WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 07:05 PM EDT

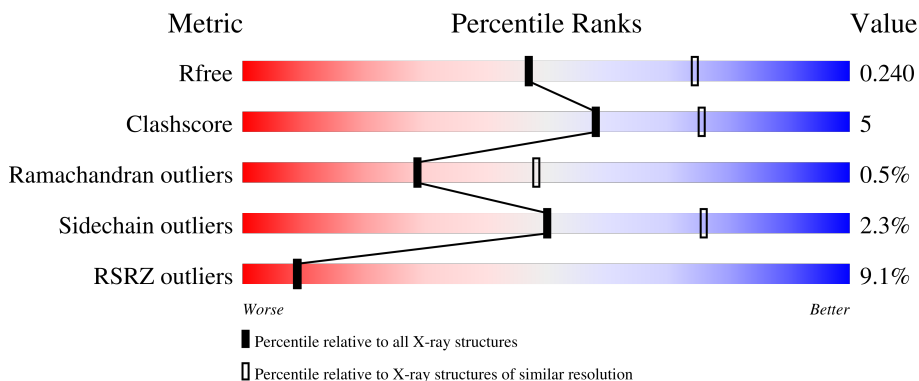|		
PDB ID	:	5KWW
Title	:	Crystal Structure of Inhibitor JNJ-53718678 In Complex with Prefusion RSV F Glycoprotein
Authors	:	McLellan, J.S.; Battles, M.B.; Arnoult, E.; Roymans, D.; Langedijk, J.P.
Deposited on	:	2016-07-19
Resolution	:	2.50 Å(reported)

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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 2.50 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	Percentile Ranks	Value
Rfree		0.240
Clashscore		5
Ramachandran outliers		0.5%
Sidechain outliers		2.3%
RSRZ outliers		9.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	F	568	7% 66% 9% • 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	F	612	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 3562 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 Fusion glycoprotein F0, Envelope glycoprotein chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	428	Total 3318	C 2107	N 542	O 648	S 21	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	66	GLU	LYS	conflict	UNP W8RJF9
F	155	CYS	SER	conflict	UNP W8RJF9
F	190	PHE	SER	conflict	UNP W8RJF9
F	207	LEU	VAL	conflict	UNP W8RJF9
F	290	CYS	SER	conflict	UNP W8RJF9
F	514	SER	-	linker	UNP W8RJF9
F	515	ALA	-	linker	UNP W8RJF9
F	516	ILE	-	linker	UNP W8RJF9
F	517	GLY	-	linker	UNP W8RJF9
F	546	GLY	-	expression tag	UNP M1E1E4
F	547	LEU	-	expression tag	UNP M1E1E4
F	548	VAL	-	expression tag	UNP M1E1E4
F	549	PRO	-	expression tag	UNP M1E1E4
F	550	ARG	-	expression tag	UNP M1E1E4
F	551	GLY	-	expression tag	UNP M1E1E4
F	552	SER	-	expression tag	UNP M1E1E4
F	553	HIS	-	expression tag	UNP M1E1E4
F	554	HIS	-	expression tag	UNP M1E1E4
F	555	HIS	-	expression tag	UNP M1E1E4
F	556	HIS	-	expression tag	UNP M1E1E4
F	557	HIS	-	expression tag	UNP M1E1E4
F	558	HIS	-	expression tag	UNP M1E1E4
F	559	SER	-	expression tag	UNP M1E1E4
F	560	ALA	-	expression tag	UNP M1E1E4
F	561	TRP	-	expression tag	UNP M1E1E4
F	562	SER	-	expression tag	UNP M1E1E4
F	563	HIS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	564	PRO	-	expression tag	UNP M1E1E4
F	565	GLN	-	expression tag	UNP M1E1E4
F	566	PHE	-	expression tag	UNP M1E1E4
F	567	GLU	-	expression tag	UNP M1E1E4
F	568	LYS	-	expression tag	UNP M1E1E4

