



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 11:39 PM EDT

PDB ID : 5SKQ
Title : Crystal Structure of human phosphodiesterase 10 in complex with N-ethyl-6-(4-fluorophenyl)sulfanyl-N-methyl-9H-purin-2-amine
Authors : Joseph, C.; Benz, J.; Flohr, A.; Brunner, M.; Rudolph, M.G.
Deposited on : 2022-02-01
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

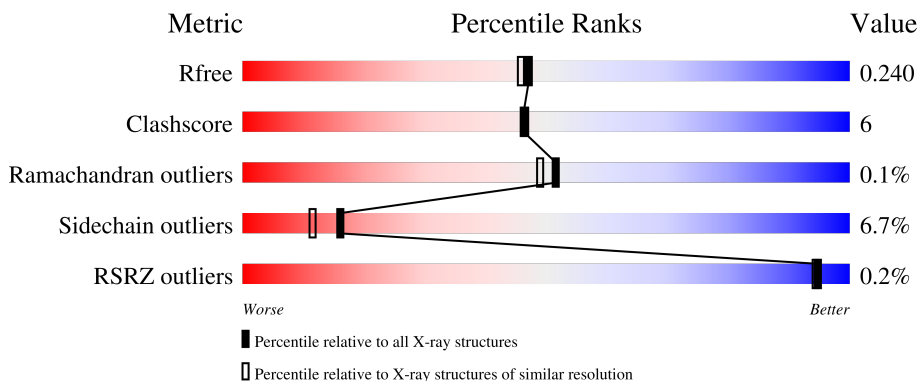
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	343	 75% 14% • 9%
1	B	343	 77% 13% • 8%
1	C	343	 78% 12% • 9%
1	D	343	 73% 17% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11008 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	Total 2565	C 1640	N 432	O 467	S 26	0	5	0
1	B	315	Total 2562	C 1637	N 437	O 463	S 25	0	2	0
1	C	313	Total 2558	C 1635	N 435	O 463	S 25	0	4	0
1	D	313	Total 2537	C 1622	N 433	O 458	S 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

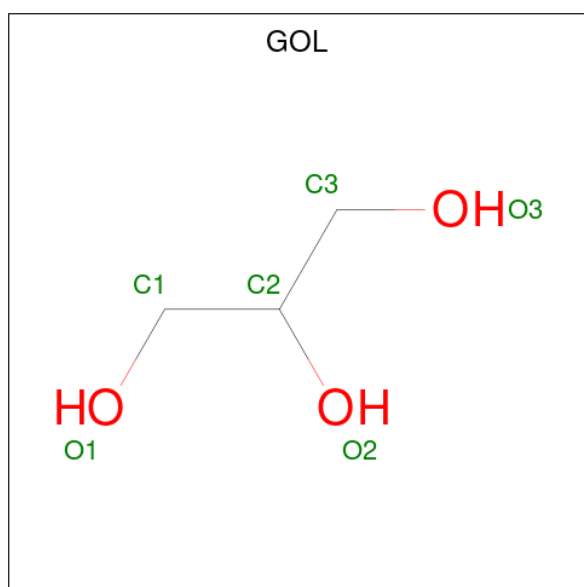
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

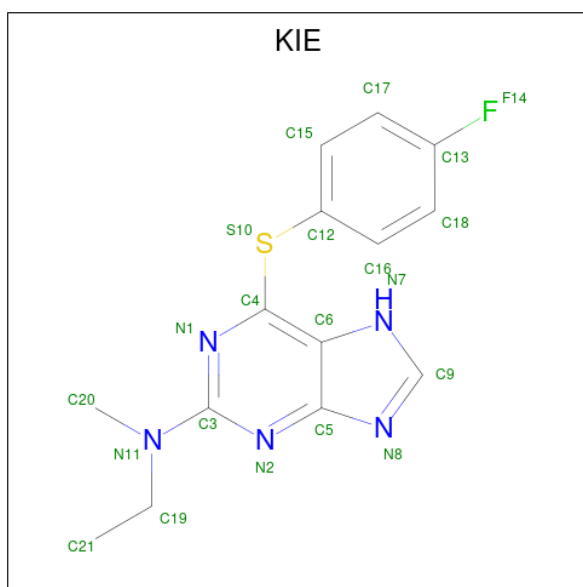
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is N-ethyl-6-[(4-fluorophenyl)sulfanyl]-N-methyl-7H-purin-2-amine (three-letter code: KIE) (formula: C₁₄H₁₄FN₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	S		
5	A	1	21	14	1	5	1	0	0
5	B	1	21	14	1	5	1	0	0
5	C	1	21	14	1	5	1	0	0

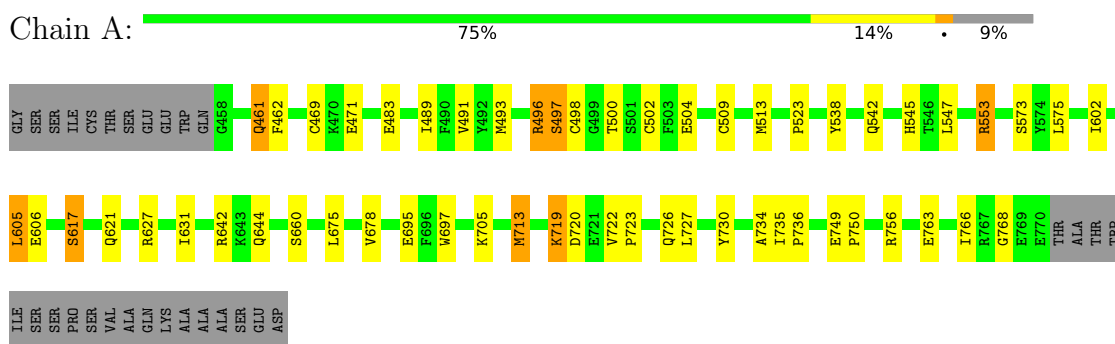
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	176	176	176	0	0
6	B	196	196	196	0	0
6	C	199	199	199	0	0
6	D	138	138	138	0	0

