wwPDB EM Validation Summary Report

Oct 16, 2024 – 12:29 AM JST

PDB ID	:	8KG5
EMDB ID	:	EMD-37210
Title	:	Prefusion RSV F Bound to Lonafarnib and D25 Fab
Authors	:	Yang, Q.; Xue, B.; Liu, F.; Peng, W.; Chen, X.
Deposited on	:	2023-08-17
Resolution	:	3.17 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

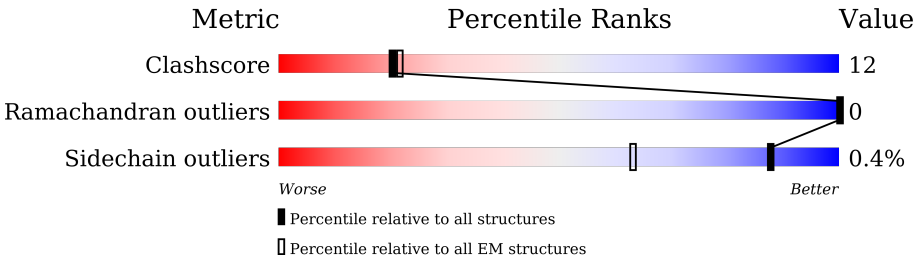
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	585	60% 17% 23%
1	B	585	59% 18% 23%
1	C	585	61% 16% 23%
2	D	231	41% 13% 46%
3	E	214	35% 14% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12307 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total 3482	C 2202	N 573	O 684	S 23	0	0
1	B	449	Total 3482	C 2202	N 573	O 684	S 23	0	0
1	C	449	Total 3482	C 2202	N 573	O 684	S 23	0	0

