



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:22 AM UTC

PDB ID : 8U7E / pdb\_00008u7e  
Title : Structure of Sts-1 HP domain with rebamipide derivative  
Authors : Aziz, F.; Dey, R.; French, J.B.  
Deposited on : 2023-09-15  
Resolution : 2.63 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](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>.

---

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

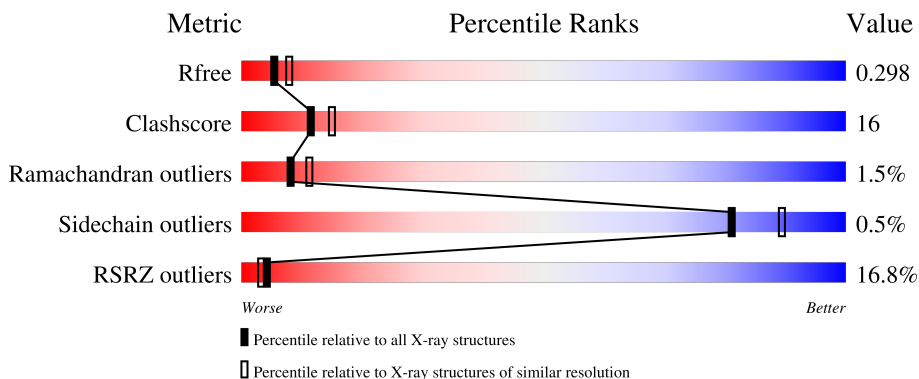
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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.



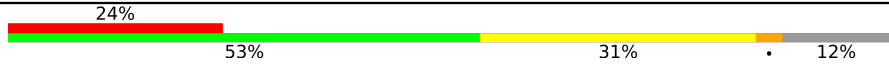
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	A	287	 10% 64% 23% • 12%
1	B	287	 8% 66% 21% • 10%
1	C	287	 13% 61% 27% • 11%
1	D	287	 12% 65% 23% • 11%
1	E	287	 23% 60% 27% • 12%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	287	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into four segments: a red segment (24%), a green segment (53%), a yellow segment (31%), and a grey segment (12%). The percentages are labeled above or below the corresponding segments.</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21773 atoms, of which 10391 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 Ubiquitin-associated and SH3 domain-containing protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	253	3666	1212	1775	322	342	15	0	0	0
1	B	257	3725	1226	1811	331	342	15	0	0	0
1	C	256	3768	1231	1843	331	349	14	0	0	0
1	D	255	3653	1204	1762	327	346	14	0	0	0
1	E	253	3361	1134	1575	316	323	13	0	0	0
1	F	253	3433	1155	1625	314	325	14	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLN	-	expression tag	UNP Q8TF42
A	353	GLY	-	expression tag	UNP Q8TF42
A	354	HIS	-	expression tag	UNP Q8TF42
A	355	MET	-	expression tag	UNP Q8TF42
A	356	ALA	-	expression tag	UNP Q8TF42
A	357	SER	-	expression tag	UNP Q8TF42
A	358	MET	-	expression tag	UNP Q8TF42
A	359	THR	-	expression tag	UNP Q8TF42
A	360	GLY	-	expression tag	UNP Q8TF42
A	361	GLY	-	expression tag	UNP Q8TF42
A	362	GLN	-	expression tag	UNP Q8TF42
A	363	GLN	-	expression tag	UNP Q8TF42
A	364	MET	-	expression tag	UNP Q8TF42
A	365	GLY	-	expression tag	UNP Q8TF42
A	366	ARG	-	expression tag	UNP Q8TF42
A	367	GLY	-	expression tag	UNP Q8TF42
A	368	SER	-	expression tag	UNP Q8TF42

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	352	GLN	-	expression tag	UNP Q8TF42
B	353	GLY	-	expression tag	UNP Q8TF42
B	354	HIS	-	expression tag	UNP Q8TF42
B	355	MET	-	expression tag	UNP Q8TF42
B	356	ALA	-	expression tag	UNP Q8TF42
B	357	SER	-	expression tag	UNP Q8TF42
B	358	MET	-	expression tag	UNP Q8TF42
B	359	THR	-	expression tag	UNP Q8TF42
B	360	GLY	-	expression tag	UNP Q8TF42
B	361	GLY	-	expression tag	UNP Q8TF42
B	362	GLN	-	expression tag	UNP Q8TF42
B	363	GLN	-	expression tag	UNP Q8TF42
B	364	MET	-	expression tag	UNP Q8TF42
B	365	GLY	-	expression tag	UNP Q8TF42
B	366	ARG	-	expression tag	UNP Q8TF42
B	367	GLY	-	expression tag	UNP Q8TF42
B	368	SER	-	expression tag	UNP Q8TF42
C	352	GLN	-	expression tag	UNP Q8TF42
C	353	GLY	-	expression tag	UNP Q8TF42
C	354	HIS	-	expression tag	UNP Q8TF42
C	355	MET	-	expression tag	UNP Q8TF42
C	356	ALA	-	expression tag	UNP Q8TF42
C	357	SER	-	expression tag	UNP Q8TF42
C	358	MET	-	expression tag	UNP Q8TF42
C	359	THR	-	expression tag	UNP Q8TF42
C	360	GLY	-	expression tag	UNP Q8TF42
C	361	GLY	-	expression tag	UNP Q8TF42
C	362	GLN	-	expression tag	UNP Q8TF42
C	363	GLN	-	expression tag	UNP Q8TF42
C	364	MET	-	expression tag	UNP Q8TF42
C	365	GLY	-	expression tag	UNP Q8TF42
C	366	ARG	-	expression tag	UNP Q8TF42
C	367	GLY	-	expression tag	UNP Q8TF42
C	368	SER	-	expression tag	UNP Q8TF42
D	352	GLN	-	expression tag	UNP Q8TF42
D	353	GLY	-	expression tag	UNP Q8TF42
D	354	HIS	-	expression tag	UNP Q8TF42
D	355	MET	-	expression tag	UNP Q8TF42
D	356	ALA	-	expression tag	UNP Q8TF42
D	357	SER	-	expression tag	UNP Q8TF42
D	358	MET	-	expression tag	UNP Q8TF42
D	359	THR	-	expression tag	UNP Q8TF42

