WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 02:26 PM EDT

PDB ID	:	6XFV
Title	:	CRYSTAL STRUCTURE OF RAR-RELATED ORPHAN RECEPTOR C IN COMPLEX WITH A NOVEL INVERSE AGONIST
Authors	:	Sack, J.S.
Deposited on	:	2020-06-16
Resolution	:	2.15 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
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 ⓘ) were used in the production of this report:

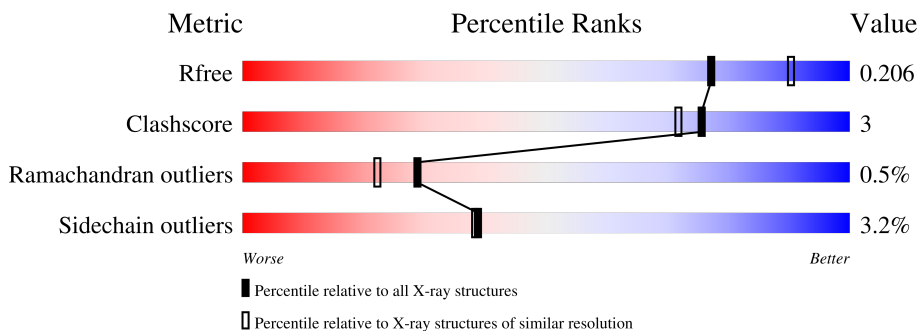|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.15 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		0.206
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		3.2%

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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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%

Mol	Chain	Length	Quality of chain
1	A	265	75% 8% 17%
1	B	265	74% 9% 17%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3685 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 Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total 1769	C 1117	N 320	O 318	S 14	0	0	0
1	B	221	Total 1765	C 1119	N 311	O 321	S 14	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	MET	-	expression tag	UNP P51449
A	224	GLY	-	expression tag	UNP P51449
A	225	SER	-	expression tag	UNP P51449
A	226	SER	-	expression tag	UNP P51449
A	227	HIS	-	expression tag	UNP P51449
A	228	HIS	-	expression tag	UNP P51449
A	229	HIS	-	expression tag	UNP P51449
A	230	HIS	-	expression tag	UNP P51449
A	231	HIS	-	expression tag	UNP P51449
A	232	HIS	-	expression tag	UNP P51449
A	233	SER	-	expression tag	UNP P51449
A	234	SER	-	expression tag	UNP P51449
A	235	GLY	-	expression tag	UNP P51449
A	236	LEU	-	expression tag	UNP P51449
A	237	VAL	-	expression tag	UNP P51449
A	238	PRO	-	expression tag	UNP P51449
A	239	ARG	-	expression tag	UNP P51449
A	240	GLY	-	expression tag	UNP P51449
A	241	SER	-	expression tag	UNP P51449
A	242	HIS	-	expression tag	UNP P51449
A	243	MET	-	expression tag	UNP P51449
B	223	MET	-	expression tag	UNP P51449
B	224	GLY	-	expression tag	UNP P51449
B	225	SER	-	expression tag	UNP P51449
B	226	SER	-	expression tag	UNP P51449

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Chain	Residue	Modelled	Actual	Comment	Reference
B	227	HIS	-	expression tag	UNP P51449
B	228	HIS	-	expression tag	UNP P51449
B	229	HIS	-	expression tag	UNP P51449
B	230	HIS	-	expression tag	UNP P51449
B	231	HIS	-	expression tag	UNP P51449
B	232	HIS	-	expression tag	UNP P51449
B	233	SER	-	expression tag	UNP P51449
B	234	SER	-	expression tag	UNP P51449
B	235	GLY	-	expression tag	UNP P51449
B	236	LEU	-	expression tag	UNP P51449
B	237	VAL	-	expression tag	UNP P51449
B	238	PRO	-	expression tag	UNP P51449
B	239	ARG	-	expression tag	UNP P51449
B	240	GLY	-	expression tag	UNP P51449
B	241	SER	-	expression tag	UNP P51449
B	242	HIS	-	expression tag	UNP P51449
B	243	MET	-	expression tag	UNP P51449

