



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:44 PM UTC

PDB ID : 8UDV / pdb_00008udv
Title : The X-RAY co-crystal structure of human FGFR3 V555M and Compound 17
Authors : Tyhonas, J.S.; Arnold, L.D.; Cox, J.; Franovic, A.; Gardiner, E.; Grandinetti, K.; Kania, R.; Kanouni, T.; Lardy, M.; Li, C.; Martin, E.S.; Miller, N.; Mohan, A.; Murphy, E.A.; Perez, M.; Soroceanu, L.; Timple, N.; Uryu, S.; Womble, S.; Kaldor, S.W.
Deposited on : 2023-09-29
Resolution : 2.35 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

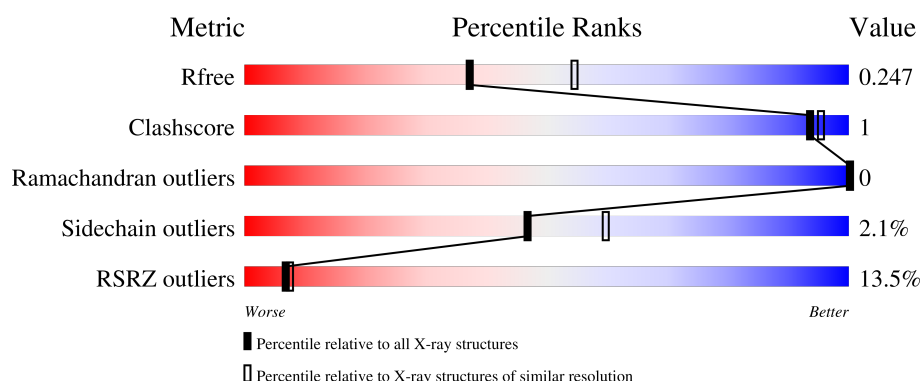
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	297	9% 91% 6%
1	B	297	15% 91% 5%
1	C	297	14% 87% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13691 atoms, of which 6624 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 Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	279	Total	C	H	N	O	S	2233	0	0
			4438	1403	2233	383	400	19			
1	B	281	Total	C	H	N	O	S	2246	0	0
			4462	1408	2246	385	404	19			
1	C	269	Total	C	H	N	O	S	2145	0	0
			4268	1354	2145	364	386	19			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	MET	-	initiating methionine	UNP P22607
A	555	MET	VAL	engineered mutation	UNP P22607
A	?	-	PRO	deletion	UNP P22607
A	?	-	PRO	deletion	UNP P22607
A	?	-	GLY	deletion	UNP P22607
A	?	-	LEU	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	TYR	deletion	UNP P22607
A	?	-	SER	deletion	UNP P22607
A	?	-	PHE	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	THR	deletion	UNP P22607
A	?	-	CYS	deletion	UNP P22607
A	?	-	LYS	deletion	UNP P22607
A	572	SER	PRO	conflict	UNP P22607
A	573	GLY	PRO	conflict	UNP P22607
A	757	HIS	-	expression tag	UNP P22607
A	758	HIS	-	expression tag	UNP P22607
A	759	HIS	-	expression tag	UNP P22607
A	760	HIS	-	expression tag	UNP P22607
A	761	HIS	-	expression tag	UNP P22607
A	762	HIS	-	expression tag	UNP P22607
B	454	MET	-	initiating methionine	UNP P22607

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Chain	Residue	Modelled	Actual	Comment	Reference
B	555	MET	VAL	engineered mutation	UNP P22607
B	?	-	PRO	deletion	UNP P22607
B	?	-	PRO	deletion	UNP P22607
B	?	-	GLY	deletion	UNP P22607
B	?	-	LEU	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	TYR	deletion	UNP P22607
B	?	-	SER	deletion	UNP P22607
B	?	-	PHE	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	THR	deletion	UNP P22607
B	?	-	CYS	deletion	UNP P22607
B	?	-	LYS	deletion	UNP P22607
B	572	SER	PRO	conflict	UNP P22607
B	573	GLY	PRO	conflict	UNP P22607
B	757	HIS	-	expression tag	UNP P22607
B	758	HIS	-	expression tag	UNP P22607
B	759	HIS	-	expression tag	UNP P22607
B	760	HIS	-	expression tag	UNP P22607
B	761	HIS	-	expression tag	UNP P22607
B	762	HIS	-	expression tag	UNP P22607
C	454	MET	-	initiating methionine	UNP P22607
C	555	MET	VAL	engineered mutation	UNP P22607
C	?	-	PRO	deletion	UNP P22607
C	?	-	PRO	deletion	UNP P22607
C	?	-	GLY	deletion	UNP P22607
C	?	-	LEU	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	TYR	deletion	UNP P22607
C	?	-	SER	deletion	UNP P22607
C	?	-	PHE	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	THR	deletion	UNP P22607
C	?	-	CYS	deletion	UNP P22607
C	?	-	LYS	deletion	UNP P22607
C	572	SER	PRO	conflict	UNP P22607
C	573	GLY	PRO	conflict	UNP P22607
C	757	HIS	-	expression tag	UNP P22607
C	758	HIS	-	expression tag	UNP P22607
C	759	HIS	-	expression tag	UNP P22607
C	760	HIS	-	expression tag	UNP P22607
C	761	HIS	-	expression tag	UNP P22607