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
A	155	CYS	SER	conflict	UNP P03420
A	190	PHE	SER	conflict	UNP P03420
A	207	LEU	VAL	conflict	UNP P03420
A	290	CYS	SER	conflict	UNP P03420
A	379	VAL	ILE	conflict	UNP P03420
A	447	VAL	MET	conflict	UNP P03420
A	514	GLY	-	linker	UNP P03420
A	515	SER	-	linker	UNP P03420
A	544	GLY	-	expression tag	UNP P10104
A	545	LEU	-	expression tag	UNP P10104
A	546	GLU	-	expression tag	UNP P10104
A	547	VAL	-	expression tag	UNP P10104
A	548	LEU	-	expression tag	UNP P10104
A	549	PHE	-	expression tag	UNP P10104
A	550	GLN	-	expression tag	UNP P10104
A	551	GLY	-	expression tag	UNP P10104
A	552	PRO	-	expression tag	UNP P10104
A	553	GLY	-	expression tag	UNP P10104
A	554	GLY	-	expression tag	UNP P10104
A	555	TRP	-	expression tag	UNP P10104
A	556	SER	-	expression tag	UNP P10104
A	557	HIS	-	expression tag	UNP P10104
A	558	PRO	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	559	GLN	-	expression tag	UNP P10104
A	560	PHE	-	expression tag	UNP P10104
A	561	GLU	-	expression tag	UNP P10104
A	562	LYS	-	expression tag	UNP P10104
A	563	GLY	-	expression tag	UNP P10104
A	564	GLY	-	expression tag	UNP P10104
A	565	GLY	-	expression tag	UNP P10104
A	566	SER	-	expression tag	UNP P10104
A	567	GLY	-	expression tag	UNP P10104
A	568	GLY	-	expression tag	UNP P10104
A	569	GLY	-	expression tag	UNP P10104
A	570	SER	-	expression tag	UNP P10104
A	571	GLY	-	expression tag	UNP P10104
A	572	GLY	-	expression tag	UNP P10104
A	573	SER	-	expression tag	UNP P10104
A	574	ALA	-	expression tag	UNP P10104
A	575	TRP	-	expression tag	UNP P10104
A	576	SER	-	expression tag	UNP P10104
A	577	HIS	-	expression tag	UNP P10104
A	578	PRO	-	expression tag	UNP P10104
A	579	GLN	-	expression tag	UNP P10104
A	580	PHE	-	expression tag	UNP P10104
A	581	GLU	-	expression tag	UNP P10104
A	582	LYS	-	expression tag	UNP P10104
A	583	GLY	-	expression tag	UNP P10104
A	584	GLY	-	expression tag	UNP P10104
A	585	SER	-	expression tag	UNP P10104
B	102	ALA	PRO	conflict	UNP P03420
B	155	CYS	SER	conflict	UNP P03420
B	190	PHE	SER	conflict	UNP P03420
B	207	LEU	VAL	conflict	UNP P03420
B	290	CYS	SER	conflict	UNP P03420
B	379	VAL	ILE	conflict	UNP P03420
B	447	VAL	MET	conflict	UNP P03420
B	514	GLY	-	linker	UNP P03420
B	515	SER	-	linker	UNP P03420
B	544	GLY	-	expression tag	UNP P10104
B	545	LEU	-	expression tag	UNP P10104
B	546	GLU	-	expression tag	UNP P10104
B	547	VAL	-	expression tag	UNP P10104
B	548	LEU	-	expression tag	UNP P10104
B	549	PHE	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	550	GLN	-	expression tag	UNP P10104
B	551	GLY	-	expression tag	UNP P10104
B	552	PRO	-	expression tag	UNP P10104
B	553	GLY	-	expression tag	UNP P10104
B	554	GLY	-	expression tag	UNP P10104
B	555	TRP	-	expression tag	UNP P10104
B	556	SER	-	expression tag	UNP P10104
B	557	HIS	-	expression tag	UNP P10104
B	558	PRO	-	expression tag	UNP P10104
B	559	GLN	-	expression tag	UNP P10104
B	560	PHE	-	expression tag	UNP P10104
B	561	GLU	-	expression tag	UNP P10104
B	562	LYS	-	expression tag	UNP P10104
B	563	GLY	-	expression tag	UNP P10104
B	564	GLY	-	expression tag	UNP P10104
B	565	GLY	-	expression tag	UNP P10104
B	566	SER	-	expression tag	UNP P10104
B	567	GLY	-	expression tag	UNP P10104
B	568	GLY	-	expression tag	UNP P10104
B	569	GLY	-	expression tag	UNP P10104
B	570	SER	-	expression tag	UNP P10104
B	571	GLY	-	expression tag	UNP P10104
B	572	GLY	-	expression tag	UNP P10104
B	573	SER	-	expression tag	UNP P10104
B	574	ALA	-	expression tag	UNP P10104
B	575	TRP	-	expression tag	UNP P10104
B	576	SER	-	expression tag	UNP P10104
B	577	HIS	-	expression tag	UNP P10104
B	578	PRO	-	expression tag	UNP P10104
B	579	GLN	-	expression tag	UNP P10104
B	580	PHE	-	expression tag	UNP P10104
B	581	GLU	-	expression tag	UNP P10104
B	582	LYS	-	expression tag	UNP P10104
B	583	GLY	-	expression tag	UNP P10104
B	584	GLY	-	expression tag	UNP P10104
B	585	SER	-	expression tag	UNP P10104
C	102	ALA	PRO	conflict	UNP P03420
C	155	CYS	SER	conflict	UNP P03420
C	190	PHE	SER	conflict	UNP P03420
C	207	LEU	VAL	conflict	UNP P03420
C	290	CYS	SER	conflict	UNP P03420
C	379	VAL	ILE	conflict	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
C	447	VAL	MET	conflict	UNP P03420
C	514	GLY	-	linker	UNP P03420
C	515	SER	-	linker	UNP P03420
C	544	GLY	-	expression tag	UNP P10104
C	545	LEU	-	expression tag	UNP P10104
C	546	GLU	-	expression tag	UNP P10104
C	547	VAL	-	expression tag	UNP P10104
C	548	LEU	-	expression tag	UNP P10104
C	549	PHE	-	expression tag	UNP P10104
C	550	GLN	-	expression tag	UNP P10104
C	551	GLY	-	expression tag	UNP P10104
C	552	PRO	-	expression tag	UNP P10104
C	553	GLY	-	expression tag	UNP P10104
C	554	GLY	-	expression tag	UNP P10104
C	555	TRP	-	expression tag	UNP P10104
C	556	SER	-	expression tag	UNP P10104
C	557	HIS	-	expression tag	UNP P10104
C	558	PRO	-	expression tag	UNP P10104
C	559	GLN	-	expression tag	UNP P10104
C	560	PHE	-	expression tag	UNP P10104
C	561	GLU	-	expression tag	UNP P10104
C	562	LYS	-	expression tag	UNP P10104
C	563	GLY	-	expression tag	UNP P10104
C	564	GLY	-	expression tag	UNP P10104
C	565	GLY	-	expression tag	UNP P10104
C	566	SER	-	expression tag	UNP P10104
C	567	GLY	-	expression tag	UNP P10104
C	568	GLY	-	expression tag	UNP P10104
C	569	GLY	-	expression tag	UNP P10104
C	570	SER	-	expression tag	UNP P10104
C	571	GLY	-	expression tag	UNP P10104
C	572	GLY	-	expression tag	UNP P10104
C	573	SER	-	expression tag	UNP P10104
C	574	ALA	-	expression tag	UNP P10104
C	575	TRP	-	expression tag	UNP P10104
C	576	SER	-	expression tag	UNP P10104
C	577	HIS	-	expression tag	UNP P10104
C	578	PRO	-	expression tag	UNP P10104
C	579	GLN	-	expression tag	UNP P10104
C	580	PHE	-	expression tag	UNP P10104
C	581	GLU	-	expression tag	UNP P10104
C	582	LYS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	583	GLY	-	expression tag	UNP P10104
C	584	GLY	-	expression tag	UNP P10104
C	585	SER	-	expression tag	UNP P10104