*Continued on next page...*

*Continued from previous page...*

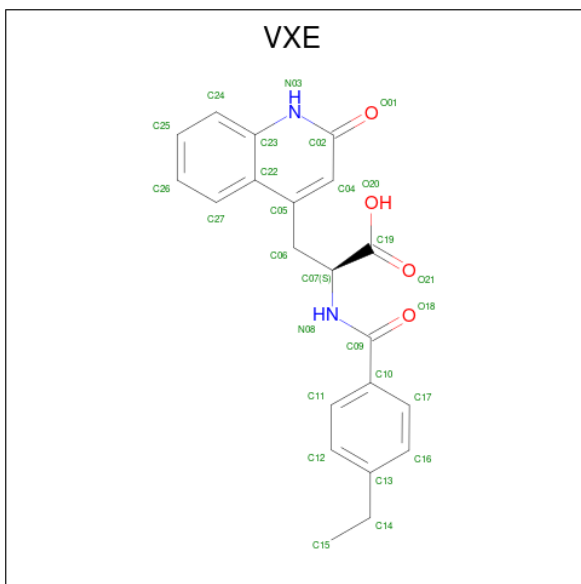
Chain	Residue	Modelled	Actual	Comment	Reference
D	360	GLY	-	expression tag	UNP Q8TF42
D	361	GLY	-	expression tag	UNP Q8TF42
D	362	GLN	-	expression tag	UNP Q8TF42
D	363	GLN	-	expression tag	UNP Q8TF42
D	364	MET	-	expression tag	UNP Q8TF42
D	365	GLY	-	expression tag	UNP Q8TF42
D	366	ARG	-	expression tag	UNP Q8TF42
D	367	GLY	-	expression tag	UNP Q8TF42
D	368	SER	-	expression tag	UNP Q8TF42
E	352	GLN	-	expression tag	UNP Q8TF42
E	353	GLY	-	expression tag	UNP Q8TF42
E	354	HIS	-	expression tag	UNP Q8TF42
E	355	MET	-	expression tag	UNP Q8TF42
E	356	ALA	-	expression tag	UNP Q8TF42
E	357	SER	-	expression tag	UNP Q8TF42
E	358	MET	-	expression tag	UNP Q8TF42
E	359	THR	-	expression tag	UNP Q8TF42
E	360	GLY	-	expression tag	UNP Q8TF42
E	361	GLY	-	expression tag	UNP Q8TF42
E	362	GLN	-	expression tag	UNP Q8TF42
E	363	GLN	-	expression tag	UNP Q8TF42
E	364	MET	-	expression tag	UNP Q8TF42
E	365	GLY	-	expression tag	UNP Q8TF42
E	366	ARG	-	expression tag	UNP Q8TF42
E	367	GLY	-	expression tag	UNP Q8TF42
E	368	SER	-	expression tag	UNP Q8TF42
F	352	GLN	-	expression tag	UNP Q8TF42
F	353	GLY	-	expression tag	UNP Q8TF42
F	354	HIS	-	expression tag	UNP Q8TF42
F	355	MET	-	expression tag	UNP Q8TF42
F	356	ALA	-	expression tag	UNP Q8TF42
F	357	SER	-	expression tag	UNP Q8TF42
F	358	MET	-	expression tag	UNP Q8TF42
F	359	THR	-	expression tag	UNP Q8TF42
F	360	GLY	-	expression tag	UNP Q8TF42
F	361	GLY	-	expression tag	UNP Q8TF42
F	362	GLN	-	expression tag	UNP Q8TF42
F	363	GLN	-	expression tag	UNP Q8TF42
F	364	MET	-	expression tag	UNP Q8TF42
F	365	GLY	-	expression tag	UNP Q8TF42
F	366	ARG	-	expression tag	UNP Q8TF42
F	367	GLY	-	expression tag	UNP Q8TF42

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	368	SER	-	expression tag	UNP Q8TF42

- Molecule 2 is N-(4-ethylbenzoyl)-3-(2-oxo-1,2-dihydroquinolin-4-yl)-L-alanine (CCD ID: VXE) (formula: C<sub>21</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			27	21	2	4		
2	C	1	Total	C	N	O	0	0
			27	21	2	4		
2	D	1	Total	C	N	O	0	0
			27	21	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	18	Total	O	0	0
			18	18		
3	C	25	Total	O	0	0
			25	25		
3	D	4	Total	O	0	0
			4	4		
3	E	1	Total	O	0	0
			1	1		

Continued on next page...

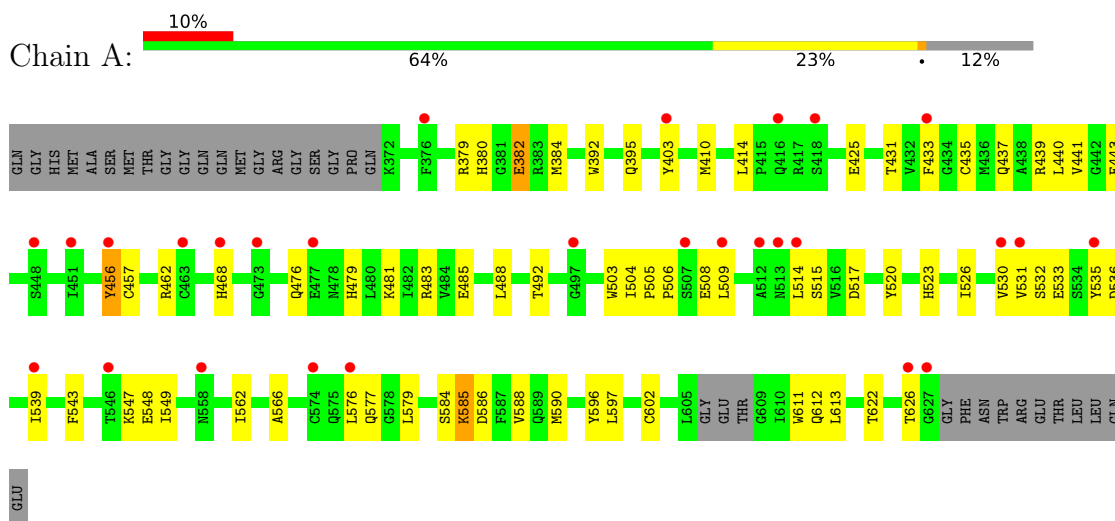
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	F	12	Total	O	0	0
			12	12		

