



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:53 PM GMT

PDB ID : 5EA5
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

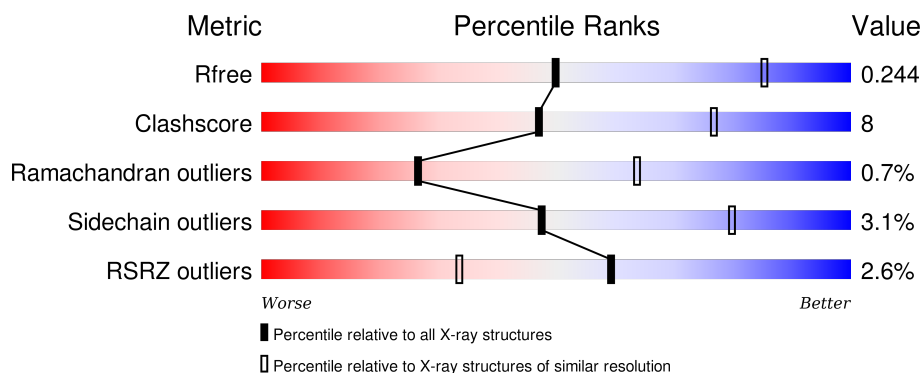
1 Overall quality at a glance

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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

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
3	TM3	F	602	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TAR	F	604	-	-	-	X

2 Entry composition

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
1	F	426	Total	C	N	O	S	0	0	0
			3297	2090	539	647	21			

There are 62 discrepancies between the modelled and reference sequences:

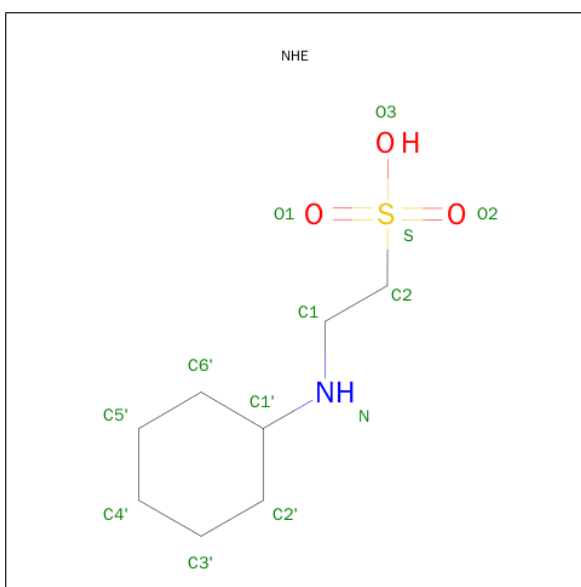
Chain	Residue	Modelled	Actual	Comment	Reference
F	102	ALA	PRO	variant	UNP P03420
F	155	CYS	SER	engineered mutation	UNP P03420
F	190	PHE	SER	engineered mutation	UNP P03420
F	207	LEU	VAL	engineered mutation	UNP P03420
F	290	CYS	SER	engineered mutation	UNP P03420
F	379	VAL	ILE	variant	UNP P03420
F	447	VAL	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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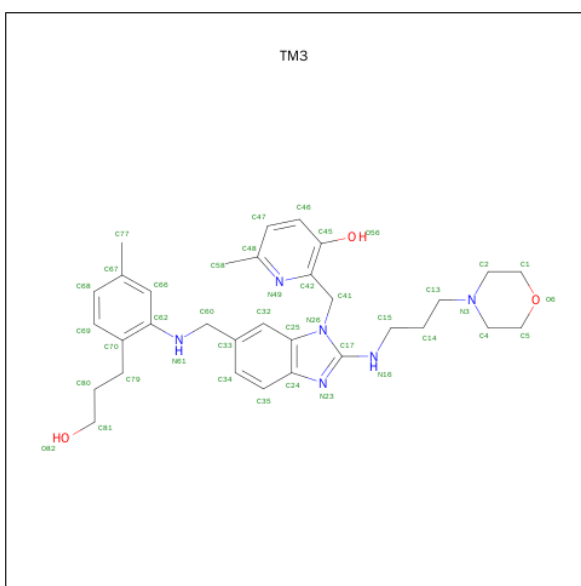
Chain	Residue	Modelled	Actual	Comment	Reference
F	534	ASP	-	expression tag	UNP P03420
F	535	GLY	-	expression tag	UNP P03420
F	536	GLU	-	expression tag	UNP P03420
F	537	TRP	-	expression tag	UNP P03420
F	538	VAL	-	expression tag	UNP P03420
F	539	LEU	-	expression tag	UNP P03420
F	540	LEU	-	expression tag	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 2-[[6-[[[2-(3-hydroxypropyl)-5-methylphenyl]amino]methyl]-2-[[3-(4-morpholinyl)propyl]amino]-1H-benzimidazol-1-yl]methyl]-6-methyl-3-pyridinol (three-letter code: TM3) (formula: $C_{32}H_{42}N_6O_3$).



