



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:18 AM UTC

PDB ID : 5NSQ / pdb_00005nsq
Title : Structure of Leucyl aminopeptidase from Trypanosoma brucei in complex with Actinonin
Authors : Timm, J.; Wilson, K.
Deposited on : 2017-04-26
Resolution : 3.00 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

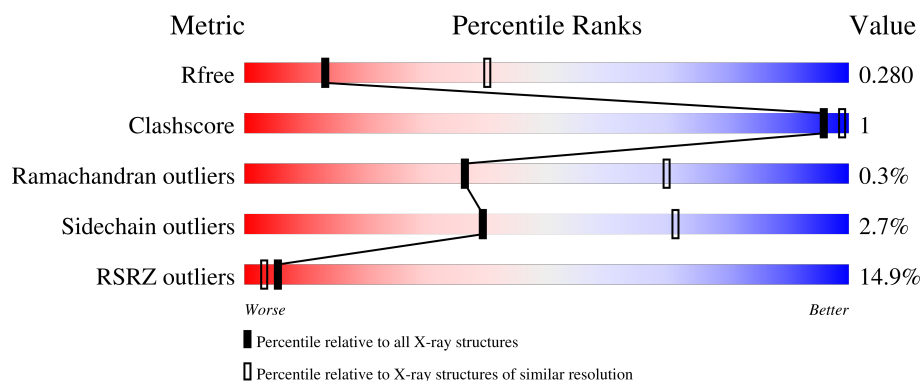
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	521	3% 95% 5%
1	B	521	3% 95% 5%
1	C	521	3% 94% 5%
1	D	521	38% 94% 5%
1	E	521	4% 94% 5%

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Mol	Chain	Length	Quality of chain
1	F	521	37% 94% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22720 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 Aminopeptidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	2	0
			3775	2391	637	725	22			
1	B	519	Total	C	N	O	S	0	2	0
			3789	2398	639	730	22			
1	C	518	Total	C	N	O	S	0	1	0
			3795	2402	643	728	22			
1	D	519	Total	C	N	O	S	0	0	0
			3738	2369	631	717	21			
1	E	519	Total	C	N	O	S	0	1	0
			3769	2389	635	723	22			
1	F	515	Total	C	N	O	S	0	0	0
			3646	2308	619	697	22			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	THR	conflict	UNP Q385B0
A	125	UNK	ALA	conflict	UNP Q385B0
A	139	THR	ALA	conflict	UNP Q385B0
B	32	ALA	THR	conflict	UNP Q385B0
B	125	UNK	ALA	conflict	UNP Q385B0
B	139	THR	ALA	conflict	UNP Q385B0
C	32	ALA	THR	conflict	UNP Q385B0
C	125	UNK	ALA	conflict	UNP Q385B0
C	139	THR	ALA	conflict	UNP Q385B0
D	32	ALA	THR	conflict	UNP Q385B0
D	125	UNK	ALA	conflict	UNP Q385B0
D	139	THR	ALA	conflict	UNP Q385B0
E	32	ALA	THR	conflict	UNP Q385B0
E	125	UNK	ALA	conflict	UNP Q385B0
E	139	THR	ALA	conflict	UNP Q385B0
F	32	ALA	THR	conflict	UNP Q385B0
F	125	UNK	ALA	conflict	UNP Q385B0

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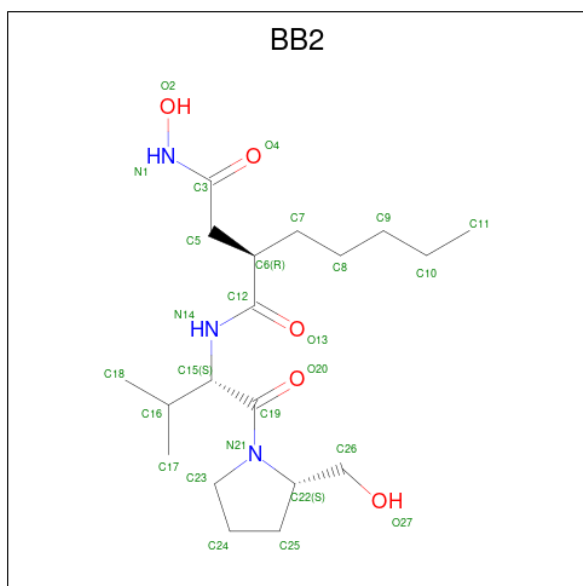
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Chain	Residue	Modelled	Actual	Comment	Reference
F	139	THR	ALA	conflict	UNP Q385B0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is ACTINONIN (CCD ID: BB2) (formula: C₁₉H₃₅N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	19	3	5		
3	B	1	Total	C	N	O	0	0
			27	19	3	5		
3	C	1	Total	C	N	O	0	0
			27	19	3	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			27	19	3	5		
3	E	1	Total	C	N	O	0	0
			27	19	3	5		
3	F	1	Total	C	N	O	0	0
			27	19	3	5		