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
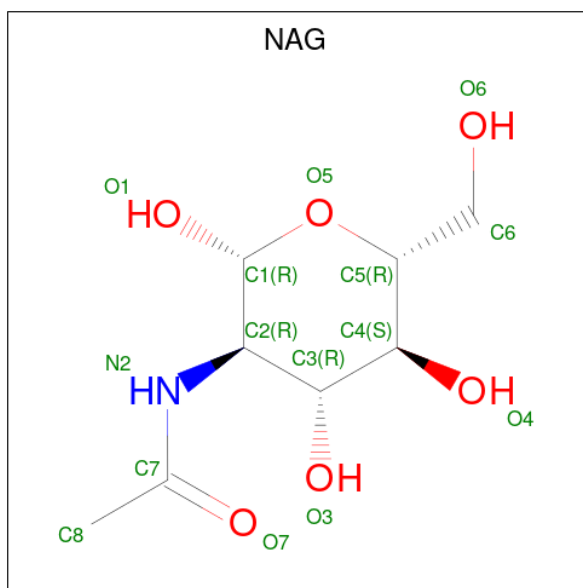
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).
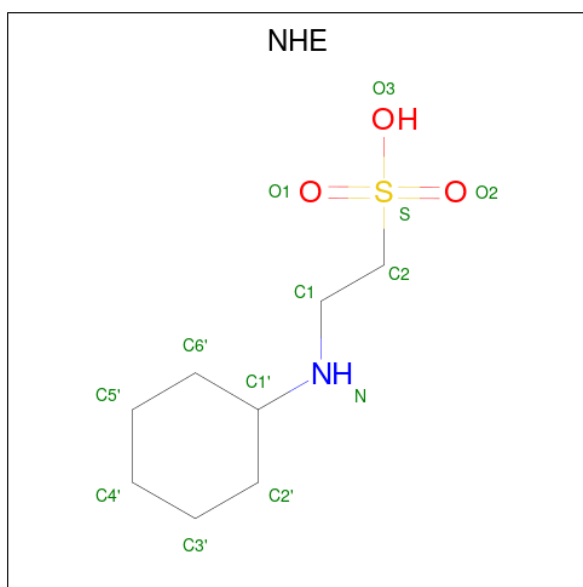
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0

- Molecule 5 is 3-[[5-chloranyl-1-(3-methylsulfonylpropyl)indol-2-yl]methyl]-1-[2,2,2-tris(fluoranyl)ethyl]imidazo[4,5-c]pyridin-2-one (three-letter code: 6YA) (formula: $C_{21}H_{20}ClF_3N_4O_3S$).
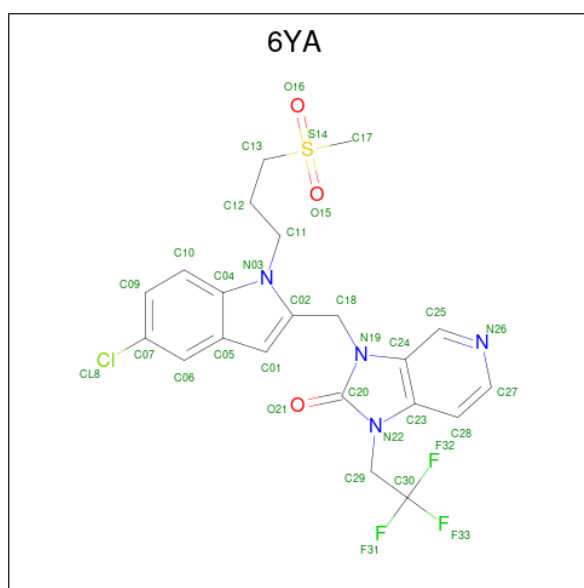
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	F	1	Total 33	C 21	Cl 1	F 3	N 4	O 3	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	134	Total 134	O 134	0	0