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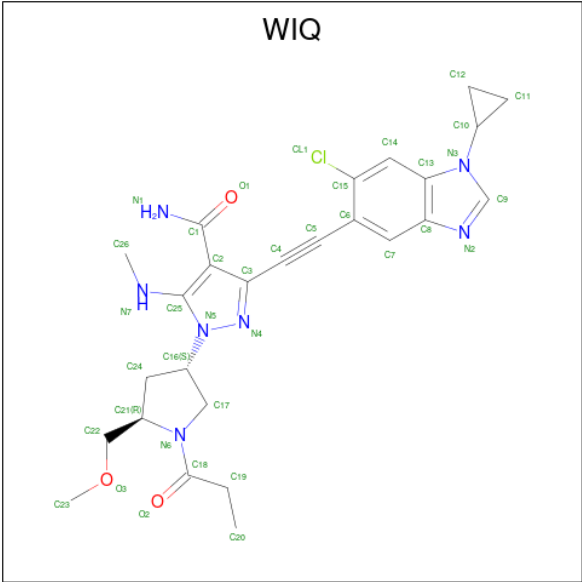
Chain	Residue	Modelled	Actual	Comment	Reference
C	762	HIS	-	expression tag	UNP P22607

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



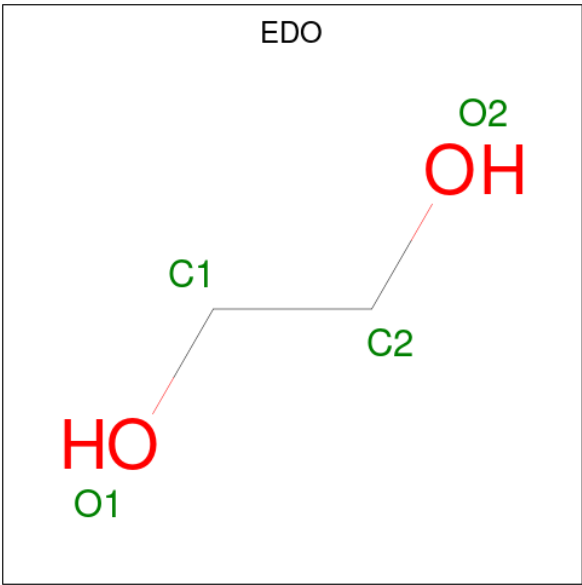
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3-[(6-chloro-1-cyclopropyl-1H-benzimidazol-5-yl)ethynyl]-1-[(3S,5S)-5-(methoxymethyl)-1-(prop-2-enyl)pyrrolidin-3-yl]-5-(methylamino)-1H-pyrazole-4-carboxamide (CCD ID: WIQ) (formula: C₂₆H₃₀ClN₇O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			37	26	1	7	3		
3	B	1	Total	C	Cl	N	O	0	0
			37	26	1	7	3		
3	C	1	Total	C	Cl	N	O	0	0
			37	26	1	7	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		

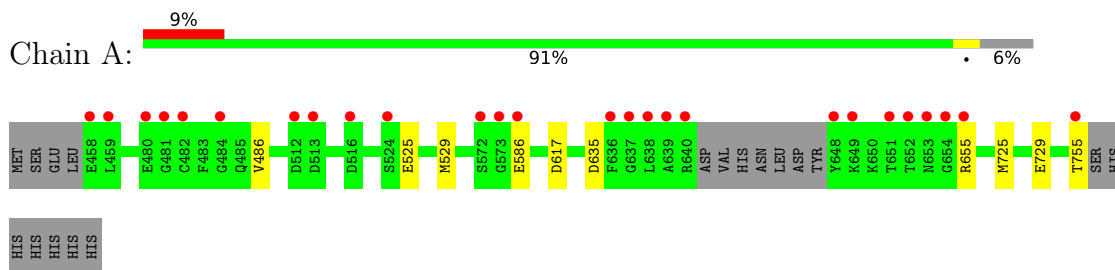
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total 141	O 141	0	0
5	B	142	Total 142	O 142	0	0
5	C	90	Total 90	O 90	0	0

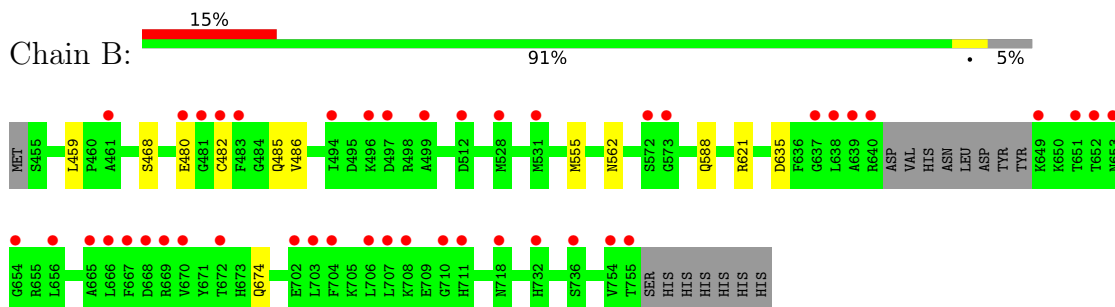
3 Residue-property plots [i](#)

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.

