



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:35 PM UTC

PDB ID : 5EA5 / pdb\_00005ea5  
Title : Crystal Structure of Inhibitor TMC-353121 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 : 3.05 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

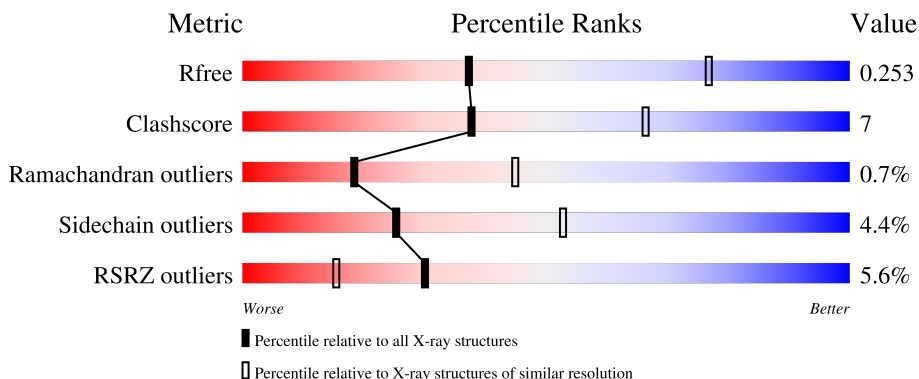
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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  $\geq 3$ , 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	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3366 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
			Total	C	N	O	S			
1	F	426	3297	2090	539	647	21	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

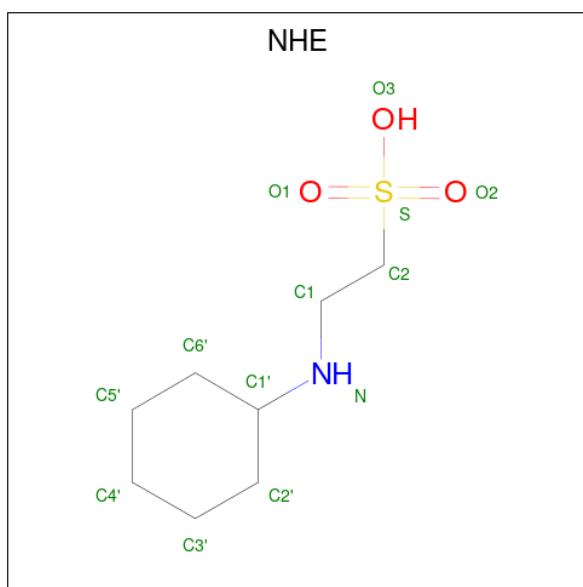
Chain	Residue	Modelled	Actual	Comment	Reference
F	102	ALA	PRO	variant	UNP P03420
F	155	CYS	SER	engineered mutation	UNP P03420
F	190	PHE	SER	engineered mutation	UNP P03420
F	207	LEU	VAL	engineered mutation	UNP P03420
F	290	CYS	SER	engineered mutation	UNP P03420
F	379	VAL	ILE	variant	UNP P03420
F	447	VAL	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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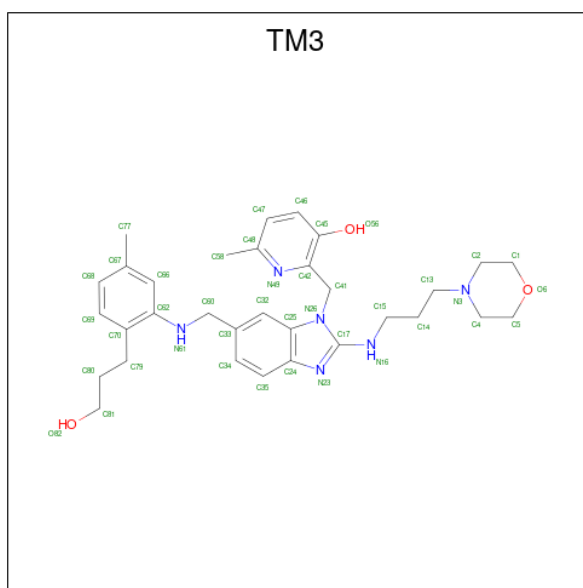
Chain	Residue	Modelled	Actual	Comment	Reference
F	534	ASP	-	expression tag	UNP P03420
F	535	GLY	-	expression tag	UNP P03420
F	536	GLU	-	expression tag	UNP P03420
F	537	TRP	-	expression tag	UNP P03420
F	538	VAL	-	expression tag	UNP P03420
F	539	LEU	-	expression tag	UNP P03420
F	540	LEU	-	expression tag	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 (CCD ID: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