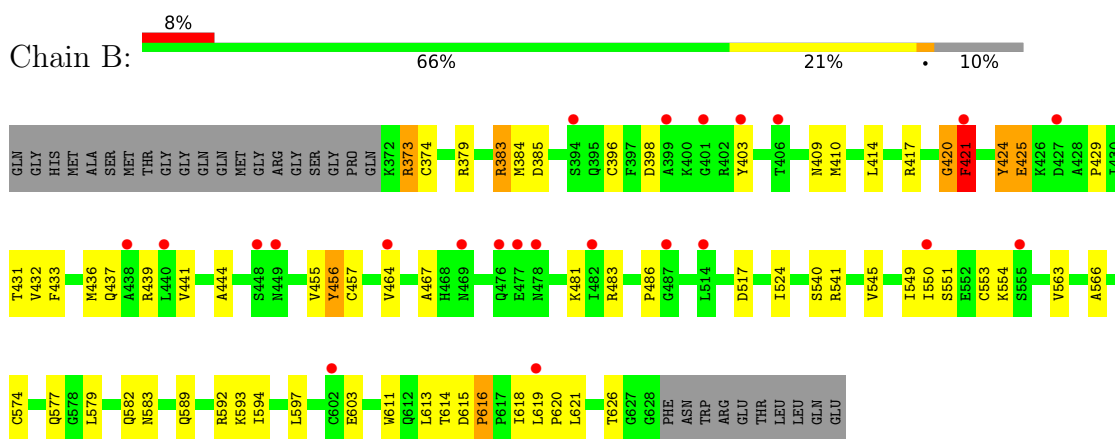
### 3 Residue-property plots

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.

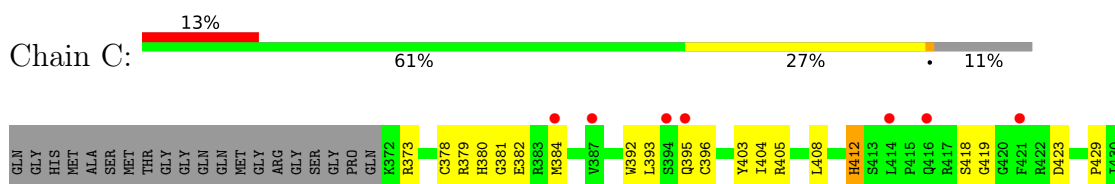
- Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B