- Molecule 2 is 1-(4-{(3S,4S)-4-[4-(1,1,1,3,3,3-hexafluoro-2-hydroxypropan-2-yl)phenyl]-3-methyl-3-phenylpyrrolidine-1-carbonyl}piperidin-1-yl)ethan-1-one (three-letter code: V27) (formula: $C_{28}H_{30}F_6N_2O_3$) (labeled as "Ligand of Interest" by depositor).
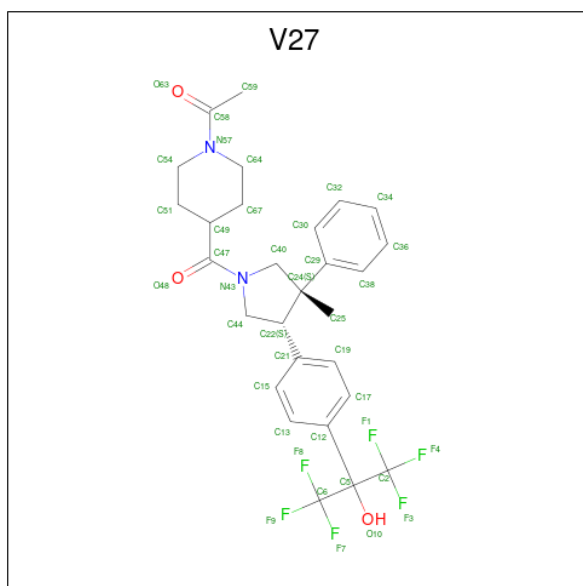
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			39	28	6	2	3		
2	B	1	Total	C	F	N	O	0	0
			39	28	6	2	3		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total O 38 38		0	0
3	B	35	Total O 35 35		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. 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. 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: Nuclear receptor ROR-gamma

Chain A:
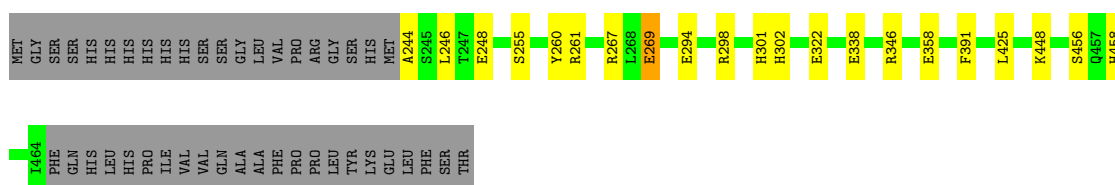
• Molecule 1: Nuclear receptor ROR-gamma

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	97.87Å 97.87Å 130.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.93 – 2.15 48.93 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.93-2.15) 99.8 (48.93-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
R, R_{free}	0.253 , 0.277 0.191 , 0.206	Depositor DCC
R_{free} test set	1925 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.7	EDS
L-test for twinning[2]	$< |L| > = 0.38, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3685	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: V27

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	0.44	0/1803	0.56	0/2427
1	B	0.45	0/1799	0.55	0/2425
All	All	0.45	0/3602	0.55	0/4852

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	A	1769	0	1728	9	0
1	B	1765	0	1729	13	0
2	A	39	0	0	3	0
2	B	39	0	0	1	0
3	A	38	0	0	2	0
3	B	35	0	0	3	0
All	All	3685	0	3457	22	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 3.

The worst 5 of 22 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:B:346:ARG:HD3	3:B:606:HOH:O	1.79	0.82
1:B:259:SER:HB2	3:B:618:HOH:O	1.81	0.80
1:B:415:LYS:O	1:B:419:GLU:HG3	1.81	0.79
1:A:458:HIS:NE2	2:A:500:V27:O10	2.35	0.59
1:B:338:GLU:HB3	1:B:451:LEU:HD21	1.86	0.55

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	219/265 (83%)	210 (96%)	8 (4%)	1 (0%)	29	22
1	B	219/265 (83%)	210 (96%)	8 (4%)	1 (0%)	29	22
All	All	438/530 (83%)	420 (96%)	16 (4%)	2 (0%)	29	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	449	GLY
1	A	246	LEU

