Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 01:04 AM EDT

PDB ID	:	7K0V
Title	:	Crystal structure of bRaf in complex with inhibitor GNE-0749
Authors	:	Yin, J.; Eigenbrot, C.E.; Wang, W.
Deposited on	:	2020-09-06
Resolution	:	1.93 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:

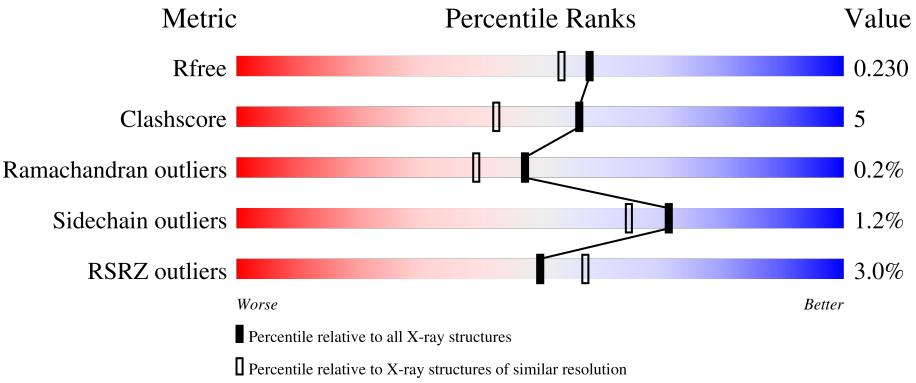
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	288	84% 7% 9%
1	B	288	3% 82% 9% • 8%
1	C	288	4% 77% 14% • 7%
1	D	288	2% 81% 12% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9083 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 Non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2096	1331	371	381	13			
1	B	264	Total	C	N	O	S	0	0	0
			2108	1337	376	382	13			
1	C	267	Total	C	N	O	S	0	1	0
			2143	1356	384	390	13			
1	D	271	Total	C	N	O	S	0	0	0
			2172	1377	386	396	13			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	initiating methionine	UNP H7C560
A	437	HIS	-	expression tag	UNP H7C560
A	438	HIS	-	expression tag	UNP H7C560
A	439	HIS	-	expression tag	UNP H7C560
A	440	HIS	-	expression tag	UNP H7C560
A	441	HIS	-	expression tag	UNP H7C560
A	442	GLY	-	expression tag	UNP H7C560
A	443	SER	-	expression tag	UNP H7C560
A	539	LYS	HIS	conflict	UNP H7C560
A	543	ALA	ILE	conflict	UNP H7C560
A	544	SER	ILE	conflict	UNP H7C560
A	551	LYS	ILE	conflict	UNP H7C560
A	562	ARG	GLN	conflict	UNP H7C560
A	588	ASN	LEU	conflict	UNP H7C560
A	630	SER	LYS	conflict	UNP H7C560
A	667	GLU	PHE	conflict	UNP H7C560
A	673	SER	TYR	conflict	UNP H7C560
A	688	ARG	ALA	conflict	UNP H7C560
A	706	SER	LEU	conflict	UNP H7C560
A	709	ARG	GLN	conflict	UNP H7C560
A	713	GLU	SER	conflict	UNP H7C560

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Chain	Residue	Modelled	Actual	Comment	Reference
A	716	GLU	LEU	conflict	UNP H7C560
A	720	GLU	SER	conflict	UNP H7C560
A	722	SER	PRO	conflict	UNP H7C560
A	723	GLY	LYS	conflict	UNP H7C560
B	436	MET	-	initiating methionine	UNP H7C560
B	437	HIS	-	expression tag	UNP H7C560
B	438	HIS	-	expression tag	UNP H7C560
B	439	HIS	-	expression tag	UNP H7C560
B	440	HIS	-	expression tag	UNP H7C560
B	441	HIS	-	expression tag	UNP H7C560
B	442	GLY	-	expression tag	UNP H7C560
B	443	SER	-	expression tag	UNP H7C560
B	539	LYS	HIS	conflict	UNP H7C560
B	543	ALA	ILE	conflict	UNP H7C560
B	544	SER	ILE	conflict	UNP H7C560
B	551	LYS	ILE	conflict	UNP H7C560
B	562	ARG	GLN	conflict	UNP H7C560
B	588	ASN	LEU	conflict	UNP H7C560
B	630	SER	LYS	conflict	UNP H7C560
B	667	GLU	PHE	conflict	UNP H7C560
B	673	SER	TYR	conflict	UNP H7C560
B	688	ARG	ALA	conflict	UNP H7C560
B	706	SER	LEU	conflict	UNP H7C560
B	709	ARG	GLN	conflict	UNP H7C560
B	713	GLU	SER	conflict	UNP H7C560
B	716	GLU	LEU	conflict	UNP H7C560
B	720	GLU	SER	conflict	UNP H7C560
B	722	SER	PRO	conflict	UNP H7C560
B	723	GLY	LYS	conflict	UNP H7C560
C	436	MET	-	initiating methionine	UNP H7C560
C	437	HIS	-	expression tag	UNP H7C560
C	438	HIS	-	expression tag	UNP H7C560
C	439	HIS	-	expression tag	UNP H7C560
C	440	HIS	-	expression tag	UNP H7C560
C	441	HIS	-	expression tag	UNP H7C560
C	442	GLY	-	expression tag	UNP H7C560
C	443	SER	-	expression tag	UNP H7C560
C	539	LYS	HIS	conflict	UNP H7C560
C	543	ALA	ILE	conflict	UNP H7C560
C	544	SER	ILE	conflict	UNP H7C560
C	551	LYS	ILE	conflict	UNP H7C560
C	562	ARG	GLN	conflict	UNP H7C560