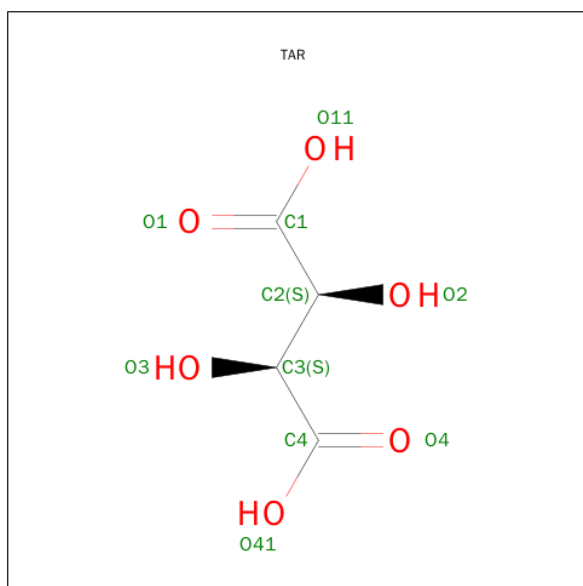
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			41	32	6	3		

- 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		

- Molecule 5 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).

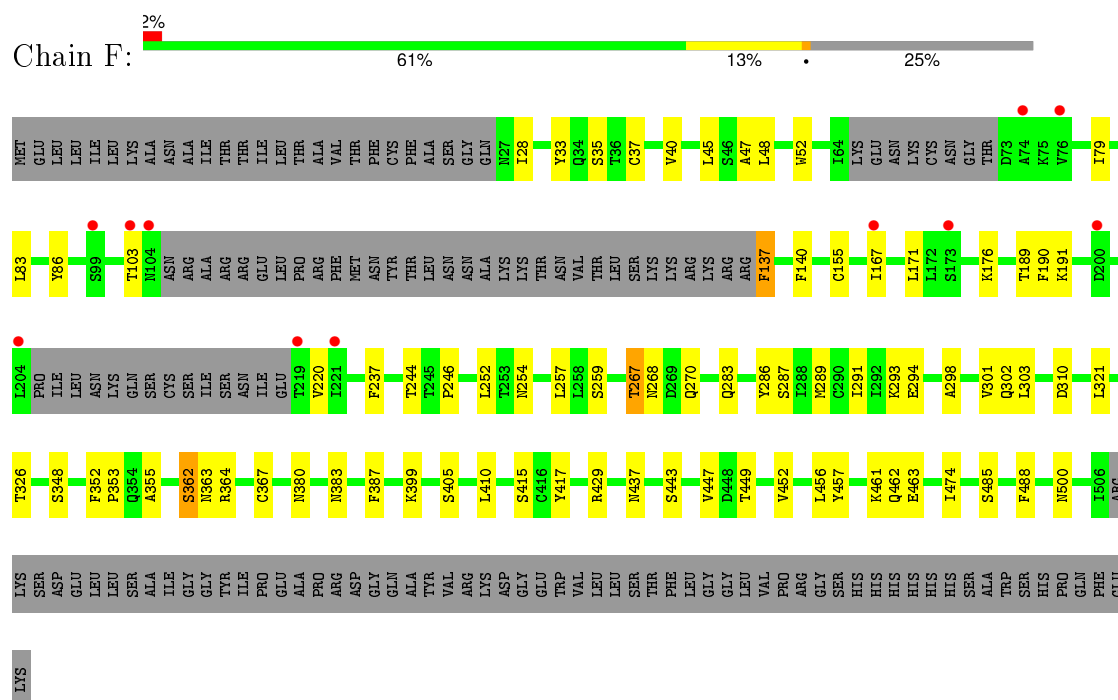


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			10	4	6		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	169.86 Å 169.86 Å 169.86 Å 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) 94.4 (49.03-3.05)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.07 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.248 0.223 , 0.244	Depositor DCC
R_{free} test set	791 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 16545 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3366	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NHE, TM3, SO4, TAR

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	0.33	0/3345	0.49	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

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	43	0
2	F	13	0	17	2	0
3	F	41	0	42	11	0
4	F	5	0	0	0	0
5	F	10	0	4	2	0
All	All	3366	0	3394	51	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 8.

The worst 5 of 51 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:602:TM3:H66	3:F:602:TM3:H32	1.57	0.87
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
3:F:602:TM3:C66	3:F:602:TM3:H32	2.21	0.69
1:F:399:LYS:HG3	1:F:485:SER:HB2	1.82	0.62

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%)	26	64

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%)	375 (97%)	12 (3%)	47	80

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	326	THR
1	F	348	SER
1	F	443	SER
1	F	267	THR
