

Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2022 – 08:11 PM EDT

PDB ID : 5SKE

Title : Crystal Structure of human phosphodiesterase 10 in complex with 2-tert-but

yl-5-(pyrimidin-5-ylamino)-N-[3-(trifluoromethoxy)phenyl]pyrimidine-4-carbo

xamide

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Deposited on : 2022-02-01

Resolution : 2.20 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

Mol Probity : 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)

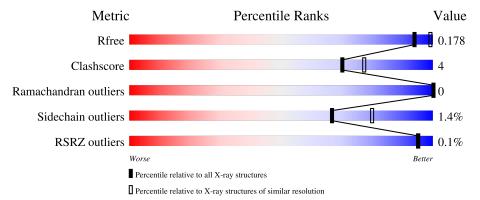
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 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	80%	11%	9%
1	В	343	84%	7%	8%
1	С	343	82%	9%	9%
1	D	343	84%	6% •	10%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10773 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	
1	Λ	313	Total	С	N	О	S	0	1	0
1	A	313	2549	1629	435	461	24		1	U
1	В	315	Total	С	N	О	S	0	1	0
1	Б	319	2559	1635	437	463	24	0	1	U
1	С	212	Total	С	N	О	S	0	2	0
1		313	2557	1634	438	461	24	U		U
1	D	310	Total	С	N	О	S	0	0	0
1	D	310	2519	1612	429	454	24	U		U

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
В	447	GLY	-	expression tag	UNP Q9Y233
В	448	SER	-	expression tag	UNP Q9Y233
С	447	GLY	-	expression tag	UNP Q9Y233
С	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).

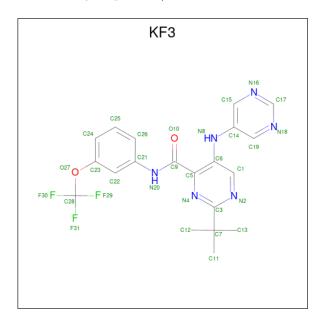
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0



•	Molecule 3 is	MAGNESIUM ION	(three-letter code:	MG)	(formula: Mg).
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

• Molecule 4 is 2-tert-butyl-5-[(pyrimidin-5-yl)amino]-N-[3-(trifluoromethoxy)phenyl]pyrimidi ne-4-carboxamide (three-letter code: KF3) (formula: $C_{20}H_{19}F_3N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	Λ	1	Total	С	F	N	О	0	0	
4	А	1	31	20	3	6	2	0	0	
4	R	1	Total	С	F	N	О	0	0	
4	D	1	31	20	3	6	2	0	U	
4	C	1	Total	С	F	N	О	0	0	
4	C	1	31	20	3	6	2	0	0	
4	D	1	Total	С	F	N	О	0	0	
4	ש	1	31	20	3	6	2		U	

• Molecule 5 is water.



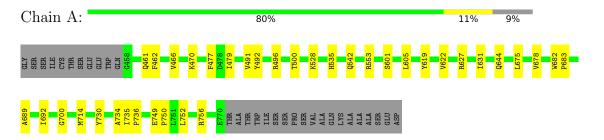
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	118	Total O 118 118	0	0
5	В	136	Total O 136 136	0	0
5	С	127	Total O 127 127	0	0
5	D	76	Total O 76 76	0	0



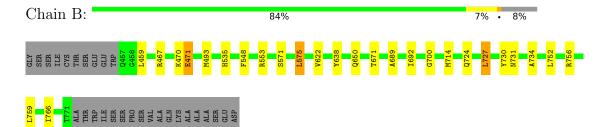
3 Residue-property plots (i)

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.

