



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:43 am BST

PDB ID : 4CQE
Title : B-Raf Kinase V600E mutant in complex with a diarylthiazole B-Raf Inhibitor
Authors : Casale, E.; Fasolini, M.; Pulici, M.; Traquandi, G.; Marchionni, C.; Modugno, M.; Lupi, R.; Amboldi, N.; Colombo, N.; Corti, L.; Gasparri, F.; Pastori, W.; Sclaro, A.; Donati, D.; Felder, E.; Galvani, A.; Isacchi, A.; Pesenti, E.; Ciomei, M.
Deposited on : 2014-02-14
Resolution : 2.30 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 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 : 2.11
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) : 2.11

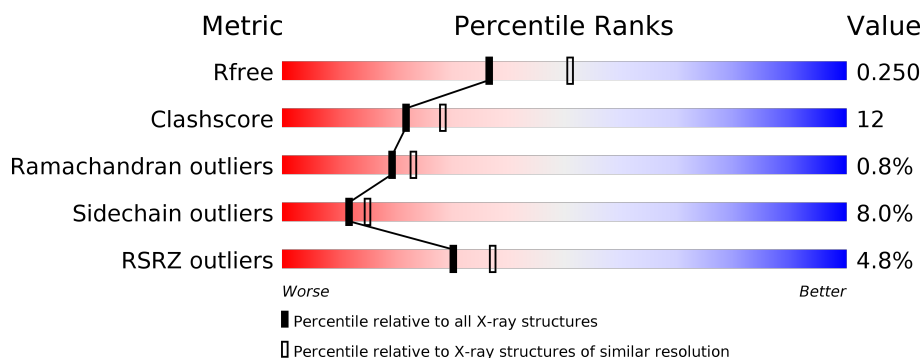
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	278	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	278	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4141 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 SLC45A3-BRAF FUSION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2003	1269	359	362	13			
1	B	248	Total	C	N	O	S	0	0	0
			1989	1261	356	360	12			

There are 38 discrepancies between the modelled and reference sequences:

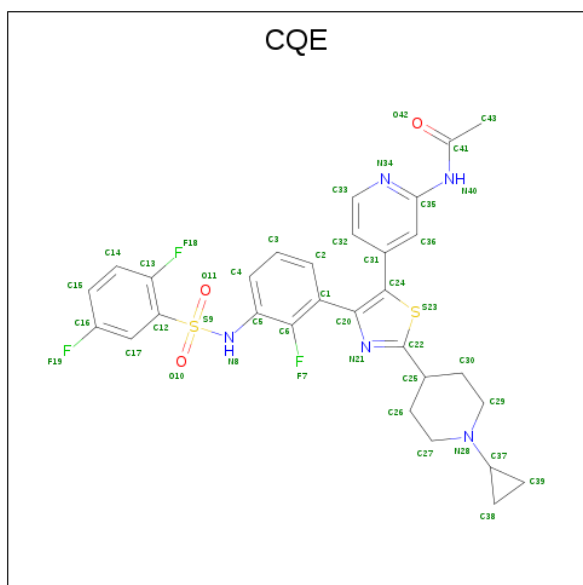
Chain	Residue	Modelled	Actual	Comment	Reference
A	446	GLY	-	expression tag	UNP D7PBN4
A	447	PRO	-	expression tag	UNP D7PBN4
A	543	ALA	ILE	engineered mutation	UNP D7PBN4
A	544	SER	ILE	engineered mutation	UNP D7PBN4
A	551	LYS	ILE	engineered mutation	UNP D7PBN4
A	562	ARG	GLN	engineered mutation	UNP D7PBN4
A	588	ASN	LEU	engineered mutation	UNP D7PBN4
A	600	GLU	VAL	engineered mutation	UNP D7PBN4
A	630	SER	LYS	engineered mutation	UNP D7PBN4
A	667	GLU	PHE	engineered mutation	UNP D7PBN4
A	673	SER	TYR	engineered mutation	UNP D7PBN4
A	688	ARG	ALA	engineered mutation	UNP D7PBN4
A	706	SER	LEU	engineered mutation	UNP D7PBN4
A	709	ARG	GLN	engineered mutation	UNP D7PBN4
A	713	GLU	SER	engineered mutation	UNP D7PBN4
A	716	GLU	LEU	engineered mutation	UNP D7PBN4
A	720	GLU	SER	engineered mutation	UNP D7PBN4
A	722	SER	PRO	engineered mutation	UNP D7PBN4
A	723	GLY	LYS	engineered mutation	UNP D7PBN4
B	446	GLY	-	expression tag	UNP D7PBN4
B	447	PRO	-	expression tag	UNP D7PBN4
B	543	ALA	ILE	engineered mutation	UNP D7PBN4
B	544	SER	ILE	engineered mutation	UNP D7PBN4
B	551	LYS	ILE	engineered mutation	UNP D7PBN4
B	562	ARG	GLN	engineered mutation	UNP D7PBN4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	588	ASN	LEU	engineered mutation	UNP D7PBN4
B	600	GLU	VAL	engineered mutation	UNP D7PBN4
B	630	SER	LYS	engineered mutation	UNP D7PBN4
B	667	GLU	PHE	engineered mutation	UNP D7PBN4
B	673	SER	TYR	engineered mutation	UNP D7PBN4
B	688	ARG	ALA	engineered mutation	UNP D7PBN4
B	706	SER	LEU	engineered mutation	UNP D7PBN4
B	709	ARG	GLN	engineered mutation	UNP D7PBN4
B	713	GLU	SER	engineered mutation	UNP D7PBN4
B	716	GLU	LEU	engineered mutation	UNP D7PBN4
B	720	GLU	SER	engineered mutation	UNP D7PBN4
B	722	SER	PRO	engineered mutation	UNP D7PBN4
B	723	GLY	LYS	engineered mutation	UNP D7PBN4