3 Residue-property plots ⓘ

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: Fusion glycoprotein F0, Envelope glycoprotein chimera
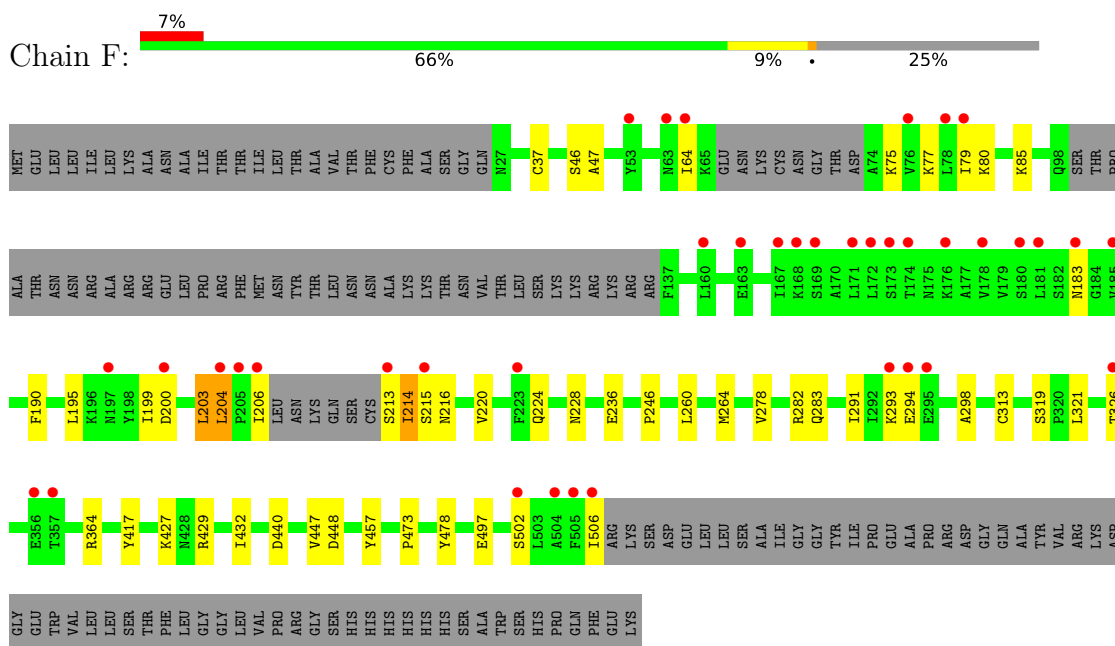
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	169.99Å 169.99Å 169.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.76 – 2.50 56.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (53.76-2.50) 95.5 (56.66-2.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.239 0.214 , 0.240	Depositor DCC
R_{free} test set	1478 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.5	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3562	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 6YA, SO4, NAG, NHE

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	F	0.30	0/3366	0.46	0/4560

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	F	3318	0	3363	29	0
2	F	14	0	13	1	0
3	F	13	0	17	0	0
4	F	50	0	0	6	0
5	F	33	0	0	0	0
6	F	134	0	0	11	0
All	All	3562	0	3393	33	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 5.

