



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:33 pm BST

PDB ID : 5EA4
Title : Crystal Structure of Inhibitor JNJ-49153390 in Complex with Prefusion RSV F Glycoprotein
Authors : Battles, M.B.; McLellan, J.S.; Arnoult, E.; Roymans, D.; Langedijk, J.P.
Deposited on : 2015-10-15
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

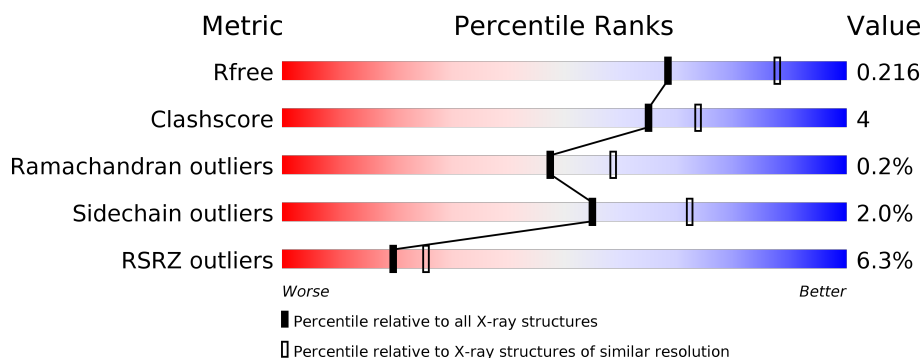
1 Overall quality at a glance

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	F	568	<div> <div>5%</div> <div>68%</div> <div>9%</div> <div>22%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3735 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	443	Total	C	N	O	S	0	0	0
			3424	2168	561	673	22			

There are 62 discrepancies between the modelled and reference sequences:

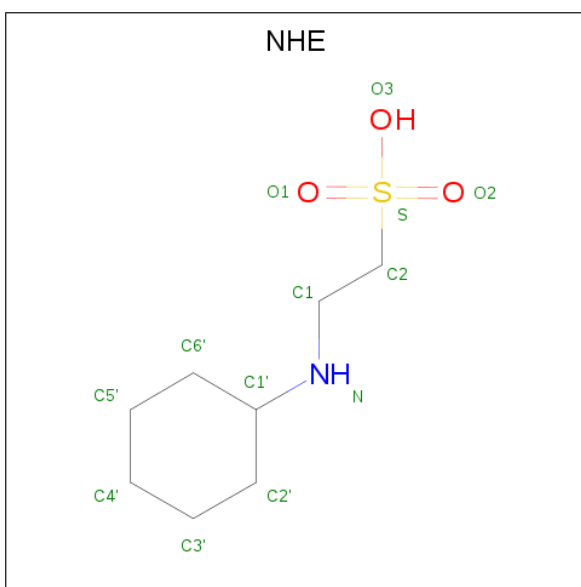
Chain	Residue	Modelled	Actual	Comment	Reference
F	102	ALA	PRO	variant	UNP P03420
F	155	CYS	SER	engineered mutation	UNP P03420
F	190	PHE	SER	engineered mutation	UNP P03420
F	207	LEU	VAL	engineered mutation	UNP P03420
F	290	CYS	SER	engineered mutation	UNP P03420
F	379	VAL	ILE	variant	UNP P03420
F	447	VAL	MET	variant	UNP P03420
F	514	SER	-	expression tag	UNP P03420
F	515	ALA	-	expression tag	UNP P03420
F	516	ILE	-	expression tag	UNP P03420
F	517	GLY	-	expression tag	UNP P03420
F	518	GLY	-	expression tag	UNP P03420
F	519	TYR	-	expression tag	UNP P03420
F	520	ILE	-	expression tag	UNP P03420
F	521	PRO	-	expression tag	UNP P03420
F	522	GLU	-	expression tag	UNP P03420
F	523	ALA	-	expression tag	UNP P03420
F	524	PRO	-	expression tag	UNP P03420
F	525	ARG	-	expression tag	UNP P03420
F	526	ASP	-	expression tag	UNP P03420
F	527	GLY	-	expression tag	UNP P03420
F	528	GLN	-	expression tag	UNP P03420
F	529	ALA	-	expression tag	UNP P03420
F	530	TYR	-	expression tag	UNP P03420
F	531	VAL	-	expression tag	UNP P03420
F	532	ARG	-	expression tag	UNP P03420
F	533	LYS	-	expression tag	UNP P03420