1	F	437	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	354	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 carbohydrates 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	2.40	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TM3	F	602	-	41,45,45	5.28	24 (58%)	50,61,61	1.40	9 (18%)
4	SO4	F	603	-	4,4,4	0.26	0	6,6,6	0.09	0
5	TAR	F	604	-	3,9,9	0.56	0	6,12,12	1.23	1 (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	-	-	0/7/15/15	0/1/1/1
3	TM3	F	602	-	-	0/18/28/28	0/5/5/5
4	SO4	F	603	-	-	0/0/0/0	0/0/0/0
5	TAR	F	604	-	-	0/4/12/12	0/0/0/0

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	TM3	C13-N3	-9.02	1.26	1.47
3	F	602	TM3	C2-N3	-3.06	1.38	1.47
3	F	602	TM3	C4-N3	-2.98	1.39	1.47
2	F	601	NHE	O2-S	2.10	1.51	1.45
2	F	601	NHE	O1-S	2.29	1.51	1.45

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	NHE	O3-S-O2	-4.38	101.56	111.26
3	F	602	TM3	C60-C33-C32	-3.80	116.11	121.81
5	F	604	TAR	C4-C3-C2	-2.49	108.24	113.35
3	F	602	TM3	C66-C62-C70	-2.26	118.20	121.12
3	F	602	TM3	C33-C60-N61	-2.12	108.49	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	NHE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	602	TM3	11	0
5	F	604	TAR	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	426/568 (75%)	-0.23	11 (2%) 59 33	35, 70, 149, 207	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	104	ASN	3.3
1	F	103	THR	3.1
1	F	219	THR	3.0
1	F	74	ALA	2.5
1	F	76	VAL	2.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	TM3	F	602	41/41	0.86	0.29	4.76	51,61,78,79	41

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	TAR	F	604	10/10	0.84	0.44	4.45	110,112,112,113	0
2	NHE	F	601	13/13	0.96	0.25	-0.15	74,76,80,92	0
4	SO4	F	603	5/5	0.91	0.36	-	145,145,146,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.