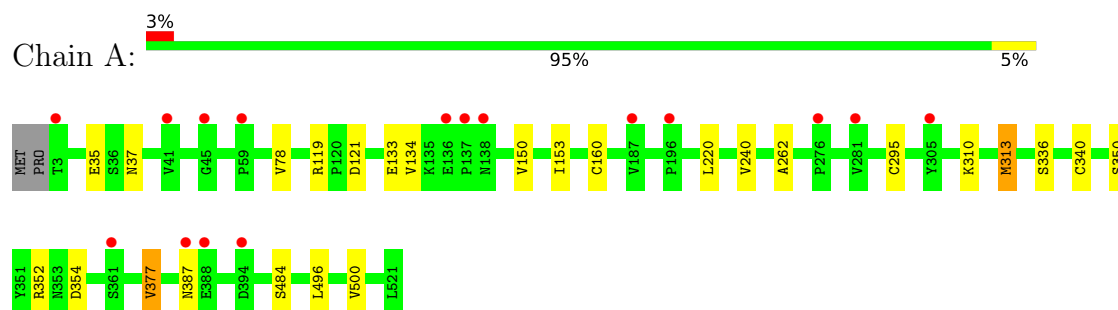
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	6	Total	O	0	0
			6	6		
4	C	8	Total	O	0	0
			8	8		
4	D	1	Total	O	0	0
			1	1		
4	E	9	Total	O	0	0
			9	9		
4	F	2	Total	O	0	0
			2	2		

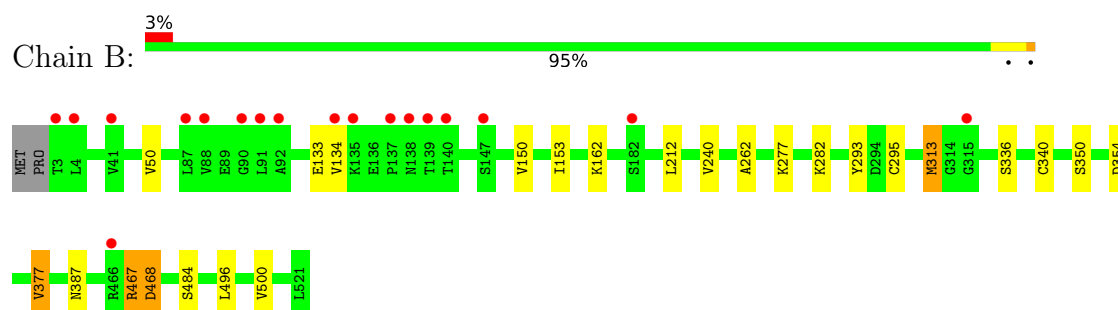
3 Residue-property plots [i](#)

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.