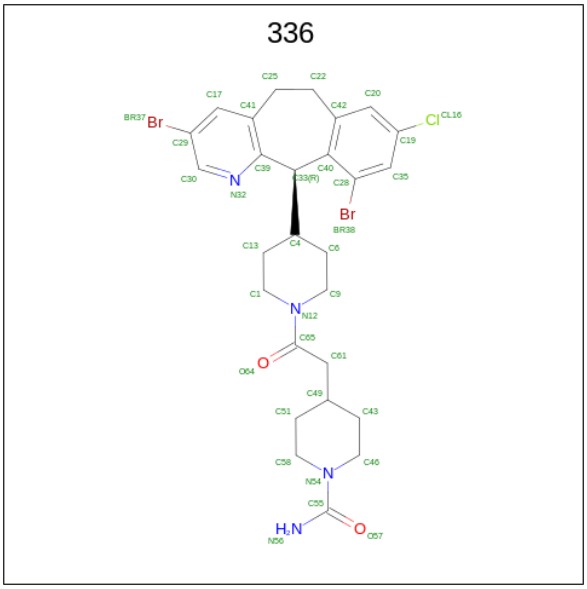
- Molecule 2 is a protein called D25 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	124	Total	C	N	O	S	0	0
			950	605	159	181	5		

- Molecule 3 is a protein called D25 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	106	Total	C	N	O	S	0	0
			803	505	130	165	3		

- Molecule 4 is 4-{2-[4-(3,10-DIBROMO-8-CHLORO-6,11-DIHYDRO-5H-BENZO[5,6]CYCLOHEPTA[1,2-B]PYRIDIN-11-YL)PIPERIDIN-1-YL]-2-OXOETHYL}PIPERIDINE-1-CARBOXAMIDE (three-letter code: 336) (formula: $C_{27}H_{31}Br_2ClN_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	Br	C	Cl	N	O	0
			36	2	27	1	4	2	
4	B	1	Total	Br	C	Cl	N	O	0
			36	2	27	1	4	2	

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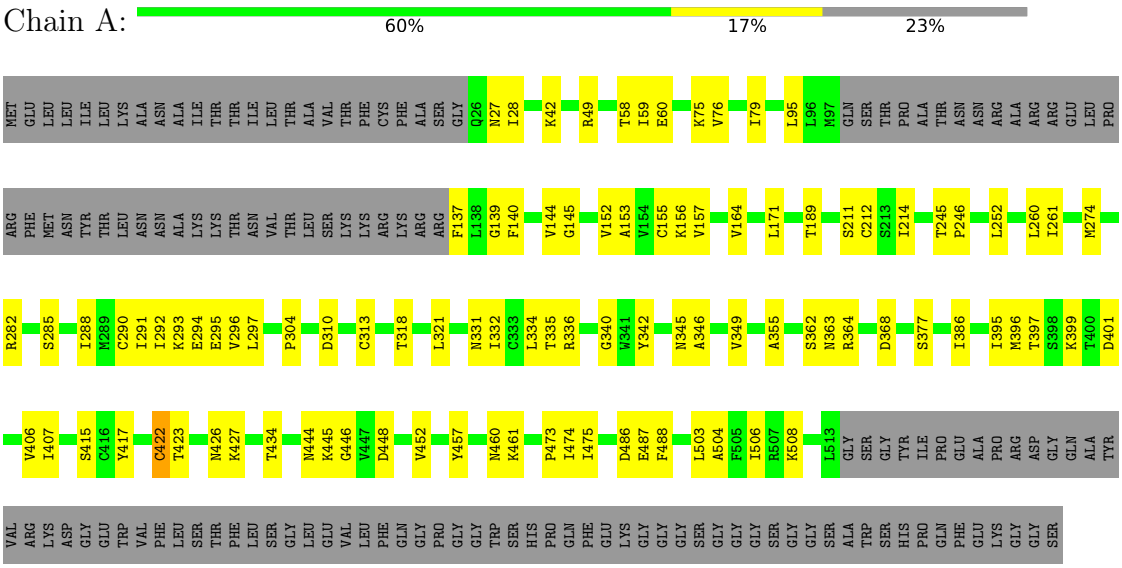
Mol	Chain	Residues	Atoms						AltConf
			Total	Br	C	Cl	N	O	
4	C	1	36	2	27	1	4	2	0

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. 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.