- Molecule 2 is N-{4-[2-(1-cyclopropylpiperidin-4-yl)-4-(3-{[(2,5-difluorophenyl)sulfonyl]amino}-2-fluorophenyl)-1,3-thiazol-5-yl]pyridin-2-yl}acetamide (three-letter code: CQE) (formula: C₃₀H₂₈F₃N₅O₃S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			43	30	3	5	3	2		
2	B	1	Total	C	F	N	O	S	0	0
			43	30	3	5	3	2		

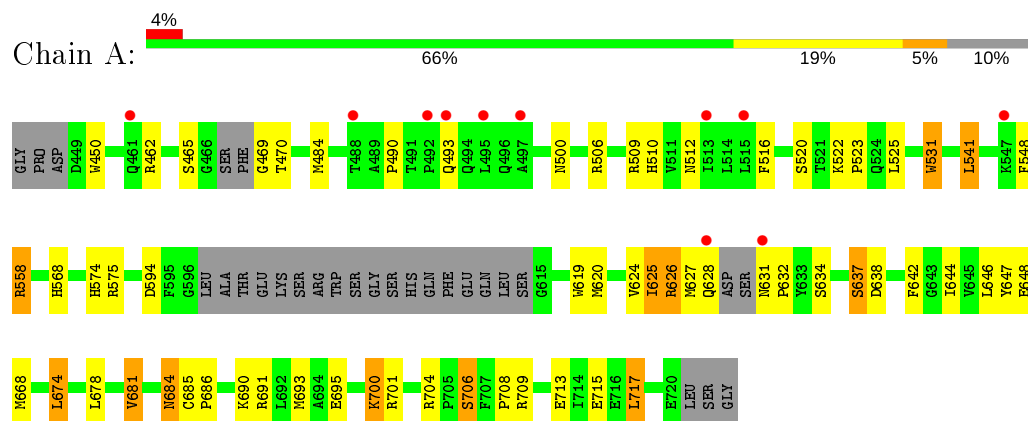
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	22	Total 22	O 22	0	0

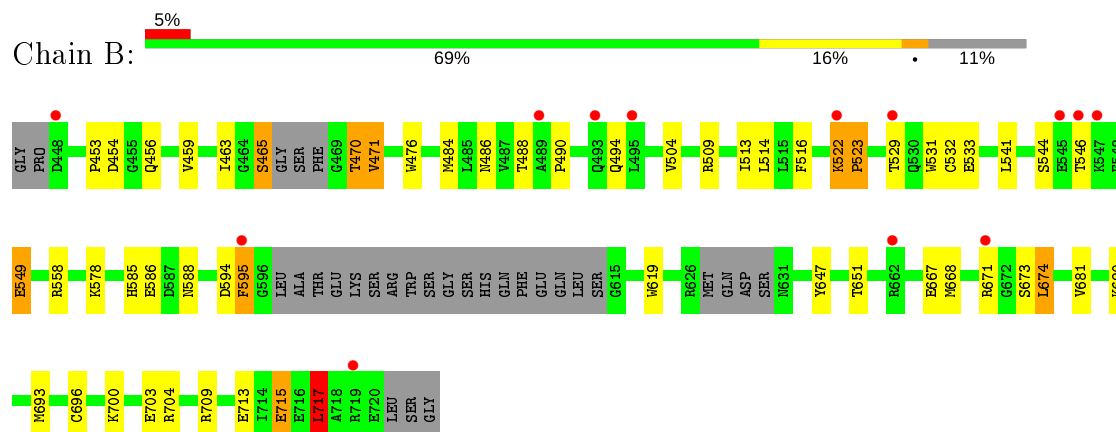
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: SLC45A3-BRAF FUSION PROTEIN



• Molecule 1: SLC45A3-BRAF FUSION PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.60 Å 105.94 Å 109.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 38.13 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.30) 99.5 (38.13-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.255 0.208 , 0.250	Depositor DCC
R_{free} test set	1414 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4141	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CQE