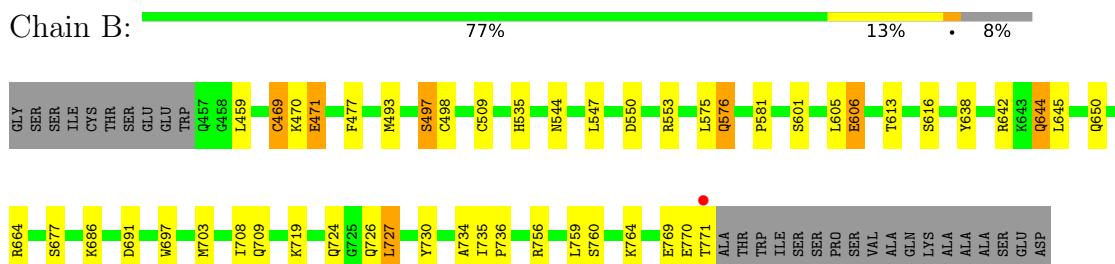
3 Residue-property plots i

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.

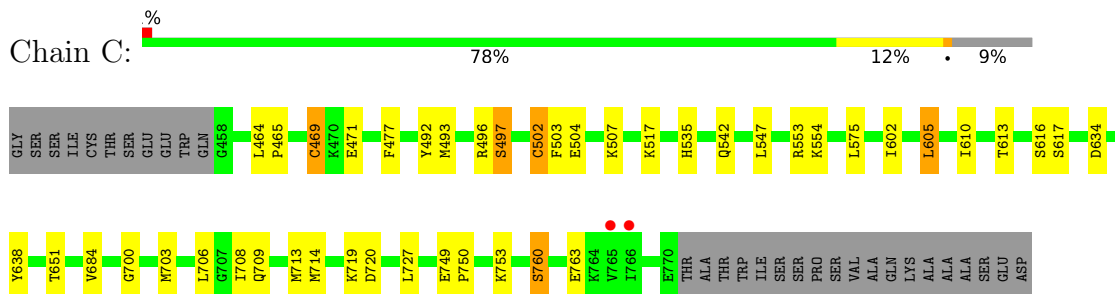
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- 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



GLY	W456	R467	L468	C469	R470	E471	E483	W486	Y492	M493	R496	S497	C498	Q499	T500	S501	C502	F503	E504	K517	H545	R553	K554	L575	Q576	L605	T613	S616	S617	V622	I625																	
I626	R627	I631	Y638	Y649	T671	L675	C676	S677	V678	T688	W697	Q709	P710	I711	P712	M713	M714	K719	D720	E721	V722	P723	Q724	L727	Y730	A734	I735	P736	P746	L752	R756	Q761	W762	E763	K764	V765	I766	R767	C768	GLU	GLU	THR	ALA					
THR	TRP	ILE	SER	SER	PRO	SER	VAL	ALA	GLN	LYS	ALA	ALA	ALA	SER	GLU	ASP																																

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	135.50Å 135.50Å 235.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.64 – 2.00 43.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	54.5 (43.64-2.00) 54.6 (43.64-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.169 , 0.235 0.178 , 0.240	Depositor DCC
R_{free} test set	3306 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11008	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.76	0/2631	0.86	0/3559
1	B	0.75	0/2619	0.88	0/3543
1	C	0.74	0/2621	0.85	0/3545
1	D	0.74	0/2588	0.88	1/3502 (0.0%)
All	All	0.75	0/10459	0.87	1/14149 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	498	CYS	CA-CB-SG	6.66	125.99	114.00