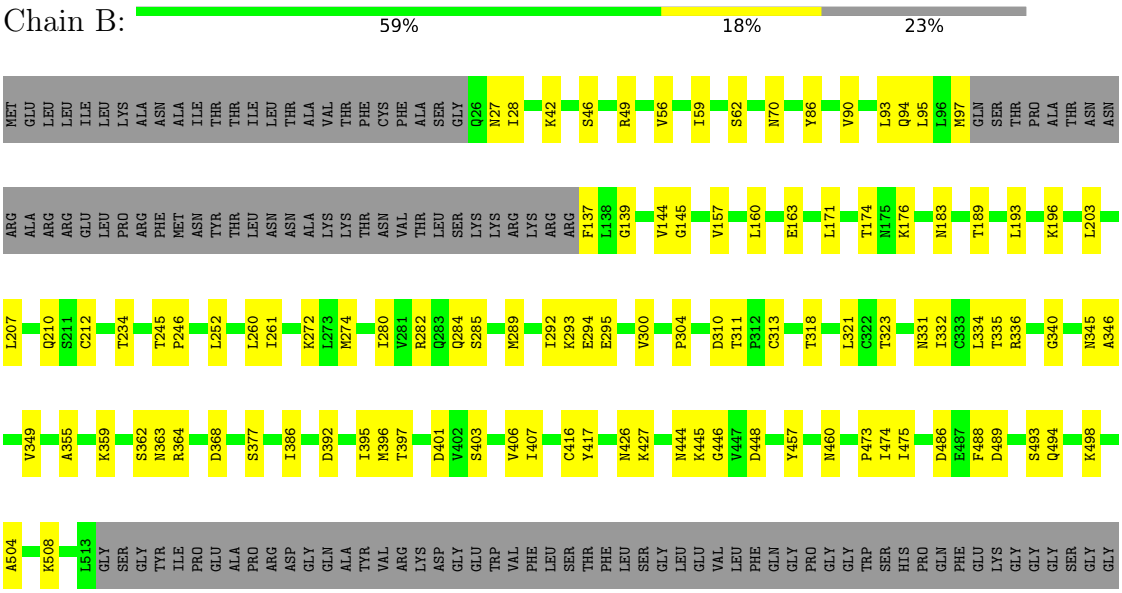
• Molecule 1: Fusion glycoprotein F0,Fibritin

Chain A:



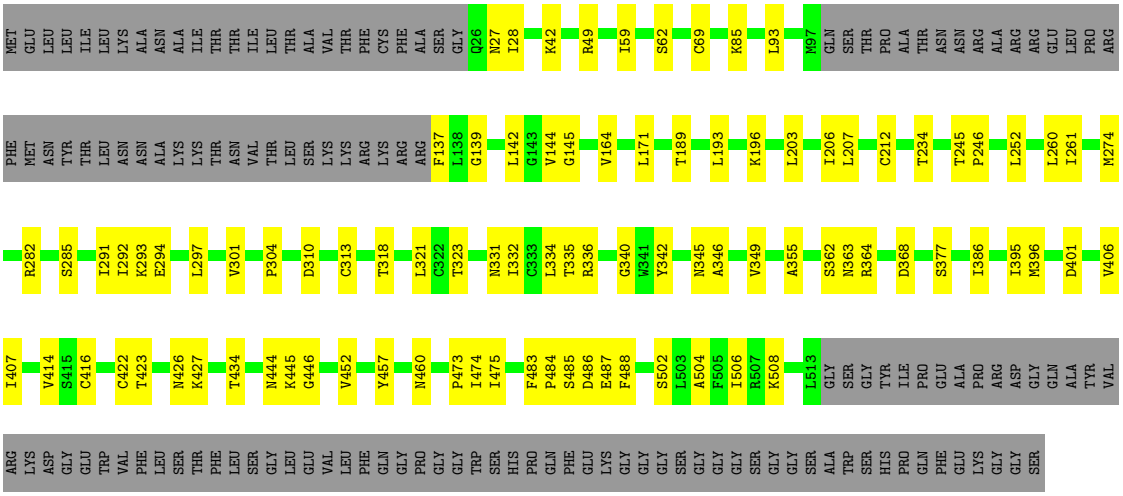
• Molecule 1: Fusion glycoprotein F0,Fibritin