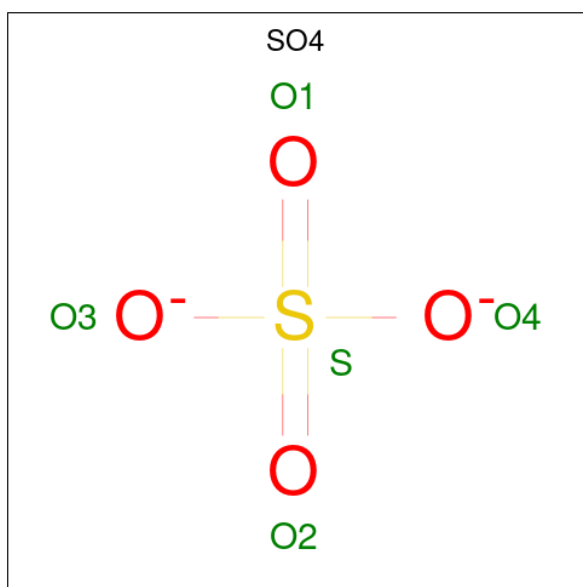
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	F	1	13	8	1	3	1	0	0

- Molecule 3 is 2-[[6-[[[2-(3-hydroxypropyl)-5-methylphenyl]amino]methyl]-2-[[3-(4-morpholinyl)propyl]amino]-1H-benzimidazol-1-yl]methyl]-6-methyl-3-pyridinol (CCD ID: TM3) (formula: C<sub>32</sub>H<sub>42</sub>N<sub>6</sub>O<sub>3</sub>).



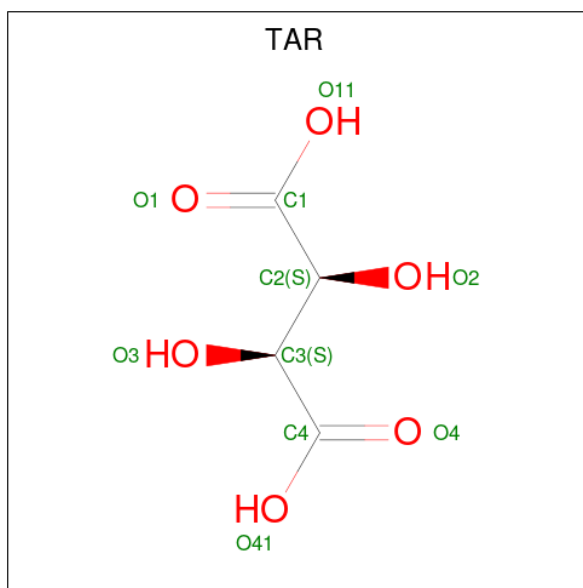
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	F	1	41	32	6	3	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula:  $C_4H_6O_6$ ).