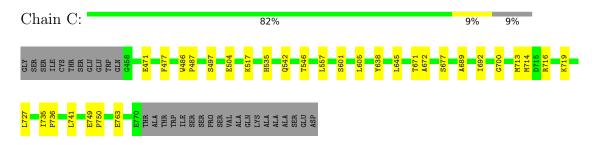
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



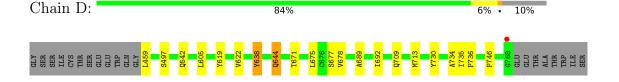
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



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



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





SER PRO SER VAL ALA GLN LYS ALA ALA ALA ALA ALA ALA ALA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	135.09Å 135.09Å 235.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.46 - 2.20 $43.46 - 2.20$	Depositor EDS
% Data completeness	99.9 (43.46-2.20)	Depositor
(in resolution range)	97.6 (43.46-2.20)	EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) > 1$	1.19 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D	0.177 , 0.215	Depositor
R, R_{free}	0.157 , 0.178	DCC
R_{free} test set	4068 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 27.2	EDS
L-test for twinning ²	$< L >=0.38, < L^2>=0.21$	Xtriage
Estimated twinning fraction	0.447 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.467 for H, K, L 0.533 for K, H, -L	Depositor
Outliers	0 of 81212 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10773	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: KF3, CME, ZN, MG

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.63	0/2603	0.67	0/3521	
1	В	0.63	0/2613	0.67	0/3535	
1	С	0.63	0/2614	0.67	0/3535	
1	D	0.64	0/2570	0.68	0/3478	
All	All	0.63	0/10400	0.67	0/14069	

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	2549	0	2524	24	0
1	В	2559	0	2528	16	0
1	С	2557	0	2537	20	0
1	D	2519	0	2496	13	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	С	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	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	0	0	0
4	В	31	0	0	2	0
4	С	31	0	0	3	0
4	D	31	0	0	3	0
5	A	118	0	0	0	0
5	В	136	0	0	1	0
5	С	127	0	0	1	0
5	D	76	0	0	0	0
All	All	10773	0	10085	74	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 (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.65	0.79
1:C:677:SER:OG	4:C:803:KF3:N18	2.18	0.76
1:B:724:GLN:NE2	5:B:901:HOH:O	2.15	0.70
1:C:689:ALA:O	1:C:692:ILE:HG22	1.92	0.69
1:D:644:GLN:HE21	1:D:644:GLN:HA	1.58	0.66
1:D:713:MET:SD	4:D:803:KF3:C25	2.87	0.62
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.11	0.62
1:C:546:THR:OG1	5:C:901:HOH:O	2.16	0.60
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.84	0.60
1:B:467:ARG:O	1:B:471:GLU:HB2	2.02	0.59
1:A:461:GLN:HE21	1:A:461:GLN:HA	1.71	0.56
1:A:689:ALA:HA	1:A:692:ILE:HG22	1.88	0.56
1:A:542:GLN:NE2	1:A:542:GLN:HA	2.20	0.55
1:B:727:LEU:HD22	1:B:731:ASN:ND2	2.22	0.55
1:B:548:PHE:O	1:B:553:ARG:NH1	2.40	0.55
1:C:497:SER:OG	1:C:557:LEU:HD11	2.07	0.55
1:D:713:MET:SD	4:D:803:KF3:C26	2.96	0.54
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.43	0.54
1:B:689:ALA:O	1:B:692:ILE:HG22	2.10	0.51
1:A:749:GLU:N	1:A:750:PRO:CD	2.74	0.51
1:A:689:ALA:O	1:A:692:ILE:HG22	2.11	0.50
1:A:479:ILE:HD11	1:A:528:LYS:HG3	1.93	0.50