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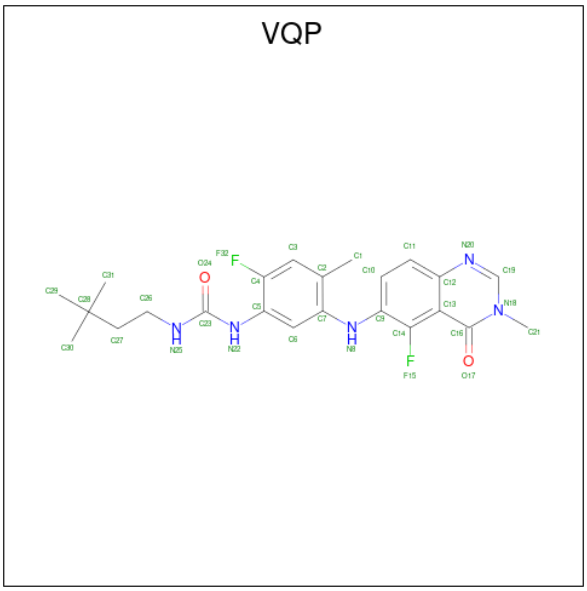
Chain	Residue	Modelled	Actual	Comment	Reference
C	588	ASN	LEU	conflict	UNP H7C560
C	630	SER	LYS	conflict	UNP H7C560
C	667	GLU	PHE	conflict	UNP H7C560
C	673	SER	TYR	conflict	UNP H7C560
C	688	ARG	ALA	conflict	UNP H7C560
C	706	SER	LEU	conflict	UNP H7C560
C	709	ARG	GLN	conflict	UNP H7C560
C	713	GLU	SER	conflict	UNP H7C560
C	716	GLU	LEU	conflict	UNP H7C560
C	720	GLU	SER	conflict	UNP H7C560
C	722	SER	PRO	conflict	UNP H7C560
C	723	GLY	LYS	conflict	UNP H7C560
D	436	MET	-	initiating methionine	UNP H7C560
D	437	HIS	-	expression tag	UNP H7C560
D	438	HIS	-	expression tag	UNP H7C560
D	439	HIS	-	expression tag	UNP H7C560
D	440	HIS	-	expression tag	UNP H7C560
D	441	HIS	-	expression tag	UNP H7C560
D	442	GLY	-	expression tag	UNP H7C560
D	443	SER	-	expression tag	UNP H7C560
D	539	LYS	HIS	conflict	UNP H7C560
D	543	ALA	ILE	conflict	UNP H7C560
D	544	SER	ILE	conflict	UNP H7C560
D	551	LYS	ILE	conflict	UNP H7C560
D	562	ARG	GLN	conflict	UNP H7C560
D	588	ASN	LEU	conflict	UNP H7C560
D	630	SER	LYS	conflict	UNP H7C560
D	667	GLU	PHE	conflict	UNP H7C560
D	673	SER	TYR	conflict	UNP H7C560
D	688	ARG	ALA	conflict	UNP H7C560
D	706	SER	LEU	conflict	UNP H7C560
D	709	ARG	GLN	conflict	UNP H7C560
D	713	GLU	SER	conflict	UNP H7C560
D	716	GLU	LEU	conflict	UNP H7C560
D	720	GLU	SER	conflict	UNP H7C560
D	722	SER	PRO	conflict	UNP H7C560
D	723	GLY	LYS	conflict	UNP H7C560

- Molecule 2 is N-(3,3-dimethylbutyl)-N'-{2-fluoro-5-[(5-fluoro-3-methyl-4-oxo-3,4-dihydroquinazolin-6-yl)amino]-4-methylphenyl}urea (three-letter code: VQP) (formula: $C_{23}H_{27}F_2N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C F N O 32 23 2 5 2	0	0
2	B	1	Total C F N O 32 23 2 5 2	0	0
2	C	1	Total C F N O 32 23 2 5 2	0	0
2	D	1	Total C F N O 32 23 2 5 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	133	Total O 133 133	0	0
4	B	85	Total O 85 85	0	0
4	C	115	Total O 115 115	0	0

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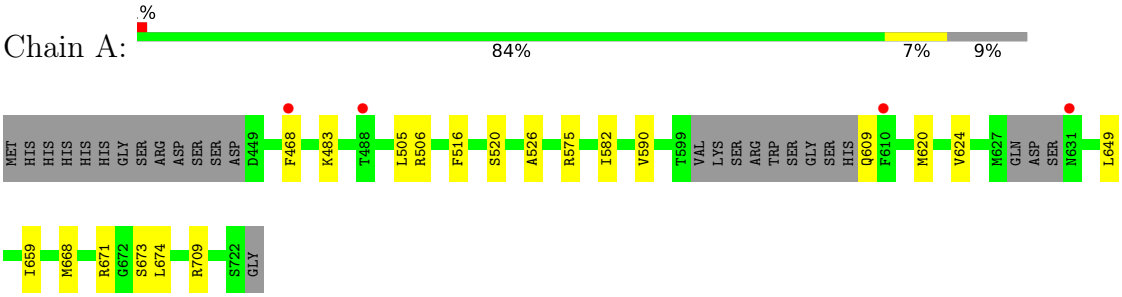
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	101	Total O 101 101	0	0

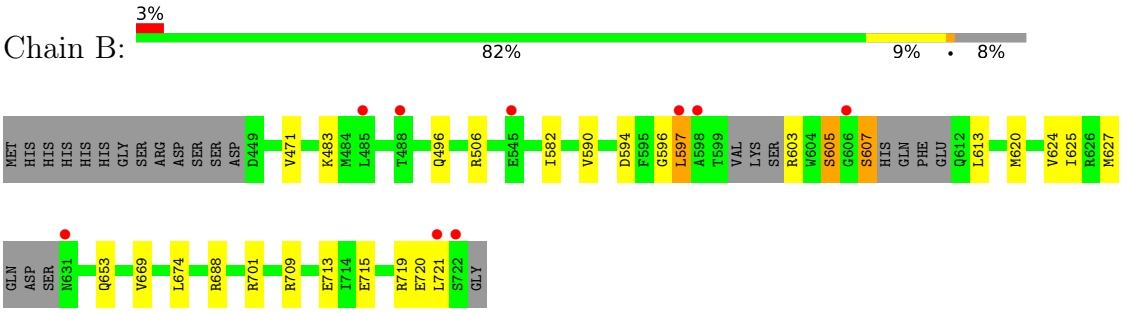
3 Residue-property plots (i)

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.