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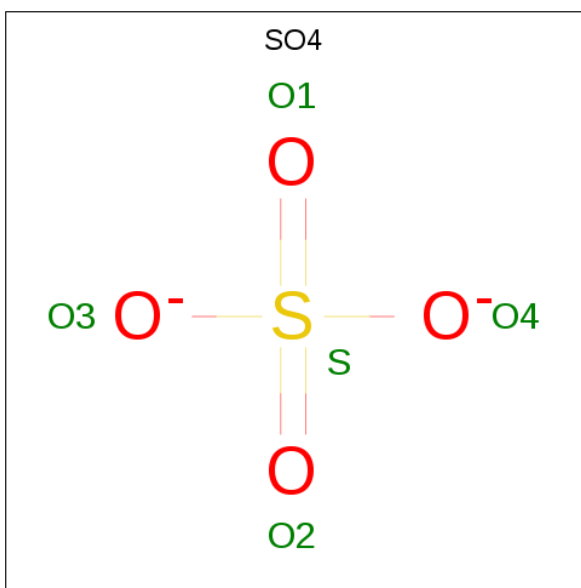
Chain	Residue	Modelled	Actual	Comment	Reference
F	534	ASP	-	expression tag	UNP P03420
F	535	GLY	-	expression tag	UNP P03420
F	536	GLU	-	expression tag	UNP P03420
F	537	TRP	-	expression tag	UNP P03420
F	538	VAL	-	expression tag	UNP P03420
F	539	LEU	-	expression tag	UNP P03420
F	540	LEU	-	expression tag	UNP P03420
F	541	SER	-	expression tag	UNP P03420
F	542	THR	-	expression tag	UNP P03420
F	543	PHE	-	expression tag	UNP P03420
F	544	LEU	-	expression tag	UNP P03420
F	545	GLY	-	expression tag	UNP P03420
F	546	GLY	-	expression tag	UNP P03420
F	547	LEU	-	expression tag	UNP P03420
F	548	VAL	-	expression tag	UNP P03420
F	549	PRO	-	expression tag	UNP P03420
F	550	ARG	-	expression tag	UNP P03420
F	551	GLY	-	expression tag	UNP P03420
F	552	SER	-	expression tag	UNP P03420
F	553	HIS	-	expression tag	UNP P03420
F	554	HIS	-	expression tag	UNP P03420
F	555	HIS	-	expression tag	UNP P03420
F	556	HIS	-	expression tag	UNP P03420
F	557	HIS	-	expression tag	UNP P03420
F	558	HIS	-	expression tag	UNP P03420
F	559	SER	-	expression tag	UNP P03420
F	560	ALA	-	expression tag	UNP P03420
F	561	TRP	-	expression tag	UNP P03420
F	562	SER	-	expression tag	UNP P03420
F	563	HIS	-	expression tag	UNP P03420
F	564	PRO	-	expression tag	UNP P03420
F	565	GLN	-	expression tag	UNP P03420
F	566	PHE	-	expression tag	UNP P03420
F	567	GLU	-	expression tag	UNP P03420
F	568	LYS	-	expression tag	UNP P03420

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



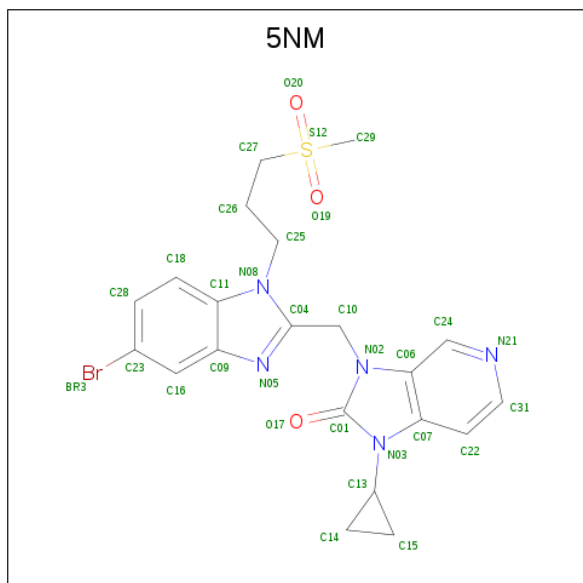
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 3-[[5-bromanyl-1-(3-methylsulfonylpropyl)benzimidazol-2-yl]methyl]-1-cyclopropyl-imidazo[4,5-c]pyridin-2-one (three-letter code: 5NM) (formula: C₂₁H₂₂BrN₅O₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	F	1	Total	Br	C	N	O	S	0	1	
			31	1	21	5	3	1			