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Continued from prev		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}\ (\mathring{\rm A})$	$overlap (\AA)$
1:C:497:SER:HA	1:C:542:GLN:HE22	1.77	0.50
1:B:727:LEU:HD23	1:B:759:LEU:HD11	1.94	0.50
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.94	0.49
1:A:461:GLN:HE22	1:A:500:THR:HG21	1.75	0.49
1:B:752:LEU:HD21	1:B:756[B]:ARG:NH2	2.28	0.49
1:C:716:ARG:O	1:C:719:LYS:HG3	2.14	0.48
1:B:727:LEU:HD12	1:B:766:ILE:HD13	1.95	0.48
1:A:461:GLN:HA	1:A:461:GLN:NE2	2.29	0.48
1:C:601:SER:O	1:C:605:LEU:HD13	2.15	0.47
1:C:497:SER:HA	1:C:542:GLN:NE2	2.30	0.47
4:B:803:KF3:O10	4:B:803:KF3:N8	2.47	0.47
1:C:700:GLY:HA3	1:C:714:MET:O	2.16	0.46
1:D:675:LEU:O	1:D:678:VAL:HG22	2.14	0.46
1:C:486:TRP:N	1:C:487:PRO:CD	2.79	0.46
4:B:803:KF3:F29	4:B:803:KF3:C22	2.54	0.46
1:D:689:ALA:HA	1:D:692:ILE:HG22	1.97	0.46
1:C:672:ALA:CB	1:C:741:LEU:HD22	2.46	0.45
1:A:461:GLN:HE22	1:A:500:THR:HG22	1.80	0.45
1:C:689:ALA:HA	1:C:692:ILE:HG22	1.99	0.45
1:D:619:TYR:O	1:D:622:VAL:HG12	2.17	0.45
1:A:675:LEU:O	1:A:678:VAL:HG22	2.16	0.45
1:C:749:GLU:HB3	1:C:750:PRO:HD3	1.99	0.45
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.52	0.44
1:A:627:ARG:O	1:A:631:ILE:HG12	2.17	0.44
1:B:638:TYR:CD1	1:B:671:THR:HG21	2.52	0.44
1:A:601:SER:O	1:A:605:LEU:HD13	2.18	0.44
1:B:727:LEU:HD22	1:B:731:ASN:HD21	1.83	0.44
1:C:477:PHE:HB3	1:C:535:HIS:CE1	2.52	0.44
1:A:700:GLY:HA3	1:A:714:MET:O	2.18	0.44
1:A:462:PHE:CE1	1:A:491:VAL:HG11	2.53	0.43
1:D:735:ILE:HB	1:D:736:PRO:HD3	1.99	0.43
1:A:752:LEU:HD21	1:A:756[B]:ARG:NH2	2.34	0.43
1:C:645:LEU:HD23	1:C:645:LEU:HA	1.90	0.43
1:A:682:TRP:N	1:A:683:PRO:CD	2.82	0.43
1:B:470:LYS:HE2	1:D:746:PRO:CG	2.43	0.42
1:C:727:LEU:HD21	1:C:763:GLU:HG3	2.00	0.42
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.02	0.42
1:B:730:TYR:HA	1:B:734:ALA:HB3	2.01	0.42
1:A:466:VAL:HG13	1:A:470:LYS:HE3	2.01	0.42
1:C:713:MET:SD	4:C:803:KF3:C25	3.08	0.42
1:B:700:GLY:HA3	1:B:714:MET:O	2.20	0.42



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance} ({ m \AA})$	overlap (Å)
1:B:493:MET:SD	1:B:535:HIS:HA	2.60	0.41
1:D:497:SER:HA	1:D:542:GLN:NE2	2.35	0.41
1:A:466:VAL:CG1	1:A:470:LYS:HE3	2.50	0.41
1:B:571:SER:O	1:B:575:LEU:HD23	2.20	0.41
1:A:619:TYR:O	1:A:622:VAL:HG12	2.21	0.41
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.56	0.41
1:C:689:ALA:O	1:C:692:ILE:CG2	2.67	0.41
1:D:638:TYR:CD1	1:D:671:THR:HG21	2.56	0.41
1:D:677:SER:OG	4:D:803:KF3:N18	2.54	0.41
1:C:735:ILE:HB	1:C:736:PRO:HD3	2.02	0.40
4:C:803:KF3:C19	4:C:803:KF3:C1	2.99	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	Perce	ntiles
1	A	311/343~(91%)	305 (98%)	6 (2%)	0	100	100
1	В	313/343~(91%)	307 (98%)	6 (2%)	0	100	100
1	\mathbf{C}	312/343~(91%)	306 (98%)	6 (2%)	0	100	100
1	D	307/343~(90%)	300 (98%)	7 (2%)	0	100	100
All	All	$1243/1372 \ (91\%)$	1218 (98%)	25 (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	282/305~(92%)	280 (99%)	2 (1%)	84 91
1	В	282/305~(92%)	276 (98%)	6 (2%)	53 67
1	С	283/305 (93%)	280 (99%)	3 (1%)	73 85
1	D	279/305~(92%)	274 (98%)	5 (2%)	59 72
All	All	1126/1220 (92%)	1110 (99%)	16 (1%)	67 80