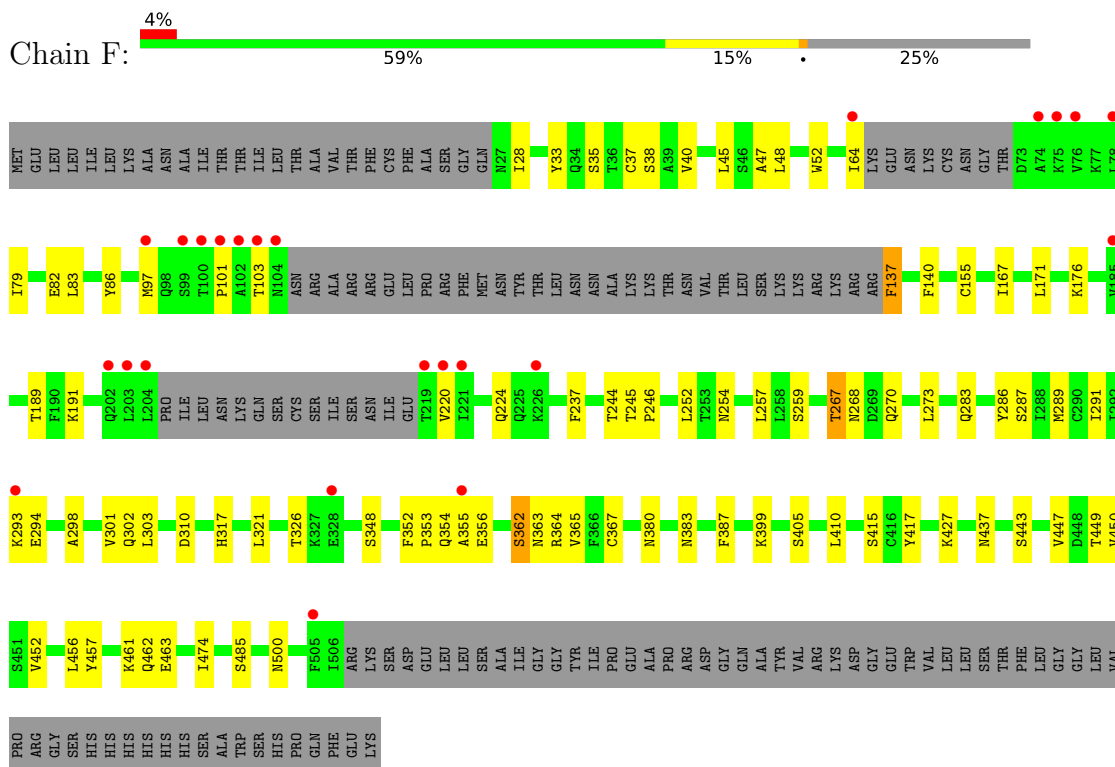


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			10	4	6		

### 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: Fusion glycoprotein F0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.86Å 169.86Å 169.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.05 49.03 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.03-3.05) 94.3 (49.03-3.05)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.07Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.214 , 0.248 0.221 , 0.253	Depositor DCC
$R_{free}$ test set	791 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 78.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TM3, SO4, TAR, 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	0.40	0/3345	0.78	0/4534

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 [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	3297	0	3331	46	0
2	F	13	0	17	2	0
3	F	41	0	42	3	0
4	F	5	0	0	0	0
5	F	10	0	4	2	0
All	All	3366	0	3394	47	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 7.

All (47) 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:246:PRO:HB3	1:F:283:GLN:HA	1.67	0.75
1:F:140:PHE:CG	3:F:602:TM3:H69	2.26	0.70
1:F:399:LYS:HG3	1:F:485:SER:HB2	1.82	0.62
1:F:293:LYS:HG2	1:F:294:GLU:HG3	1.83	0.60
1:F:137:PHE:N	5:F:604:TAR:HO3	2.02	0.58
1:F:167:ILE:HG23	1:F:189:THR:HG21	1.88	0.56
1:F:33:TYR:HE2	1:F:40:VAL:HG23	1.73	0.53
1:F:140:PHE:CE2	3:F:602:TM3:H68	2.43	0.53
1:F:415:SER:HB3	1:F:417:TYR:HE2	1.73	0.53
1:F:79:ILE:HD11	1:F:220:VAL:HG22	1.90	0.52
