



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2026 – 04:09 PM EDT

PDB ID : 12IT / pdb_000012it
Title : Thrombin inhibited with D-Phe-Pro-Gln-Chloromethylketone
Authors : Friet, T.; Mohammed, B.M.; Sukumar, N.; Di Cera, E.
Deposited on : 2026-04-07
Resolution : 1.68 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

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 Phenix2.2
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.2
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

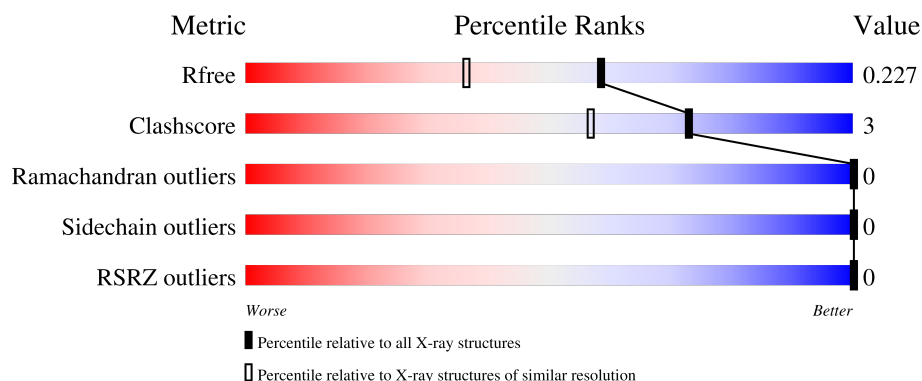
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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 $\leq 5\%$. 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	49	45% 10% 45%
1	C	49	53% . 43%
2	B	273	87% . 9%
2	D	273	81% 10% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4891 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	27	Total	C	N	O	S	0	0	0
			223	139	36	47	1			
1	C	28	Total	C	N	O	S	0	0	0
			231	145	37	48	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			2010	1281	356	359	14			
2	D	249	Total	C	N	O	S	0	0	0
			2018	1288	357	359	14			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	580	TYR	-	expression tag	UNP P00734
B	581	LEU	-	expression tag	UNP P00734
B	582	GLU	-	expression tag	UNP P00734
B	583	ASP	-	expression tag	UNP P00734
B	584	GLN	-	expression tag	UNP P00734
B	585	VAL	-	expression tag	UNP P00734
B	586	ASP	-	expression tag	UNP P00734
B	587	PRO	-	expression tag	UNP P00734
B	588	ARG	-	expression tag	UNP P00734
B	589	LEU	-	expression tag	UNP P00734
B	590	ILE	-	expression tag	UNP P00734
B	591	ASP	-	expression tag	UNP P00734
B	592	GLY	-	expression tag	UNP P00734
B	593	LYS	-	expression tag	UNP P00734
D	580	TYR	-	expression tag	UNP P00734
D	581	LEU	-	expression tag	UNP P00734

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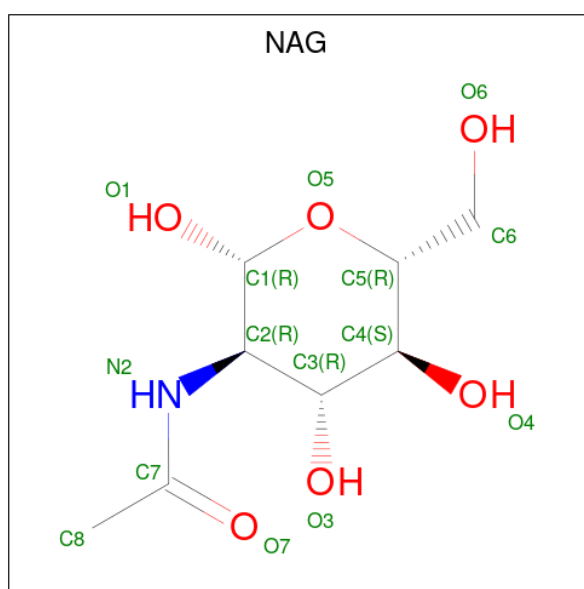
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Chain	Residue	Modelled	Actual	Comment	Reference
D	582	GLU	-	expression tag	UNP P00734
D	583	ASP	-	expression tag	UNP P00734
D	584	GLN	-	expression tag	UNP P00734
D	585	VAL	-	expression tag	UNP P00734
D	586	ASP	-	expression tag	UNP P00734
D	587	PRO	-	expression tag	UNP P00734
D	588	ARG	-	expression tag	UNP P00734
D	589	LEU	-	expression tag	UNP P00734
D	590	ILE	-	expression tag	UNP P00734
D	591	ASP	-	expression tag	UNP P00734
D	592	GLY	-	expression tag	UNP P00734
D	593	LYS	-	expression tag	UNP P00734