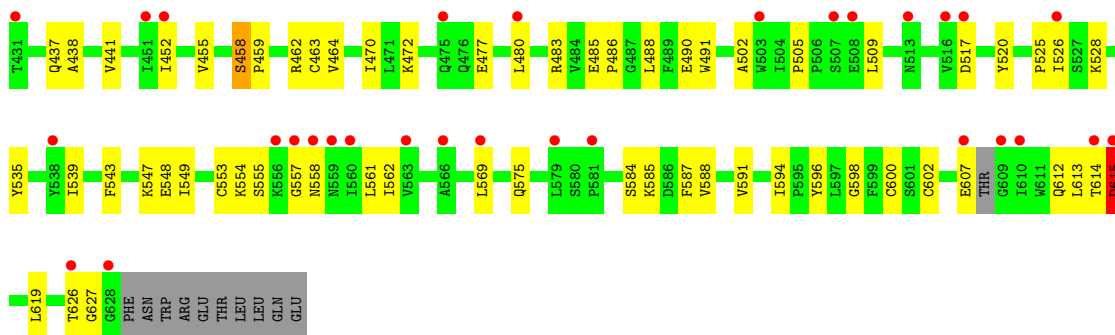


- Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B

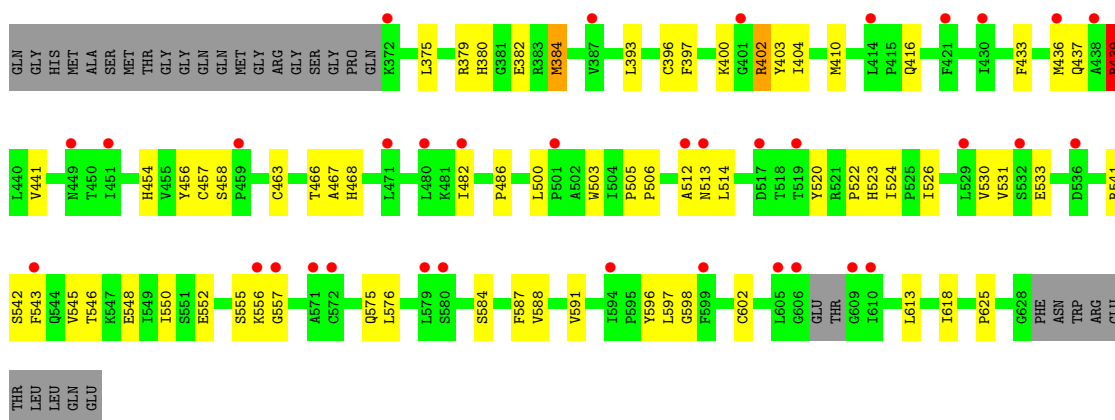


- Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B

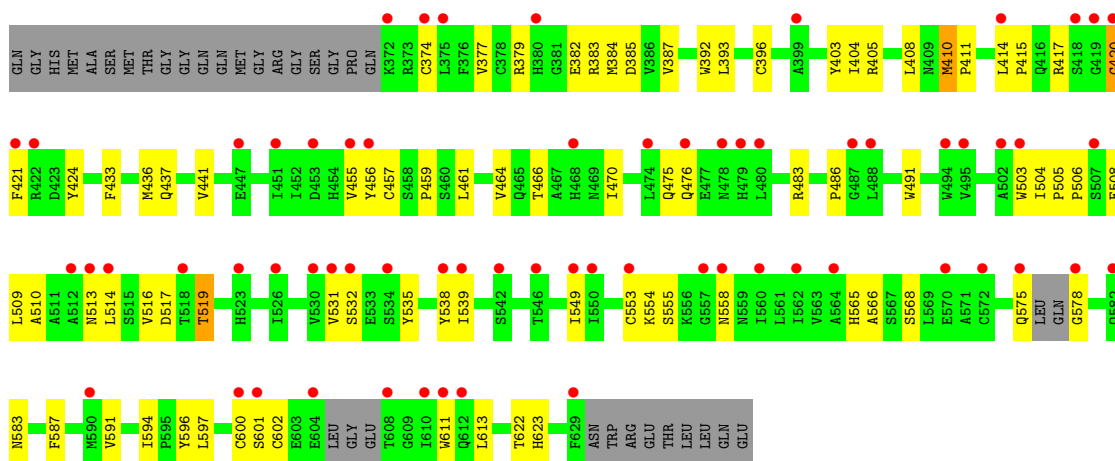




• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B



• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B



• Molecule 1: Ubiquitin-associated and SH3 domain-containing protein B





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.78Å 122.70Å 99.94Å 90.00° 112.62° 90.00°	Depositor
Resolution (Å)	92.26 – 2.63 92.26 – 2.63	Depositor EDS
% Data completeness (in resolution range)	95.5 (92.26-2.63) 95.7 (92.26-2.63)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.62Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.215 , 0.298 0.221 , 0.298	Depositor DCC
$R_{free}$ test set	2491 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtrriage
Anisotropy	0.883	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 75.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: VXE

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	0.73	2/1939 (0.1%)	1.01	8/2650 (0.3%)
1	B	0.78	2/1963 (0.1%)	1.26	23/2681 (0.9%)
1	C	0.73	3/1973 (0.2%)	0.93	3/2689 (0.1%)
1	D	0.64	1/1939 (0.1%)	0.89	4/2652 (0.2%)
1	E	0.55	1/1829 (0.1%)	0.83	1/2507 (0.0%)
1	F	0.76	3/1854 (0.2%)	0.97	8/2545 (0.3%)
All	All	0.71	12/11497 (0.1%)	1.00	47/15724 (0.3%)

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	B	0	1
1	D	0	2
1	F	0	1
All	All	0	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	384	MET	SD-CE	11.99	2.09	1.79
1	B	425	GLU	CB-CG	8.18	1.76	1.52
1	F	384	MET	CB-CG	6.95	1.73	1.52
1	C	412	HIS	CA-CB	6.34	1.63	1.53
1	F	485	GLU	CD-OE2	6.25	1.37	1.25

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	ARG	NE-CZ-NH2	-17.98	103.02	119.20
1	B	425	GLU	CG-CD-OE1	13.40	149.23	118.40
1	B	373	ARG	CG-CD-NE	-11.95	85.70	112.00
1	F	384	MET	CG-SD-CE	-10.80	77.15	100.90
1	E	594	ILE	N-CA-C	10.29	117.48	108.63

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	420	GLY	Peptide
1	D	439	ARG	Sidechain
1	D	625	PRO	Peptide
1	F	384	MET	Mainchain

## 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	A	1891	1775	1776	54	0
1	B	1914	1811	1811	63	0
1	C	1925	1843	1846	53	0
1	D	1891	1762	1762	48	0
1	E	1786	1575	1575	62	0
1	F	1808	1625	1625	85	0
2	A	27	0	0	0	0
2	C	27	0	0	0	0
2	D	27	0	0	0	0
3	A	26	0	0	0	0
3	B	18	0	0	0	0
3	C	25	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
3	F	12	0	0	1	0
All	All	11382	10391	10395	349	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 16.

The worst 5 of 349 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:425:GLU:CG	1:B:425:GLU:CB	1.77	1.62
1:F:384:MET:SD	1:F:384:MET:CE	2.09	1.40
1:F:384:MET:CE	1:F:384:MET:CG	2.43	0.97
1:F:378:CYS:HB2	1:F:599:PHE:HB2	1.48	0.95
1:F:384:MET:HG3	1:F:431:THR:HG22	1.55	0.87

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	A	249/287 (87%)	226 (91%)	23 (9%)	0	100	100
1	B	255/287 (89%)	229 (90%)	26 (10%)	0	100	100
1	C	252/287 (88%)	224 (89%)	23 (9%)	5 (2%)	6	8
1	D	251/287 (88%)	219 (87%)	32 (13%)	0	100	100
1	E	247/287 (86%)	218 (88%)	24 (10%)	5 (2%)	6	8
1	F	249/287 (87%)	212 (85%)	24 (10%)	13 (5%)	1	1
All	All	1503/1722 (87%)	1328 (88%)	152 (10%)	23 (2%)	8	11

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	554	LYS
1	E	611	TRP
1	F	554	LYS
1	E	519	THR
1	F	515	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	A	190/249 (76%)	189 (100%)	1 (0%)	81	89
1	B	192/249 (77%)	190 (99%)	2 (1%)	68	80
1	C	200/249 (80%)	200 (100%)	0	100	100
1	D	191/249 (77%)	191 (100%)	0	100	100
1	E	162/249 (65%)	161 (99%)	1 (1%)	78	87
1	F	169/249 (68%)	168 (99%)	1 (1%)	78	87
All	All	1104/1494 (74%)	1099 (100%)	5 (0%)	81	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	TYR
1	B	421	PHE
1	B	456	TYR
1	E	583	ASN
1	F	536	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	380	HIS
1	D	523	HIS
1	C	478	ASN
1	D	476	GLN
1	C	469	ASN

### 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](#)

3 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	VXE	D	701	-	29,29,29	3.05	8 (27%)	38,40,40	2.39	11 (28%)
2	VXE	A	701	-	29,29,29	2.88	8 (27%)	38,40,40	1.94	8 (21%)
2	VXE	C	701	-	29,29,29	3.24	13 (44%)	38,40,40	2.33	11 (28%)