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	0.57	2/2042 (0.1%)	0.67	1/2747 (0.0%)
1	B	0.57	2/2028 (0.1%)	0.66	1/2729 (0.0%)
All	All	0.57	4/4070 (0.1%)	0.67	2/5476 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	TRP	CD2-CE2	5.22	1.47	1.41
1	B	476	TRP	CD2-CE2	5.04	1.47	1.41
1	B	619	TRP	CD2-CE2	5.03	1.47	1.41
1	A	450	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	717	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	704	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2003	0	2022	59	0
1	B	1989	0	2006	36	0
2	A	43	0	28	3	0
2	B	43	0	28	4	0
3	A	41	0	0	0	0
3	B	22	0	0	1	0
All	All	4141	0	4084	96	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 12.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:ASN:N	1:A:684:ASN:HD22	1.55	1.03
1:A:628:GLN:HG2	1:A:632:PRO:HG3	1.03	1.00
1:A:628:GLN:CG	1:A:632:PRO:HG3	1.93	0.98
1:A:684:ASN:HD22	1:A:684:ASN:H	1.03	0.94
1:A:664:GLN:HG2	1:A:668:MET:CE	1.97	0.93
1:B:522:LYS:HB2	1:B:523:PRO:HD3	1.53	0.91
1:A:684:ASN:ND2	1:A:684:ASN:H	1.67	0.89
1:A:700:LYS:H	1:A:700:LYS:HD2	1.37	0.89
1:A:628:GLN:HG2	1:A:632:PRO:CG	1.99	0.87
1:A:558:ARG:HG2	1:A:558:ARG:HH11	1.40	0.86
1:A:664:GLN:HG2	1:A:668:MET:HE2	1.57	0.83
1:B:667:GLU:O	1:B:671:ARG:HB2	1.82	0.80
1:A:684:ASN:N	1:A:684:ASN:ND2	2.29	0.79
1:A:510:HIS:HD2	1:A:512:ASN:H	1.28	0.78
1:B:454:ASP:HB2	1:B:522:LYS:HG3	1.68	0.75
1:A:625:ILE:C	1:A:627:MET:H	1.90	0.75
1:A:664:GLN:HG2	1:A:668:MET:HE1	1.66	0.75
1:A:647:TYR:HD2	1:A:693:MET:HE3	1.50	0.74
1:A:647:TYR:HD2	1:A:693:MET:CE	2.04	0.70
1:B:533:GLU:H	1:B:585:HIS:HD2	1.40	0.69
1:A:647:TYR:CD2	1:A:693:MET:HE3	2.28	0.69
1:A:510:HIS:CD2	1:A:512:ASN:H	2.11	0.68
1:A:531:TRP:CZ2	2:A:1721:CQE:H433	2.30	0.67
1:B:531:TRP:CZ2	2:B:1721:CQE:H433	2.28	0.67
1:A:631:ASN:N	1:A:632:PRO:CD	2.58	0.66
1:B:533:GLU:H	1:B:585:HIS:CD2	2.14	0.64
1:A:625:ILE:O	1:A:627:MET:N	2.30	0.64
1:A:594:ASP:H	2:A:1721:CQE:H8	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:VAL:HG21	1:A:690:LYS:HD2	1.81	0.63
1:A:713:GLU:O	1:A:717:LEU:HD23	1.97	0.63
1:B:522:LYS:CB	1:B:523:PRO:HD3	2.28	0.62
1:B:558:ARG:HD3	1:B:715:GLU:HG3	1.83	0.61
1:B:549:GLU:CD	1:B:549:GLU:H	2.04	0.60
1:A:706:SER:HB3	1:A:708:PRO:HD2	1.85	0.59
1:B:594:ASP:H	2:B:1721:CQE:H8	1.51	0.58
1:B:454:ASP:HB2	1:B:522:LYS:CG	2.33	0.58
1:A:558:ARG:HG2	1:A:558:ARG:NH1	2.15	0.58
1:A:631:ASN:N	1:A:632:PRO:HD3	2.18	0.58
1:B:453:PRO:HG2	1:B:456:GLN:NE2	2.19	0.57
1:A:678:LEU:HD22	1:A:693:MET:HE2	1.86	0.57
1:A:506:ARG:HG2	1:A:516:PHE:CE2	2.39	0.57
1:A:555:ASP:OD1	1:A:558:ARG:NH1	2.34	0.56
1:A:627:MET:O	1:A:628:GLN:HB2	2.04	0.56