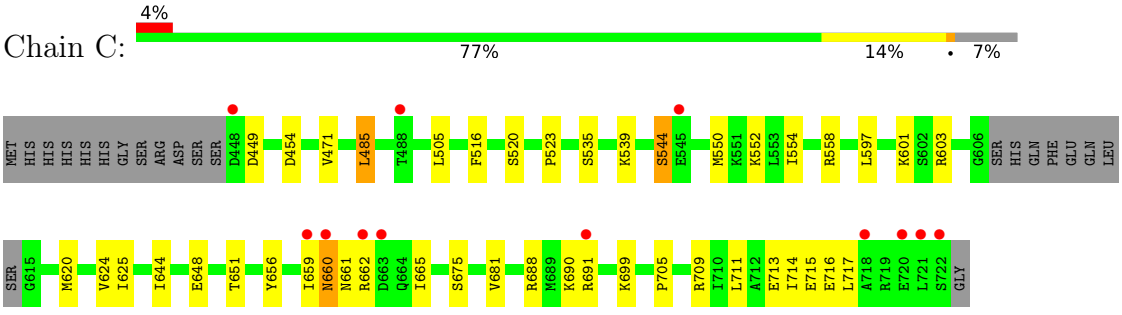
• Molecule 1: Non-specific serine/threonine protein kinase



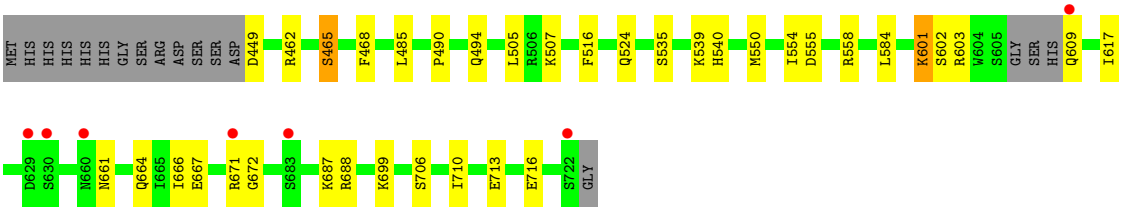
• Molecule 1: Non-specific serine/threonine protein kinase



• Molecule 1: Non-specific serine/threonine protein kinase



• Molecule 1: Non-specific serine/threonine protein kinase


MET HIS HIS HIS HIS GLY SER ARG ASP SER SER ASP D449 R462 S465 F468 L485 P490 Q494 L505 R506 K507 F516 Q524 S535 K539 H540 M550 I554 D555 R558 L584 K601 S602 R603 W604 S605 GLY SER HIS Q609 I617
D629 S630 N660 N661 Q664 I665 I666 E667 R671 G672 S683 K687 R688 K699 S706 I710 E713 E716 S722 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.25Å 115.35Å 119.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 1.93 49.27 – 1.93	Depositor EDS
% Data completeness (in resolution range)	66.7 (49.27-1.93) 66.7 (49.27-1.93)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874_final	Depositor
R, R_{free}	0.184 , 0.230 0.184 , 0.230	Depositor DCC
R_{free} test set	2972 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9083	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/2137	0.56	0/2876
1	B	0.37	0/2149	0.56	0/2891
1	C	0.37	0/2186	0.54	0/2943
1	D	0.36	0/2216	0.52	0/2984
All	All	0.37	0/8688	0.54	0/11694

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

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	2096	0	2121	14	0
1	B	2108	0	2133	22	1
1	C	2143	0	2166	30	1
1	D	2172	0	2194	24	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	1	0
4	A	133	0	0	5	0
4	B	85	0	0	4	0
4	C	115	0	0	2	0
4	D	101	0	0	3	0
All	All	9083	0	8614	86	1

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 5.