All (33) 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)
4:F:612:SO4:O4	6:F:701:HOH:O	1.93	0.86
1:F:429:ARG:NH2	6:F:708:HOH:O	2.18	0.77
1:F:246:PRO:HB3	1:F:283:GLN:HA	1.68	0.76
1:F:200:ASP:HA	1:F:204:LEU:HG	1.68	0.75
1:F:429:ARG:O	6:F:702:HOH:O	2.04	0.74
4:F:606:SO4:O4	6:F:703:HOH:O	2.05	0.74
1:F:206:ILE:HG12	1:F:213:SER:HB2	1.69	0.73
1:F:75:LYS:HB2	1:F:214:ILE:HG23	1.72	0.72
4:F:605:SO4:O2	6:F:704:HOH:O	2.10	0.68
1:F:440:ASP:OD2	6:F:705:HOH:O	2.11	0.67
1:F:478:TYR:O	6:F:706:HOH:O	2.12	0.66
1:F:417:TYR:O	6:F:707:HOH:O	2.16	0.60
1:F:432:ILE:HD11	1:F:447:VAL:HG22	1.84	0.58
1:F:46:SER:HB3	1:F:313:CYS:SG	2.47	0.55
1:F:293:LYS:NZ	1:F:294:GLU:OE2	2.37	0.54
1:F:321:LEU:HD11	1:F:473:PRO:HB3	1.89	0.53
1:F:79:ILE:HD11	1:F:220:VAL:HA	1.92	0.52
1:F:77:LYS:HA	1:F:80:LYS:HD2	1.91	0.51
1:F:236:GLU:OE1	6:F:709:HOH:O	2.19	0.50
1:F:497:GLU:HG2	2:F:601:NAG:H81	1.93	0.50
1:F:199:ILE:HA	1:F:203:LEU:HB2	1.93	0.49
1:F:220:VAL:O	1:F:224:GLN:HG3	2.14	0.47
1:F:427:LYS:HG3	1:F:448:ASP:CG	2.36	0.46
1:F:260:LEU:O	1:F:264:MET:HG3	2.18	0.43
1:F:47:ALA:HB2	1:F:364:ARG:HD2	1.99	0.43
1:F:326:THR:N	4:F:610:SO4:O1	2.45	0.43
1:F:37:CYS:SG	1:F:319:SER:HB3	2.58	0.42
1:F:85:LYS:NZ	4:F:611:SO4:O3	2.48	0.42
1:F:291:ILE:HG22	1:F:298:ALA:HB3	2.01	0.42
4:F:612:SO4:O3	6:F:710:HOH:O	2.19	0.41
1:F:278:VAL:O	1:F:282:ARG:HG3	2.20	0.41
1:F:215:SER:OG	1:F:216:ASN:N	2.54	0.41
1:F:448:ASP:O	6:F:711:HOH:O	2.22	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	F	420/568 (74%)	402 (96%)	16 (4%)	2 (0%)	29	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	183	ASN
1	F	214	ILE

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	F	390/510 (76%)	381 (98%)	9 (2%)	50	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	64	ILE
1	F	190	PHE
1	F	195	LEU
1	F	203	LEU
1	F	204	LEU
1	F	228	ASN
1	F	457	TYR
1	F	502	SER
1	F	506	ILE

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 ⓘ

13 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	SO4	F	604	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	F	609	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	F	606	-	4,4,4	0.13	0	6,6,6	0.10	0
4	SO4	F	612	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	F	603	-	4,4,4	0.17	0	6,6,6	0.06	0
4	SO4	F	608	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	F	605	-	4,4,4	0.14	0	6,6,6	0.09	0
4	SO4	F	607	-	4,4,4	0.14	0	6,6,6	0.05	0
3	NHE	F	602	-	13,13,13	1.43	2 (15%)	16,17,17	1.96	5 (31%)
4	SO4	F	610	-	4,4,4	0.15	0	6,6,6	0.05	0
5	6YA	F	613	-	32,36,36	1.93	9 (28%)	48,55,55	2.07	15 (31%)
4	SO4	F	611	-	4,4,4	0.13	0	6,6,6	0.06	0
2	NAG	F	601	1	14,14,15	0.21	0	17,19,21	0.66	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
3	NHE	F	602	-	-	3/7/15/15	0/1/1/1
5	6YA	F	613	-	-	3/16/16/16	0/4/4/4
2	NAG	F	601	1	-	3/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	613	6YA	C28-C23	5.52	1.48	1.39
5	F	613	6YA	C20-N19	3.76	1.43	1.38
5	F	613	6YA	C06-C07	3.51	1.43	1.36
5	F	613	6YA	C29-C30	3.01	1.54	1.50
3	F	602	NHE	C2-S	2.94	1.81	1.77
5	F	613	6YA	C10-C09	2.69	1.42	1.36
5	F	613	6YA	C20-N22	2.66	1.41	1.38
3	F	602	NHE	O1-S	2.49	1.52	1.45
5	F	613	6YA	C29-N22	-2.23	1.44	1.47
5	F	613	6YA	C25-C24	2.15	1.42	1.39
5	F	613	6YA	C23-N22	2.15	1.43	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	613	6YA	O16-S14-O15	-7.51	101.03	117.09
5	F	613	6YA	O16-S14-C13	4.67	111.61	108.34
3	F	602	NHE	O3-S-O2	-4.13	101.18	111.27
5	F	613	6YA	O15-S14-C13	3.95	111.11	108.34
3	F	602	NHE	O3-S-C2	3.90	112.08	105.77
5	F	613	6YA	C02-C18-N19	-3.76	108.22	113.00
3	F	602	NHE	O2-S-C2	3.50	111.13	106.92
5	F	613	6YA	C27-N26-C25	3.06	122.14	116.85
5	F	613	6YA	C28-C23-C24	-2.95	116.53	120.92
3	F	602	NHE	O1-S-C2	2.77	110.25	106.92
5	F	613	6YA	C18-C02-N03	2.74	126.00	122.05
5	F	613	6YA	F32-C30-C29	-2.53	107.98	112.13
3	F	602	NHE	C1-N-C1'	-2.52	109.19	114.14
5	F	613	6YA	O16-S14-C17	2.45	111.37	108.91
5	F	613	6YA	C18-C02-C01	-2.42	126.10	129.24
5	F	613	6YA	C18-N19-C20	2.37	126.62	122.81
5	F	613	6YA	C28-C23-N22	2.22	135.17	130.51
5	F	613	6YA	C23-N22-C20	-2.21	107.76	110.05
5	F	613	6YA	C29-N22-C20	2.06	125.67	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	613	6YA	O15-S14-C17	2.03	110.94	108.91