1:B:668:MET:HG2	1:B:671:ARG:HH12	1.70	0.56
1:B:595:PHE:CD1	1:B:595:PHE:N	2.74	0.56
1:A:490:PRO:HG3	1:A:525:LEU:HD21	1.89	0.55
1:A:625:ILE:C	1:A:627:MET:N	2.60	0.55
1:A:574:HIS:O	1:A:575:ARG:HB2	2.08	0.54
1:B:696:CYS:O	1:B:704:ARG:HD2	2.08	0.54
1:A:462:ARG:NH1	1:A:465:SER:OG	2.41	0.53
1:B:595:PHE:HD1	1:B:595:PHE:N	2.07	0.52
1:B:700:LYS:HE3	1:B:703:GLU:OE2	2.09	0.52
1:A:462:ARG:HD2	1:A:470:THR:HG21	1.92	0.52
1:A:558:ARG:HD3	1:A:715:GLU:HG3	1.92	0.52
1:A:620:MET:CE	1:A:624:VAL:HG12	2.40	0.52
1:A:647:TYR:CD2	1:A:693:MET:CE	2.88	0.51
1:B:463:ILE:HB	1:B:471:VAL:HG22	1.92	0.51
1:B:681:VAL:HG21	1:B:690:LYS:HD2	1.92	0.51
1:A:541:LEU:HD23	1:A:648:GLU:HB3	1.93	0.51
1:A:642:PHE:CE2	1:A:646:LEU:HD11	2.46	0.51
1:A:626:ARG:C	1:A:628:GLN:H	2.13	0.50
2:A:1721:CQE:H36	2:A:1721:CQE:O42	2.12	0.50
1:A:681:VAL:CG2	1:A:690:LYS:HD2	2.42	0.50
1:B:532:CYS:HA	1:B:585:HIS:CD2	2.47	0.50
1:A:469:GLY:HA3	1:A:484:MET:O	2.12	0.50
1:B:713:GLU:O	1:B:717:LEU:HB3	2.10	0.50
1:A:668:MET:HB3	1:A:674:LEU:HB2	1.92	0.49
1:A:619:TRP:HA	1:A:644:ILE:HG13	1.95	0.49
1:B:522:LYS:HB2	1:B:523:PRO:CD	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:MET:HE2	1:A:624:VAL:HG12	1.95	0.48
2:B:1721:CQE:H36	2:B:1721:CQE:O42	2.13	0.48
1:B:544:SER:OG	1:B:546:THR:OG1	2.32	0.47
1:B:667:GLU:HG3	1:B:671:ARG:HH11	1.79	0.47
1:B:465:SER:HB3	1:B:470:THR:HB	1.97	0.46
1:B:490:PRO:HA	1:B:494:GLN:NE2	2.30	0.46
1:A:548:PHE:CB	1:A:553:LEU:HD13	2.46	0.46
1:A:678:LEU:O	1:A:681:VAL:HG13	2.16	0.46
1:A:509:ARG:HD3	1:B:516:PHE:O	2.16	0.45
1:A:522:LYS:HG3	1:A:523:PRO:HA	1.98	0.44
1:B:647:TYR:CZ	1:B:651:THR:HG21	2.53	0.44
1:A:691:ARG:O	1:A:695:GLU:HG2	2.18	0.44
1:B:532:CYS:HA	1:B:585:HIS:HD2	1.82	0.43
1:A:516:PHE:O	1:B:509:ARG:HD3	2.18	0.43
1:A:634:SER:H	1:A:637:SER:HG	1.65	0.42
1:B:647:TYR:HD1	1:B:693:MET:HE1	1.85	0.42
1:A:548:PHE:HB3	1:A:553:LEU:HD13	2.02	0.42
1:A:568:HIS:HE1	1:A:638:ASP:OD2	2.02	0.42
1:B:522:LYS:HG2	3:B:2002:HOH:O	2.19	0.42
1:B:668:MET:HB3	1:B:674:LEU:HB2	2.00	0.42
1:B:558:ARG:CD	1:B:715:GLU:HG3	2.47	0.42
1:A:651:THR:HG22	1:A:681:VAL:HA	2.03	0.41
1:B:513:ILE:O	1:B:514:LEU:C	2.58	0.41
2:B:1721:CQE:C1	2:B:1721:CQE:H32	2.51	0.41
1:A:685:CYS:O	1:A:686:PRO:C	2.60	0.41
1:B:522:LYS:CB	1:B:523:PRO:CD	2.98	0.40
1:A:626:ARG:C	1:A:628:GLN:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	242/278 (87%)	227 (94%)	13 (5%)	2 (1%)	19	23
1	B	240/278 (86%)	233 (97%)	5 (2%)	2 (1%)	19	23
All	All	482/556 (87%)	460 (95%)	18 (4%)	4 (1%)	19	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	ARG
1	B	522	LYS
1	B	523	PRO
1	A	493	GLN