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	2565	0	2539	38	0
1	B	2562	0	2533	34	0
1	C	2558	0	2539	24	0
1	D	2537	0	2509	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	2	0
5	A	21	0	0	4	0
5	B	21	0	0	2	0
5	C	21	0	0	1	0
6	A	176	0	0	6	0
6	B	196	0	0	10	0
6	C	199	0	0	8	0
6	D	138	0	0	4	0
All	All	11008	0	10128	128	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 (128) 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:469[B]:CYS:SG	6:C:1078:HOH:O	2.12	1.07
1:B:606:GLU:HG2	6:B:1064:HOH:O	1.59	1.02
1:A:461:GLN:NE2	1:A:461:GLN:HA	1.76	0.96
5:C:803:KIE:C16	5:C:803:KIE:N1	2.33	0.87
1:B:644:GLN:HE21	1:B:644:GLN:HA	1.45	0.82
1:A:726:GLN:NE2	5:A:804:KIE:N8	2.27	0.81
1:A:642:ARG:NH2	6:A:901:HOH:O	2.12	0.81
1:C:553:ARG:NH1	6:C:902:HOH:O	2.16	0.77
1:C:493:MET:O	1:C:497:SER:HB2	1.84	0.77
1:B:493:MET:O	1:B:497:SER:HB2	1.84	0.77
1:A:713:MET:SD	5:A:804:KIE:C19	2.74	0.76
1:C:760:SER:OG	6:C:901:HOH:O	2.03	0.75
1:A:726:GLN:HE22	5:A:804:KIE:C9	2.00	0.75
1:D:469:CYS:SG	6:D:1030:HOH:O	2.46	0.72
1:A:469[A]:CYS:SG	6:A:1016:HOH:O	2.46	0.72
1:B:726:GLN:NE2	5:B:803:KIE:N8	2.38	0.67
1:B:703:MET:HE1	1:B:708:ILE:HG21	1.76	0.66
5:A:804:KIE:C16	5:A:804:KIE:N1	2.57	0.65
1:B:691:ASP:OD2	6:B:902:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:MET:O	1:A:497:SER:HB2	1.96	0.64
1:B:550:ASP:OD1	6:B:901:HOH:O	2.15	0.64
1:B:644:GLN:HA	1:B:644:GLN:NE2	2.14	0.63
1:C:651:THR:HG23	6:C:1082:HOH:O	1.99	0.63
1:B:770:GLU:HG3	1:B:771:THR:N	2.15	0.62
5:B:803:KIE:C16	5:B:803:KIE:N1	2.62	0.61
1:A:727:LEU:HD21	1:A:763:GLU:HG3	1.83	0.61
1:A:553:ARG:CD	6:A:1020:HOH:O	2.49	0.61
1:B:727:LEU:HD23	1:B:759:LEU:HD11	1.81	0.61
1:D:622:VAL:HA	1:D:625:ILE:HD12	1.84	0.59
1:A:461:GLN:NE2	1:A:500:THR:HG21	2.17	0.59
1:D:493:MET:O	1:D:497:SER:CB	2.50	0.59
1:A:553:ARG:HD3	6:A:1020:HOH:O	2.02	0.58
1:D:727:LEU:HD12	1:D:766:ILE:CD1	2.33	0.58
1:B:644:GLN:HE21	1:B:644:GLN:CA	2.14	0.58
1:D:498:CYS:HB2	1:D:553:ARG:HB3	1.85	0.58
1:B:697:TRP:CZ2	1:B:719:LYS:HG2	2.39	0.58
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.86	0.57
1:D:675:LEU:O	1:D:678:VAL:HG22	2.05	0.57
1:C:749:GLU:HB3	1:C:750:PRO:HD3	1.87	0.57
1:B:509:CME:HB2	6:B:1066:HOH:O	2.04	0.56
1:D:627:ARG:O	1:D:631:ILE:HG12	2.05	0.56
1:A:461:GLN:NE2	1:A:500:THR:CG2	2.69	0.56
1:D:727:LEU:CD1	1:D:766:ILE:HD12	2.36	0.56
1:D:752:LEU:HD21	1:D:756:ARG:NH2	2.21	0.55
1:A:496:ARG:HD3	1:A:538:TYR:OH	2.07	0.55
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.41	0.55
1:A:461:GLN:NE2	1:A:461:GLN:CA	2.59	0.55
1:A:489:ILE:O	1:A:493:MET:HG3	2.06	0.55
1:B:764:LYS:HD3	1:B:769:GLU:HG2	1.87	0.55
1:C:727:LEU:HD21	1:C:763:GLU:HG3	1.89	0.54
1:C:602:ILE:HA	1:C:605:LEU:HD22	1.88	0.54
1:D:711:ILE:HD11	1:D:713:MET:HE2	1.88	0.54
1:B:470:LYS:HG3	1:B:471:GLU:N	2.24	0.53
1:D:467:ARG:O	1:D:471:GLU:HB2	2.09	0.53
1:B:544:ASN:HB3	1:B:547:LEU:HD22	1.90	0.52
1:A:483[A]:GLU:H	4:A:803:GOL:H31	1.74	0.52
1:A:483[B]:GLU:H	4:A:803:GOL:H31	1.74	0.52
1:B:756[B]:ARG:HD2	6:B:989:HOH:O	2.08	0.52
1:D:677:SER:HB2	1:D:688:THR:HG21	1.91	0.52
1:B:727:LEU:HD23	1:B:759:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:LYS:HE2	6:C:1028:HOH:O	2.11	0.51
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.92	0.50
1:A:749:GLU:N	1:A:750:PRO:CD	2.75	0.50