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	553	ARG
1	A	644	GLN
1	В	459	LEU
1	В	471	GLU
1	В	575	LEU
1	В	622	VAL
1	В	650	GLN
1	В	727	LEU
1	С	471	GLU
1	С	504	GLU
1	С	517	LYS
1	D	459	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 (20) 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	В	484	ASN
1	В	604	GLN
1	В	650	GLN



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Mol	Chain	Res	Type
1	В	731	ASN
1	С	542	GLN
1	С	604	GLN
1	С	743	GLN
1	D	484	ASN
1	D	542	GLN
1	D	604	GLN
1	D	621	GLN
1	D	644	GLN
1	D	731	ASN
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	Chain	Chain	Chain	Chain	Res	Link	Bond lengths			Bond angles		
Moi Type	nes		Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2					
1	CME	D	509	1	8,9,10	0.45	0	5,9,11	0.24	0				
1	CME	С	509	1	8,9,10	0.53	0	5,9,11	0.47	0				
1	CME	В	509	1	8,9,10	0.49	0	5,9,11	0.26	0				
1	CME	A	509	1	8,9,10	0.51	0	5,9,11	0.31	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	-	1/5/8/10	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	С	509	1	-	3/5/8/10	_
1	CME	В	509	1	-	0/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	С	509	CME	CE-SD-SG-CB
1	A	509	CME	CZ-CE-SD-SG
1	D	509	CME	CZ-CE-SD-SG
1	С	509	CME	SD-CE-CZ-OH
1	С	509	CME	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

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	Type	Chain	Res	Link	Во	ond leng	$ ag{ths}$	В	ond ang	les
		Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
	4	KF3	В	803	-	33,33,33	1.43	4 (12%)	43,48,48	1.25	3 (6%)
	4	KF3	A	803	-	33,33,33	1.45	4 (12%)	43,48,48	1.39	4 (9%)



Ma	Trino	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
Mol T	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	KF3	D	803	-	33,33,33	1.44	4 (12%)	43,48,48	1.28	3 (6%)
4	KF3	С	803	-	33,33,33	1.38	4 (12%)	43,48,48	1.46	6 (13%)

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	KF3	В	803	-	-	2/23/23/23	0/3/3/3
4	KF3	A	803	-	-	2/23/23/23	0/3/3/3
4	KF3	D	803	-	-	2/23/23/23	0/3/3/3
4	KF3	С	803	-	-	2/23/23/23	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
4	В	803	KF3	C3-N2	3.75	1.38	1.33
4	A	803	KF3	C3-N2	3.68	1.38	1.33
4	С	803	KF3	C1-C6	3.62	1.45	1.39
4	С	803	KF3	C3-N2	3.47	1.38	1.33
4	D	803	KF3	C3-N2	3.47	1.38	1.33
4	В	803	KF3	C1-C6	3.29	1.44	1.39
4	D	803	KF3	C1-C6	3.25	1.44	1.39
4	A	803	KF3	C1-C6	3.17	1.44	1.39
4	D	803	KF3	C15-C14	2.96	1.44	1.39
4	В	803	KF3	C19-C14	2.62	1.44	1.39
4	A	803	KF3	C15-C14	2.60	1.44	1.39
4	В	803	KF3	C15-C14	2.32	1.43	1.39
4	С	803	KF3	C22-C21	2.28	1.43	1.39
4	A	803	KF3	C19-C14	2.27	1.43	1.39
4	D	803	KF3	C26-C21	2.18	1.42	1.39
4	С	803	KF3	C26-C21	2.02	1.42	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
4	С	803	KF3	N2-C3-N4	-5.76	124.11	130.06
4	A	803	KF3	N2-C3-N4	-5.52	124.35	130.06
4	D	803	KF3	N2-C3-N4	-5.45	124.43	130.06
4	В	803	KF3	N2-C3-N4	-4.28	125.64	130.06