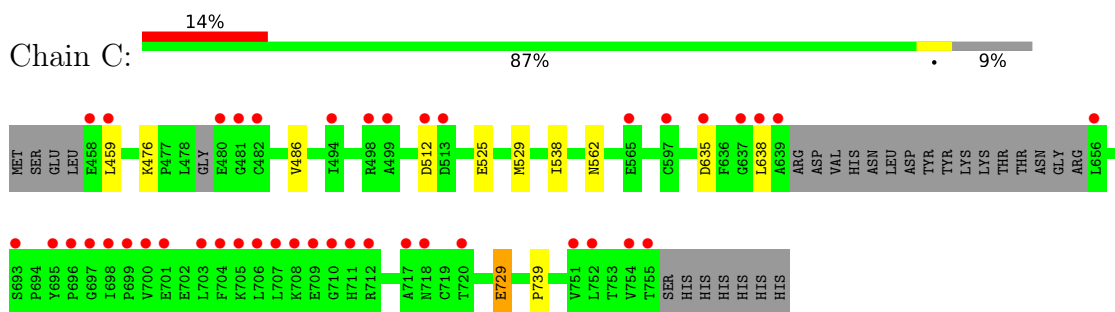
- Molecule 1: Fibroblast growth factor receptor 3



- Molecule 1: Fibroblast growth factor receptor 3



- Molecule 1: Fibroblast growth factor receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.66Å 54.51Å 128.72Å 90.00° 120.22° 90.00°	Depositor
Resolution (Å)	34.74 – 2.35 34.74 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.6 (34.74-2.35) 97.5 (34.74-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.236 , 0.261 0.228 , 0.247	Depositor DCC
R_{free} test set	2148 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13691	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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: WIQ, EDO, SO4

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	0.58	0/2249	1.03	0/3034
1	B	0.61	0/2259	1.05	2/3047 (0.1%)
1	C	0.60	0/2165	1.05	2/2922 (0.1%)
All	All	0.60	0/6673	1.05	4/9003 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	GLU	CB-CG-CD	6.47	123.61	112.60
1	C	729	GLU	CB-CG-CD	5.71	122.31	112.60
1	B	562	ASN	CA-CB-CG	5.39	117.99	112.60
1	C	562	ASN	CA-CB-CG	5.01	117.61	112.60

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	2205	2233	2233	5	0
1	B	2216	2246	2246	5	0
1	C	2123	2145	2145	5	0
2	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	1	0
2	C	10	0	0	0	0
3	A	37	0	0	3	0
3	B	37	0	0	4	0
3	C	37	0	0	4	0
4	C	4	0	6	0	0
5	A	141	0	0	0	0
5	B	142	0	0	1	0
5	C	90	0	0	0	0
All	All	7067	6624	6630	18	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 1.

All (18) 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:486:VAL:HG12	3:C:1004:WIQ:CL1	2.30	0.68
1:C:486:VAL:CG1	3:C:1004:WIQ:CL1	2.82	0.64
1:B:588:GLN:HG2	5:B:1002:HOH:O	1.99	0.62
1:C:729:GLU:HG3	1:C:739:PRO:HD3	1.88	0.54
1:B:555:MET:SD	3:B:803:WIQ:C14	3.02	0.47
1:A:486:VAL:CG2	3:A:1003:WIQ:CL1	3.00	0.46
1:B:468:SER:OG	2:B:802:SO4:O1	2.32	0.46
3:C:1004:WIQ:N1	3:C:1004:WIQ:C4	2.79	0.46
3:A:1003:WIQ:C4	3:A:1003:WIQ:N1	2.79	0.45
1:B:486:VAL:CG2	3:B:803:WIQ:CL1	3.01	0.45
1:A:617:ASP:OD1	1:A:655:ARG:NH2	2.50	0.45
3:B:803:WIQ:N1	3:B:803:WIQ:C4	2.80	0.45
1:C:486:VAL:HG11	3:C:1004:WIQ:CL1	2.52	0.45
1:A:486:VAL:HG22	3:A:1003:WIQ:CL1	2.56	0.43
1:A:725:MET:O	1:A:729:GLU:HG2	2.19	0.42
1:B:486:VAL:HG22	3:B:803:WIQ:CL1	2.57	0.42
1:C:525:GLU:O	1:C:529:MET:HG2	2.21	0.41
1:A:525:GLU:O	1:A:529:MET:HG2	2.21	0.41

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	275/297 (93%)	272 (99%)	3 (1%)	0	100	100
1	B	277/297 (93%)	273 (99%)	4 (1%)	0	100	100
1	C	263/297 (89%)	260 (99%)	3 (1%)	0	100	100
All	All	815/891 (92%)	805 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	236/254 (93%)	233 (99%)	3 (1%)	61	73
1	B	238/254 (94%)	232 (98%)	6 (2%)	42	54
1	C	228/254 (90%)	222 (97%)	6 (3%)	40	53
All	All	702/762 (92%)	687 (98%)	15 (2%)	47	60

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	586	GLU
1	A	635	ASP
1	A	755	THR
1	B	459	LEU
1	B	482	CYS