1:C:503:PHE:CE2	1:C:610:ILE:HD12	2.46	0.50
1:C:651:THR:CG2	6:C:1082:HOH:O	2.56	0.50
1:A:553:ARG:HD2	6:A:1020:HOH:O	2.12	0.50
1:A:498:CYS:SG	1:A:502[A]:CYS:CB	2.99	0.50
1:A:509:CME:O	1:A:513:MET:HG2	2.12	0.50
1:B:601:SER:O	1:B:605:LEU:HD13	2.12	0.49
1:B:727:LEU:CD2	1:B:759:LEU:HD11	2.42	0.49
1:B:730:TYR:HA	1:B:734:ALA:HB3	1.94	0.49
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.95	0.49
1:D:493:MET:O	1:D:497:SER:HB3	2.12	0.48
1:C:703:MET:HE1	1:C:708:ILE:HG21	1.96	0.48
1:D:502:CYS:HB2	1:D:554:LYS:HE2	1.96	0.47
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.96	0.47
1:D:761:GLN:HE22	1:D:764:LYS:NZ	2.13	0.47
1:A:627:ARG:O	1:A:631:ILE:HG12	2.15	0.47
1:D:493:MET:O	1:D:497:SER:HB2	2.14	0.47
1:A:461:GLN:HE22	1:A:500:THR:HG22	1.79	0.47
1:A:462:PHE:CE1	1:A:491:VAL:HG11	2.50	0.46
1:D:735:ILE:HB	1:D:736:PRO:HD3	1.95	0.46
1:C:477:PHE:HB3	1:C:535:HIS:CE1	2.51	0.46
1:C:502:CYS:HB3	1:C:554:LYS:HE2	1.98	0.46
1:D:724:GLN:HB2	6:D:968:HOH:O	2.15	0.46
1:C:492:TYR:CE2	1:C:496:ARG:HD2	2.51	0.46
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.30	0.46
1:B:724:GLN:NE2	6:B:909:HOH:O	2.41	0.46
1:B:697:TRP:CH2	1:B:719:LYS:HG2	2.51	0.46
1:B:581:PRO:O	6:B:903:HOH:O	2.21	0.45
1:A:617:SER:O	1:A:621:GLN:HG3	2.17	0.45
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.99	0.44
1:A:705:LYS:HG2	1:C:684:VAL:HG22	2.00	0.44
1:A:756:ARG:NH1	6:A:911:HOH:O	2.44	0.44
1:B:469[A]:CYS:HB3	6:B:1068:HOH:O	2.18	0.44
1:B:471:GLU:HB3	1:B:477:PHE:CD1	2.52	0.44
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.32	0.43
1:B:756[B]:ARG:CD	6:B:989:HOH:O	2.66	0.43
1:A:523:PRO:HD2	1:A:695:GLU:HG2	2.01	0.43
1:B:497:SER:O	1:B:553:ARG:HD2	2.19	0.43
1:C:700:GLY:HA3	1:C:714:MET:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:713:MET:HE2	1:D:714:MET:HG3	2.00	0.42
1:A:735:ILE:N	1:A:736:PRO:HD2	2.34	0.42
1:C:634:ASP:OD2	6:C:903:HOH:O	2.22	0.42
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.54	0.42
1:B:498:CYS:HB3	1:B:553:ARG:HB3	2.00	0.42
1:D:766:ILE:HG22	1:D:766:ILE:O	2.18	0.42
1:D:727:LEU:CD1	1:D:766:ILE:CD1	2.96	0.41
1:D:722:VAL:HB	1:D:723:PRO:HD3	2.01	0.41
1:A:719:LYS:O	1:A:722:VAL:HG23	2.20	0.41
1:D:697:TRP:CZ2	1:D:719:LYS:HG3	2.54	0.41
1:C:602:ILE:O	1:C:605:LEU:HB2	2.21	0.41
1:D:638:TYR:CD1	1:D:671:THR:HG21	2.56	0.41
1:A:766:ILE:C	1:A:768:GLY:H	2.24	0.41
1:B:645:LEU:HD21	1:B:664:ARG:CB	2.51	0.41
1:B:576:GLN:HB2	6:B:1065:HOH:O	2.21	0.41
1:D:545:HIS:HA	6:D:997:HOH:O	2.21	0.41
1:D:714:MET:CE	6:D:988:HOH:O	2.68	0.41
1:A:697:TRP:CH2	1:A:719:LYS:HG2	2.55	0.41
1:C:464:LEU:O	1:C:465:PRO:C	2.58	0.41
1:C:469[A]:CYS:HB3	6:C:1078:HOH:O	2.20	0.41
1:C:706:LEU:HD23	1:C:706:LEU:HA	1.93	0.40
1:A:542:GLN:NE2	1:A:542:GLN:HA	2.36	0.40
1:D:483:GLU:HG3	1:D:486:TRP:CZ3	2.57	0.40
1:D:762:TRP:O	1:D:766:ILE:HG13	2.21	0.40
1:A:675:LEU:O	1:A:678:VAL:HG22	2.22	0.40
1:B:493:MET:SD	1:B:535:HIS:HA	2.61	0.40
1:B:735:ILE:N	1:B:736:PRO:CD	2.85	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	315/343 (92%)	302 (96%)	12 (4%)	1 (0%)	41	37
1	B	314/343 (92%)	302 (96%)	12 (4%)	0	100	100
1	C	314/343 (92%)	303 (96%)	11 (4%)	0	100	100
1	D	310/343 (90%)	298 (96%)	12 (4%)	0	100	100
All	All	1253/1372 (91%)	1205 (96%)	47 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	HIS

