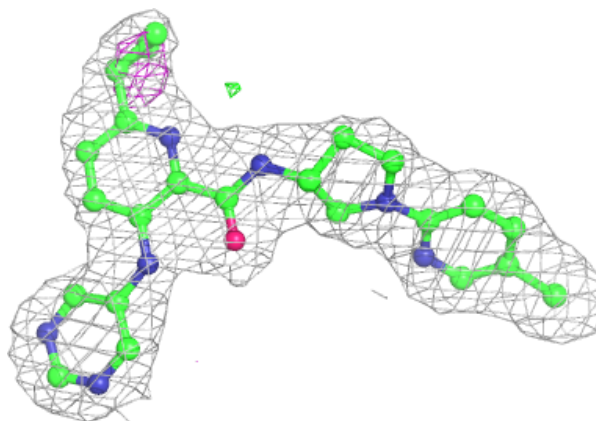
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	IKK	A	803	31/31	0.98	0.10	33,36,39,41	0
4	IKK	B	803	31/31	0.98	0.09	32,34,38,39	0
4	IKK	C	803	31/31	0.98	0.10	30,35,42,44	0
4	IKK	D	803	31/31	0.98	0.08	37,40,48,50	0
3	MG	C	802	1/1	0.99	0.09	27,27,27,27	0
3	MG	D	802	1/1	0.99	0.07	32,32,32,32	0
3	MG	A	802	1/1	0.99	0.08	28,28,28,28	0
2	ZN	C	801	1/1	1.00	0.11	32,32,32,32	0
2	ZN	D	801	1/1	1.00	0.11	35,35,35,35	0
2	ZN	A	801	1/1	1.00	0.11	32,32,32,32	0
3	MG	B	802	1/1	1.00	0.08	27,27,27,27	0
2	ZN	B	801	1/1	1.00	0.11	32,32,32,32	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 IKK A 803:**

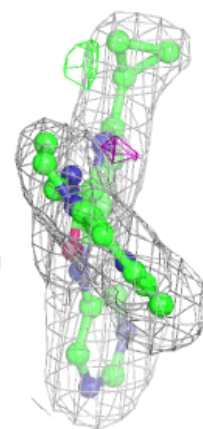
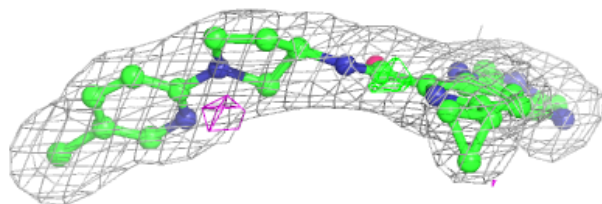
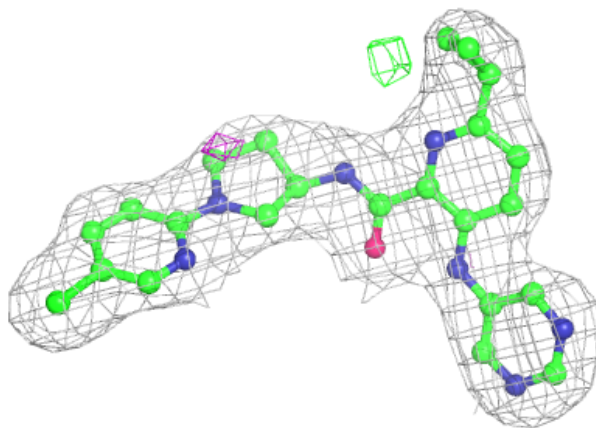
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





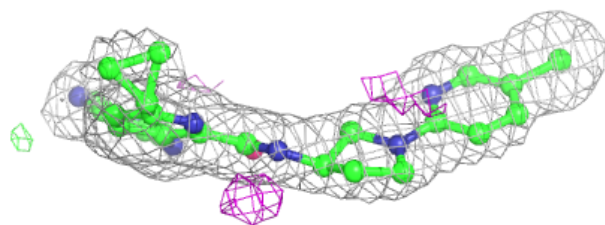
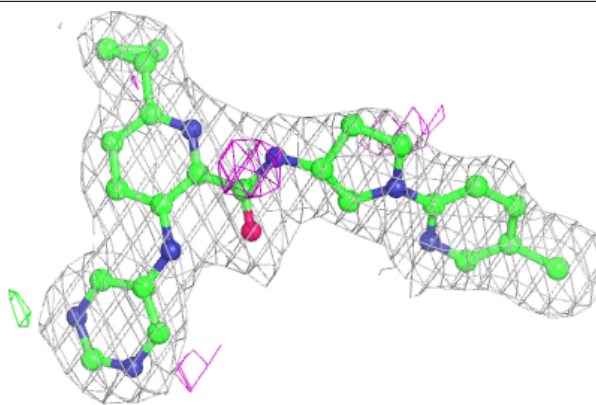
**Electron density around IKK B 803:**

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

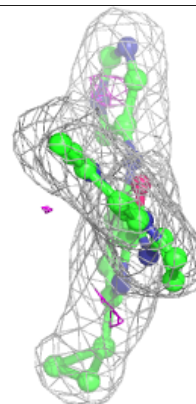
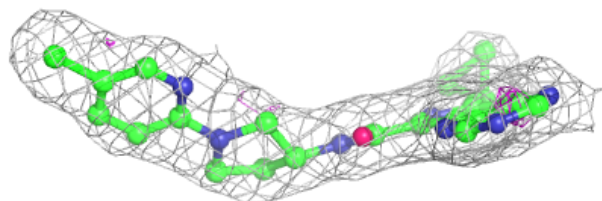
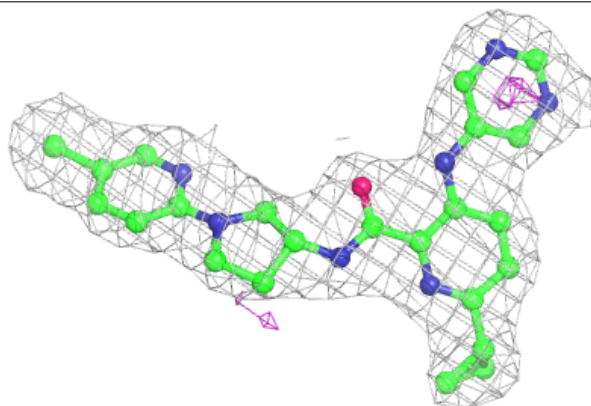


**Electron density around IKK C 803:**

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

**Electron density around IKK D 803:**

$2mF_o-DF_c$  (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.