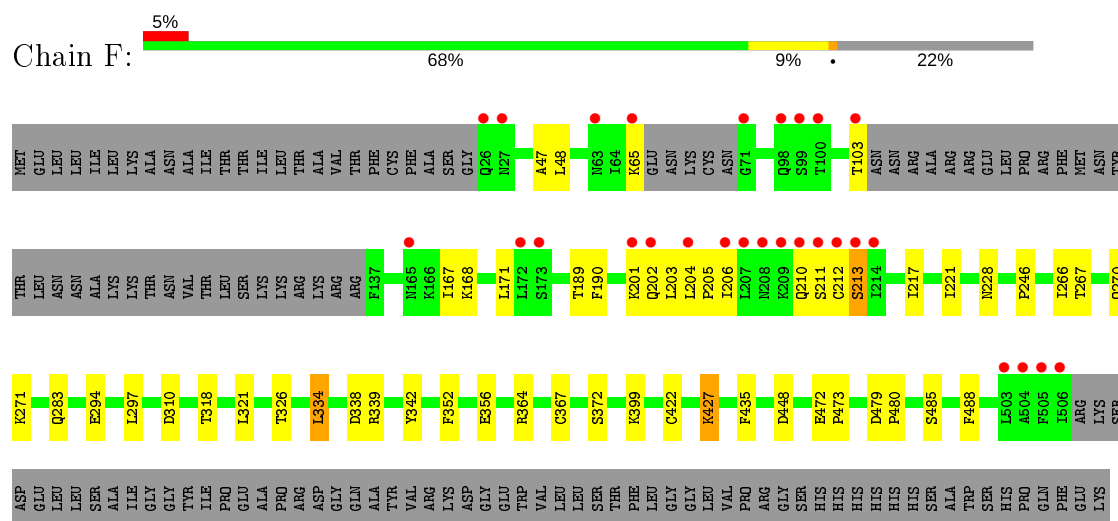
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	242	Total O 242 242	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: Fusion glycoprotein F0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	168.37Å 168.37Å 168.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.30 48.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.60-2.30) 93.3 (48.60-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.214 0.186 , 0.216	Depositor DCC
R_{free} test set	1848 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3735	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, SO4, 5NM

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	0/3474	0.47	1/4709 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	334	LEU	CA-CB-CG	6.52	130.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	213	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3424	0	3467	28	0
2	F	13	0	17	0	0
3	F	25	0	0	1	0
4	F	31	0	22	1	0
5	F	242	0	0	4	1
All	All	3735	0	3506	29	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 4.