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Mol	Chain	Res	Type
1	B	485	GLN
1	B	621	ARG
1	B	635	ASP
1	B	674	GLN
1	C	459	LEU
1	C	476	LYS
1	C	512	ASP
1	C	538	ILE
1	C	635	ASP
1	C	638	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	622	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
4	EDO	C	1003	-	3,3,3	0.23	0	2,2,2	0.23	0
2	SO4	A	1002	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	A	1001	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	B	801	-	4,4,4	0.28	0	6,6,6	0.50	0
3	WIQ	C	1004	1	41,41,41	1.14	3 (7%)	47,60,60	2.31	6 (12%)
2	SO4	C	1002	-	4,4,4	0.30	0	6,6,6	0.37	0
2	SO4	A	1004	-	4,4,4	0.25	0	6,6,6	0.24	0
2	SO4	B	802	-	4,4,4	0.25	0	6,6,6	0.41	0
2	SO4	C	1001	-	4,4,4	0.28	0	6,6,6	0.33	0
3	WIQ	B	803	1	41,41,41	1.26	4 (9%)	47,60,60	2.00	11 (23%)
3	WIQ	A	1003	1	41,41,41	1.00	1 (2%)	47,60,60	2.17	6 (12%)

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
3	WIQ	B	803	1	-	9/26/42/42	0/5/5/5
3	WIQ	C	1004	1	-	7/26/42/42	0/5/5/5
4	EDO	C	1003	-	-	0/1/1/1	-
3	WIQ	A	1003	1	-	7/26/42/42	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	WIQ	C20-C19	-5.22	1.29	1.51
3	C	1004	WIQ	C20-C19	-5.06	1.30	1.51
3	A	1003	WIQ	C20-C19	-4.80	1.31	1.51
3	C	1004	WIQ	C3-N4	3.22	1.37	1.33
3	B	803	WIQ	C3-N4	3.16	1.37	1.33
3	B	803	WIQ	C10-N3	-2.53	1.42	1.46
3	B	803	WIQ	C19-C18	-2.36	1.47	1.51
3	C	1004	WIQ	C2-C3	-2.04	1.38	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1004	WIQ	C20-C19-C18	9.61	129.52	112.69
3	A	1003	WIQ	C20-C19-C18	8.41	127.43	112.69
3	C	1004	WIQ	C2-C3-N4	-7.57	106.66	112.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	WIQ	C2-C3-N4	-7.43	106.78	112.85
3	B	803	WIQ	C20-C19-C18	6.86	124.71	112.69
3	B	803	WIQ	C2-C3-N4	-5.92	108.01	112.85
3	B	803	WIQ	C17-C16-N5	5.14	117.31	112.48
3	C	1004	WIQ	C3-N4-N5	5.12	108.69	103.81
3	A	1003	WIQ	C3-N4-N5	4.89	108.47	103.81
3	A	1003	WIQ	C17-C16-N5	4.55	116.76	112.48
3	C	1004	WIQ	C17-C16-N5	4.41	116.62	112.48
3	B	803	WIQ	C3-N4-N5	3.95	107.58	103.81
3	C	1004	WIQ	C25-C2-C3	3.93	108.54	103.93
3	A	1003	WIQ	C25-C2-C3	3.38	107.89	103.93
3	B	803	WIQ	C13-N3-C9	2.83	108.83	106.26
3	C	1004	WIQ	C25-N5-N4	-2.58	109.14	112.12
3	B	803	WIQ	C25-C2-C3	2.44	106.79	103.93
3	B	803	WIQ	C10-N3-C9	-2.44	123.11	128.01
3	A	1003	WIQ	C25-N5-N4	-2.26	109.51	112.12
3	B	803	WIQ	N3-C9-N2	-2.08	110.98	113.94
3	B	803	WIQ	C25-N5-N4	-2.03	109.78	112.12
3	B	803	WIQ	C21-C24-C16	2.02	106.09	95.10
3	B	803	WIQ	C16-C17-N6	2.01	105.06	102.82

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	WIQ	C3-C4-C5-C6
3	C	1004	WIQ	C3-C4-C5-C6
3	B	803	WIQ	N6-C18-C19-C20
3	A	1003	WIQ	C24-C21-C22-O3
3	B	803	WIQ	C24-C21-C22-O3
3	C	1004	WIQ	C24-C21-C22-O3
3	A	1003	WIQ	C11-C10-N3-C13
3	B	803	WIQ	C11-C10-N3-C13
3	C	1004	WIQ	C11-C10-N3-C13
3	B	803	WIQ	C3-C4-C5-C6
3	C	1004	WIQ	C4-C5-C6-C15
3	B	803	WIQ	C4-C5-C6-C15
3	A	1003	WIQ	N6-C21-C22-O3
3	B	803	WIQ	N6-C21-C22-O3
3	C	1004	WIQ	N6-C21-C22-O3
3	A	1003	WIQ	C4-C5-C6-C15
3	B	803	WIQ	O2-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	B	803	WIQ	C4-C5-C6-C7
3	C	1004	WIQ	C4-C5-C6-C7
3	A	1003	WIQ	C12-C10-N3-C13
3	B	803	WIQ	C12-C10-N3-C13
3	C	1004	WIQ	C12-C10-N3-C13
3	A	1003	WIQ	C4-C5-C6-C7