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	286/305 (94%)	268 (94%)	18 (6%)	18	13
1	B	283/305 (93%)	264 (93%)	19 (7%)	16	11
1	C	285/305 (93%)	265 (93%)	20 (7%)	15	10
1	D	280/305 (92%)	259 (92%)	21 (8%)	13	9
All	All	1134/1220 (93%)	1056 (93%)	78 (7%)	16	11

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	471[A]	GLU
1	A	471[B]	GLU
1	A	496	ARG
1	A	497	SER
1	A	504	GLU
1	A	547	LEU
1	A	553	ARG
1	A	573	SER
1	A	575	LEU

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Mol	Chain	Res	Type
1	A	605	LEU
1	A	606	GLU
1	A	617	SER
1	A	644	GLN
1	A	660	SER
1	A	713	MET
1	A	719	LYS
1	A	720	ASP
1	B	459	LEU
1	B	469[A]	CYS
1	B	469[B]	CYS
1	B	471	GLU
1	B	497	SER
1	B	575	LEU
1	B	576	GLN
1	B	606	GLU
1	B	613	THR
1	B	616	SER
1	B	638	TYR
1	B	642	ARG
1	B	644	GLN
1	B	650	GLN
1	B	677	SER
1	B	686	LYS
1	B	709	GLN
1	B	727	LEU
1	B	760	SER
1	C	469[A]	CYS
1	C	469[B]	CYS
1	C	471	GLU
1	C	497	SER
1	C	502	CYS
1	C	504	GLU
1	C	517	LYS
1	C	547	LEU
1	C	575	LEU
1	C	605	LEU
1	C	613	THR
1	C	616	SER
1	C	617	SER
1	C	638	TYR
1	C	709	GLN

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Mol	Chain	Res	Type
1	C	713	MET
1	C	719	LYS
1	C	720	ASP
1	C	753	LYS
1	C	760	SER
1	D	457	GLN
1	D	459	LEU
1	D	460	MET
1	D	463	THR
1	D	471	GLU
1	D	498	CYS
1	D	500	THR
1	D	504	GLU
1	D	517	LYS
1	D	575	LEU
1	D	576	GLN
1	D	605	LEU
1	D	613	THR
1	D	616	SER
1	D	617	SER
1	D	649	TYR
1	D	709	GLN
1	D	720	ASP
1	D	727	LEU
1	D	766	ILE
1	D	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	726	GLN
1	A	743	GLN
1	A	761	GLN
1	B	484	ASN
1	B	495	HIS
1	B	576	GLN
1	B	604	GLN

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Mol	Chain	Res	Type
1	B	621	GLN
1	B	644	GLN
1	B	650	GLN
1	B	726	GLN
1	C	542	GLN
1	C	576	GLN
1	C	604	GLN
1	C	621	GLN
1	C	743	GLN
1	D	484	ASN
1	D	542	GLN
1	D	576	GLN
1	D	604	GLN
1	D	609	ASN
1	D	621	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	0.50	0	5,9,11	0.73	0
1	CME	C	509	1	8,9,10	0.51	0	5,9,11	1.27	0
1	CME	B	509	1	8,9,10	0.47	0	5,9,11	0.96	0
1	CME	A	509	1	8,9,10	0.50	0	5,9,11	0.58	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	C	509	1	-	1/5/8/10	-
1	CME	B	509	1	-	1/5/8/10	-
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	B	509	CME	SD-CE-CZ-OH
1	D	509	CME	SD-CE-CZ-OH
1	C	509	CME	CE-SD-SG-CB
1	A	509	CME	CZ-CE-SD-SG
1	D	509	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	509	CME	1	0
1	A	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
5	KIE	C	803	-	21,23,23	1.50	3 (14%)	19,32,32	2.23	6 (31%)
5	KIE	B	803	-	21,23,23	1.11	1 (4%)	19,32,32	2.37	9 (47%)
4	GOL	A	803	-	5,5,5	0.16	0	5,5,5	0.44	0
5	KIE	A	804	-	21,23,23	1.01	1 (4%)	19,32,32	2.18	8 (42%)

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
5	KIE	C	803	-	-	2/9/10/10	0/3/3/3
5	KIE	B	803	-	-	5/9/10/10	0/3/3/3
4	GOL	A	803	-	-	2/4/4/4	-
5	KIE	A	804	-	-	2/9/10/10	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	803	KIE	C4-N1	4.43	1.34	1.31
5	B	803	KIE	C4-C6	-3.45	1.37	1.43
5	C	803	KIE	C5-N8	2.70	1.39	1.34
5	C	803	KIE	C4-C6	-2.50	1.39	1.43
5	A	804	KIE	C17-C13	2.03	1.41	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	803	KIE	C12-S10-C4	-5.08	86.06	104.22
5	B	803	KIE	C20-N11-C3	4.99	126.14	121.27
5	A	804	KIE	C18-C13-C17	-4.58	116.74	122.83
5	C	803	KIE	C3-N2-C5	4.20	120.05	115.28
5	B	803	KIE	C16-C18-C13	4.08	122.58	118.36
5	A	804	KIE	C15-C17-C13	3.96	122.45	118.36
5	A	804	KIE	C3-N2-C5	3.45	119.19	115.28
5	C	803	KIE	C21-C19-N11	-3.42	93.99	110.73
5	B	803	KIE	C6-C4-N1	-3.40	117.01	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	803	KIE	C19-N11-C3	-3.25	116.17	120.90
5	C	803	KIE	F14-C13-C17	-3.17	113.16	118.54
5	A	804	KIE	F14-C13-C17	3.00	123.64	118.54
5	B	803	KIE	C18-C16-C12	-2.92	116.98	120.50
5	A	804	KIE	C16-C18-C13	2.84	121.30	118.36
5	B	803	KIE	C21-C19-N11	-2.80	97.00	110.73
5	C	803	KIE	C20-N11-C3	2.70	123.91	121.27
5	B	803	KIE	C12-S10-C4	-2.50	95.28	104.22
5	A	804	KIE	C12-S10-C4	-2.49	95.33	104.22
5	A	804	KIE	C20-N11-C3	-2.40	118.93	121.27
5	B	803	KIE	C15-C17-C13	-2.25	116.03	118.36
5	C	803	KIE	F14-C13-C18	2.22	122.31	118.54
5	A	804	KIE	C17-C15-C12	-2.04	118.04	120.50
5	B	803	KIE	C5-C6-N7	2.02	111.50	109.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	KIE	C21-C19-N11-C20
5	B	803	KIE	C21-C19-N11-C20
5	C	803	KIE	C21-C19-N11-C20
5	B	803	KIE	N1-C3-N11-C19
5	B	803	KIE	C21-C19-N11-C3
5	C	803	KIE	C21-C19-N11-C3
4	A	803	GOL	O1-C1-C2-C3
5	B	803	KIE	N2-C3-N11-C19
4	A	803	GOL	O1-C1-C2-O2
5	A	804	KIE	C21-C19-N11-C3
5	B	803	KIE	N1-C3-N11-C20