All (29) 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:F:485:SER:OG	5:F:701:HOH:O	1.86	0.93
3:F:606:SO4:O2	5:F:702:HOH:O	2.00	0.79
1:F:246:PRO:HB3	1:F:283:GLN:HA	1.75	0.69
1:F:168:LYS:NZ	1:F:294:GLU:O	2.27	0.67
1:F:201:LYS:O	1:F:203:LEU:N	2.27	0.66
1:F:210:GLN:O	1:F:213:SER:N	2.28	0.65
1:F:167:ILE:HG23	1:F:189:THR:HG21	1.85	0.58
1:F:267:THR:HG23	1:F:270:GLN:H	1.71	0.54
1:F:356:GLU:H	1:F:356:GLU:CD	2.11	0.54
1:F:47:ALA:HB2	1:F:364:ARG:HD2	1.90	0.53
1:F:228:ASN:ND2	5:F:710:HOH:O	2.37	0.53
1:F:310:ASP:OD1	1:F:364:ARG:NH1	2.38	0.50
1:F:488:PHE:HB2	4:F:607[A]:5NM:C16	2.41	0.50
1:F:318:THR:OG1	1:F:339:ARG:HD3	2.11	0.50
1:F:321:LEU:HD11	1:F:473:PRO:HB3	1.93	0.49
1:F:211:SER:HA	1:F:212:CYS:HA	1.44	0.47
1:F:217:ILE:O	1:F:221:ILE:HG12	2.17	0.45
1:F:171:LEU:HD11	1:F:189:THR:HG22	2.00	0.44
1:F:266:ILE:HG13	1:F:271:LYS:HG3	2.00	0.43
1:F:422:CYS:HB2	1:F:435:PHE:HB2	2.00	0.43
1:F:352:PHE:CE2	1:F:372:SER:HB3	2.53	0.43
1:F:399:LYS:HE3	1:F:399:LYS:HB3	1.80	0.42
1:F:48:LEU:HD22	1:F:367:CYS:HB2	2.01	0.41
1:F:204:LEU:N	1:F:205:PRO:HD2	2.35	0.41
1:F:65:LYS:HG3	1:F:65:LYS:H	1.74	0.41
1:F:339:ARG:HD2	5:F:876:HOH:O	2.20	0.41
1:F:427:LYS:HB2	1:F:448:ASP:OD2	2.21	0.40
1:F:338:ASP:HB2	1:F:342:TYR:OH	2.22	0.40
1:F:479:ASP:HA	1:F:480:PRO:HD3	1.91	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)
5:F:714:HOH:O	5:F:862:HOH:O[5_555]	2.01	0.19

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	F	437/568 (77%)	423 (97%)	13 (3%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	202	GLN

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	F	403/510 (79%)	395 (98%)	8 (2%)	55 72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	103	THR
1	F	190	PHE

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Mol	Chain	Res	Type
1	F	206	ILE
1	F	297	LEU
1	F	326	THR
1	F	334	LEU
1	F	427	LYS
1	F	472	GLU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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	5NM	F	607[A]	-	24,35,35	5.04	12 (50%)	27,53,53	2.08	6 (22%)
3	SO4	F	606	-	4,4,4	0.15	0	6,6,6	0.09	0
2	NHE	F	601	-	13,13,13	1.44	3 (23%)	16,17,17	1.93	4 (25%)
3	SO4	F	605	-	4,4,4	0.15	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	603	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	F	604	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	F	602	-	4,4,4	0.12	0	6,6,6	0.17	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
4	5NM	F	607[A]	-	-	0/11/17/17	0/5/5/5
2	NHE	F	601	-	-	2/7/15/15	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	607[A]	5NM	C22-C31	11.43	1.52	1.36
4	F	607[A]	5NM	C16-C09	9.56	1.56	1.41
4	F	607[A]	5NM	C24-N21	9.00	1.48	1.32
4	F	607[A]	5NM	C16-C23	8.69	1.50	1.36
4	F	607[A]	5NM	C18-C11	8.07	1.57	1.41
4	F	607[A]	5NM	C18-C28	6.64	1.50	1.36
4	F	607[A]	5NM	C28-C23	5.11	1.48	1.38
4	F	607[A]	5NM	C31-N21	5.01	1.48	1.33
4	F	607[A]	5NM	C22-C07	4.78	1.50	1.41
4	F	607[A]	5NM	C01-N03	4.08	1.45	1.35
4	F	607[A]	5NM	C01-N02	3.90	1.44	1.35
2	F	601	NHE	C2-S	3.02	1.81	1.77
4	F	607[A]	5NM	C10-N02	-2.46	1.44	1.48
2	F	601	NHE	O1-S	2.40	1.52	1.45
2	F	601	NHE	O2-S	2.15	1.51	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	607[A]	5NM	O20-S12-O19	-6.97	102.19	117.09
2	F	601	NHE	O2-S-C2	4.79	112.69	106.92
4	F	607[A]	5NM	O20-S12-C27	3.98	111.13	108.34
2	F	601	NHE	O3-S-O2	-3.84	101.89	111.27
4	F	607[A]	5NM	O19-S12-C27	3.50	110.80	108.34
4	F	607[A]	5NM	O20-S12-C29	3.26	112.18	108.91
2	F	601	NHE	O1-S-C2	3.13	110.68	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	607[A]	5NM	C22-C31-N21	-3.06	119.83	123.81
2	F	601	NHE	O3-S-C2	2.78	110.26	105.77
4	F	607[A]	5NM	O19-S12-C29	2.70	111.62	108.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