1:F:79:ILE:HG12	1:F:220:VAL:HG13	1.91	0.52
1:F:463:GLU:H	1:F:463:GLU:CD	2.18	0.52
1:F:415:SER:HB3	1:F:417:TYR:CE2	2.45	0.51
1:F:380:ASN:OD1	1:F:383:ASN:ND2	2.43	0.51
1:F:137:PHE:N	5:F:604:TAR:O3	2.42	0.51
1:F:171:LEU:HD13	1:F:191:LYS:HB2	1.92	0.51
1:F:244:THR:OG1	1:F:287:SER:HB3	2.11	0.50
1:F:405:SER:HB2	1:F:452:VAL:HG21	1.94	0.50
1:F:97:MET:HE1	1:F:101:PRO:HD3	1.94	0.50
1:F:171:LEU:HD11	1:F:189:THR:HG22	1.95	0.49
1:F:176:LYS:NZ	1:F:259:SER:HB2	2.28	0.49
1:F:140:PHE:CZ	3:F:602:TM3:H68	2.48	0.49
1:F:52:TRP:CE3	1:F:302:GLN:HG2	2.48	0.48
1:F:267:THR:HG23	1:F:270:GLN:H	1.78	0.47
1:F:252:LEU:HD23	1:F:257:LEU:HD13	1.95	0.47
1:F:291:ILE:HG22	1:F:298:ALA:HB3	1.95	0.47
1:F:48:LEU:HD22	1:F:367:CYS:HB2	1.95	0.47
1:F:35:SER:O	1:F:474:ILE:HG23	2.15	0.47
1:F:267:THR:OG1	1:F:268:ASN:N	2.49	0.46
1:F:28:ILE:HG22	1:F:410:LEU:HD11	1.97	0.46
1:F:37:CYS:HB2	1:F:321:LEU:HD13	1.98	0.45
1:F:449:THR:HB	1:F:456:LEU:HD11	1.99	0.45
1:F:301:VAL:HG12	1:F:303:LEU:HG	2.00	0.44
1:F:82:GLU:CD	1:F:224:GLN:HG2	2.43	0.44
1:F:83:LEU:O	1:F:86:TYR:HB3	2.18	0.44
1:F:447:VAL:O	1:F:461:LYS:NZ	2.35	0.43
1:F:245:THR:HA	1:F:246:PRO:C	2.43	0.43
1:F:405:SER:HB3	1:F:457:TYR:CE1	2.54	0.43
1:F:362:SER:OG	1:F:363:ASN:N	2.52	0.42
2:F:601:NHE:HC12	2:F:601:NHE:H2'1	1.52	0.42
1:F:47:ALA:HB2	1:F:364:ARG:HD2	2.02	0.42
1:F:354:GLN:C	1:F:356:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:PHE:HA	1:F:353:PRO:HD2	1.95	0.42
1:F:387:PHE:CE1	2:F:601:NHE:H4'1	2.55	0.42
1:F:286:TYR:HB2	1:F:302:GLN:HB3	2.03	0.41
1:F:45:LEU:HD13	1:F:310:ASP:OD1	2.21	0.40
1:F:237:PHE:CD2	1:F:289:MET:HB2	2.56	0.40