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	186/236 (79%)	178 (96%)	8 (4%)	29	27
1	B	188/236 (80%)	184 (98%)	4 (2%)	53	57
All	All	374/472 (79%)	362 (97%)	12 (3%)	39	38

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

Mol	Chain	Res	Type
1	A	456	SER
1	B	255	SER
1	B	421	LEU
1	B	322	GLU
1	A	301	HIS

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 ⓘ

2 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	V27	B	500	-	42,42,42	0.39	0	60,66,66	0.60	1 (1%)
2	V27	A	500	-	42,42,42	0.46	0	60,66,66	0.82	1 (1%)

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	V27	B	500	-	-	8/46/71/71	0/4/4/4
2	V27	A	500	-	-	8/46/71/71	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	V27	C6-C5-C2	4.53	115.95	110.28
2	B	500	V27	C6-C5-C2	2.76	113.74	110.28

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	V27	O48-C47-N43-C40
2	A	500	V27	C49-C47-N43-C40
2	A	500	V27	O48-C47-N43-C44
2	A	500	V27	C49-C47-N43-C44
2	B	500	V27	O48-C47-N43-C40

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	V27	1	0
2	A	500	V27	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 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 V27 B 500

Bond lengths

Bond angles

Torsions

Rings

Ligand V27 A 500