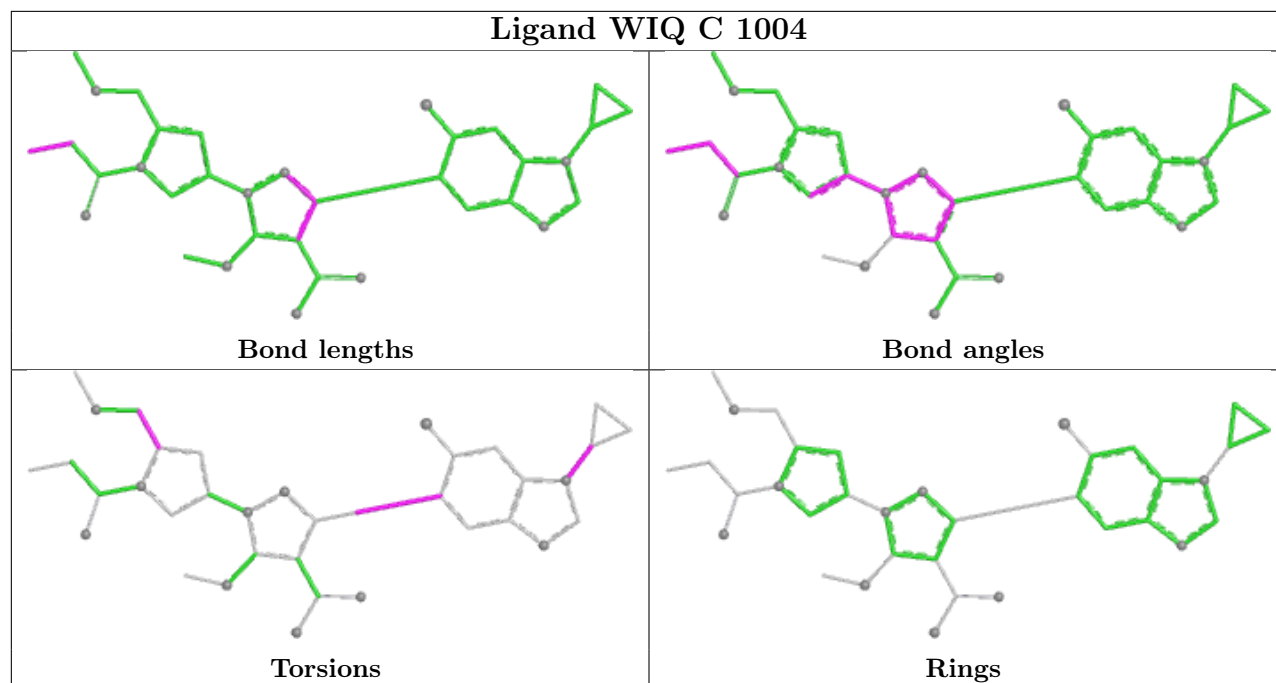
There are no ring outliers.

4 monomers are involved in 12 short contacts:

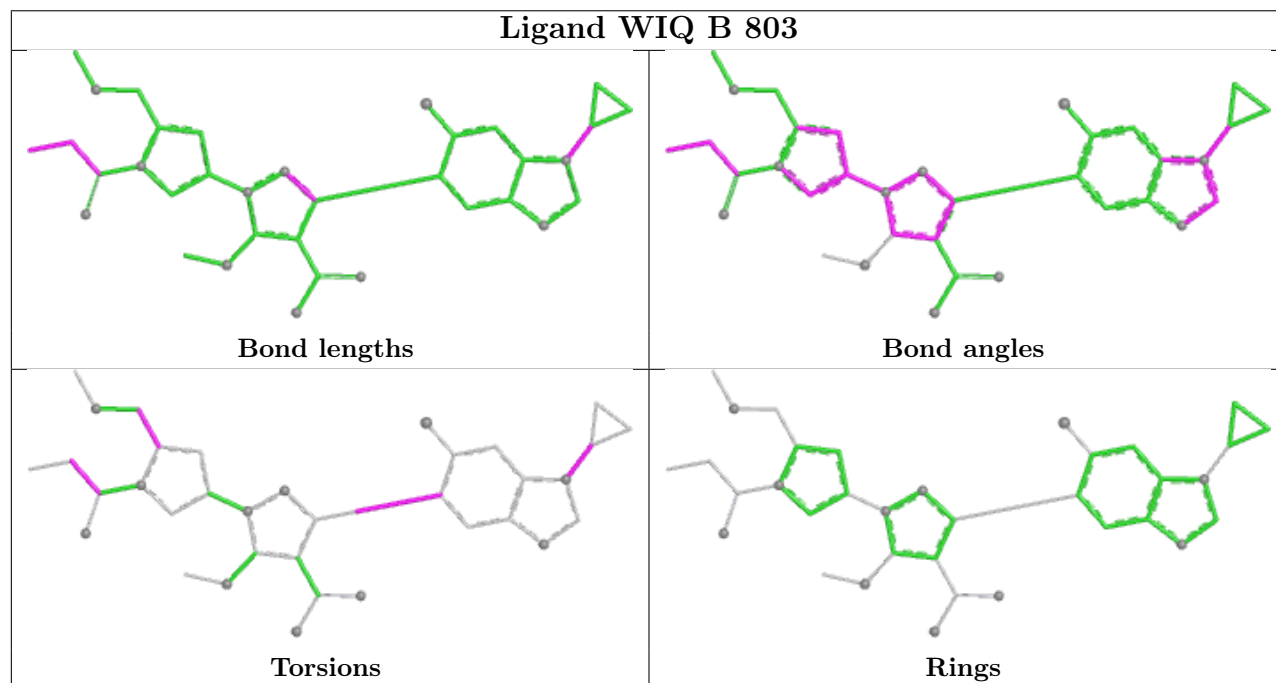
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1004	WIQ	4	0
2	B	802	SO4	1	0
3	B	803	WIQ	4	0
3	A	1003	WIQ	3	0