All (86) 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)
3:A:802:CL:CL	4:A:995:HOH:O	2.38	0.78
3:B:802:CL:CL	4:B:971:HOH:O	2.47	0.69
1:B:620:MET:SD	4:B:964:HOH:O	2.52	0.67
1:D:609:GLN:N	4:D:901:HOH:O	2.29	0.65
1:B:607:SER:HB3	1:C:603:ARG:HD2	1.78	0.65
1:B:603:ARG:N	4:B:903:HOH:O	2.32	0.62
1:C:688:ARG:HD2	1:C:691:ARG:HH11	1.64	0.62
1:A:575:ARG:HD2	1:D:603:ARG:O	2.00	0.61
1:B:605:SER:O	1:C:603:ARG:NH1	2.28	0.60
1:A:659:ILE:HD13	1:A:668:MET:HE1	1.83	0.60
1:B:483:LYS:HD3	1:B:597:LEU:HD22	1.85	0.59
1:C:675:SER:HB3	1:C:699:LYS:HZ1	1.67	0.59
1:B:594:ASP:O	1:B:597:LEU:HD23	2.04	0.57
1:B:471:VAL:HG23	1:B:597:LEU:HD11	1.86	0.57
1:D:539:LYS:NZ	4:D:903:HOH:O	2.37	0.54
1:D:535:SER:HB3	1:D:539:LYS:HD3	1.88	0.53
1:D:485:LEU:O	1:D:524:GLN:NE2	2.42	0.53
1:B:594:ASP:HB3	1:B:597:LEU:HB3	1.90	0.53
1:C:705:PRO:HB3	1:C:709:ARG:HH11	1.75	0.52
1:C:552:LYS:HE3	4:C:910:HOH:O	2.08	0.52
1:A:649:LEU:O	4:A:901:HOH:O	2.19	0.52
1:C:558:ARG:HD2	1:C:715:GLU:OE1	2.11	0.51
1:D:449:ASP:N	4:D:906:HOH:O	2.42	0.51
1:A:620:MET:HE2	1:A:624:VAL:HG12	1.91	0.51
1:C:620:MET:HE3	1:C:624:VAL:HG12	1.92	0.51
1:D:688:ARG:HD2	1:D:713:GLU:OE1	2.10	0.51
1:D:706:SER:O	1:D:710:ILE:HG13	2.11	0.50
1:A:468:PHE:CD2	1:A:483:LYS:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:LEU:HD23	1:D:490:PRO:HB3	1.93	0.49
1:B:471:VAL:CG2	1:B:597:LEU:HD11	2.41	0.49
1:C:681:VAL:HG21	1:C:690:LYS:HD2	1.94	0.49
1:D:468:PHE:HB3	1:D:494:GLN:NE2	2.28	0.49
1:D:661:ASN:HB3	1:D:664:GLN:HB2	1.96	0.47
1:D:505:LEU:HB3	1:D:516:PHE:HB2	1.95	0.47
1:D:540:HIS:CD2	1:D:584:LEU:HD12	2.50	0.47
1:A:709:ARG:NE	4:A:911:HOH:O	2.44	0.47
1:D:462:ARG:HH11	1:D:465:SER:HB2	1.80	0.47
1:C:651:THR:HG22	1:C:681:VAL:HA	1.97	0.47
1:C:539:LYS:O	1:C:544:SER:HB3	2.14	0.47
1:D:617:ILE:HD13	1:D:666:ILE:HD11	1.97	0.46
1:B:669:VAL:HG23	1:B:674:LEU:HD23	1.96	0.46
1:B:620:MET:CE	1:B:625:ILE:HG13	2.46	0.46
1:C:485:LEU:HD23	1:C:485:LEU:HA	1.84	0.46
1:B:620:MET:HE1	1:B:625:ILE:HG13	1.98	0.46
1:B:624:VAL:O	1:B:627:MET:HG3	2.16	0.46
1:B:596:GLY:O	1:B:597:LEU:HD12	2.16	0.45
1:C:601:LYS:HE3	1:C:601:LYS:HB2	1.84	0.45
1:B:613:LEU:HD13	1:D:601:LYS:NZ	2.32	0.45
1:D:555:ASP:OD1	1:D:558:ARG:NH2	2.49	0.44
1:B:506:ARG:NH2	4:B:906:HOH:O	2.43	0.44
1:C:471:VAL:HG23	1:C:597:LEU:HD11	1.99	0.44
1:A:671:ARG:NH2	1:C:625:ILE:O	2.40	0.44
1:D:550:MET:O	1:D:554:ILE:HG12	2.18	0.44
1:A:506:ARG:NE	4:A:916:HOH:O	2.50	0.44
1:B:688:ARG:NH1	1:B:713:GLU:OE1	2.51	0.43
1:C:454:ASP:OD1	1:C:523:PRO:HD3	2.18	0.43
1:D:462:ARG:NH1	1:D:465:SER:HB2	2.33	0.43
1:C:660:ASN:HA	1:C:665:ILE:HD11	2.00	0.43
1:A:668:MET:HB3	1:A:674:LEU:HB2	2.00	0.43
1:D:507:LYS:HE2	1:D:507:LYS:HB2	1.68	0.43
1:D:667:GLU:O	1:D:671:ARG:HG2	2.18	0.43
1:B:582:ILE:HG23	1:B:590:VAL:HG13	2.01	0.43
1:B:620:MET:HE2	1:B:624:VAL:HG12	2.01	0.42
1:C:659:ILE:HG22	1:C:659:ILE:O	2.19	0.42
1:C:550:MET:O	1:C:554:ILE:HG12	2.19	0.42
1:D:687:LYS:HA	1:D:687:LYS:HD3	1.57	0.42
1:D:688:ARG:HH22	1:D:716:GLU:HB3	1.84	0.42
1:A:609:GLN:O	1:B:496:GLN:NE2	2.53	0.42
1:C:644:ILE:O	1:C:648:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ILE:O	1:C:661:ASN:N	2.53	0.42
1:C:656:TYR:HA	1:C:659:ILE:HD13	2.03	0.41
1:C:688:ARG:HD2	1:C:691:ARG:NH1	2.34	0.41
1:C:691:ARG:NH1	1:C:713:GLU:OE2	2.54	0.41
1:B:715:GLU:O	1:B:719:ARG:HD2	2.21	0.41
1:C:535:SER:HB3	1:C:539:LYS:HD3	2.01	0.41
1:B:720:GLU:O	1:B:721:LEU:HD23	2.21	0.41
1:C:449:ASP:HA	4:C:958:HOH:O	2.21	0.41
1:D:672:GLY:O	1:D:699:LYS:HE3	2.21	0.41
1:A:505:LEU:HB3	1:A:516:PHE:HB2	2.03	0.41
1:A:520:SER:HB2	1:A:526:ALA:HB3	2.02	0.41
1:C:505:LEU:HB3	1:C:516:PHE:HB2	2.03	0.41
1:C:675:SER:HB3	1:C:699:LYS:NZ	2.34	0.41
1:A:582:ILE:HG23	1:A:590:VAL:HG13	2.02	0.40
1:C:711:LEU:O	1:C:715:GLU:HB2	2.21	0.40
1:C:714:ILE:HA	1:C:717:LEU:HG	2.03	0.40
1:A:673:SER:O	4:A:902:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:ARG:NH1	1:C:716:GLU:OE2[4_454]	2.15	0.05

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	256/288 (89%)	248 (97%)	8 (3%)	0	100	100
1	B	256/288 (89%)	245 (96%)	11 (4%)	0	100	100
1	C	264/288 (92%)	251 (95%)	11 (4%)	2 (1%)	19	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	267/288 (93%)	255 (96%)	12 (4%)	0	100 100
All	All	1043/1152 (90%)	999 (96%)	42 (4%)	2 (0%)	47 39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	660	ASN
1	C	662	ARG

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	230/253 (91%)	230 (100%)	0	100 100
1	B	231/253 (91%)	226 (98%)	5 (2%)	52 39
1	C	235/253 (93%)	232 (99%)	3 (1%)	69 62
1	D	239/253 (94%)	236 (99%)	3 (1%)	69 62
All	All	935/1012 (92%)	924 (99%)	11 (1%)	71 64

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

Mol	Chain	Res	Type
1	B	597	LEU
1	B	605	SER
1	B	607	SER
1	B	653	GLN
1	B	701	ARG
1	C	485	LEU
1	C	520	SER
1	C	544	SER
1	D	465	SER
1	D	601	LYS
1	D	602	SER

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
2	VQP	A	801	-	33,34,34	0.63	1 (3%)	43,50,50	1.69	10 (23%)
2	VQP	B	801	-	33,34,34	0.62	1 (3%)	43,50,50	1.61	10 (23%)
2	VQP	D	801	-	33,34,34	0.62	1 (3%)	43,50,50	1.59	8 (18%)
2	VQP	C	801	-	33,34,34	0.65	1 (3%)	43,50,50	1.37	5 (11%)