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

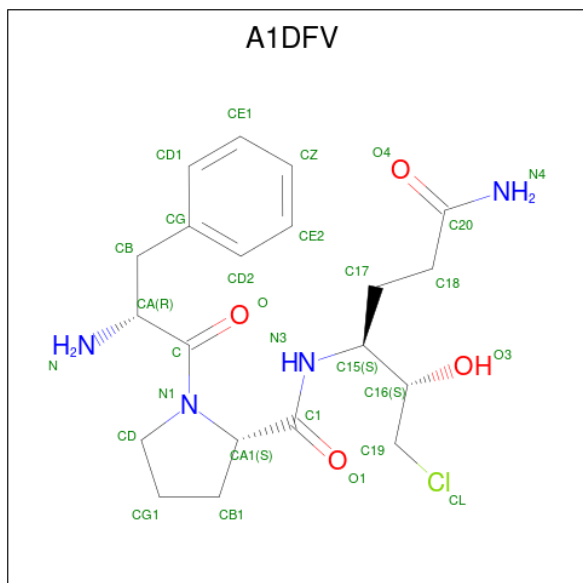
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is D-phenylalanyl-N-[(2S,3S)-6-amino-1-chloro-2-hydroxy-6-oxohexan-3-yl]-L-prolinamide (CCD ID: A1DFV) (formula: C₂₀H₂₉ClN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			28	20	4	4		
5	D	1	Total	C	N	O	0	0
			28	20	4	4		

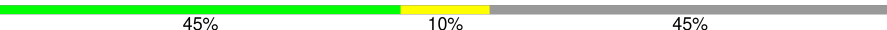
- Molecule 6 is water.

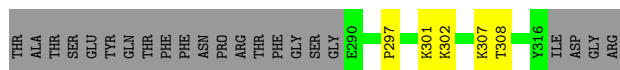
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	136	Total	O	0	0
			136	136		
6	C	22	Total	O	0	0
			22	22		
6	D	146	Total	O	0	0
			146	146		

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.

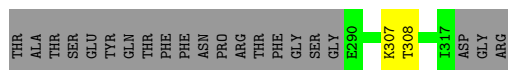
- Molecule 1: Thrombin light chain

Chain A: 



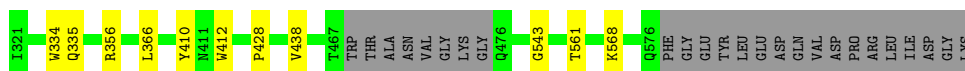
- Molecule 1: Thrombin light chain

Chain C: 



- Molecule 2: Thrombin heavy chain

Chain B: 



- Molecule 2: Thrombin heavy chain

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.23Å 86.17Å 73.69Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	34.76 – 1.68 34.76 – 1.68	Depositor EDS
% Data completeness (in resolution range)	92.6 (34.76-1.68) 92.6 (34.76-1.68)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.184 , 0.229 0.184 , 0.227	Depositor DCC
R_{free} test set	2787 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.169 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4891	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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, 0.333 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: A1DFV, NAG, NA

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	0.26	0/225	0.55	0/299
1	C	0.28	0/233	0.56	0/310
2	B	0.25	0/2061	0.48	0/2785
2	D	0.26	0/2070	0.49	0/2796
All	All	0.25	0/4589	0.50	0/6190

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	A	223	0	217	3	0
1	C	231	0	228	1	0
2	B	2010	0	1987	7	0
2	D	2018	0	1992	18	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	14	0	13	1	0
4	D	14	0	13	0	0
5	B	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	28	0	0	0	0
6	A	19	0	0	0	0
6	B	136	0	0	0	0
6	C	22	0	0	0	0
6	D	146	0	0	1	0
All	All	4891	0	4450	29	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.