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	VXE	D	701	-	-	2/18/18/18	0/3/3/3
2	VXE	A	701	-	-	2/18/18/18	0/3/3/3
2	VXE	C	701	-	-	2/18/18/18	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	VXE	C02-N03	8.65	1.48	1.37
2	C	701	VXE	C02-N03	8.58	1.47	1.37
2	A	701	VXE	C02-N03	8.30	1.47	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	VXE	C23-N03	8.14	1.53	1.39
2	C	701	VXE	C23-N03	7.84	1.53	1.39

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	VXE	C02-C04-C05	-7.26	118.66	122.51
2	C	701	VXE	C04-C02-N03	6.39	120.99	115.89
2	A	701	VXE	C23-N03-C02	-5.75	119.00	124.50
2	D	701	VXE	O01-C02-C04	-5.60	117.72	125.46
2	D	701	VXE	C04-C02-N03	5.39	120.19	115.89

There are no chirality outliers.

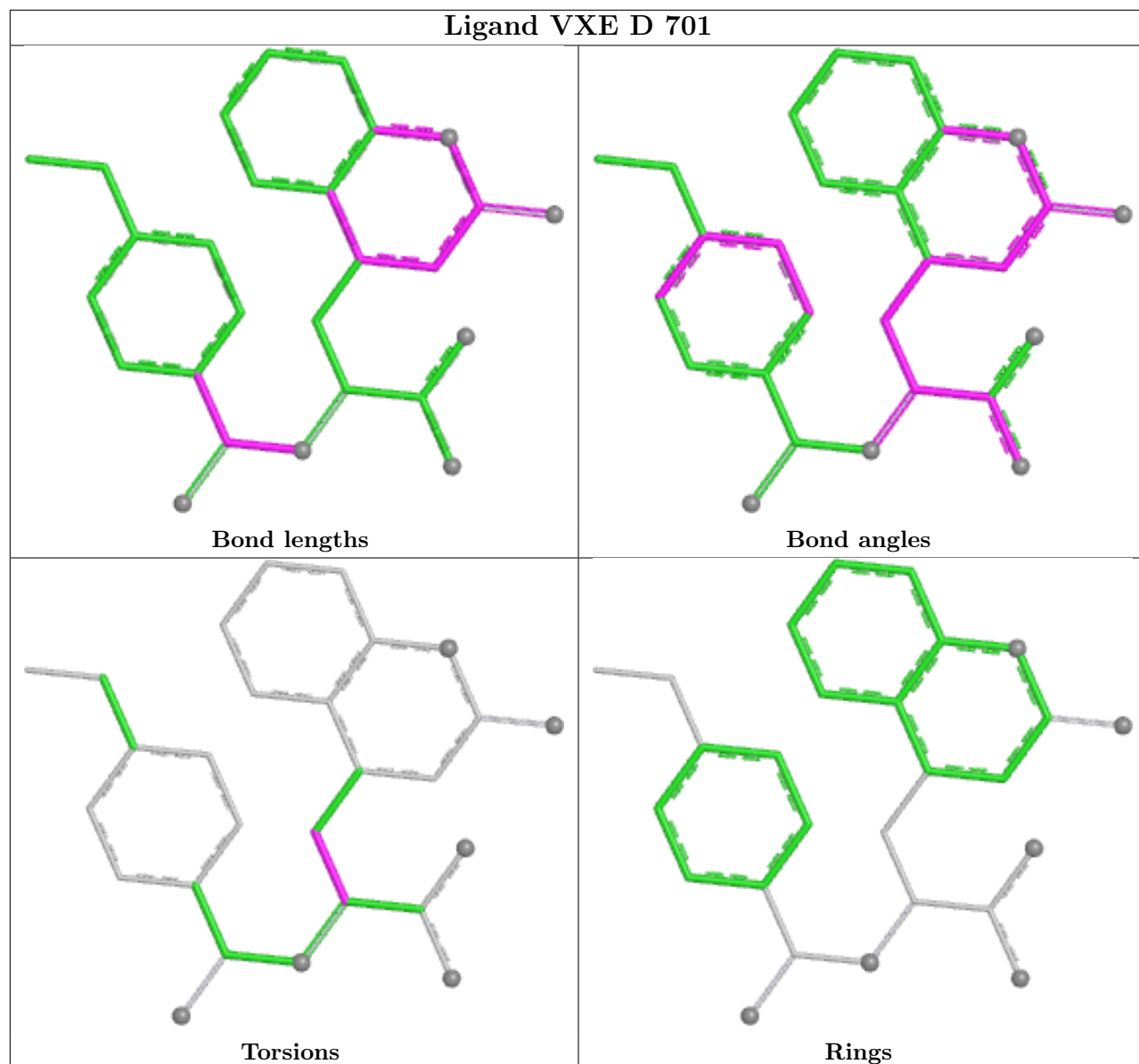
5 of 6 torsion outliers are listed below:

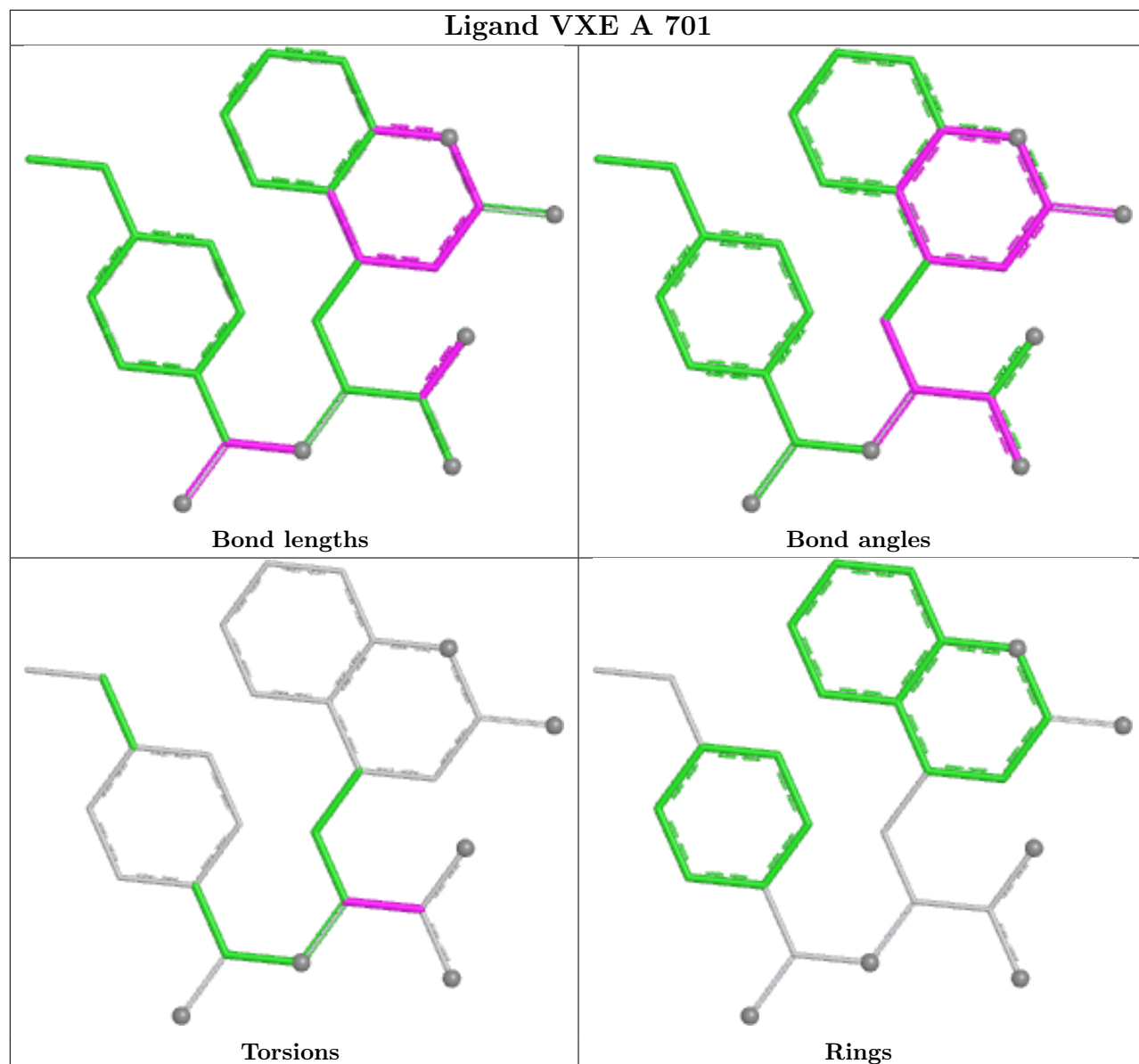
Mol	Chain	Res	Type	Atoms
2	D	701	VXE	C05-C06-C07-C19
2	D	701	VXE	C05-C06-C07-N08
2	C	701	VXE	C05-C06-C07-C19
2	C	701	VXE	C05-C06-C07-N08
2	A	701	VXE	C06-C07-C19-O20

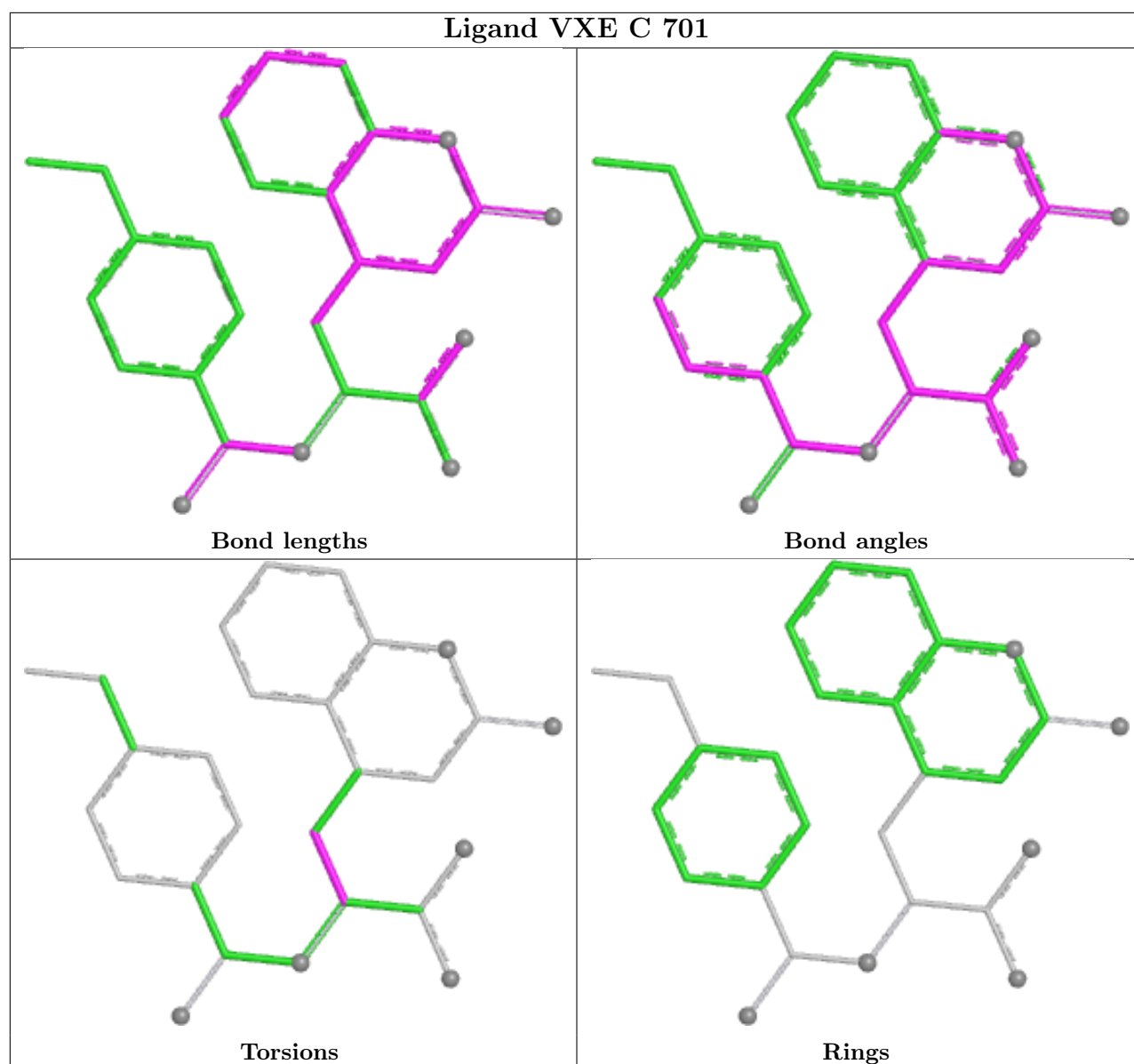
There are no ring outliers.