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	VQP	A	801	-	-	3/15/15/15	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VQP	B	801	-	-	2/15/15/15	0/3/3/3
2	VQP	D	801	-	-	3/15/15/15	0/3/3/3
2	VQP	C	801	-	-	3/15/15/15	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	VQP	C12-N20	-2.43	1.35	1.40
2	C	801	VQP	C12-N20	-2.41	1.35	1.40
2	D	801	VQP	C12-N20	-2.14	1.36	1.40
2	B	801	VQP	C12-N20	-2.12	1.36	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	VQP	C12-N20-C19	5.67	122.21	116.62
2	B	801	VQP	C12-N20-C19	5.67	122.21	116.62
2	A	801	VQP	C12-N20-C19	5.29	121.83	116.62
2	C	801	VQP	C12-N20-C19	4.62	121.17	116.62
2	A	801	VQP	C13-C12-N20	-3.50	117.57	122.54
2	A	801	VQP	C11-C12-N20	3.45	122.59	118.35
2	D	801	VQP	C11-C12-N20	3.39	122.51	118.35
2	C	801	VQP	C11-C12-N20	3.11	122.17	118.35
2	A	801	VQP	C2-C7-N8	2.92	124.22	118.70
2	B	801	VQP	C10-C9-C14	2.80	121.93	117.80
2	D	801	VQP	C13-C12-N20	-2.77	118.60	122.54
2	B	801	VQP	N18-C19-N20	-2.72	122.84	126.02
2	A	801	VQP	N22-C23-N25	2.72	118.55	113.87
2	D	801	VQP	N22-C23-N25	2.62	118.38	113.87
2	B	801	VQP	C13-C12-N20	-2.61	118.83	122.54
2	B	801	VQP	N22-C23-N25	2.52	118.21	113.87
2	B	801	VQP	C11-C12-N20	2.50	121.42	118.35
2	D	801	VQP	C4-C5-N22	-2.49	113.72	118.44
2	C	801	VQP	C13-C12-N20	-2.47	119.02	122.54
2	A	801	VQP	C6-C7-N8	-2.42	116.03	121.05
2	A	801	VQP	C1-C2-C7	2.42	123.99	121.25
2	B	801	VQP	C2-C7-N8	2.35	123.14	118.70
2	D	801	VQP	N18-C19-N20	-2.34	123.29	126.02
2	B	801	VQP	F15-C14-C13	2.26	122.90	119.95
2	A	801	VQP	C27-C26-N25	-2.23	106.50	111.28
2	B	801	VQP	C1-C2-C7	2.19	123.73	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	VQP	C6-C7-N8	-2.19	116.52	121.05
2	C	801	VQP	N22-C23-N25	2.18	117.63	113.87
2	A	801	VQP	C19-N18-C16	-2.12	119.31	122.11
2	D	801	VQP	C6-C5-N22	2.11	127.47	121.90
2	D	801	VQP	C27-C26-N25	-2.07	106.84	111.28
2	A	801	VQP	C3-C4-C5	-2.07	121.53	123.50
2	C	801	VQP	N18-C19-N20	-2.04	123.64	126.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

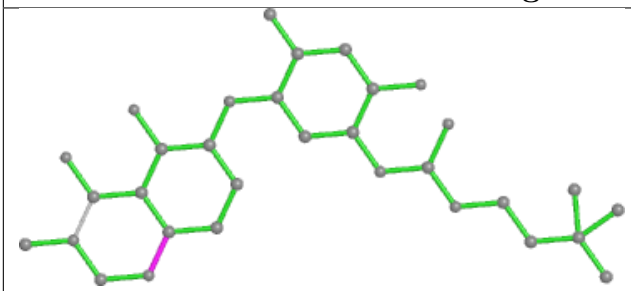
Mol	Chain	Res	Type	Atoms
2	B	801	VQP	C2-C7-N8-C9
2	A	801	VQP	C2-C7-N8-C9
2	A	801	VQP	C6-C7-N8-C9
2	B	801	VQP	C6-C7-N8-C9
2	D	801	VQP	C2-C7-N8-C9
2	C	801	VQP	C2-C7-N8-C9
2	D	801	VQP	C6-C7-N8-C9
2	C	801	VQP	C6-C7-N8-C9
2	C	801	VQP	C4-C5-N22-C23
2	D	801	VQP	C4-C5-N22-C23
2	A	801	VQP	C4-C5-N22-C23

There are no ring outliers.

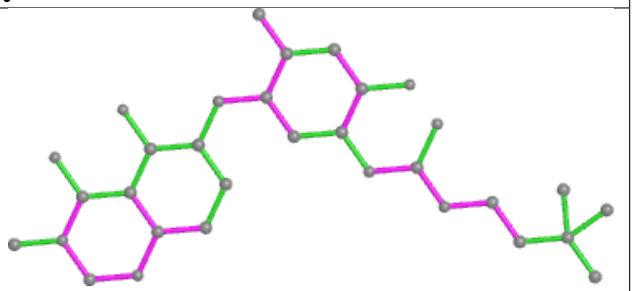
No monomer is involved in short contacts.

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.