Bond lengths

Bond angles

Torsions

Rings
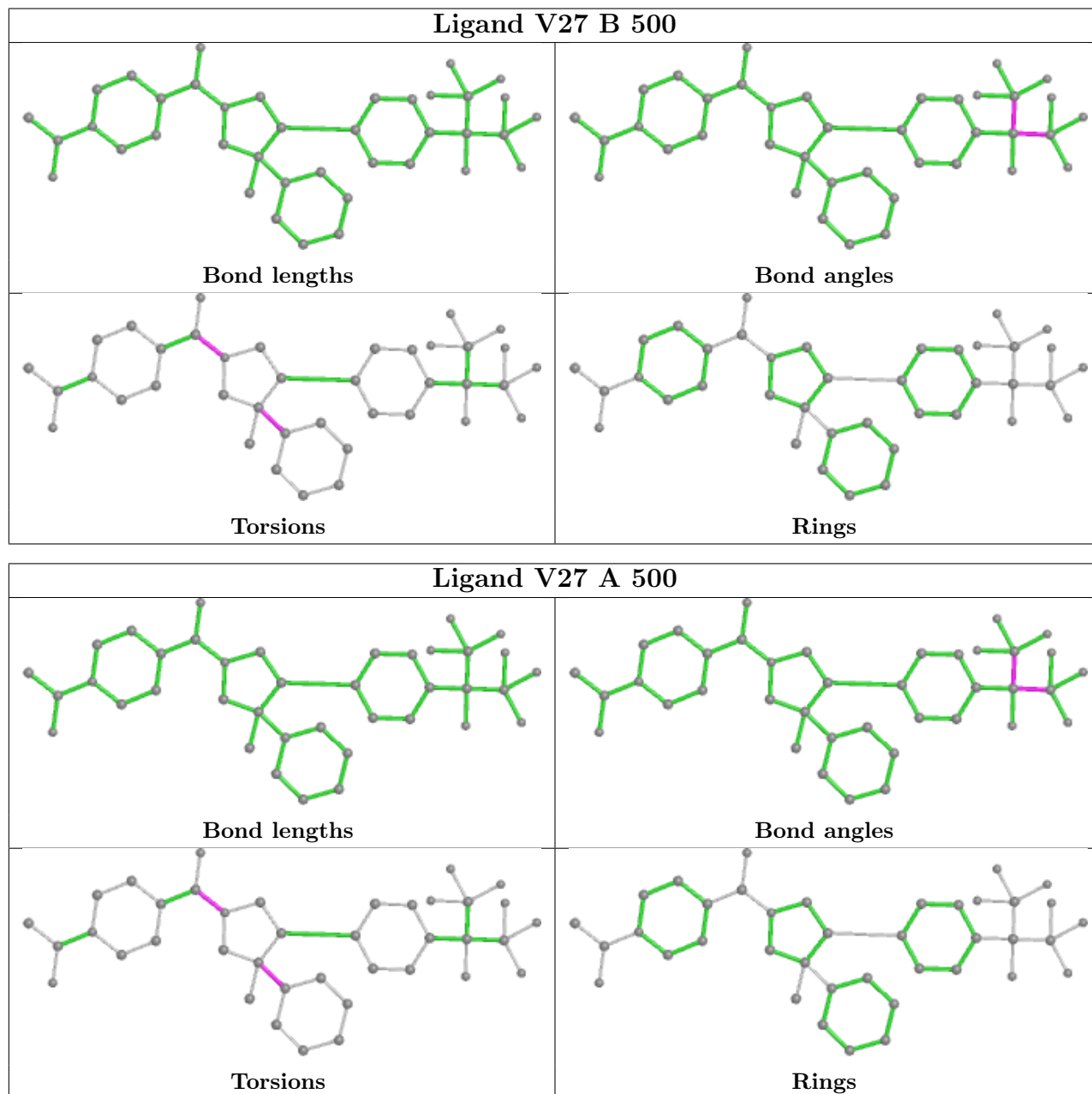
5.7 Other polymers ⓘ

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

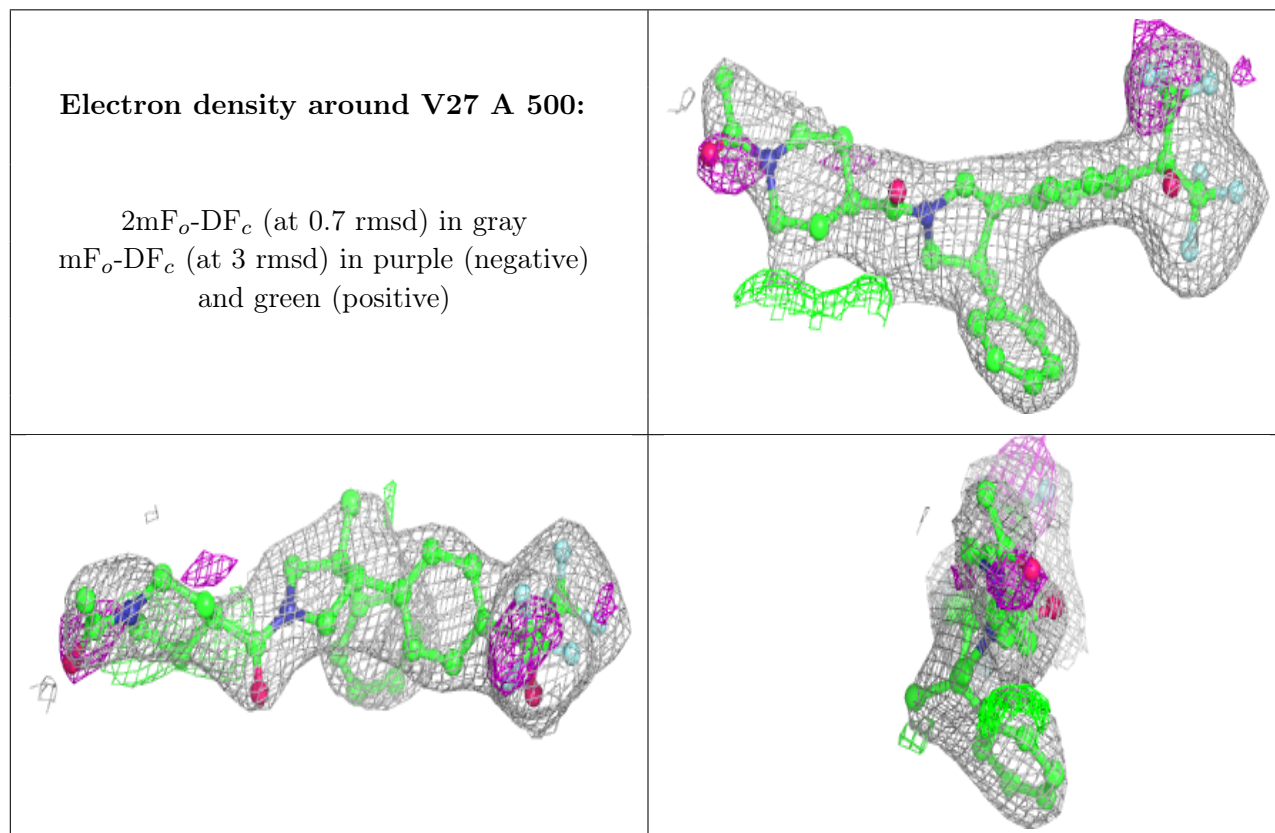Unable to reproduce the depositors R factor - this section is therefore empty.
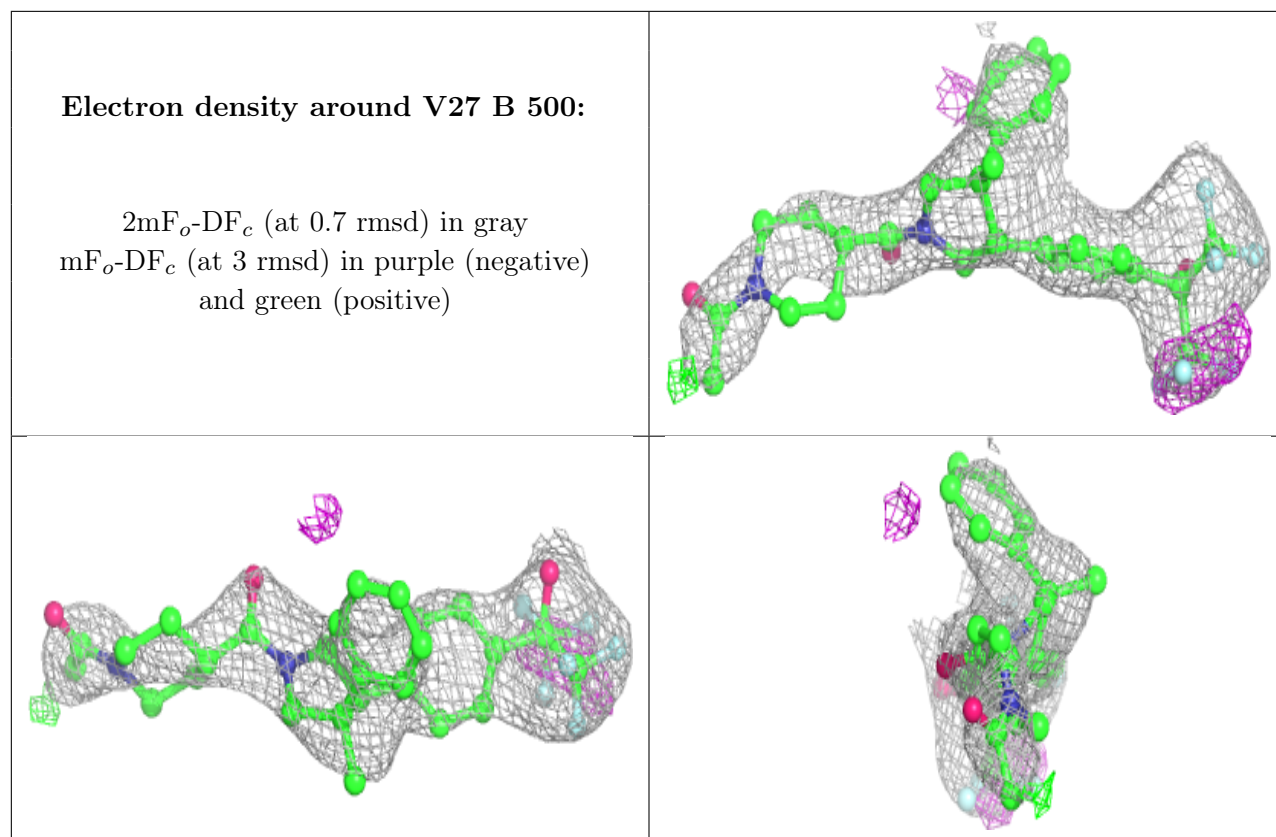
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 V27 A 500:

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

Electron density around V27 B 500:

$2mF_o$-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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.