There are no symmetry-related clashes.

## 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	418/568 (74%)	394 (94%)	21 (5%)	3 (1%)	18 45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	103	THR
1	F	355	ALA
1	F	362	SER

### 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	387/510 (76%)	370 (96%)	17 (4%)	25 53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	38	SER
1	F	64	ILE
1	F	137	PHE
1	F	155	CYS
1	F	254	ASN
1	F	267	THR
1	F	273	LEU
1	F	317	HIS
1	F	326	THR
1	F	348	SER
1	F	365	VAL
1	F	427	LYS
1	F	437	ASN
1	F	443	SER
1	F	450	VAL
1	F	462	GLN
1	F	500	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	175	ASN
1	F	240	ASN
1	F	283	GLN
1	F	494	GLN

### 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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NHE	F	601	-	13,13,13	1.36	3 (23%)	16,17,17	1.63	4 (25%)
3	TM3	F	602	-	44,45,45	5.76	26 (59%)	53,61,61	1.78	11 (20%)
4	SO4	F	603	-	4,4,4	0.23	0	6,6,6	0.10	0
5	TAR	F	604	-	9,9,9	0.99	0	12,12,12	1.31	2 (16%)

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	NHE	F	601	-	-	6/7/15/15	0/1/1/1
3	TM3	F	602	-	-	15/20/28/28	0/5/5/5
5	TAR	F	604	-	-	8/12/12/12	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	TM3	C62-C70	12.89	1.56	1.40
3	F	602	TM3	C35-C24	12.39	1.59	1.40
3	F	602	TM3	C32-C25	10.21	1.56	1.39
3	F	602	TM3	C66-C67	10.09	1.54	1.39
3	F	602	TM3	C69-C68	9.38	1.54	1.38
3	F	602	TM3	C13-N3	-9.30	1.26	1.47
3	F	602	TM3	C66-C62	8.84	1.53	1.39
3	F	602	TM3	C35-C34	8.81	1.53	1.38
3	F	602	TM3	C42-N49	8.47	1.48	1.34
3	F	602	TM3	C69-C70	8.41	1.53	1.39
3	F	602	TM3	C48-N49	7.67	1.48	1.34
3	F	602	TM3	C17-N16	7.26	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	TM3	C47-C46	6.76	1.49	1.38
3	F	602	TM3	C45-C42	6.54	1.51	1.40
3	F	602	TM3	C68-C67	6.52	1.54	1.38
3	F	602	TM3	C47-C48	5.88	1.52	1.39
3	F	602	TM3	C34-C33	5.68	1.50	1.38
3	F	602	TM3	C46-C45	5.54	1.49	1.39
3	F	602	TM3	C32-C33	5.25	1.48	1.39
3	F	602	TM3	C17-N23	4.85	1.40	1.32
3	F	602	TM3	C41-C42	3.21	1.55	1.51
3	F	602	TM3	C62-N61	3.15	1.45	1.37
3	F	602	TM3	C2-N3	-3.00	1.38	1.46
3	F	602	TM3	O56-C45	2.95	1.42	1.36
3	F	602	TM3	C4-N3	-2.91	1.39	1.46
3	F	602	TM3	C58-C48	2.90	1.56	1.50
2	F	601	NHE	C2-S	2.50	1.81	1.77
2	F	601	NHE	O1-S	2.36	1.51	1.45
2	F	601	NHE	O2-S	2.17	1.51	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	F	602	TM3	C24-C25-N26	6.82	110.94	105.55
2	F	601	NHE	O3-S-O2	-3.93	101.56	111.40
3	F	602	TM3	C32-C25-C24	-3.23	118.60	122.47
3	F	602	TM3	C41-C42-N49	3.23	121.10	115.15
3	F	602	TM3	C25-C32-C33	3.15	125.19	120.28
3	F	602	TM3	C25-C24-N23	-3.00	106.38	110.19
3	F	602	TM3	C60-C33-C34	2.80	126.64	120.94
2	F	601	NHE	O2-S-C2	2.78	110.93	106.73
2	F	601	NHE	O3-S-C2	2.74	111.38	106.00
5	F	604	TAR	O11-C1-C2	2.69	120.78	113.31
3	F	602	TM3	C58-C48-N49	2.60	120.49	116.56
3	F	602	TM3	C24-N23-C17	2.51	107.97	104.06
3	F	602	TM3	C66-C62-C70	-2.34	118.20	120.86
5	F	604	TAR	O41-C4-C3	2.30	119.70	113.31
3	F	602	TM3	C35-C24-N23	2.29	134.72	128.21
2	F	601	NHE	O1-S-C2	2.20	110.05	106.73
3	F	602	TM3	C60-C33-C32	-2.12	116.11	120.63

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	NHE	C2'-C1'-N-C1
2	F	601	NHE	C1-C2-S-O3
3	F	602	TM3	N23-C17-N16-C15
3	F	602	TM3	N26-C17-N16-C15
3	F	602	TM3	N26-C41-C42-C45
3	F	602	TM3	N26-C41-C42-N49
5	F	604	TAR	O2-C2-C3-O3
5	F	604	TAR	C1-C2-C3-O3
5	F	604	TAR	O2-C2-C3-C4
5	F	604	TAR	C1-C2-C3-C4
3	F	602	TM3	C66-C62-N61-C60
3	F	602	TM3	C70-C62-N61-C60
3	F	602	TM3	C13-C14-C15-N16
5	F	604	TAR	O1-C1-C2-O2
3	F	602	TM3	C14-C13-N3-C2
3	F	602	TM3	C14-C13-N3-C4
5	F	604	TAR	O11-C1-C2-O2
3	F	602	TM3	C79-C80-C81-O82
3	F	602	TM3	N3-C13-C14-C15
2	F	601	NHE	C2-C1-N-C1'
2	F	601	NHE	C1-C2-S-O1
2	F	601	NHE	C1-C2-S-O2
3	F	602	TM3	C70-C79-C80-C81
2	F	601	NHE	C6'-C1'-N-C1
5	F	604	TAR	O11-C1-C2-C3
3	F	602	TM3	C14-C15-N16-C17
5	F	604	TAR	O1-C1-C2-C3
3	F	602	TM3	C62-C70-C79-C80
3	F	602	TM3	C42-C41-N26-C17