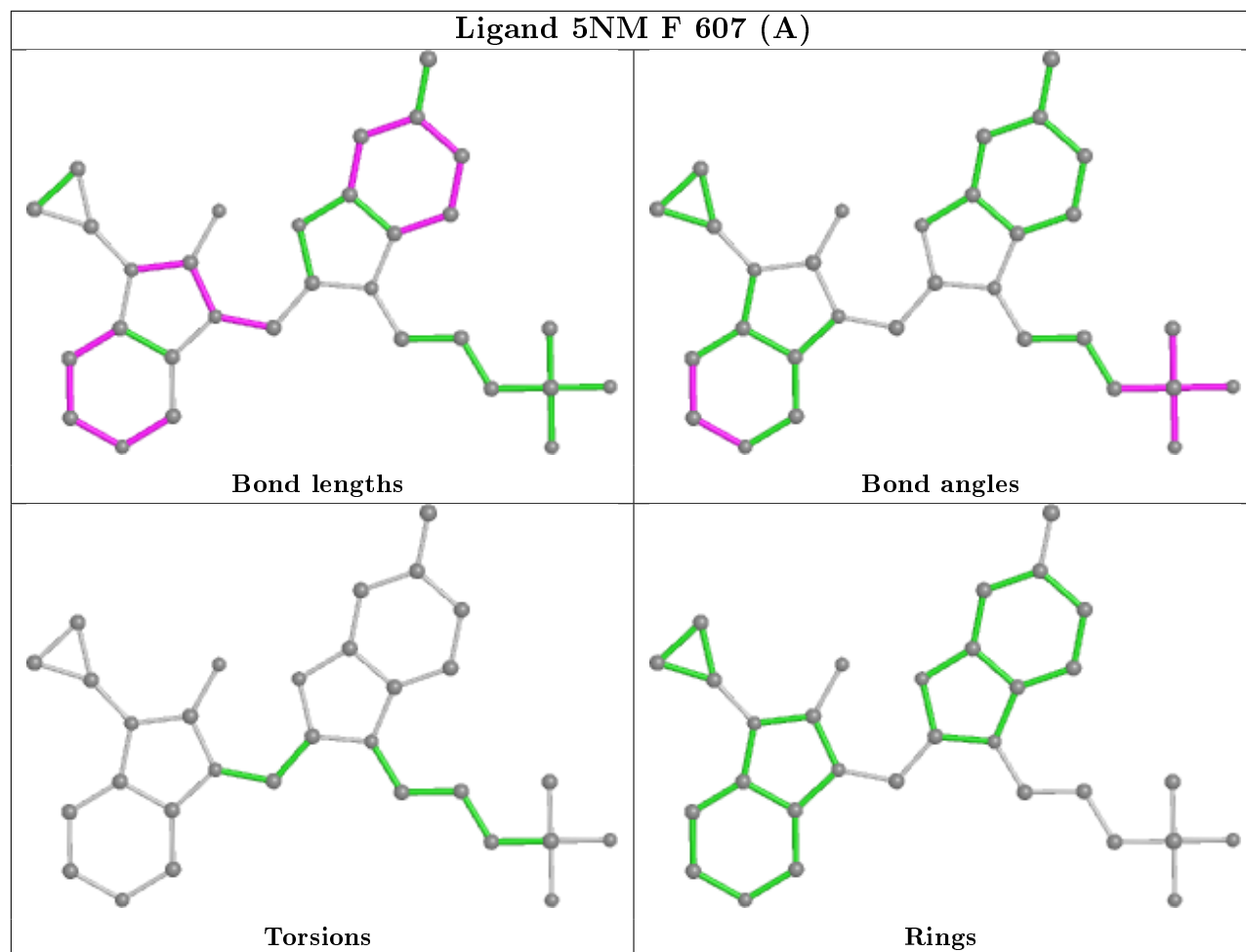
Mol	Chain	Res	Type	Atoms
2	F	601	NHE	C2'-C1'-N-C1
2	F	601	NHE	N-C1-C2-S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	607[A]	5NM	1	0
3	F	606	SO4	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	443/568 (77%)	-0.09	28 (6%) 20 25	25, 42, 100, 142	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	505	PHE	7.6
1	F	207	LEU	5.3
1	F	26	GLN	5.3
1	F	209	LYS	5.2
1	F	506	ILE	4.9
1	F	213	SER	4.3
1	F	212	CYS	4.1
1	F	208	ASN	4.0
1	F	211	SER	4.0
1	F	98	GLN	3.9
1	F	504	ALA	3.7
1	F	71	GLY	3.5
1	F	65	LYS	3.3
1	F	173	SER	3.2
1	F	204	LEU	3.2
1	F	99	SER	3.0
1	F	206	ILE	3.0
1	F	214	ILE	2.9
1	F	210	GLN	2.9
1	F	27	ASN	2.7
1	F	100	THR	2.7
1	F	103	THR	2.7
1	F	172	LEU	2.6
1	F	63	ASN	2.6
1	F	202	GLN	2.4
1	F	165	ASN	2.1
1	F	503	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	201	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