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	NHE	C1-C2-S-O1
3	F	602	NHE	C1-C2-S-O3
2	F	601	NAG	O5-C5-C6-O6
2	F	601	NAG	C4-C5-C6-O6
3	F	602	NHE	C1-C2-S-O2
5	F	613	6YA	C12-C11-N03-C04
2	F	601	NAG	C3-C2-N2-C7
5	F	613	6YA	C30-C29-N22-C20
5	F	613	6YA	N03-C02-C18-N19

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	606	SO4	1	0
4	F	612	SO4	2	0
4	F	605	SO4	1	0
4	F	610	SO4	1	0
4	F	611	SO4	1	0
2	F	601	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 6YA F 613

Bond lengths

Bond angles

Torsions

Rings
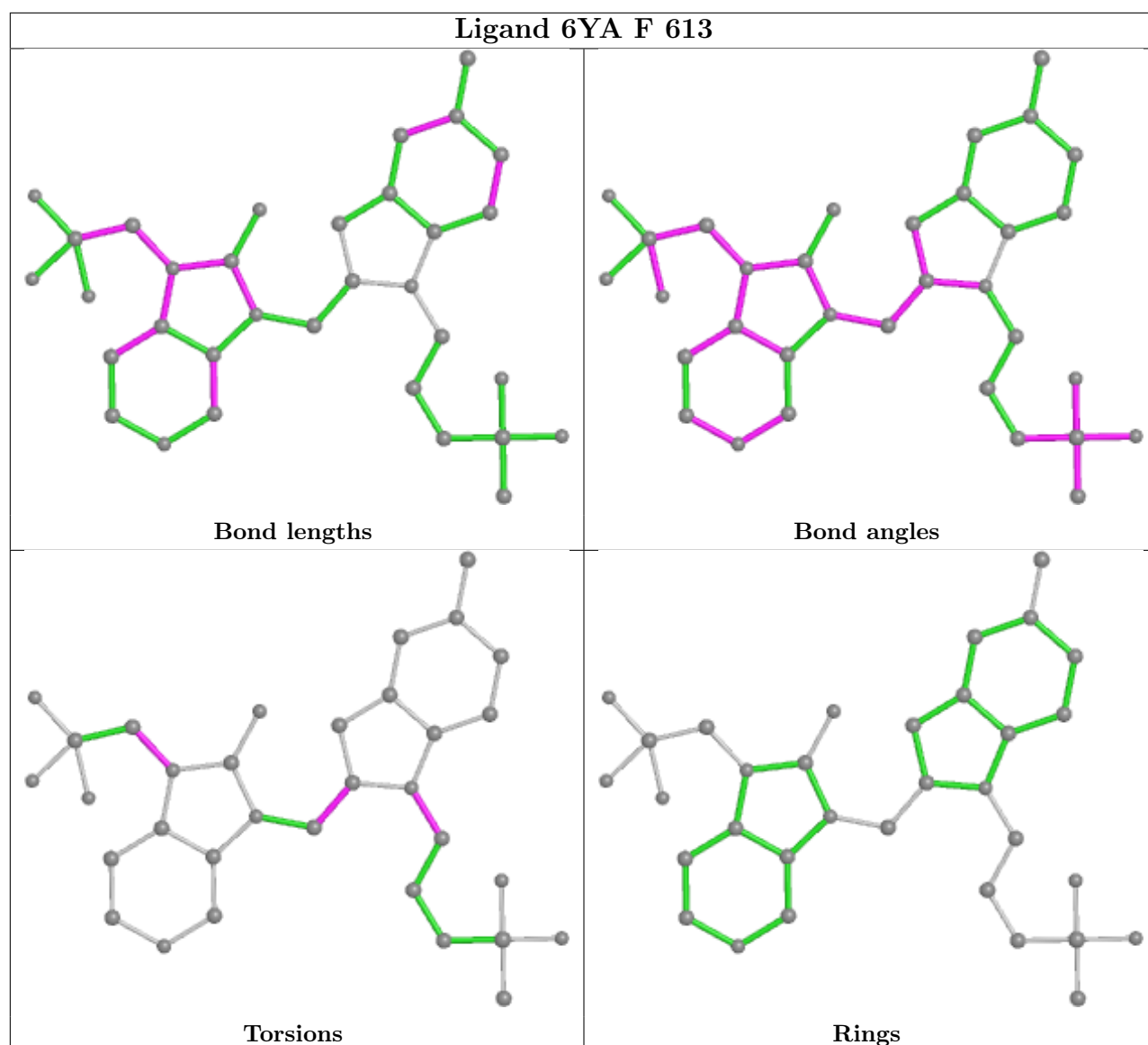
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	F	428/568 (75%)	0.24	39 (9%)	9	9	30, 50, 99, 129	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	505	PHE	6.6
1	F	183	ASN	5.0
1	F	160	LEU	5.0