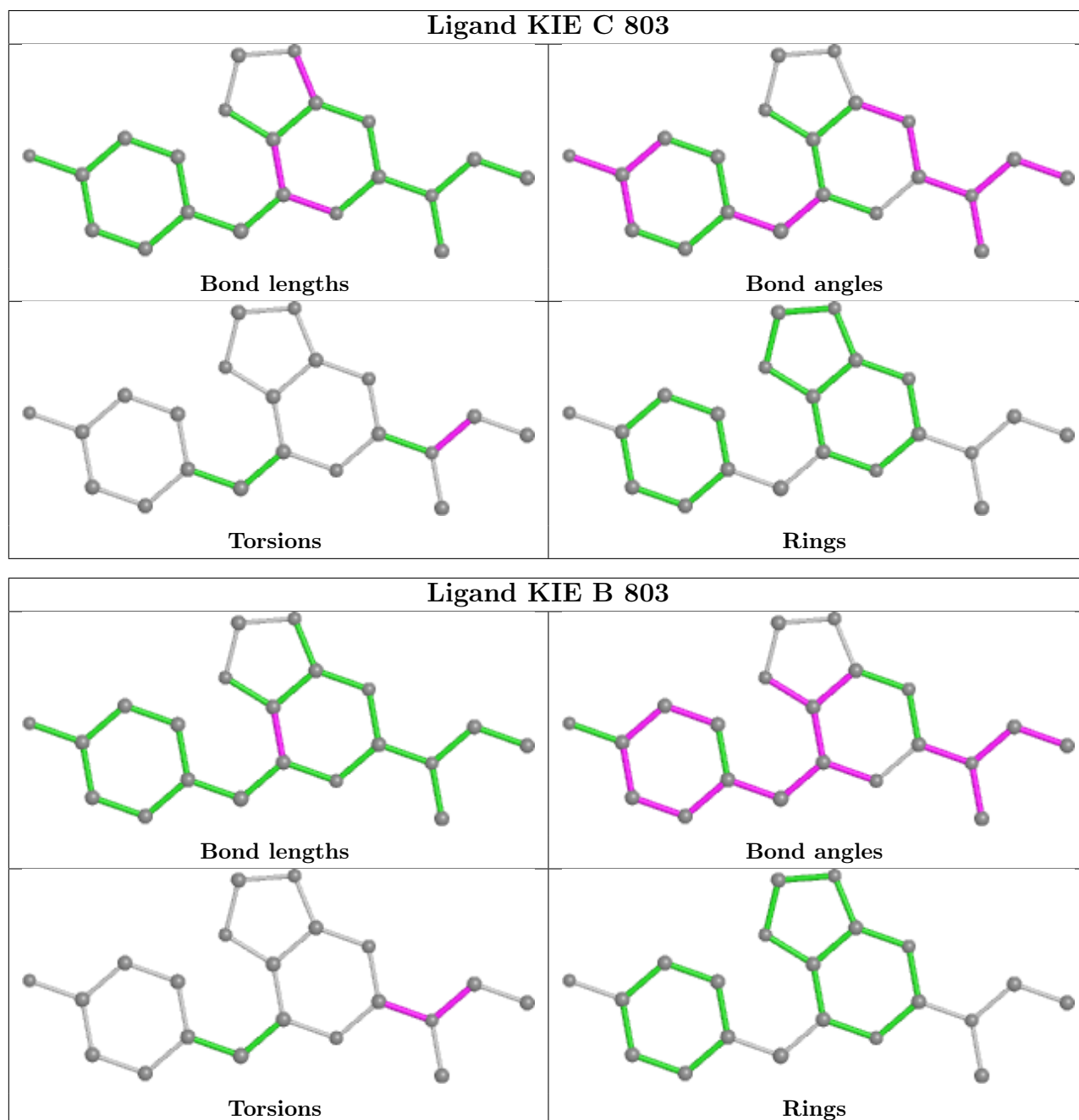
There are no ring outliers.