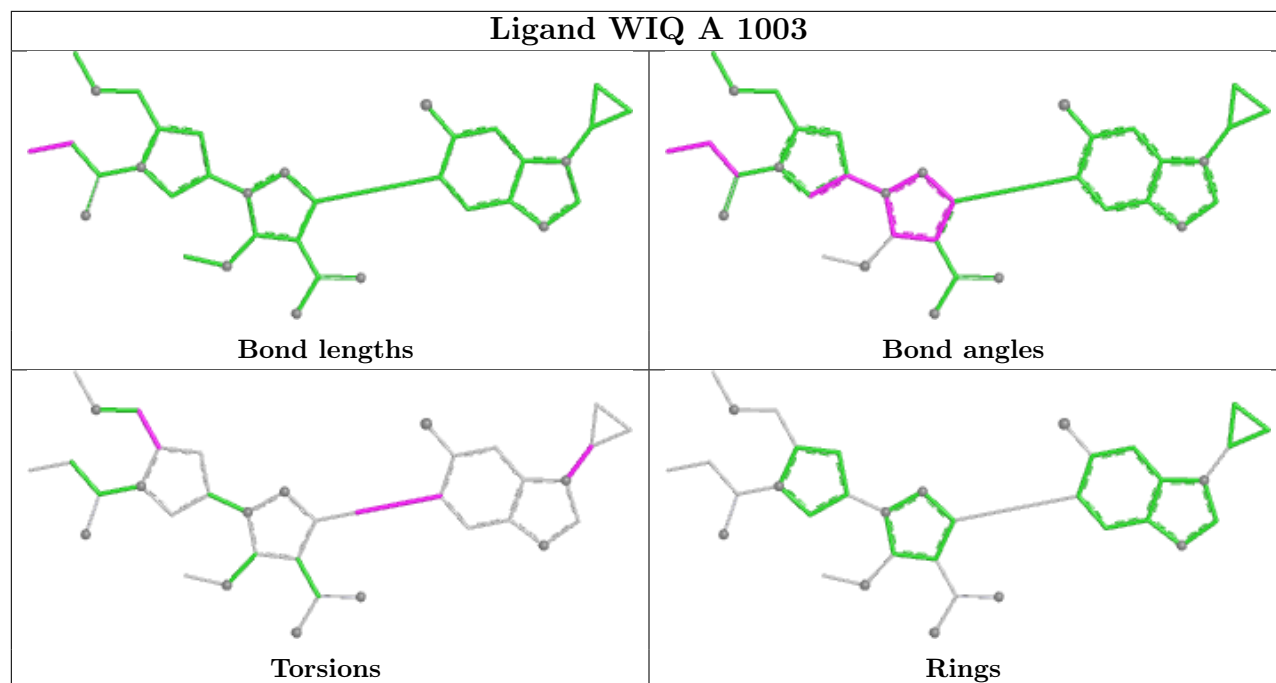
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 WIQ C 1004