Chain B:



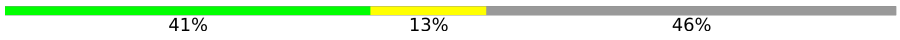
• Molecule 1: Fusion glycoprotein F0,Fibritin

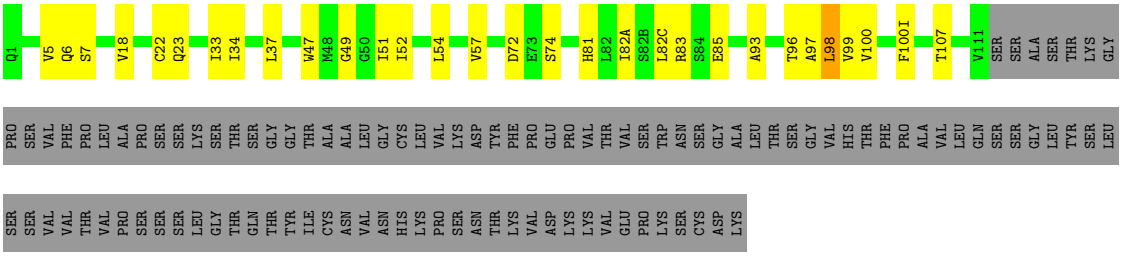
Chain C:



• Molecule 2: D25 heavy chain

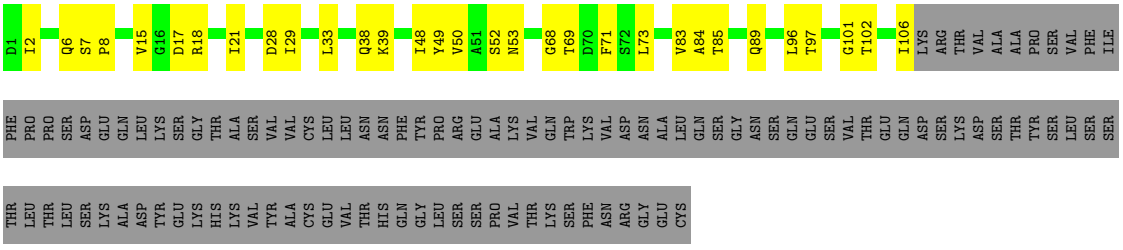
Chain D:





• Molecule 3: D25 light chain

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37059	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 336

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	0.40	0/3532	0.56	0/4784
1	B	0.39	0/3532	0.53	0/4784
1	C	0.40	0/3532	0.59	0/4784
2	D	0.33	0/974	0.48	0/1332
3	E	0.50	0/819	0.67	0/1116
All	All	0.40	0/12389	0.56	0/16800

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	3482	0	3526	77	0
1	B	3482	0	3526	85	0
1	C	3482	0	3526	82	0
2	D	950	0	933	30	0
3	E	803	0	783	25	0
4	A	36	0	31	13	0
4	B	36	0	31	11	0
4	C	36	0	31	13	0
All	All	12307	0	12387	296	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 12.

The worst 5 of 296 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:46:SER:HB3	1:B:313:CYS:SG	1.99	1.02
1:B:427:LYS:HG3	1:B:448:ASP:OD2	1.63	0.99
1:A:427:LYS:HG3	1:A:448:ASP:OD2	1.63	0.98
1:B:293:LYS:HG2	1:B:294:GLU:H	1.29	0.95
1:C:334:LEU:CD1	1:C:395:ILE:HD12	1.97	0.94

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 PDB entries followed by that with respect to all EM entries.