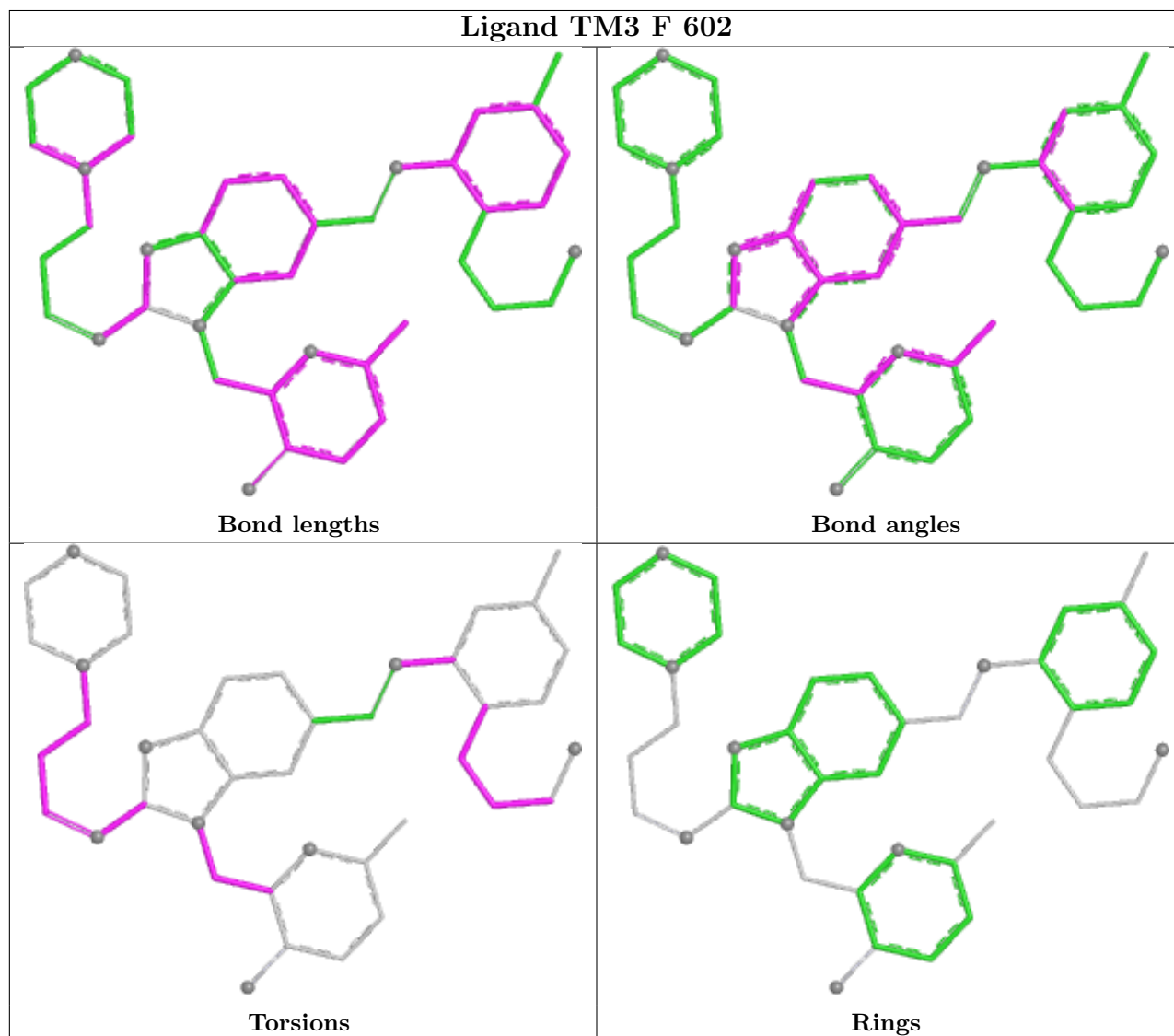
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	NHE	2	0
3	F	602	TM3	3	0
5	F	604	TAR	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	F	426/568 (75%)	0.06	24 (5%) <span style="border: 1px solid red; padding: 2px;">30</span> <span style="border: 1px solid red; padding: 2px;">15</span>	35, 70, 149, 207	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	100	THR	6.6
1	F	104	ASN	5.7
1	F	103	THR	4.1
1	F	64	ILE	3.8
1	F	102	ALA	3.5
1	F	226	LYS	3.3
1	F	101	PRO	3.1
1	F	220	VAL	3.0
1	F	221	ILE	3.0
1	F	75	LYS	3.0
1	F	355	ALA	3.0
1	F	505	PHE	3.0
1	F	78	LEU	2.8
1	F	97	MET	2.7
1	F	219	THR	2.6
1	F	76	VAL	2.6
1	F	203	LEU	2.5
1	F	328	GLU	2.5
1	F	99	SER	2.4
1	F	185	VAL	2.3
1	F	204	LEU	2.2
1	F	293	LYS	2.2
1	F	74	ALA	2.1
1	F	202	GLN	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](#)