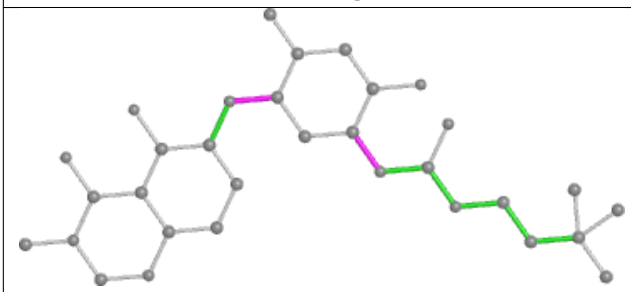
Ligand VQP A 801



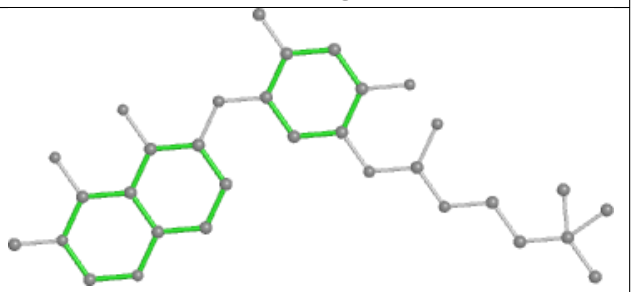
Bond lengths



Bond angles

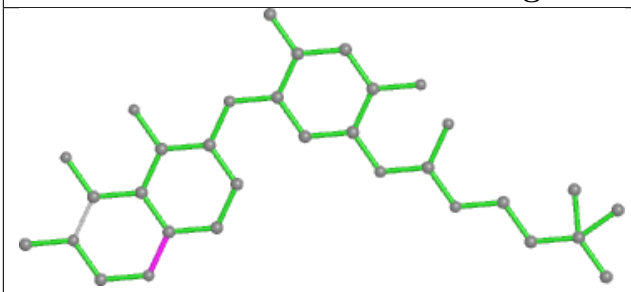


Torsions

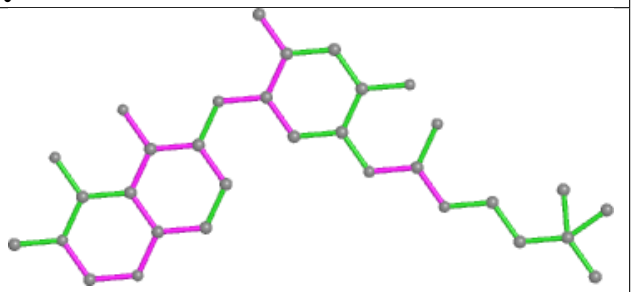


Rings

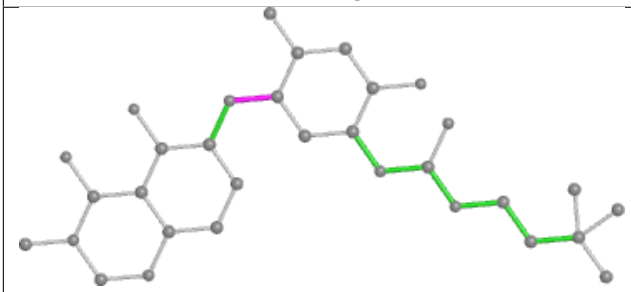
Ligand VQP B 801



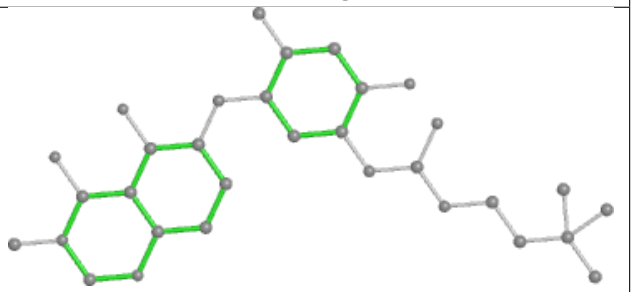
Bond lengths



Bond angles

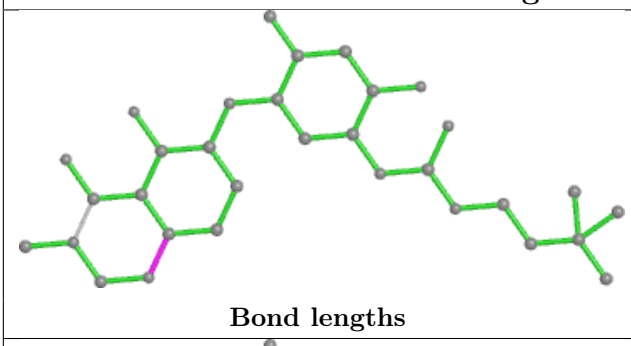


Torsions

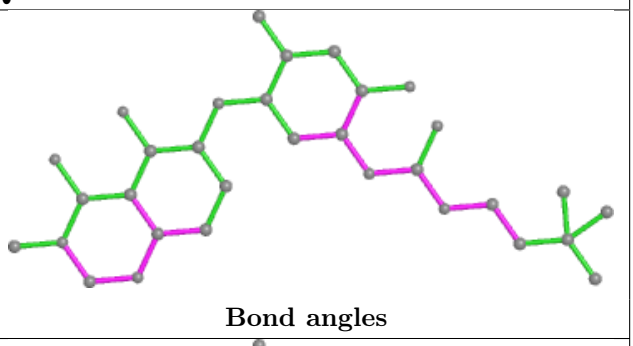


Rings

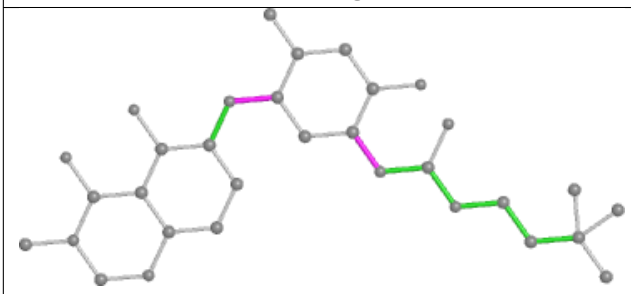
Ligand VQP D 801



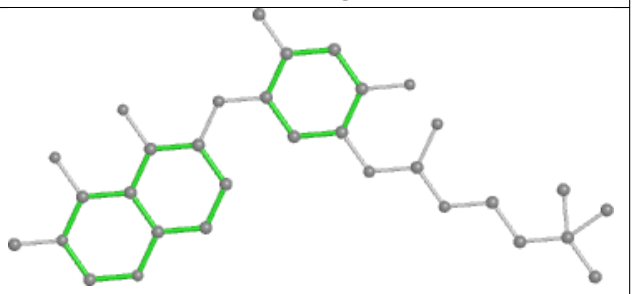
Bond lengths



Bond angles

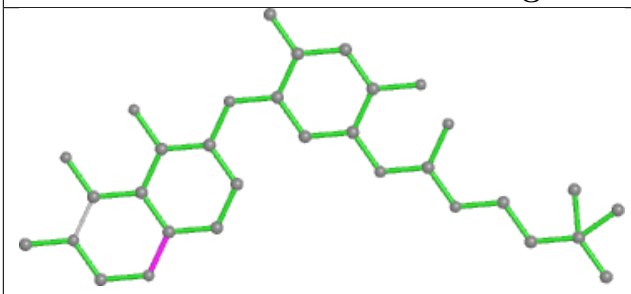


Torsions

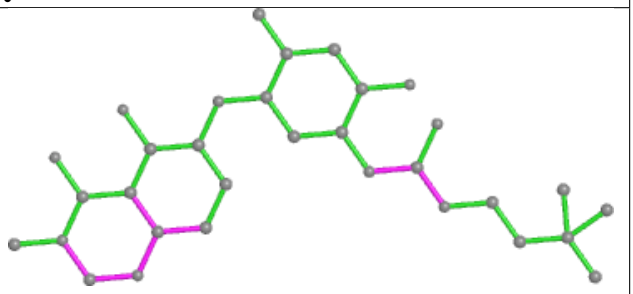


Rings

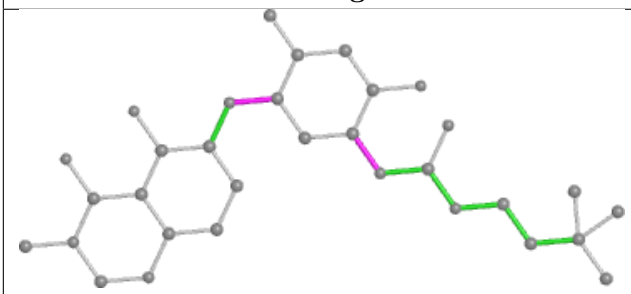
Ligand VQP C 801



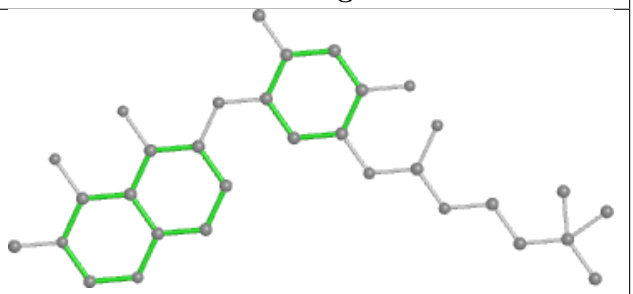
Bond lengths



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, 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	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	262/288 (90%)	0.10	4 (1%)	73 79	20, 30, 52, 81	0
1	B	264/288 (91%)	0.15	9 (3%)	45 53	23, 37, 65, 82	0
1	C	267/288 (92%)	0.10	12 (4%)	33 40	20, 35, 62, 95	0