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	803	KF3	C9-C5-N4	3.81	119.55	115.99
4	A	803	KF3	C9-C5-N4	3.43	119.20	115.99
4	С	803	KF3	C9-C5-N4	3.16	118.94	115.99
4	С	803	KF3	C7-C3-N2	2.57	121.76	117.48
4	D	803	KF3	C1-N2-C3	2.41	117.73	114.82
4	С	803	KF3	C11-C7-C3	2.34	114.83	109.57
4	A	803	KF3	C12-C7-C3	-2.18	104.67	109.57
4	В	803	KF3	F30-C28-O27	-2.12	102.27	111.71
4	A	803	KF3	C1-N2-C3	2.12	117.38	114.82
4	D	803	KF3	C9-C5-N4	2.05	117.91	115.99
4	С	803	KF3	C7-C3-N4	-2.04	114.09	117.48
4	С	803	KF3	C6-C1-N2	2.03	123.56	121.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	803	KF3	C22-C23-O27-C28
4	В	803	KF3	C24-C23-O27-C28
4	С	803	KF3	C22-C23-O27-C28
4	D	803	KF3	C22-C23-O27-C28
4	A	803	KF3	C22-C23-O27-C28
4	С	803	KF3	C24-C23-O27-C28
4	D	803	KF3	C24-C23-O27-C28
4	A	803	KF3	C24-C23-O27-C28

There are no ring outliers.

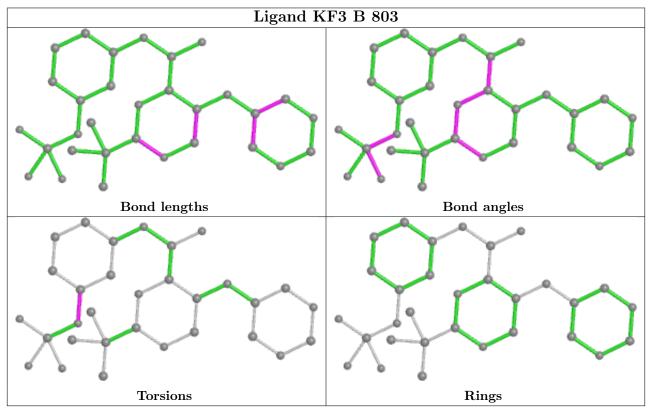
3 monomers are involved in 8 short contacts:

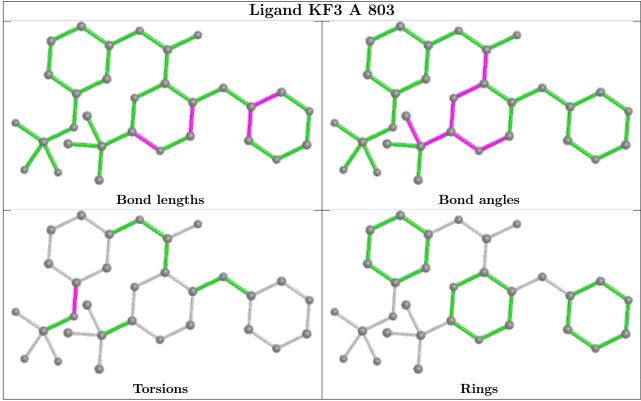
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	803	KF3	2	0
4	D	803	KF3	3	0
4	С	803	KF3	3	0