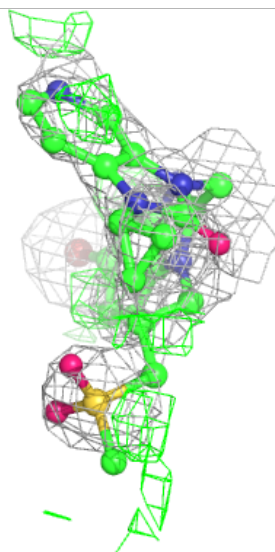
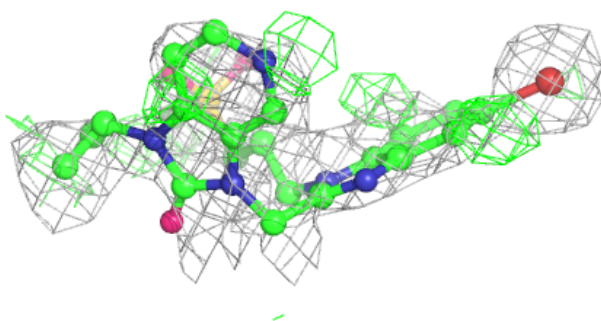
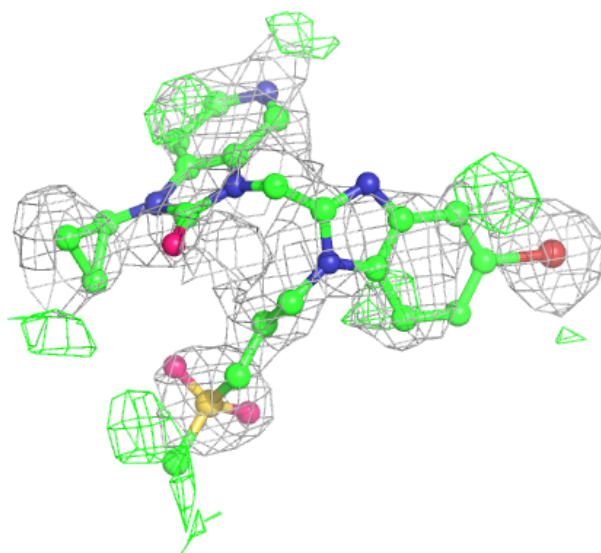
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	F	606	5/5	0.85	0.36	126,127,127,127	0
3	SO4	F	603	5/5	0.87	0.22	115,116,116,116	0
3	SO4	F	605	5/5	0.88	0.21	127,127,127,127	0
4	5NM	F	607[A]	31/31	0.91	0.28	27,37,38,38	31
3	SO4	F	604	5/5	0.94	0.20	89,90,91,91	0
2	NHE	F	601	13/13	0.97	0.20	63,65,69,99	0
3	SO4	F	602	5/5	0.97	0.24	85,86,86,87	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 5NM F 607 (A):

$2mF_o-DF_c$ (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.