1	D	271/288 (94%)	0.03	7 (2%)	56 63	23, 36, 63, 89	0
All	All	1064/1152 (92%)	0.09	32 (3%)	50 57	20, 34, 62, 95	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	597	LEU	5.5
1	B	721	LEU	5.0
1	D	671	ARG	4.6
1	A	468	PHE	4.6
1	C	721	LEU	4.3
1	C	722	SER	4.1
1	C	659	ILE	4.0
1	B	722	SER	3.6
1	C	448	ASP	3.6
1	A	631	ASN	3.5
1	B	545	GLU	3.1
1	B	598	ALA	3.0
1	C	660	ASN	3.0
1	C	488	THR	2.9
1	C	718	ALA	2.7
1	C	662	ARG	2.7
1	C	663	ASP	2.7
1	D	629	ASP	2.5
1	D	630	SER	2.5
1	B	606	GLY	2.4
1	B	485	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	691	ARG	2.4
1	D	683	SER	2.3
1	A	488	THR	2.2
1	C	545	GLU	2.2
1	B	631	ASN	2.2
1	D	660	ASN	2.1
1	C	720	GLU	2.1
1	A	610	PHE	2.1
1	B	488	THR	2.0
1	D	609	GLN	2.0
1	D	722	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

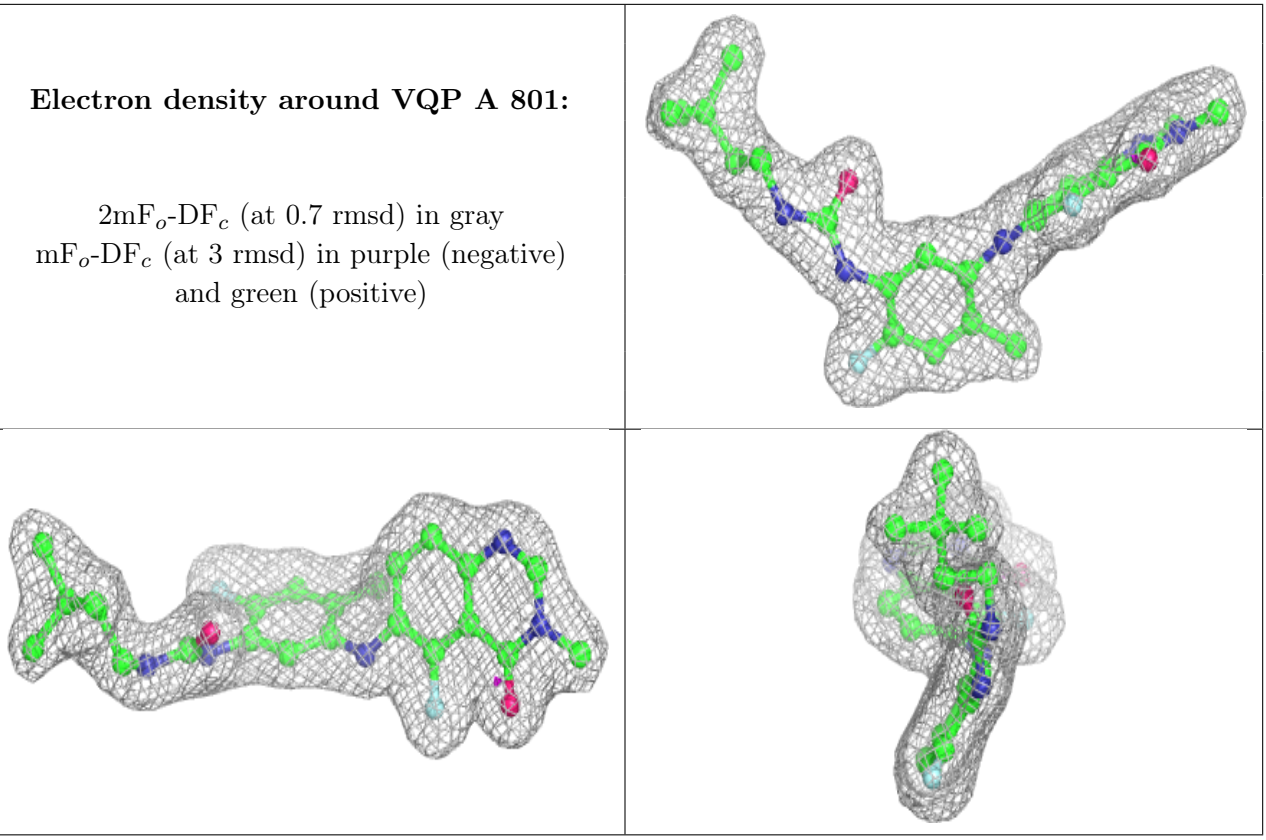
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	VQP	A	801	32/32	0.97	0.11	21,24,27,28	0
2	VQP	B	801	32/32	0.97	0.10	25,27,29,33	0
2	VQP	C	801	32/32	0.97	0.10	21,24,27,29	0
2	VQP	D	801	32/32	0.98	0.09	23,27,30,32	0
3	CL	A	802	1/1	0.99	0.14	31,31,31,31	0
3	CL	B	802	1/1	0.99	0.10	36,36,36,36	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.