5.3.2 Protein sidechains ⓘ

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	219/243 (90%)	204 (93%)	15 (7%)	16	21
1	B	218/243 (90%)	198 (91%)	20 (9%)	9	11
All	All	437/486 (90%)	402 (92%)	35 (8%)	12	15

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	ASN
1	A	520	SER
1	A	541	LEU
1	A	553	LEU
1	A	558	ARG
1	A	625	ILE
1	A	637	SER
1	A	674	LEU
1	A	681	VAL
1	A	684	ASN
1	A	700	LYS
1	A	701	ARG

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Mol	Chain	Res	Type
1	A	706	SER
1	A	709	ARG
1	A	717	LEU
1	B	459	VAL
1	B	465	SER
1	B	470	THR
1	B	471	VAL
1	B	484	MET
1	B	486	ASN
1	B	488	THR
1	B	504	VAL
1	B	529	THR
1	B	541	LEU
1	B	549	GLU
1	B	578	LYS
1	B	586	GLU
1	B	588	ASN
1	B	595	PHE
1	B	673	SER
1	B	674	LEU
1	B	709	ARG
1	B	715	GLU
1	B	717	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	493	GLN
1	A	500	ASN
1	A	510	HIS
1	A	568	HIS
1	A	684	ASN
1	B	486	ASN
1	B	494	GLN
1	B	580	ASN
1	B	585	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CQE	B	1721	-	45,48,48	3.63	15 (33%)	52,71,71	1.81	11 (21%)
2	CQE	A	1721	-	45,48,48	3.45	12 (26%)	52,71,71	2.13	13 (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
2	CQE	B	1721	-	-	4/25/43/43	0/6/6/6
2	CQE	A	1721	-	-	4/25/43/43	0/6/6/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1721	CQE	C31-C24	-13.83	1.34	1.48
2	B	1721	CQE	C1-C20	-13.35	1.36	1.49
2	A	1721	CQE	C1-C20	-12.29	1.37	1.49
2	A	1721	CQE	C31-C24	-12.12	1.36	1.48
2	A	1721	CQE	O10-S9	7.92	1.52	1.43
2	B	1721	CQE	O11-S9	7.31	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1721	CQE	O10-S9	6.78	1.51	1.43
2	A	1721	CQE	O11-S9	6.57	1.51	1.43
2	A	1721	CQE	C22-S23	-4.61	1.59	1.73
2	A	1721	CQE	F7-C6	-4.43	1.28	1.35
2	B	1721	CQE	C5-N8	-4.22	1.35	1.42
2	A	1721	CQE	C5-N8	-4.19	1.35	1.42
2	B	1721	CQE	S9-N8	-4.01	1.56	1.63
2	B	1721	CQE	C22-C25	3.32	1.57	1.50
2	B	1721	CQE	F7-C6	-3.11	1.30	1.35
2	A	1721	CQE	C33-N34	3.02	1.41	1.34
2	B	1721	CQE	F19-C16	-2.94	1.29	1.36
2	B	1721	CQE	C33-N34	2.94	1.40	1.34
2	A	1721	CQE	C39-C37	2.72	1.54	1.48
2	A	1721	CQE	F19-C16	2.66	1.42	1.36
2	A	1721	CQE	C38-C37	2.60	1.54	1.48
2	B	1721	CQE	C39-C37	2.57	1.54	1.48
2	B	1721	CQE	C12-S9	2.56	1.81	1.77
2	A	1721	CQE	C43-C41	2.39	1.55	1.50
2	B	1721	CQE	C38-C37	2.30	1.53	1.48
2	B	1721	CQE	C43-C41	2.24	1.55	1.50
2	B	1721	CQE	C22-S23	-2.06	1.67	1.73

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1721	CQE	O11-S9-O10	-5.62	112.64	119.55
2	A	1721	CQE	C16-C17-C12	5.36	120.51	116.86
2	A	1721	CQE	C35-N40-C41	-5.30	122.66	128.16
2	A	1721	CQE	C27-N28-C29	4.52	117.34	109.08
2	B	1721	CQE	C16-C17-C12	4.52	119.94	116.86
2	A	1721	CQE	O11-S9-O10	-4.32	114.24	119.55
2	A	1721	CQE	C36-C35-N34	-3.81	117.43	122.75
2	B	1721	CQE	C36-C35-N34	-3.78	117.48	122.75
2	A	1721	CQE	C33-N34-C35	3.72	122.50	117.22
2	B	1721	CQE	C35-N40-C41	-3.61	124.42	128.16
2	B	1721	CQE	C33-N34-C35	3.37	122.00	117.22
2	A	1721	CQE	C20-C1-C6	-3.27	119.47	123.56
2	B	1721	CQE	C4-C5-N8	3.24	127.37	120.88
2	A	1721	CQE	C32-C33-N34	-3.24	119.93	123.96
2	A	1721	CQE	C31-C36-C35	2.94	122.68	118.97
2	B	1721	CQE	C12-S9-N8	2.93	110.69	107.27
2	A	1721	CQE	C4-C5-N8	2.83	126.54	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1721	CQE	O10-S9-N8	2.60	113.23	106.73
2	B	1721	CQE	C32-C33-N34	-2.56	120.77	123.96
2	A	1721	CQE	C29-N28-C37	2.51	119.72	112.64
2	A	1721	CQE	C15-C16-C17	-2.48	120.07	123.29
2	A	1721	CQE	C12-S9-N8	2.38	110.05	107.27
2	B	1721	CQE	C27-N28-C29	2.19	113.07	109.08
2	B	1721	CQE	C31-C36-C35	2.03	121.53	118.97

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1721	CQE	C2-C1-C20-N21
2	B	1721	CQE	C38-C37-N28-C27
2	A	1721	CQE	C2-C1-C20-N21
2	A	1721	CQE	C38-C37-N28-C29
2	B	1721	CQE	C20-C24-C31-C36
2	A	1721	CQE	C20-C24-C31-C36
2	B	1721	CQE	C20-C24-C31-C32
2	A	1721	CQE	C20-C24-C31-C32

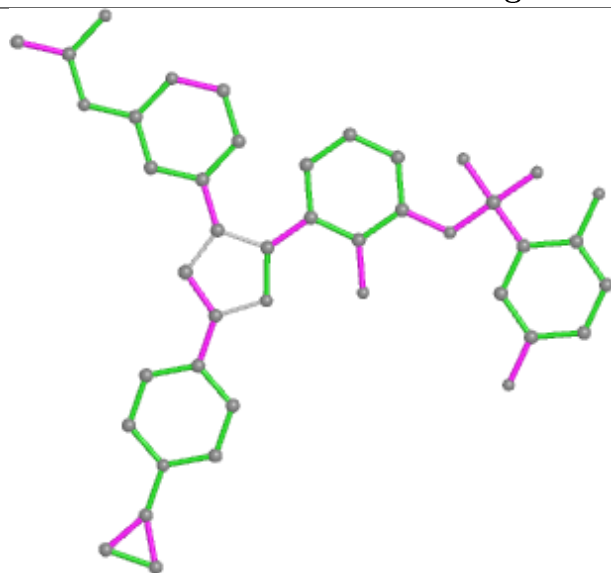
There are no ring outliers.