No monomer is involved in short contacts.

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 [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, 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	A	253/287 (88%)	0.89	28 (11%) 10 8	40, 60, 80, 92	1 (0%)
1	B	257/287 (89%)	0.96	23 (8%) 15 12	43, 65, 86, 98	0
1	C	256/287 (89%)	1.08	37 (14%) 6 5	44, 65, 98, 114	0
1	D	255/287 (88%)	1.11	35 (13%) 6 5	47, 70, 97, 120	0
1	E	253/287 (88%)	1.50	65 (25%) 1 1	54, 94, 126, 152	0
1	F	253/287 (88%)	1.52	69 (27%) 1 1	45, 82, 110, 124	0
All	All	1527/1722 (88%)	1.18	257 (16%) 4 3	40, 69, 108, 152	1 (0%)

The worst 5 of 257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	571	ALA	6.5
1	D	606	GLY	5.3
1	D	512	ALA	5.0
1	D	414	LEU	5.0
1	C	557	GLY	4.6

### 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](#)

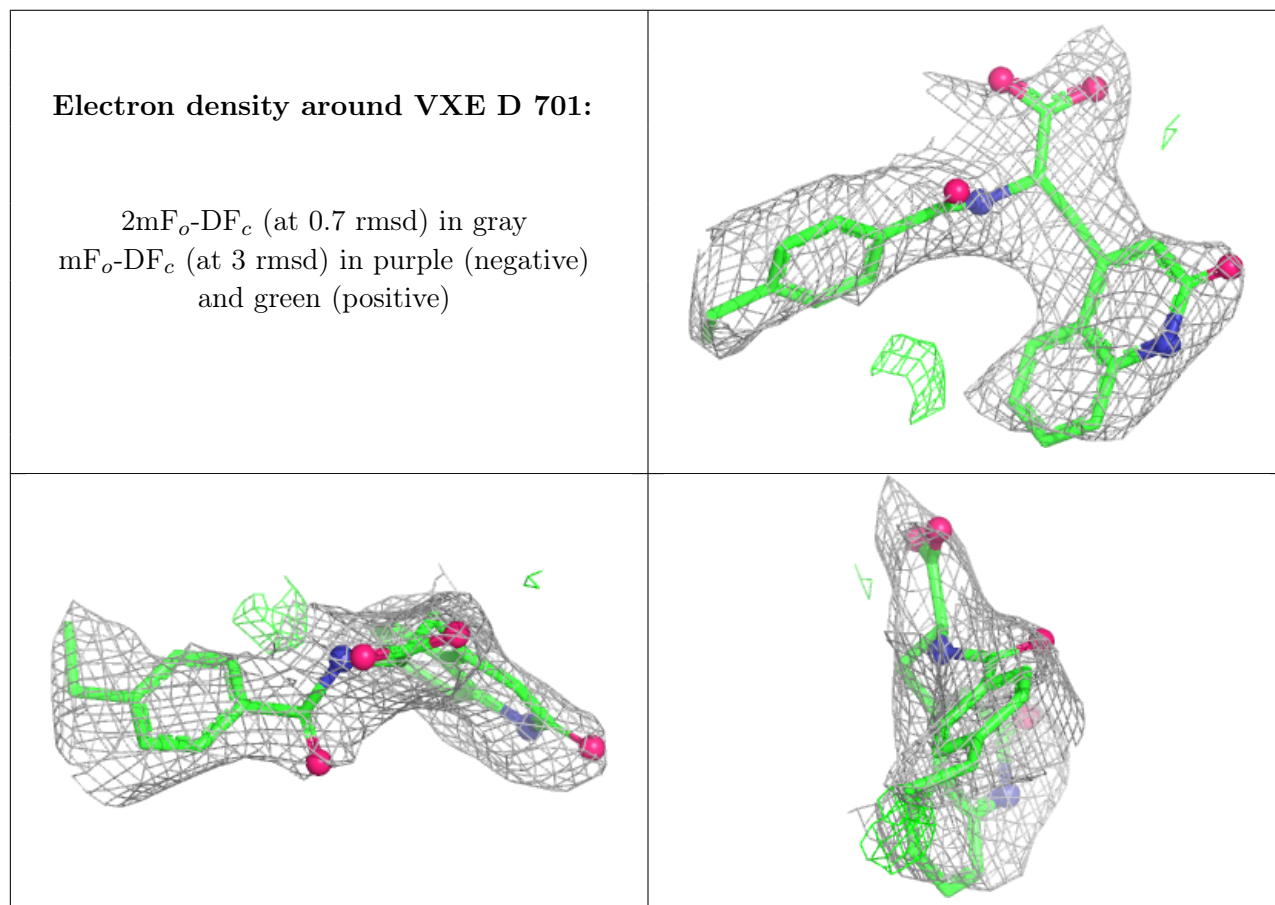
There are no oligosaccharides in this entry.