1	F	504	ALA	4.6
1	F	205	PRO	4.4
1	F	506	ILE	4.3
1	F	167	ILE	4.2
1	F	76	VAL	3.9
1	F	63	ASN	3.8
1	F	174	THR	3.7
1	F	204	LEU	3.6
1	F	172	LEU	3.5
1	F	206	ILE	3.3
1	F	79	ILE	3.2
1	F	181	LEU	3.0
1	F	64	ILE	3.0
1	F	200	ASP	3.0
1	F	78	LEU	3.0
1	F	294	GLU	2.7
1	F	223	PHE	2.7
1	F	169	SER	2.7
1	F	293	LYS	2.7
1	F	326	THR	2.5
1	F	213	SER	2.5
1	F	215	SER	2.4
1	F	356	GLU	2.4
1	F	168	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	163	GLU	2.4
1	F	197	ASN	2.4
1	F	171	LEU	2.3
1	F	53	TYR	2.3
1	F	173	SER	2.2
1	F	178	VAL	2.2
1	F	180	SER	2.2
1	F	502	SER	2.1
1	F	357	THR	2.1
1	F	295	GLU	2.1
1	F	185	VAL	2.1
1	F	176	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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.
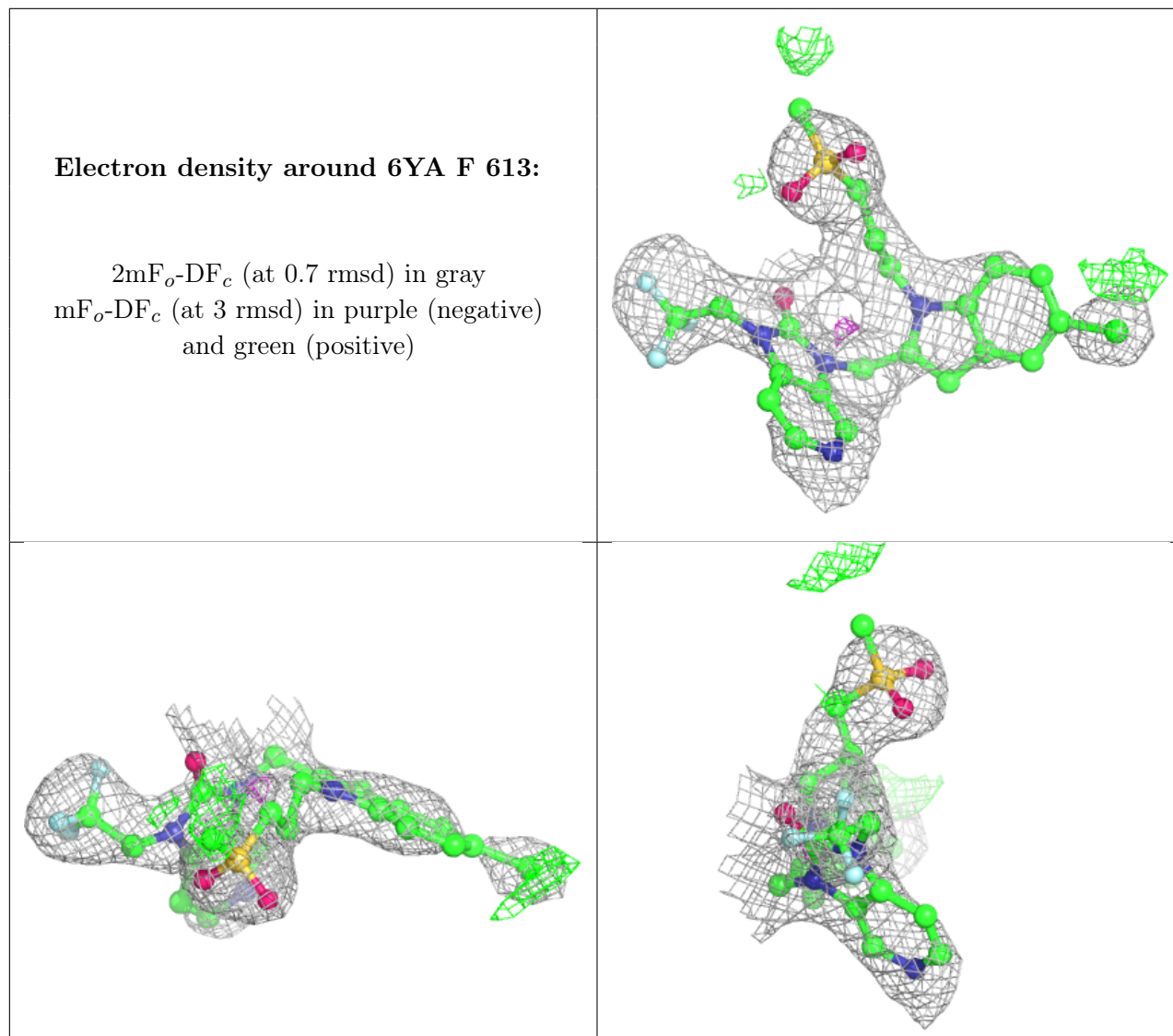
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	601	14/15	0.76	0.51	152,157,169,171	0
4	SO4	F	610	5/5	0.76	0.37	158,159,159,159	0
4	SO4	F	605	5/5	0.80	0.34	128,129,129,129	0
4	SO4	F	606	5/5	0.85	0.20	111,111,112,112	0
4	SO4	F	604	5/5	0.85	0.32	139,139,139,139	0
4	SO4	F	608	5/5	0.86	0.25	142,142,143,143	0
4	SO4	F	611	5/5	0.89	0.12	130,130,131,131	0
4	SO4	F	607	5/5	0.90	0.25	124,124,125,125	0
4	SO4	F	612	5/5	0.90	0.40	137,137,138,139	0
4	SO4	F	609	5/5	0.91	0.13	118,119,119,119	0
5	6YA	F	613	33/33	0.91	0.25	32,38,40,40	33

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	F	603	5/5	0.96	0.56	33,33,33,33	5
3	NHE	F	602	13/13	0.97	0.20	58,60,69,91	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 6YA F 613:

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.