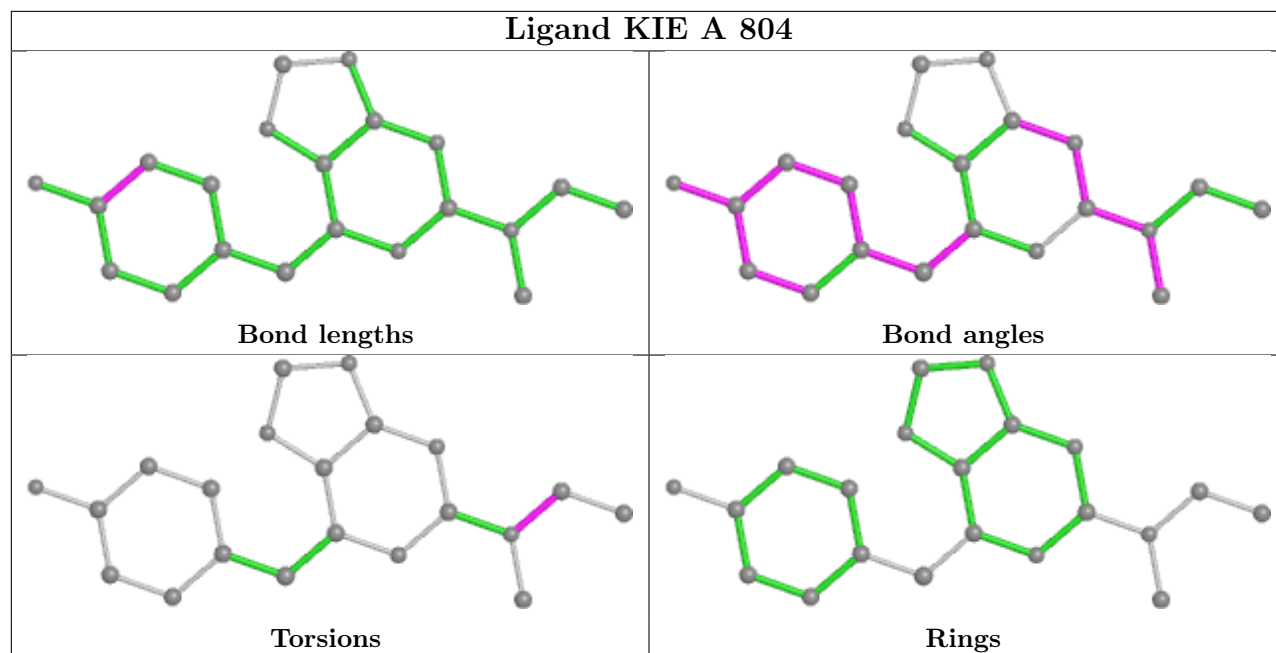
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	803	KIE	1	0
5	B	803	KIE	2	0
4	A	803	GOL	2	0
5	A	804	KIE	4	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, 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	312/343 (90%)	-0.57	0 100 100	20, 33, 54, 78	0
1	B	314/343 (91%)	-0.51	1 (0%) 94 93	20, 32, 54, 79	0
1	C	312/343 (90%)	-0.72	2 (0%) 89 88	21, 32, 53, 84	0
1	D	312/343 (90%)	-0.49	0 100 100	26, 39, 60, 82	0
All	All	1250/1372 (91%)	-0.57	3 (0%) 95 94	20, 34, 57, 84	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	771	THR	3.2
1	C	766	ILE	2.5
1	C	765	VAL	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, 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
1	CME	A	509	10/11	0.96	0.09	34,43,70,71	0
1	CME	B	509	10/11	0.96	0.10	33,42,63,71	0
1	CME	C	509	10/11	0.96	0.11	35,45,59,61	0
1	CME	D	509	10/11	0.97	0.09	36,47,63,64	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

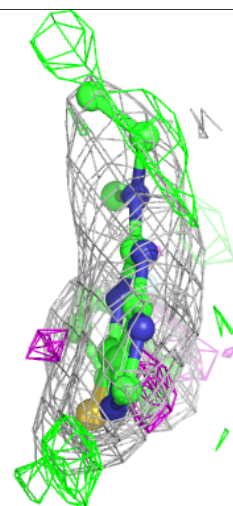
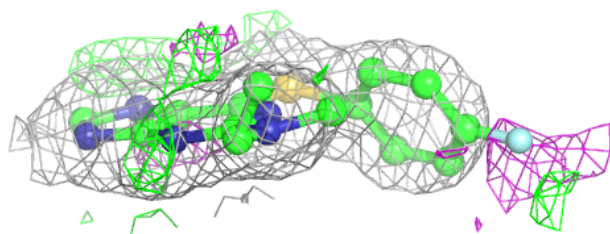
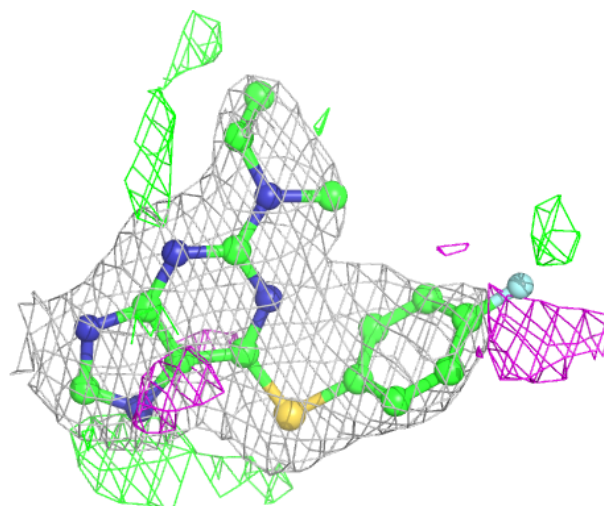
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	KIE	A	804	21/21	0.93	0.14	43,51,61,81	0
5	KIE	C	803	21/21	0.93	0.15	41,49,57,68	0
4	GOL	A	803	6/6	0.95	0.14	32,44,49,49	0
5	KIE	B	803	21/21	0.96	0.10	28,40,46,68	0
3	MG	B	802	1/1	0.99	0.07	15,15,15,15	0
3	MG	D	802	1/1	0.99	0.06	26,26,26,26	0
3	MG	A	802	1/1	0.99	0.09	20,20,20,20	0
2	ZN	C	801	1/1	1.00	0.09	28,28,28,28	0
2	ZN	D	801	1/1	1.00	0.08	33,33,33,33	0
2	ZN	A	801	1/1	1.00	0.09	28,28,28,28	0
2	ZN	B	801	1/1	1.00	0.10	26,26,26,26	0
3	MG	C	802	1/1	1.00	0.08	21,21,21,21	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.