All (29) 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)
2:D:494:LYS:HA	2:D:501:ILE:HD12	1.81	0.63
1:A:307:LYS:HG3	1:A:308:THR:HG23	1.89	0.55
2:D:397:LYS:HD3	2:D:429:VAL:HG23	1.88	0.55
2:D:410:TYR:CZ	2:D:412:TRP:HB3	2.43	0.53
2:B:543:GLY:HA2	2:B:561:THR:O	2.13	0.49
2:D:337:MET:HE3	2:D:346:LEU:HD22	1.93	0.49
2:B:410:TYR:CZ	2:B:412:TRP:HB3	2.47	0.49
1:C:307:LYS:HG3	1:C:308:THR:HG23	1.95	0.49
2:D:407:HIS:HE1	2:D:409:ARG:HE	1.62	0.48
2:D:570:ILE:O	2:D:574:ILE:HG12	2.13	0.48
2:D:337:MET:HE2	2:D:339:PHE:CE2	2.50	0.47
2:D:397:LYS:NZ	2:D:430:ALA:H	2.13	0.46
2:D:340:ARG:HD2	2:D:345:GLU:HG2	1.98	0.46
1:A:297:PRO:HA	1:A:301:LYS:HG3	1.98	0.46
2:D:464:LEU:O	2:D:465:LYS:HG3	2.17	0.44
2:D:543:GLY:HA2	2:D:561:THR:O	2.18	0.44
2:B:335:GLN:HE21	2:B:335:GLN:HB2	1.56	0.43
2:B:366:LEU:HD11	4:B:602:NAG:H82	2.00	0.43
2:D:341:LYS:HG2	2:D:380:LEU:HD23	1.99	0.43
2:D:397:LYS:HD2	6:D:791:HOH:O	2.17	0.43
2:D:397:LYS:HD3	2:D:429:VAL:CG2	2.50	0.42
2:D:388:ARG:HB2	2:D:461:TRP:CD1	2.56	0.41
2:B:334:TRP:CG	2:B:438:VAL:HB	2.55	0.41
2:D:397:LYS:HZ2	2:D:430:ALA:H	1.68	0.41
2:D:446:ALA:HA	2:D:542:MET:HE1	2.02	0.41
1:A:297:PRO:O	1:A:302:LYS:HG3	2.22	0.40
2:D:401:LEU:HD22	2:D:423:MET:HB3	2.03	0.40
2:B:356:ARG:HD3	2:B:428:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:568:LYS:HE2	2:B:568:LYS:HB3	1.93	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	A	25/49 (51%)	24 (96%)	1 (4%)	0	100	100
1	C	26/49 (53%)	25 (96%)	1 (4%)	0	100	100
2	B	244/273 (89%)	238 (98%)	6 (2%)	0	100	100
2	D	245/273 (90%)	237 (97%)	8 (3%)	0	100	100
All	All	540/644 (84%)	524 (97%)	16 (3%)	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 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	25/43 (58%)	25 (100%)	0	100	100
1	C	26/43 (60%)	26 (100%)	0	100	100
2	B	218/238 (92%)	218 (100%)	0	100	100
2	D	218/238 (92%)	218 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	487/562 (87%)	487 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	335	GLN
2	B	377	ASN
2	B	504	ASN
2	B	571	GLN
2	D	394	ASN
2	D	571	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	NAG	B	602	2	14,14,15	0.75	0	17,19,21	1.08	1 (5%)
5	A1DFV	B	603	2	28,29,30	0.18	0	36,39,40	0.59	0
4	NAG	D	602	2	14,14,15	0.78	0	17,19,21	1.03	2 (11%)
5	A1DFV	D	603	2	28,29,30	0.18	0	36,39,40	0.60	0

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	NAG	B	602	2	-	1/6/23/26	0/1/1/1
5	A1DFV	B	603	2	-	2/29/39/41	0/2/2/2
4	NAG	D	602	2	-	0/6/23/26	0/1/1/1
5	A1DFV	D	603	2	-	1/29/39/41	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	NAG	C1-O5-C5	2.25	115.20	112.19
4	B	602	NAG	C1-O5-C5	2.19	115.12	112.19
4	D	602	NAG	C3-C4-C5	-2.03	106.55	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	603	A1DFV	C17-C18-C20-O4
5	B	603	A1DFV	C17-C18-C20-N4
4	B	602	NAG	O5-C5-C6-O6
5	D	603	A1DFV	C17-C18-C20-N4