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	445/585 (76%)	422 (95%)	23 (5%)	0	100	100
1	B	445/585 (76%)	423 (95%)	22 (5%)	0	100	100
1	C	445/585 (76%)	422 (95%)	23 (5%)	0	100	100
2	D	122/231 (53%)	117 (96%)	5 (4%)	0	100	100
3	E	104/214 (49%)	91 (88%)	13 (12%)	0	100	100
All	All	1561/2200 (71%)	1475 (94%)	86 (6%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	410/517 (79%)	408 (100%)	2 (0%)	86 93
1	B	410/517 (79%)	410 (100%)	0	100 100
1	C	410/517 (79%)	408 (100%)	2 (0%)	86 93
2	D	103/196 (53%)	101 (98%)	2 (2%)	52 74
3	E	91/188 (48%)	91 (100%)	0	100 100
All	All	1424/1935 (74%)	1418 (100%)	6 (0%)	88 94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	486	ASP
2	D	98	LEU
2	D	100	VAL
1	A	487	GLU
1	A	422	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	GLN
3	E	24	GLN
1	C	183	ASN
3	E	53	ASN
2	D	6	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)

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	$\#\|Z\| > 2$
4	336	C	601	-	38,40,40	3.16	18 (47%)	48,58,58	3.26	19 (39%)
4	336	B	601	-	38,40,40	3.16	18 (47%)	48,58,58	3.26	19 (39%)
4	336	A	601	-	38,40,40	3.16	18 (47%)	48,58,58	3.26	19 (39%)

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	336	C	601	-	-	0/12/49/49	0/5/5/5
4	336	B	601	-	-	0/12/49/49	0/5/5/5
4	336	A	601	-	-	0/12/49/49	0/5/5/5

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	336	C55-N56	7.91	1.46	1.34
4	A	601	336	C55-N56	7.86	1.46	1.34
4	B	601	336	C55-N56	7.85	1.46	1.34
4	B	601	336	C65-N12	7.43	1.50	1.35
4	A	601	336	C65-N12	7.41	1.50	1.35

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	336	C6-C4-C33	-10.72	96.58	111.87
4	B	601	336	C6-C4-C33	-10.71	96.61	111.87
4	C	601	336	C6-C4-C33	-10.69	96.62	111.87
4	C	601	336	C58-N54-C46	-8.89	95.50	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	336	C58-N54-C46	-8.87	95.54	112.62

There are no chirality outliers.

There are no torsion outliers.

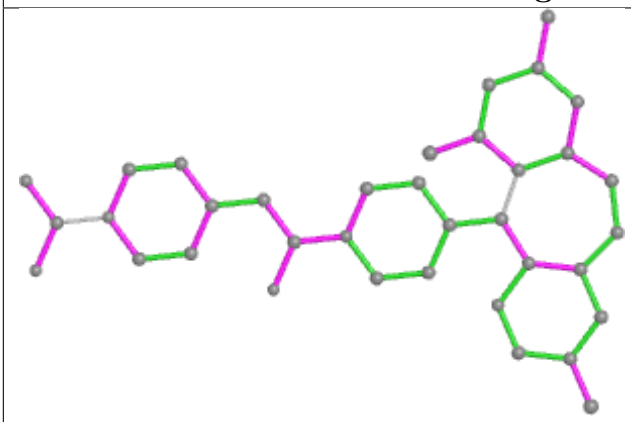
There are no ring outliers.

3 monomers are involved in 36 short contacts:

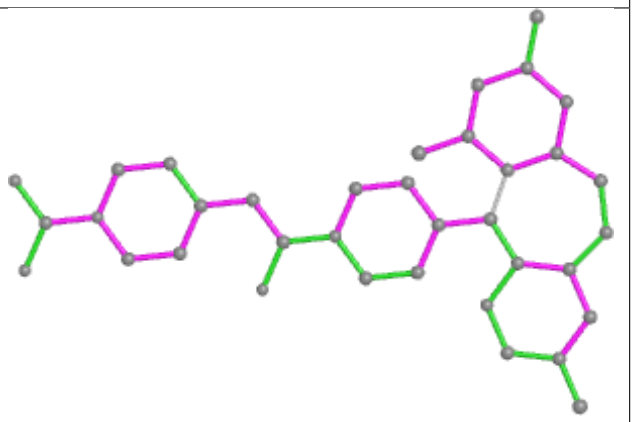
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	336	13	0
4	B	601	336	11	0
4	A	601	336	13	0

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.