## 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.

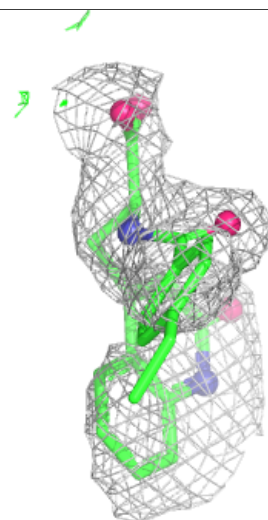
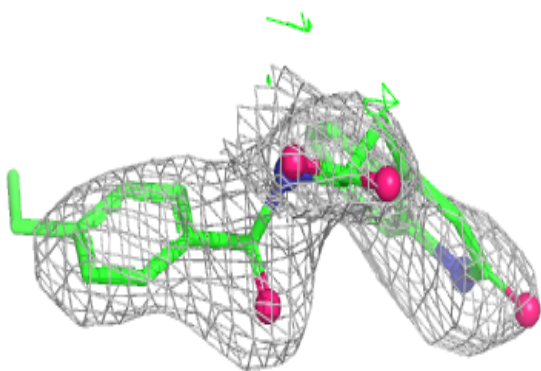
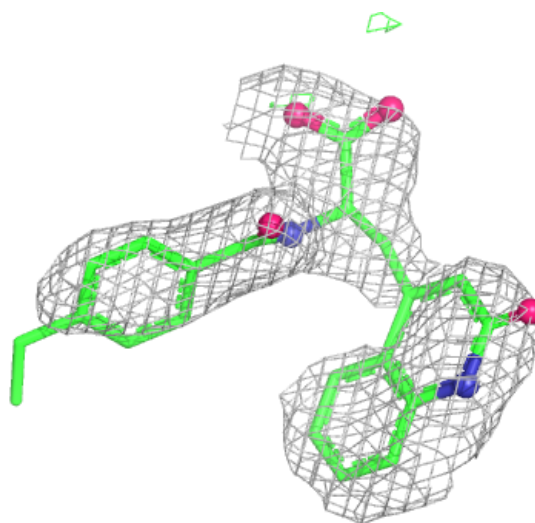
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	VXE	D	701	27/27	0.77	0.18	60,68,74,81	0
2	VXE	C	701	27/27	0.79	0.19	48,60,73,78	0
2	VXE	A	701	27/27	0.82	0.15	48,59,65,67	0

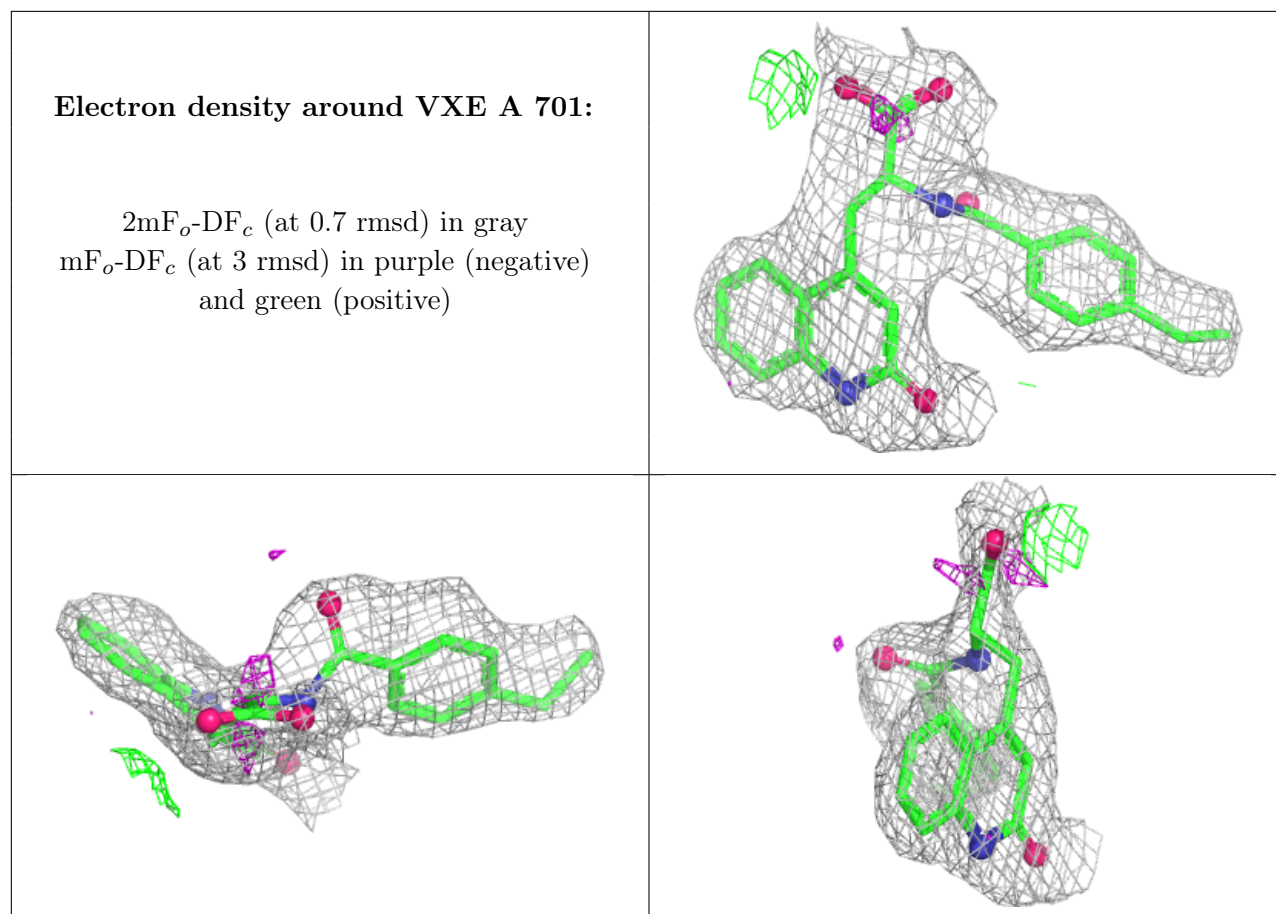
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around VXE C 701:**

$2mF_o-DF_c$  (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.