Ligand WIQ B 803





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	279/297 (93%)	0.69	26 (9%) 14 17	9, 16, 32, 41	0
1	B	281/297 (94%)	0.87	44 (15%) 5 5	9, 17, 32, 42	0
1	C	269/297 (90%)	1.02	42 (15%) 5 5	12, 20, 37, 55	0
All	All	829/891 (93%)	0.86	112 (13%) 7 7	9, 17, 34, 55	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	GLY	6.3
1	A	654	GLY	6.1
1	B	654	GLY	5.6
1	C	481	GLY	5.3
1	A	755	THR	5.3
1	C	703	LEU	5.2
1	B	666	LEU	5.1
1	B	704	PHE	5.1
1	B	702	GLU	4.8
1	C	700	VAL	4.8
1	A	651	THR	4.7
1	C	697	GLY	4.6
1	B	707	LEU	4.4
1	B	639	ALA	4.3
1	B	651	THR	4.2
1	C	656	LEU	4.1
1	A	648	TYR	4.1
1	B	482	CYS	4.1
1	A	653	ASN	4.0
1	A	640	ARG	3.9
1	C	704	PHE	3.9
1	C	755	THR	3.8
1	B	667	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	482	CYS	3.8
1	C	718	ASN	3.7
1	A	482	CYS	3.6
1	C	706	LEU	3.5
1	B	653	ASN	3.5
1	A	652	THR	3.4
1	C	480	GLU	3.4
1	B	754	VAL	3.4
1	B	528	MET	3.3
1	C	705	LYS	3.3
1	A	481	GLY	3.3
1	B	638	LEU	3.2
1	A	513	ASP	3.2
1	A	637	GLY	3.2
1	C	696	PRO	3.2
1	B	649	LYS	3.1
1	C	710	GLY	3.1
1	B	665	ALA	3.1
1	C	698	ILE	3.1
1	A	639	ALA	3.1
1	B	710	GLY	3.0
1	C	754	VAL	3.0
1	A	649	LYS	3.0
1	C	717	ALA	3.0
1	B	640	ARG	3.0
1	B	669	ARG	3.0
1	B	637	GLY	2.9
1	C	499	ALA	2.9
1	C	695	TYR	2.8
1	A	480	GLU	2.8
1	B	483	PHE	2.8
1	C	720	THR	2.8
1	C	711	HIS	2.7
1	B	531	MET	2.7
1	C	752	LEU	2.7
1	B	499	ALA	2.7
1	C	494	ILE	2.7
1	B	461	ALA	2.6
1	A	638	LEU	2.6
1	C	707	LEU	2.6
1	C	712	ARG	2.6
1	B	711	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	573	GLY	2.6
1	C	637	GLY	2.6
1	C	597	CYS	2.5
1	B	480	GLU	2.5
1	C	635	ASP	2.5
1	C	639	ALA	2.4
1	B	736	SER	2.4
1	A	458	GLU	2.4
1	C	699	PRO	2.4
1	C	751	VAL	2.4
1	A	459	LEU	2.4
1	B	668	ASP	2.3
1	C	513	ASP	2.3
1	C	708	LYS	2.3
1	B	512	ASP	2.3
1	A	655	ARG	2.3
1	B	496	LYS	2.3
1	C	512	ASP	2.3
1	B	652	THR	2.3
1	C	498	ARG	2.3
1	B	494	ILE	2.3
1	B	703	LEU	2.3
1	B	708	LYS	2.3
1	B	718	ASN	2.3
1	A	573	GLY	2.3
1	A	516	ASP	2.2
1	B	497	ASP	2.2
1	A	484	GLY	2.2
1	C	693	SER	2.2
1	B	670	VAL	2.2
1	B	732	HIS	2.2
1	C	709	GLU	2.2
1	C	638	LEU	2.2
1	A	636	PHE	2.2
1	A	586	GLU	2.2
1	C	458	GLU	2.2
1	A	572	SER	2.2
1	C	701	GLU	2.1
1	B	706	LEU	2.1
1	C	459	LEU	2.1
1	B	572	SER	2.1
1	B	755	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	524	SER	2.1
1	A	512	ASP	2.1
1	B	672	THR	2.0
1	C	565	GLU	2.0
1	B	656	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

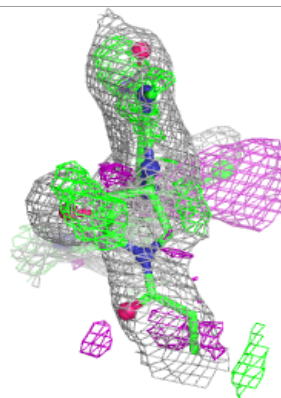
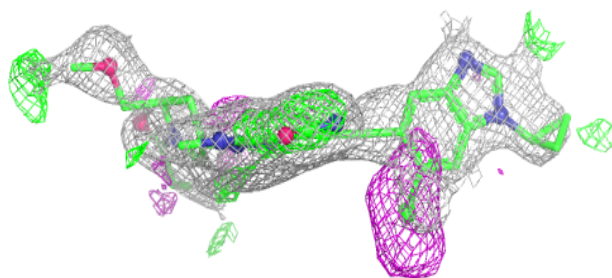
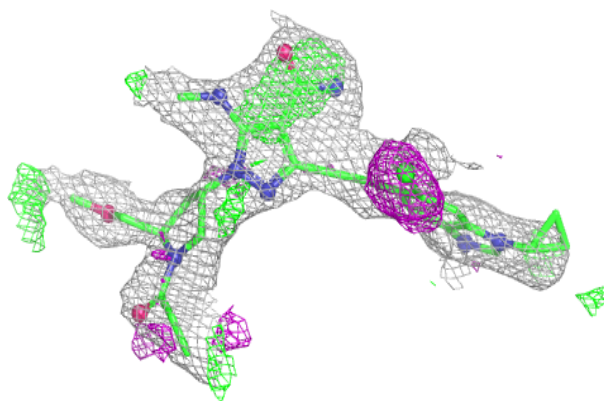
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1002	5/5	0.66	0.25	90,90,90,90	0
3	WIQ	B	803	37/37	0.69	0.24	56,58,62,62	0
2	SO4	C	1002	5/5	0.70	0.26	101,101,101,101	0
2	SO4	B	801	5/5	0.70	0.17	90,90,90,90	5
3	WIQ	A	1003	37/37	0.82	0.17	53,54,56,57	0
3	WIQ	C	1004	37/37	0.84	0.16	53,54,58,59	0
2	SO4	B	802	5/5	0.85	0.32	62,62,62,62	0
2	SO4	A	1001	5/5	0.86	0.30	59,59,59,59	5
2	SO4	C	1001	5/5	0.86	0.21	80,80,80,81	0
4	EDO	C	1003	4/4	0.89	0.11	44,44,44,44	0
2	SO4	A	1004	5/5	0.99	0.04	29,29,30,30	0