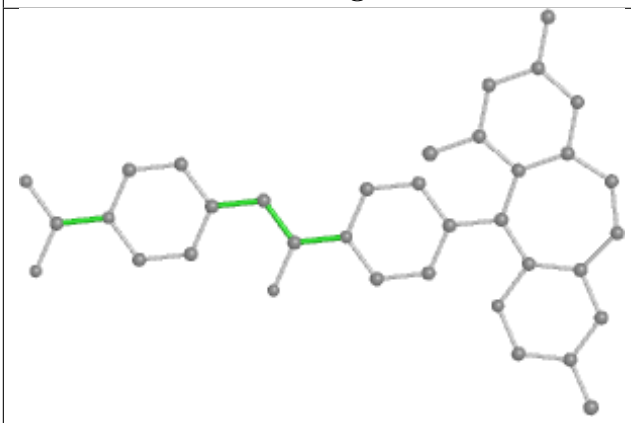
Ligand 336 C 601



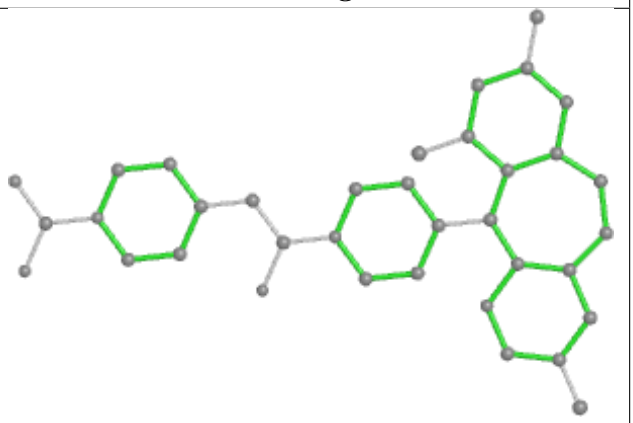
Bond lengths



Bond angles

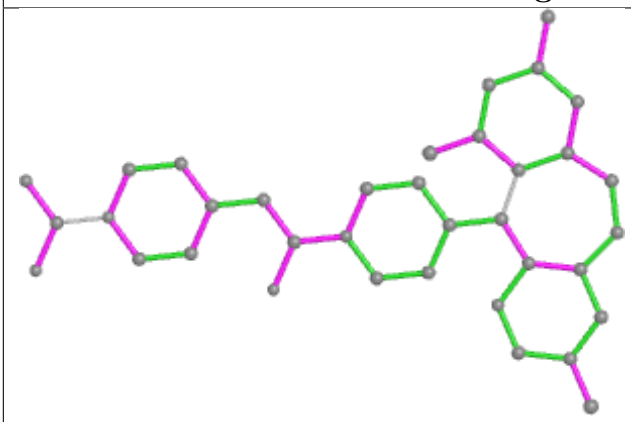


Torsions

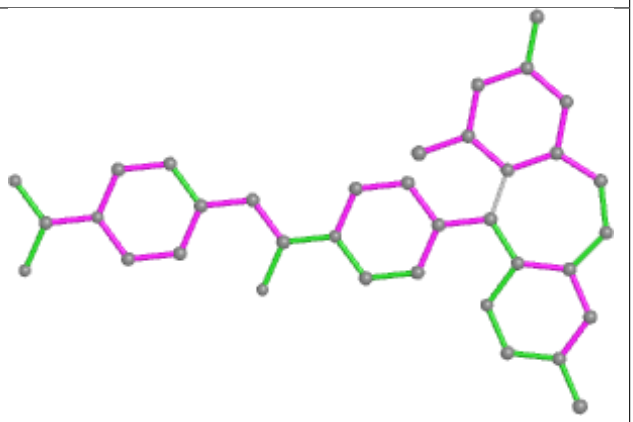


Rings