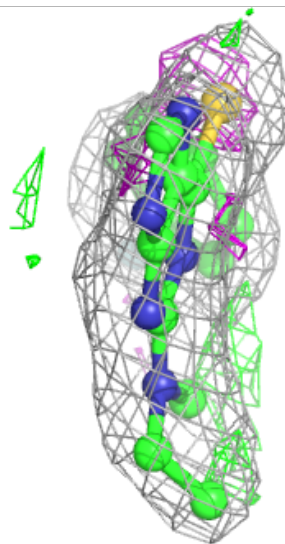
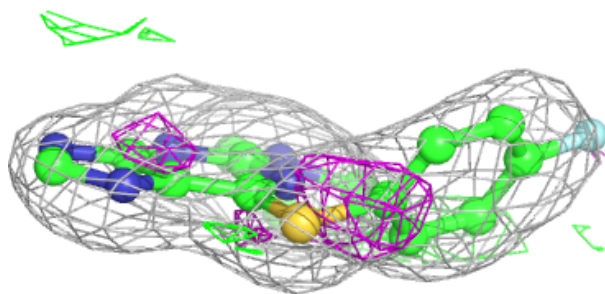
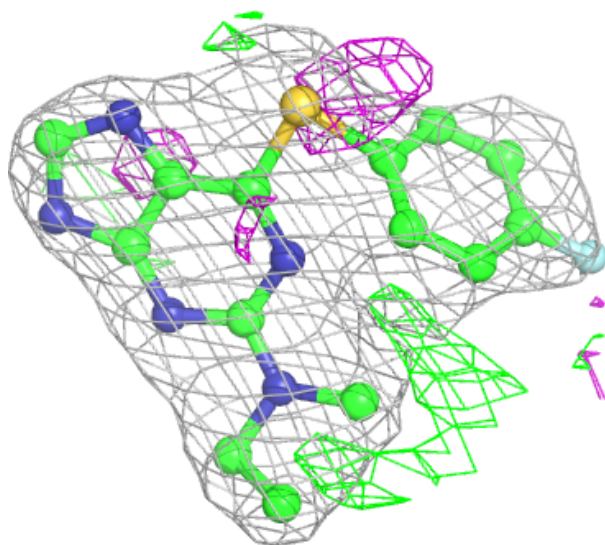
Electron density around KIE A 804:

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



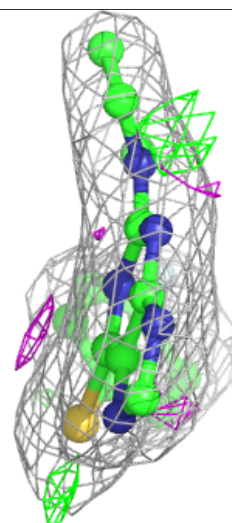
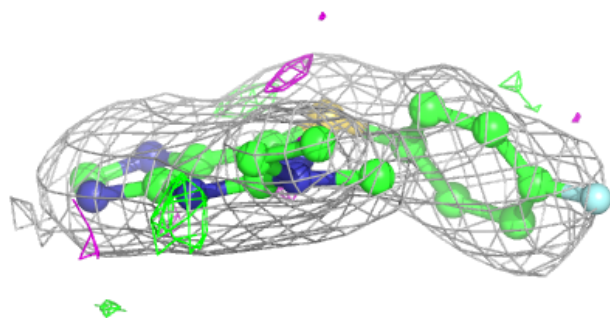
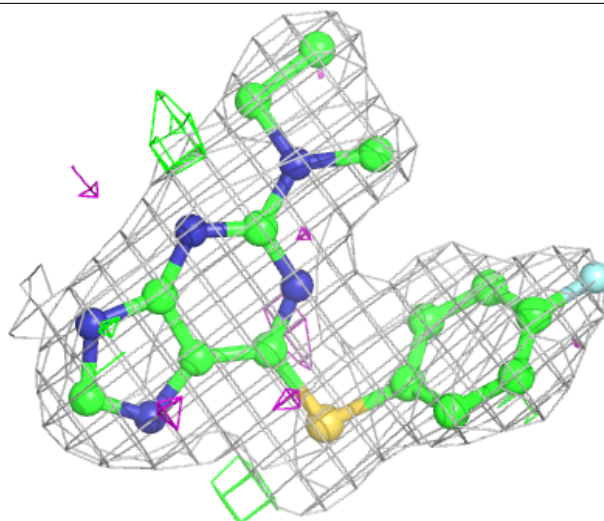
Electron density around KIE C 803:

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



Electron density around KIE 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.