2 monomers are involved in 7 short contacts:

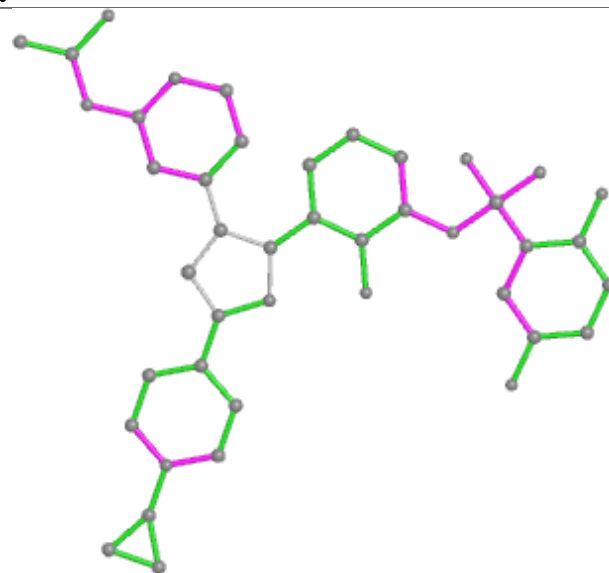
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1721	CQE	4	0
2	A	1721	CQE	3	0

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 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.