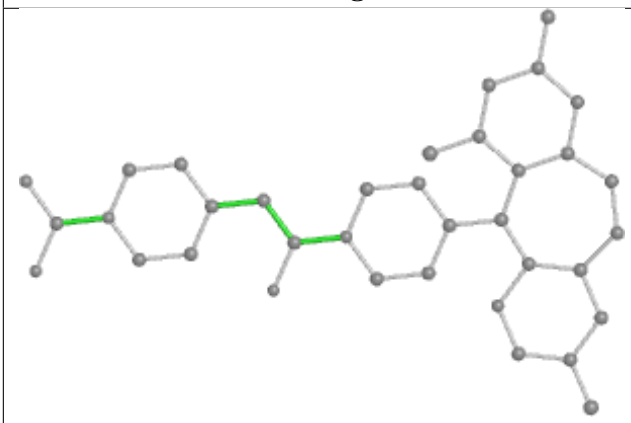
Ligand 336 B 601



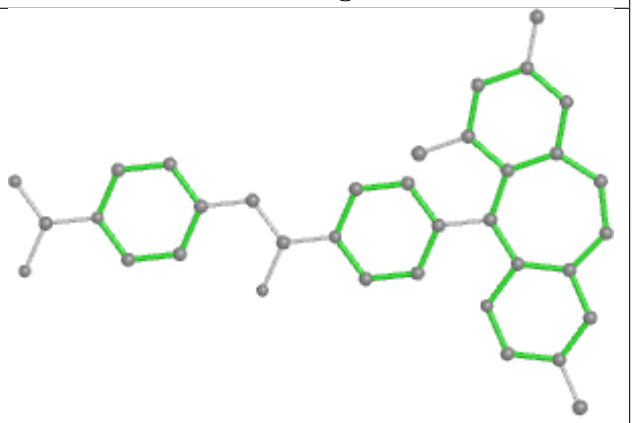
Bond lengths



Bond angles

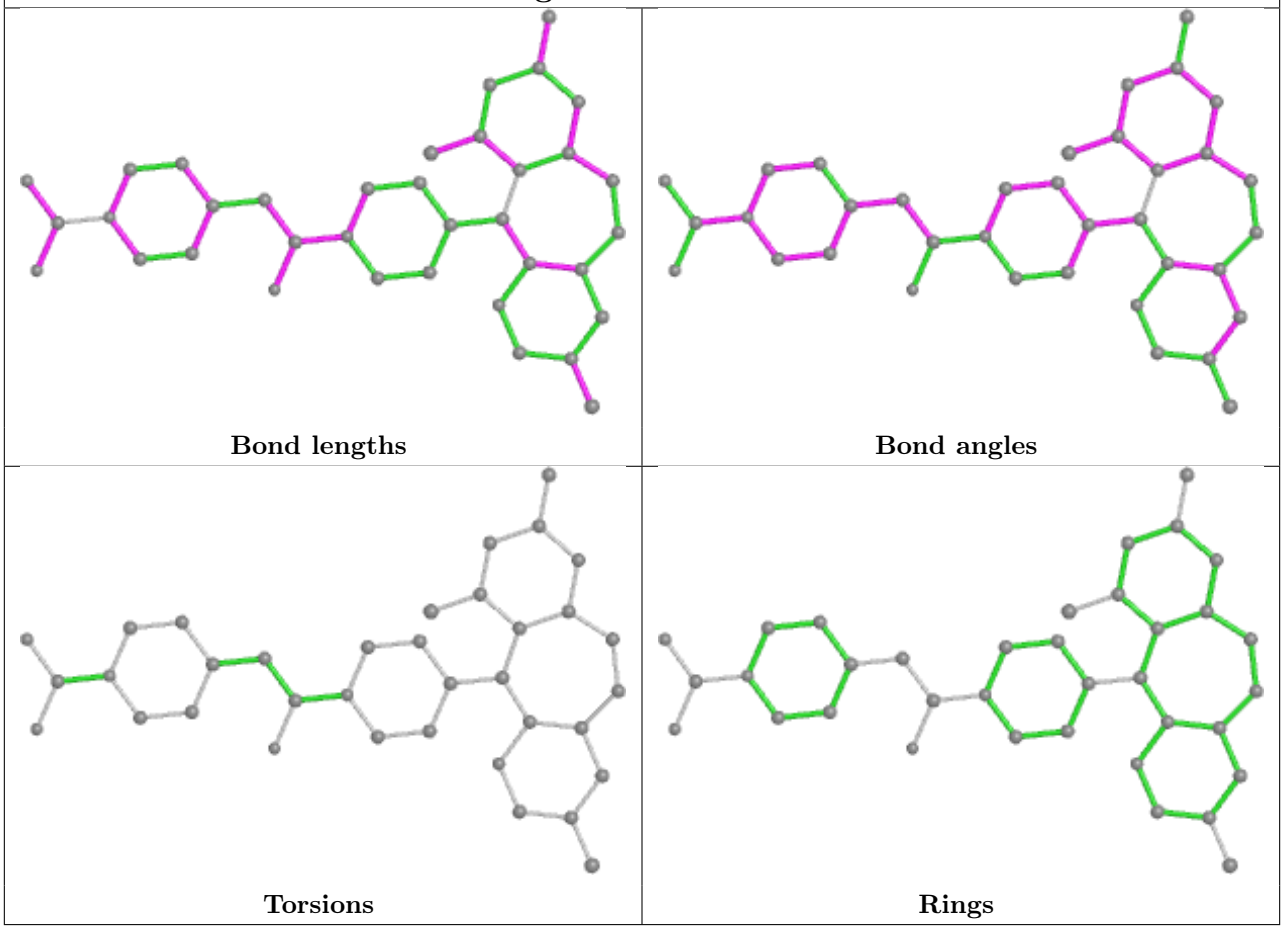


Torsions



Rings

Ligand 336 A 601



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.