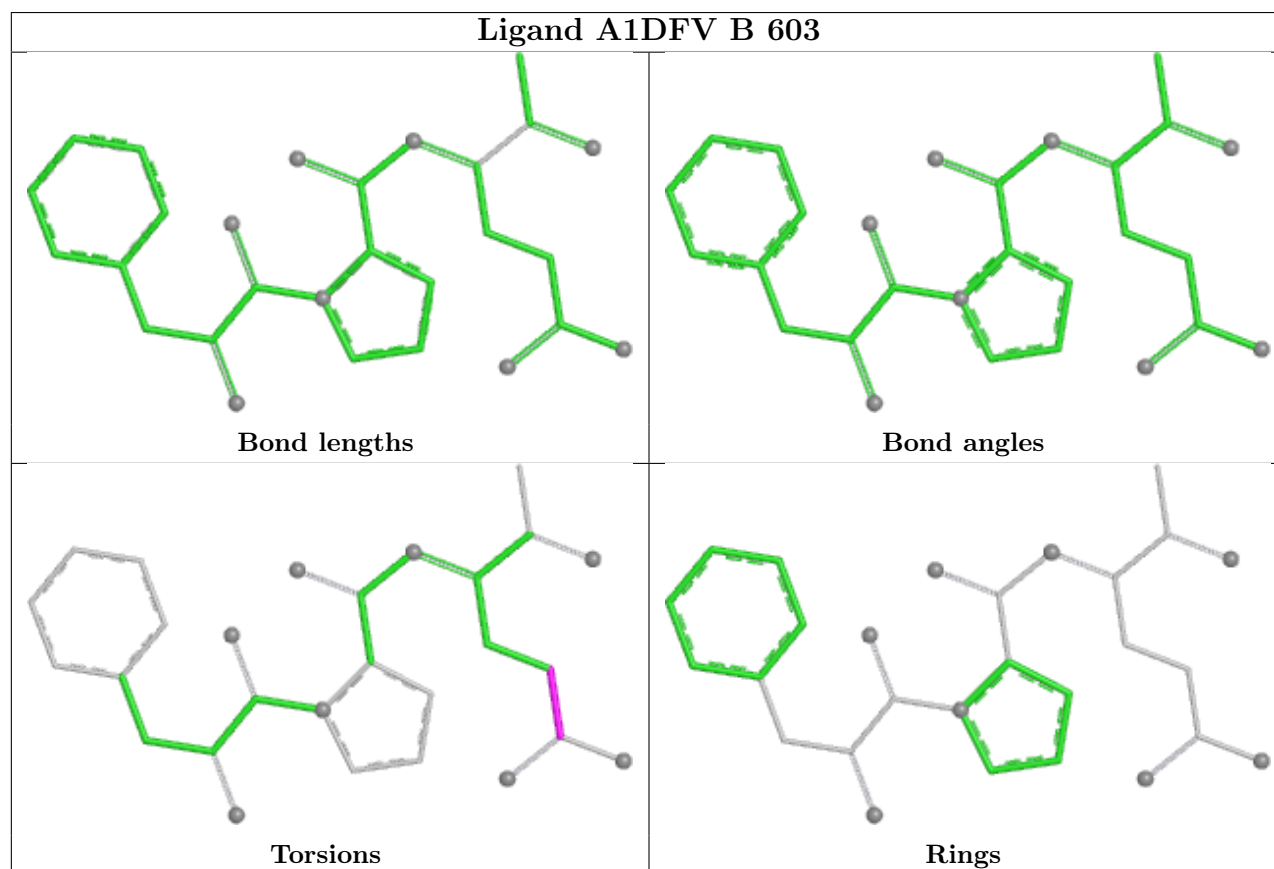
There are no ring outliers.