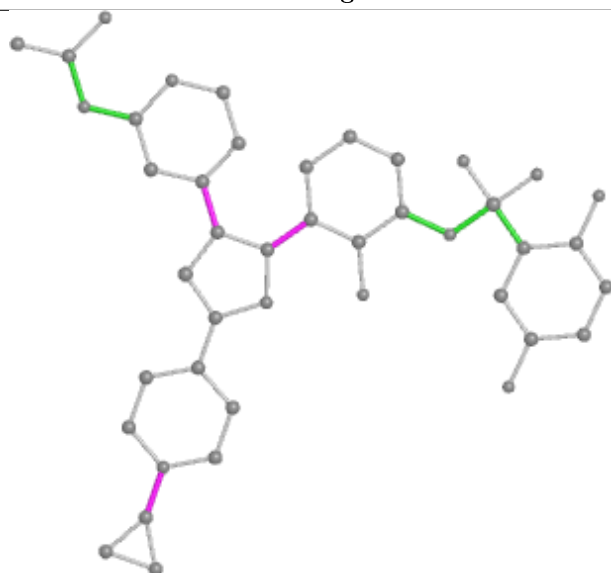
Ligand CQE B 1721



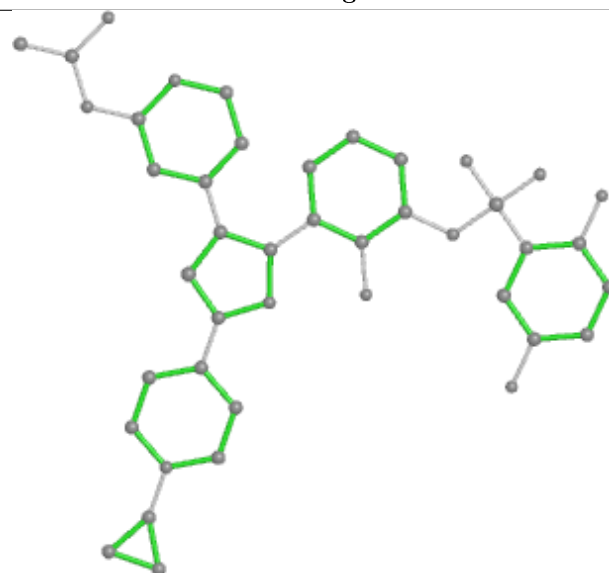
Bond lengths



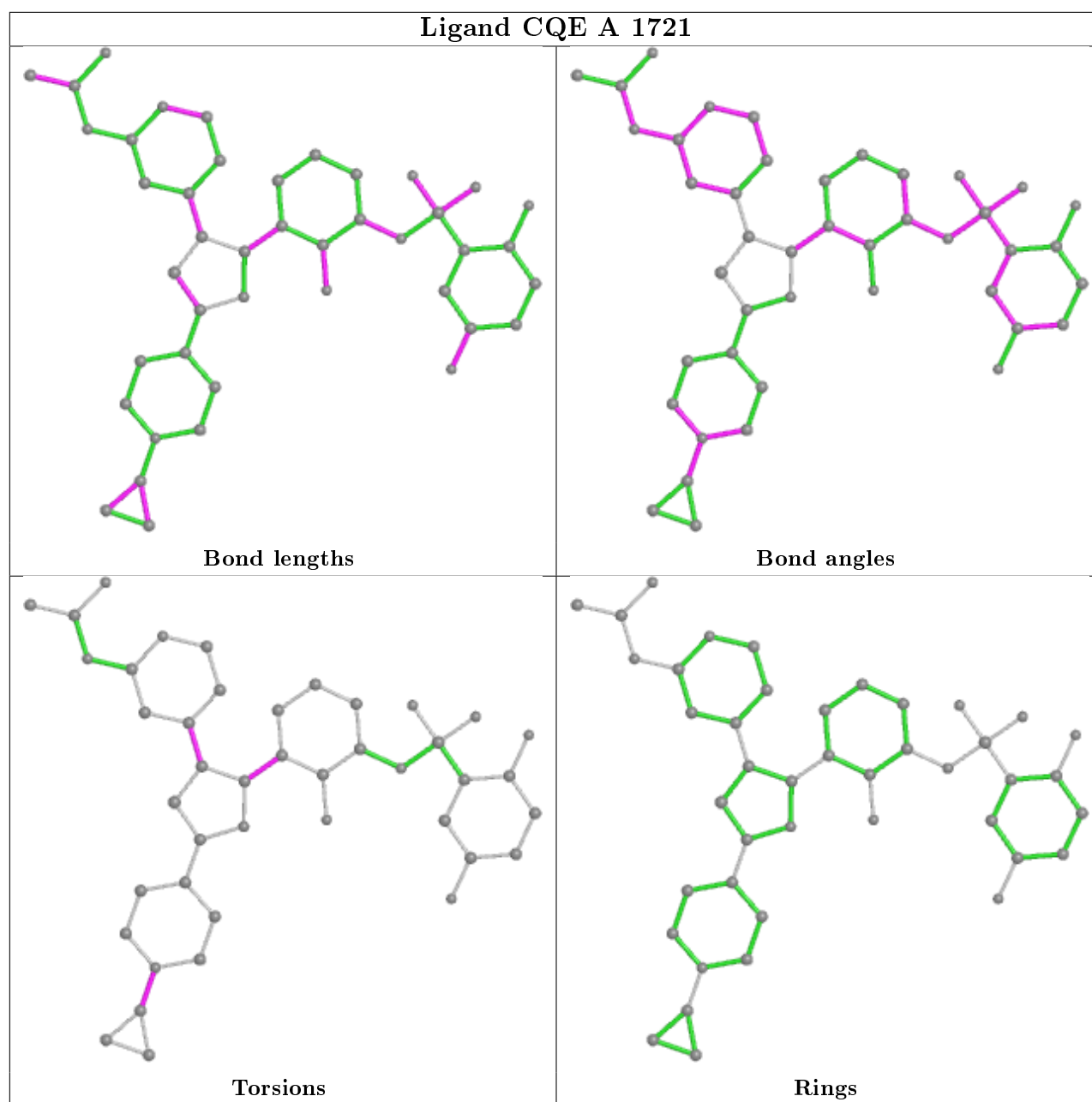
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/278 (89%)	0.33	11 (4%) 34 41	29, 47, 80, 96	0
1	B	248/278 (89%)	0.39	13 (5%) 27 34	27, 49, 81, 103	0
All	All	498/556 (89%)	0.36	24 (4%) 30 37	27, 48, 81, 103	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	631	ASN	4.4
1	B	545	GLU	4.3
1	B	719	ARG	4.1
1	B	546	THR	3.9
1	B	522	LYS	3.7
1	B	493	GLN	3.5
1	A	495	LEU	3.4
1	B	671	ARG	3.4
1	A	628	GLN	3.2
1	B	495	LEU	3.1
1	B	448	ASP	2.9
1	B	547	LYS	2.8
1	A	492	PRO	2.8
1	A	493	GLN	2.8
1	A	488	THR	2.7
1	B	662	ARG	2.6
1	A	461	GLN	2.4
1	B	529	THR	2.3
1	A	497	ALA	2.3
1	B	489	ALA	2.2
1	A	515	LEU	2.2
1	A	547	LYS	2.1
1	A	513	ILE	2.1
1	B	595	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