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

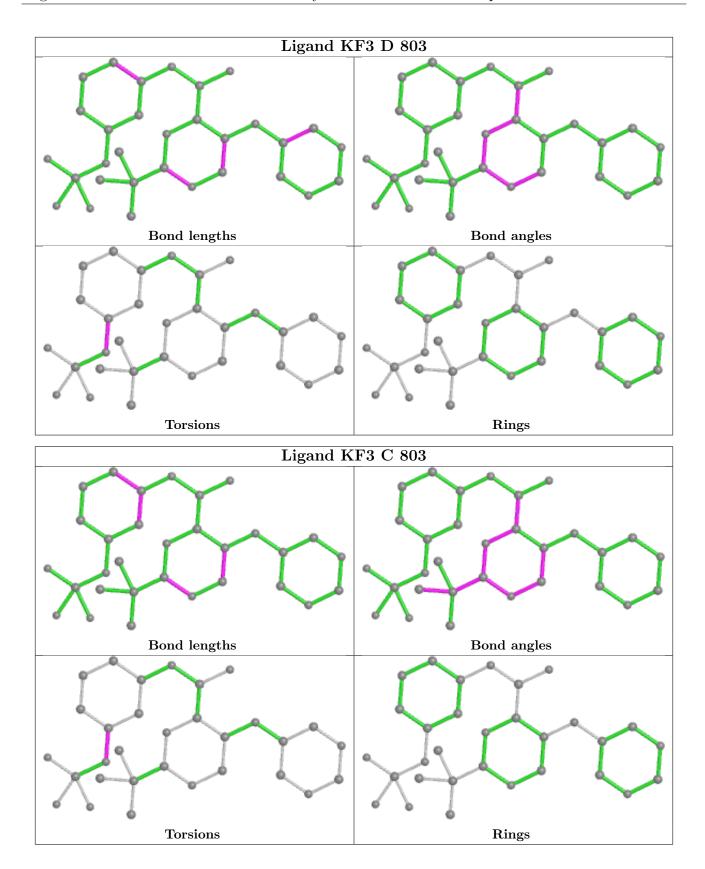


average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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^{th} 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	$\langle { m RSRZ} \rangle$	#RS	RZ>2	$OWAB(A^2)$	Q<0.9
1	A	312/343 (90%)	-0.65	0 100	100	27, 40, 64, 88	0
1	В	314/343 (91%)	-0.61	0 100	100	28, 40, 63, 90	0
1	С	312/343 (90%)	-0.63	0 100	100	29, 41, 62, 89	0
1	D	309/343 (90%)	-0.65	1 (0%)	94 93	34, 48, 66, 90	0
All	All	1247/1372 (90%)	-0.64	1 (0%)	95 95	27, 43, 65, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	768	GLY	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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	CME	A	509	10/11	0.95	0.09	45,54,68,69	0
1	CME	D	509	10/11	0.95	0.14	51,61,84,86	0
1	CME	В	509	10/11	0.96	0.12	49,58,84,87	0
1	CME	С	509	10/11	0.97	0.08	44,51,71,72	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