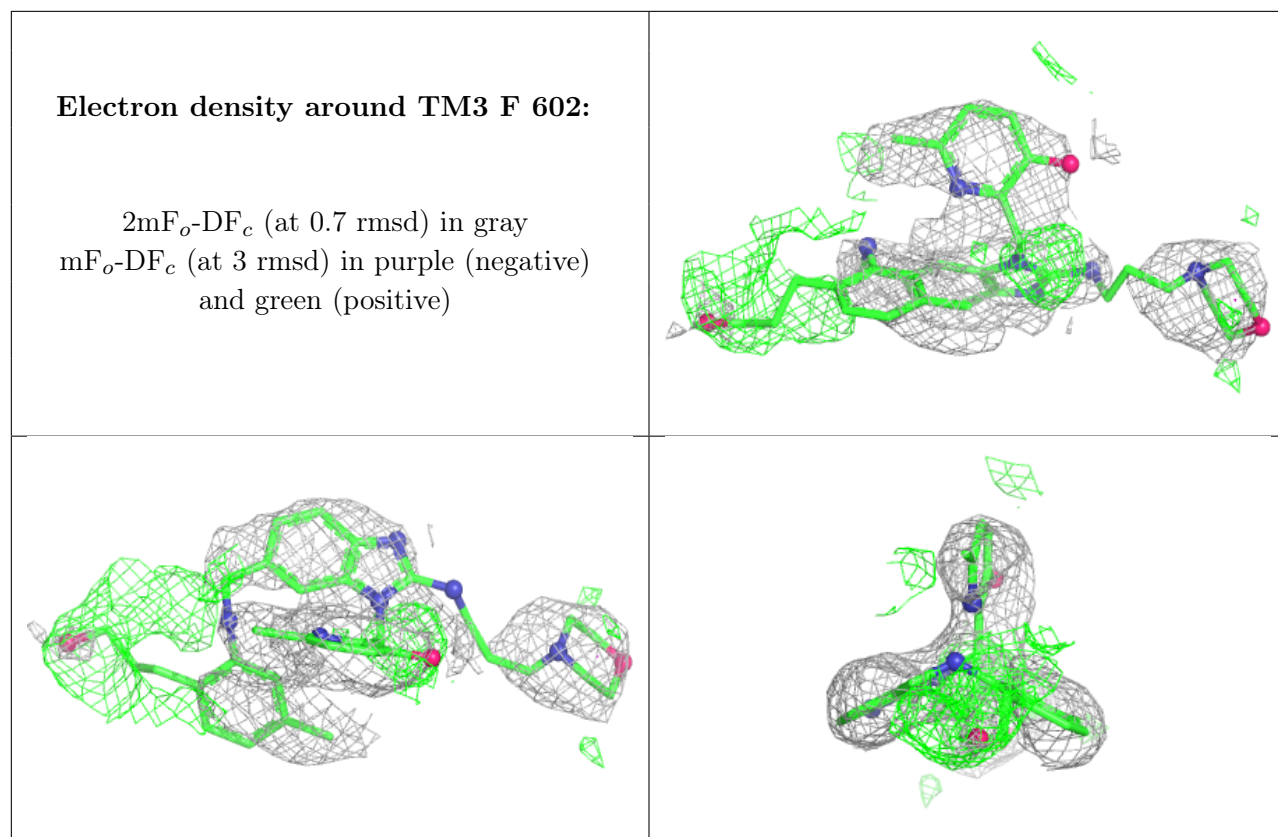
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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
5	TAR	F	604	10/10	0.73	0.19	110,112,112,113	0
3	TM3	F	602	41/41	0.89	0.21	51,61,78,79	41
4	SO4	F	603	5/5	0.91	0.11	145,145,146,148	0
2	NHE	F	601	13/13	0.95	0.12	74,76,80,92	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.