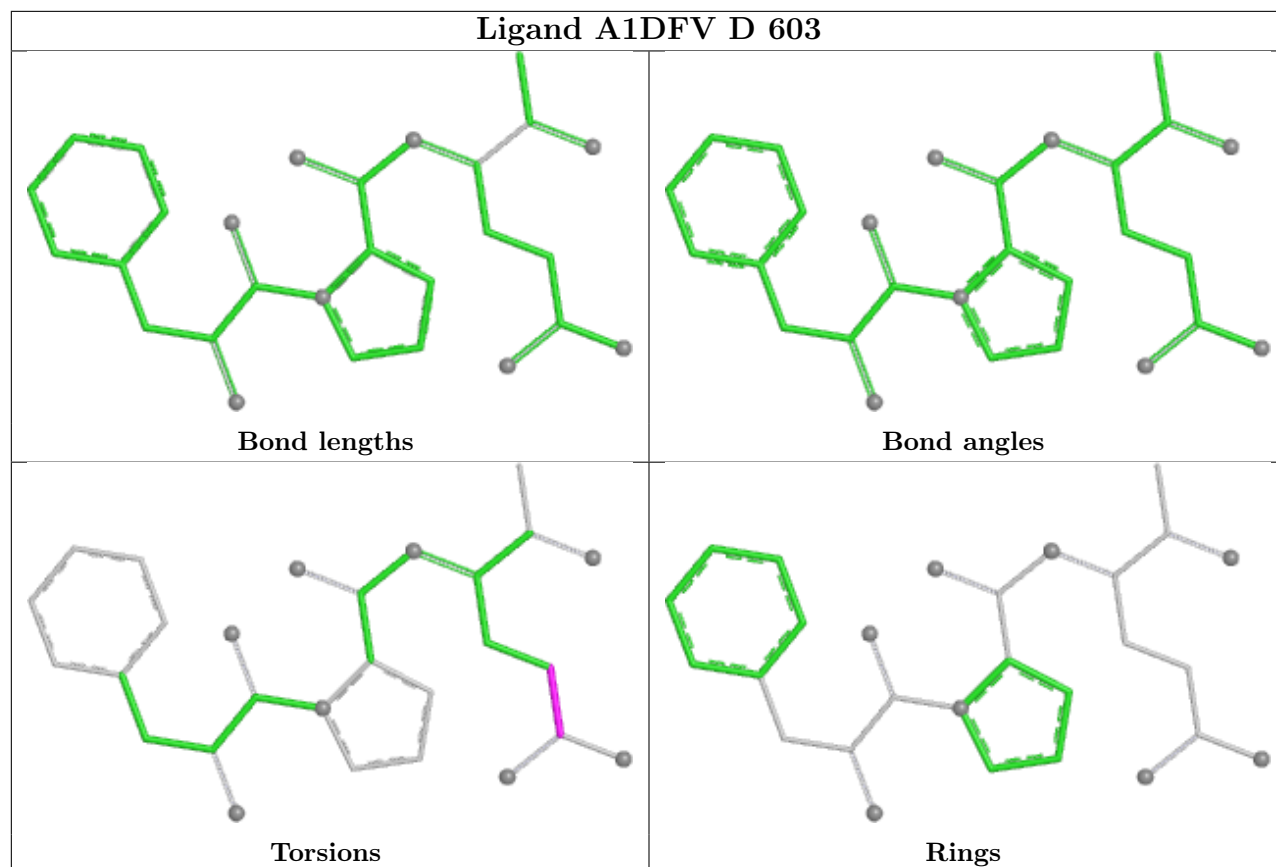
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	NAG	1	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 [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	A	27/49 (55%)	-1.41	0 100 100	11, 15, 23, 35	0
1	C	28/49 (57%)	-1.42	0 100 100	11, 16, 21, 31	0
2	B	248/273 (90%)	-1.36	0 100 100	10, 17, 31, 42	0
2	D	249/273 (91%)	-1.36	0 100 100	10, 16, 31, 43	0
All	All	552/644 (85%)	-1.36	0 100 100	10, 17, 31, 43	0

There are no RSRZ outliers to report.