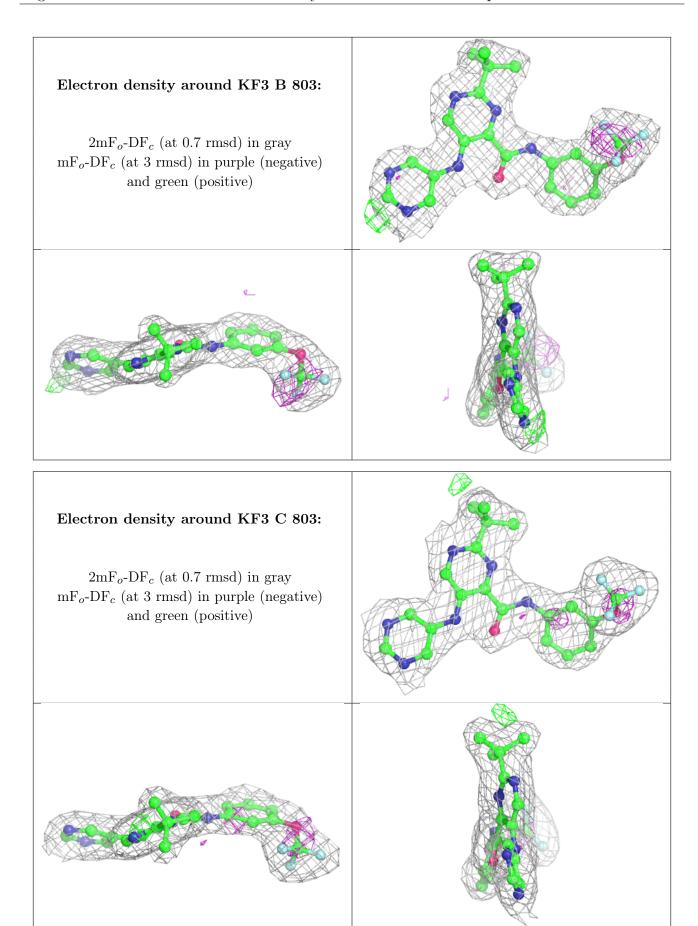
6.4 Ligands (i)

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	KF3	В	803	31/31	0.97	0.09	33,38,42,47	0
4	KF3	С	803	31/31	0.97	0.08	34,38,46,50	0
4	KF3	D	803	31/31	0.97	0.09	34,39,47,49	0
4	KF3	A	803	31/31	0.98	0.08	32,37,42,45	0
3	MG	A	802	1/1	0.99	0.09	25,25,25,25	0
3	MG	В	802	1/1	0.99	0.11	26,26,26,26	0
3	MG	С	802	1/1	0.99	0.10	27,27,27,27	0
3	MG	D	802	1/1	0.99	0.09	34,34,34,34	0
2	ZN	A	801	1/1	1.00	0.14	33,33,33,33	0
2	ZN	В	801	1/1	1.00	0.14	32,32,32,32	0
2	ZN	С	801	1/1	1.00	0.13	35,35,35,35	0
2	ZN	D	801	1/1	1.00	0.11	40,40,40,40	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.

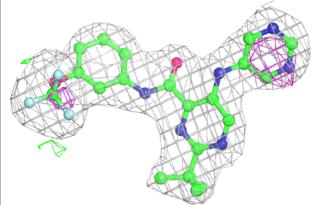


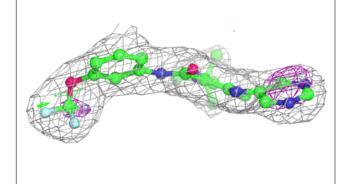


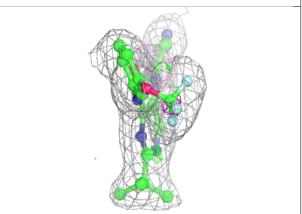


Electron density around KF3 D 803:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

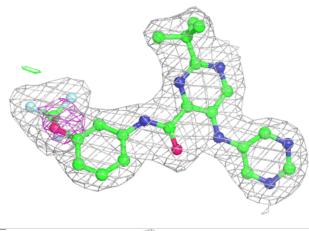


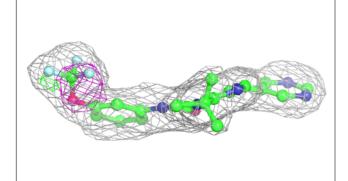


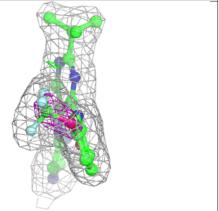


Electron density around KF3 A 803:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