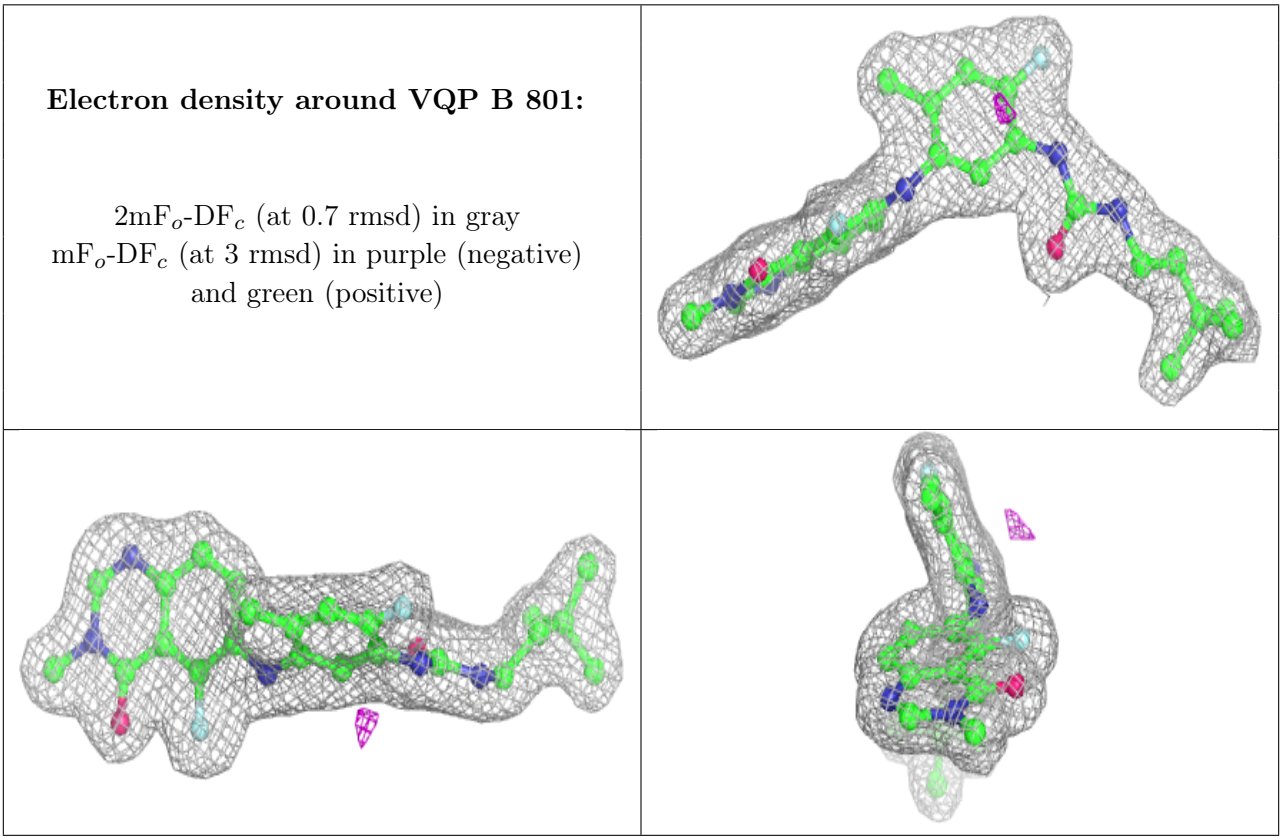
Electron density around VQP A 801:

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



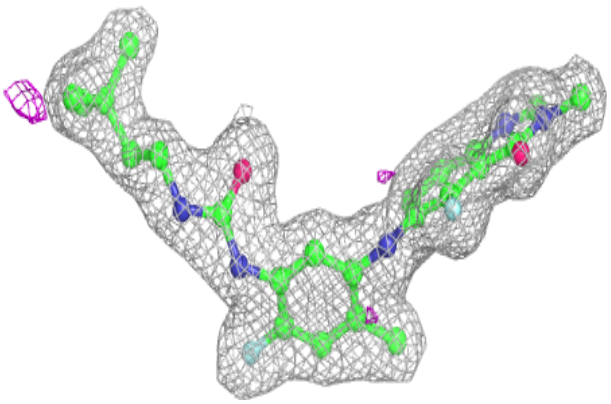
Electron density around VQP B 801:

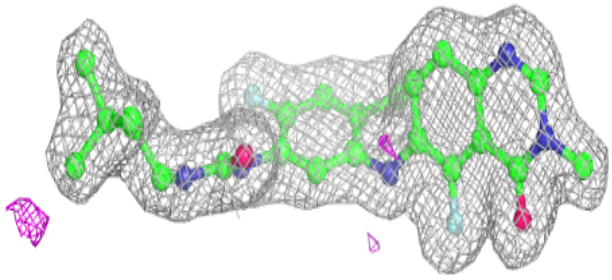
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

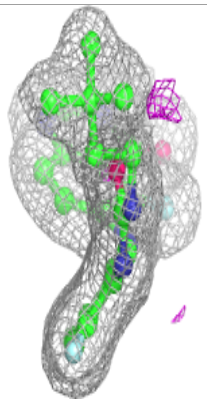


Electron density around VQP C 801:

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

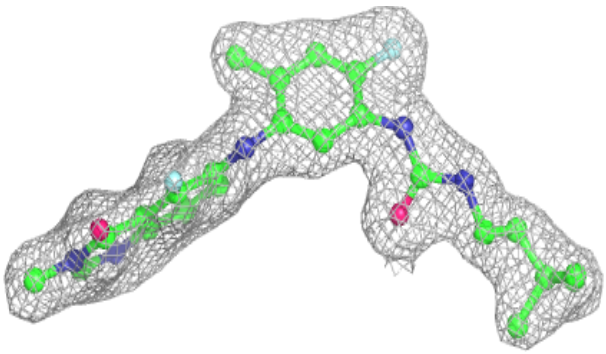


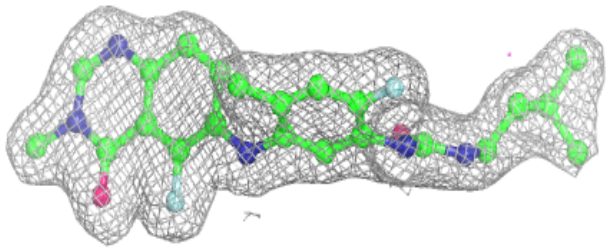


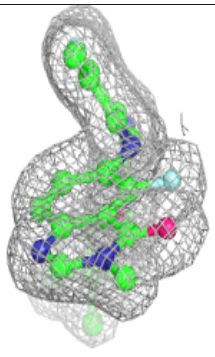


Electron density around VQP D 801:

$2mF_o$-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.