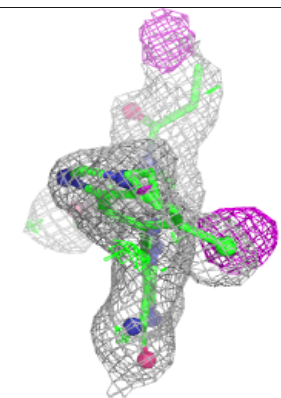
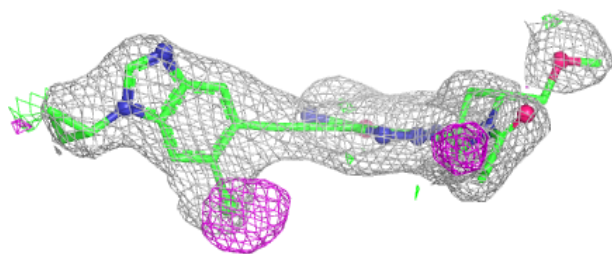
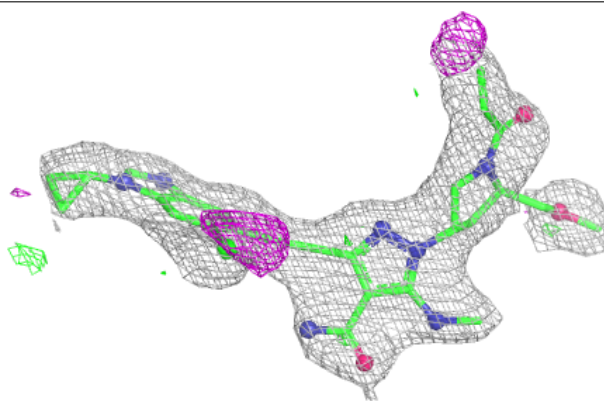
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

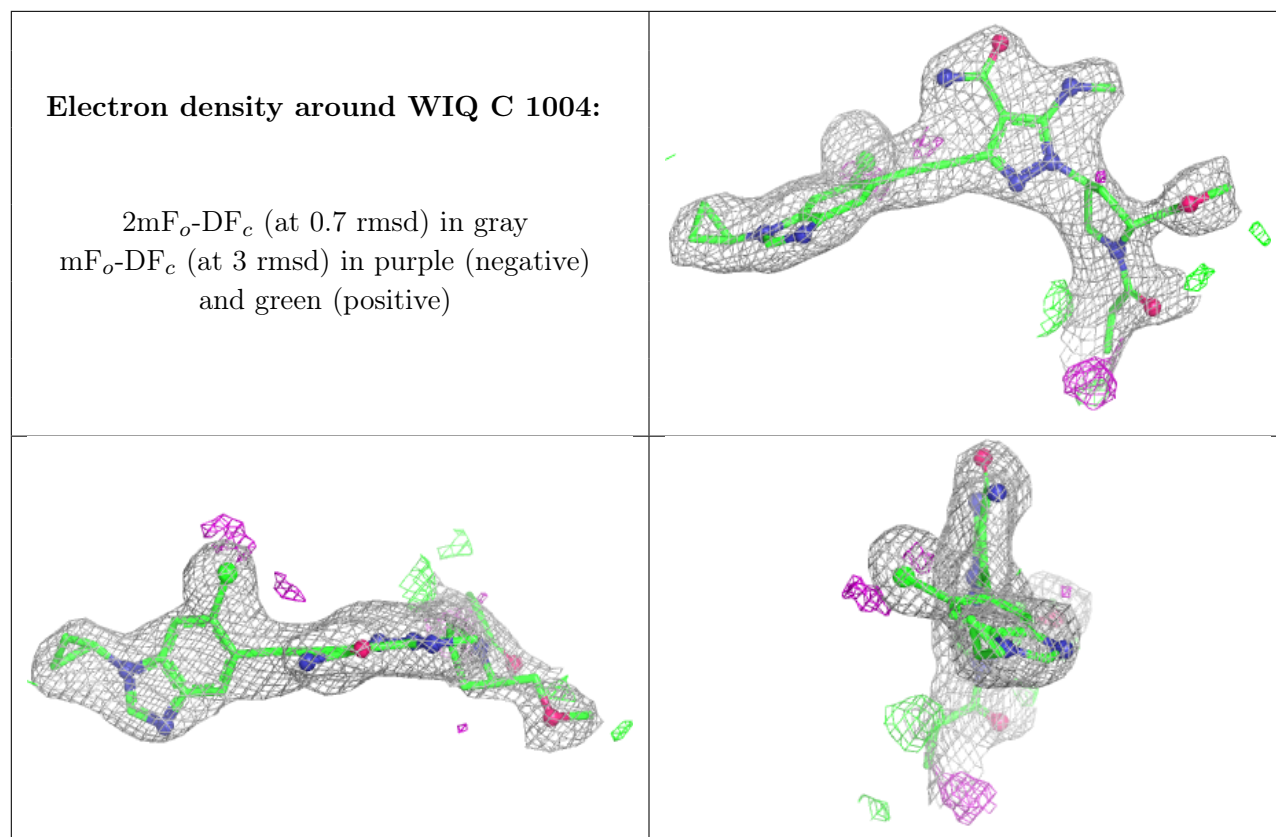
Electron density around WIQ B 803:

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

**Electron density around WIQ A 1003:**

$2mF_o-DF_c$ (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.