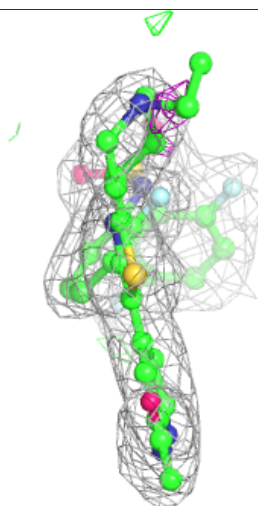
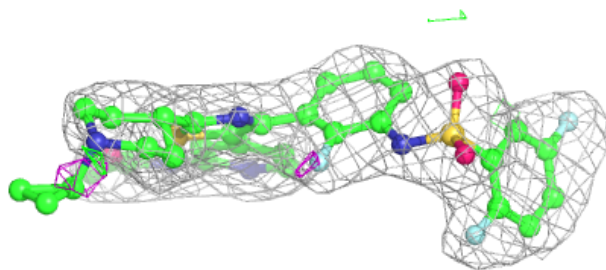
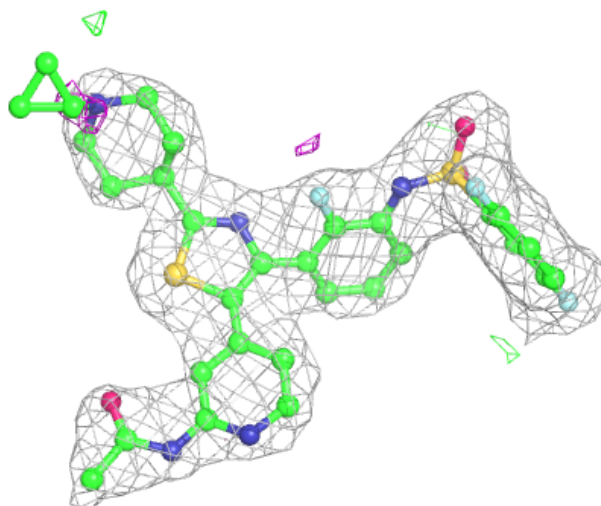
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

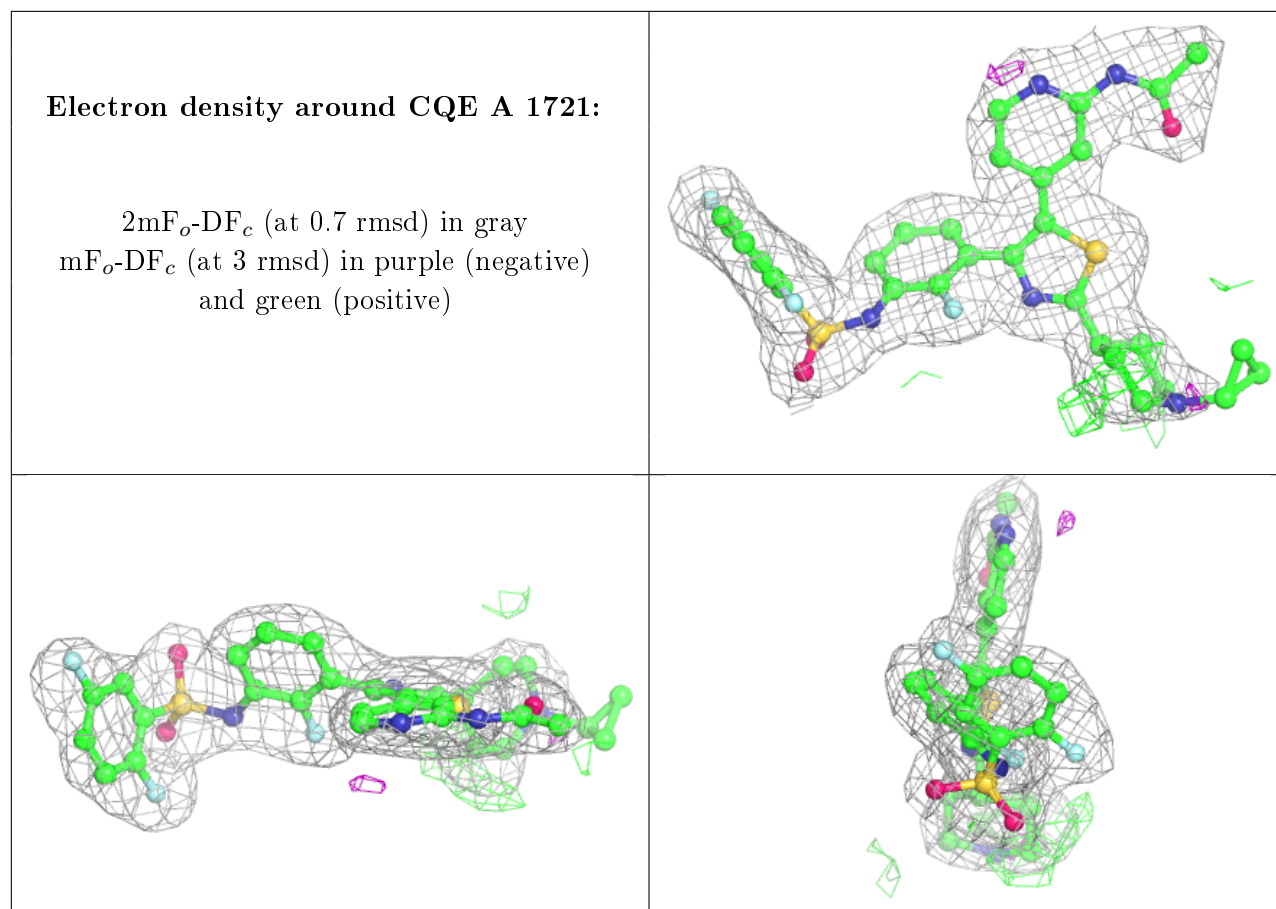
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CQE	B	1721	43/43	0.94	0.15	33,43,75,81	0
2	CQE	A	1721	43/43	0.97	0.15	28,33,70,80	0

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 CQE B 1721:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.