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, 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	B-factors(Å ²)	Q<0.9
4	NAG	B	602	14/15	0.96	0.05	28,36,47,52	0
4	NAG	D	602	14/15	0.97	0.06	29,40,49,50	0
5	A1DFV	B	603	28/29	0.99	0.03	12,16,22,24	0
5	A1DFV	D	603	28/29	0.99	0.03	13,16,22,23	0

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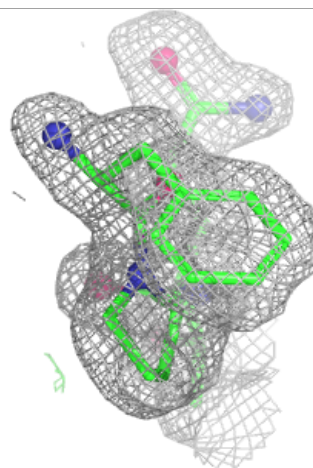
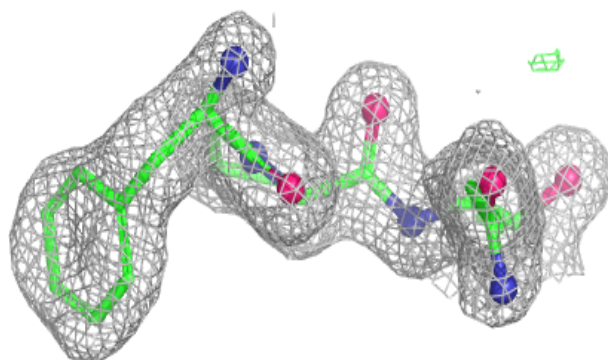
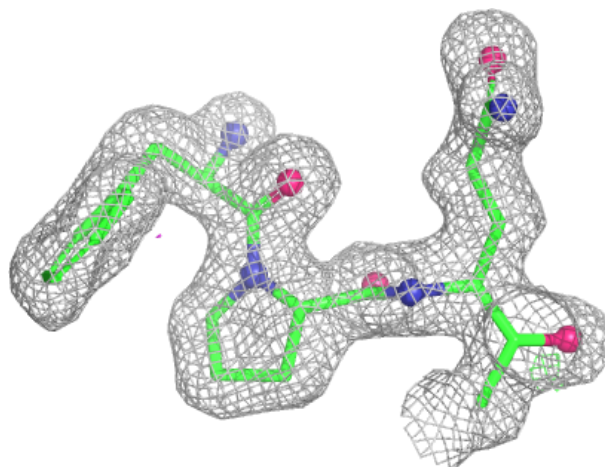
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	601	1/1	1.00	0.04	16,16,16,16	0
3	NA	D	601	1/1	1.00	0.02	15,15,15,15	0

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.

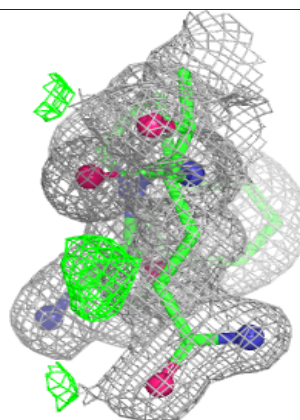
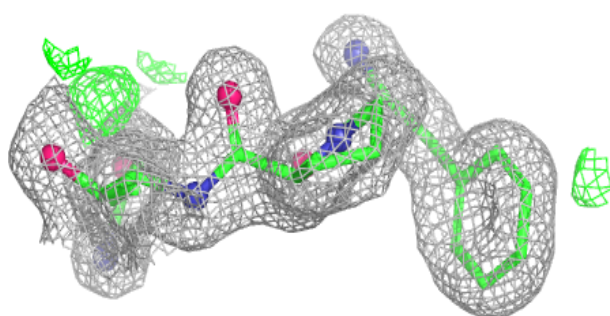
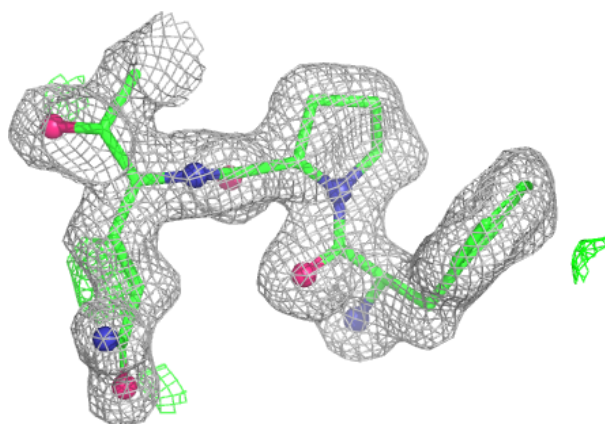
Electron density around A1DFV B 603:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1DFV D 603:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.