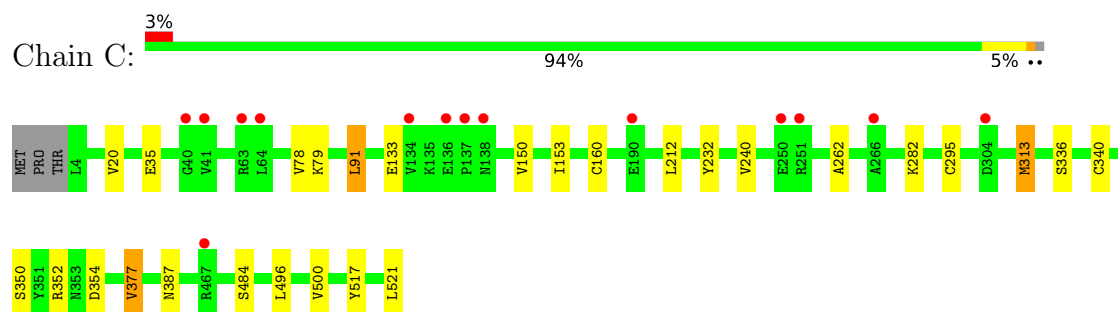
- Molecule 1: Aminopeptidase, putative



- Molecule 1: Aminopeptidase, putative

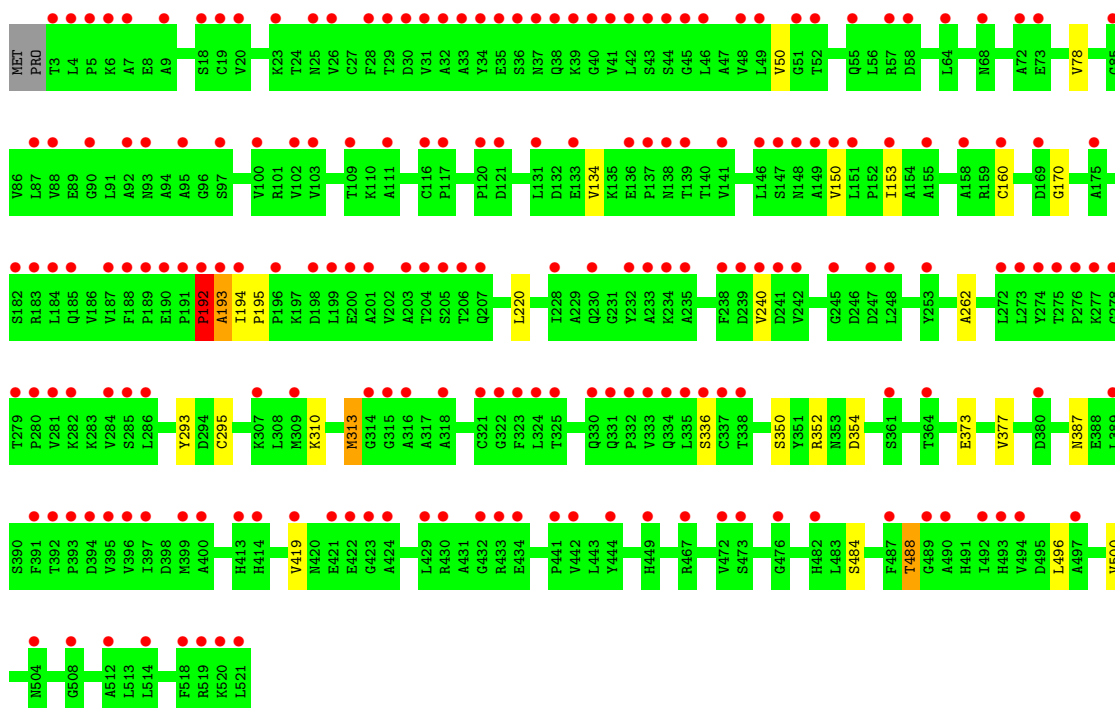


- Molecule 1: Aminopeptidase, putative

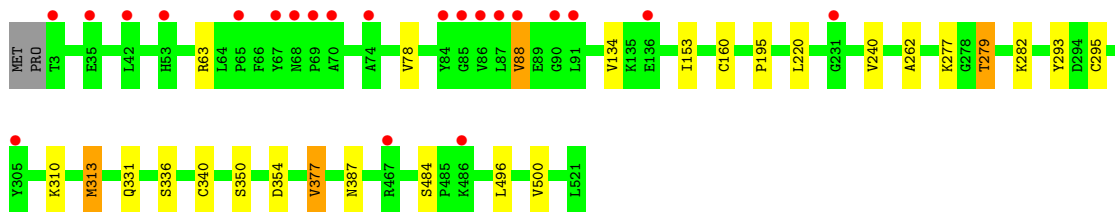


- Molecule 1: Aminopeptidase, putative

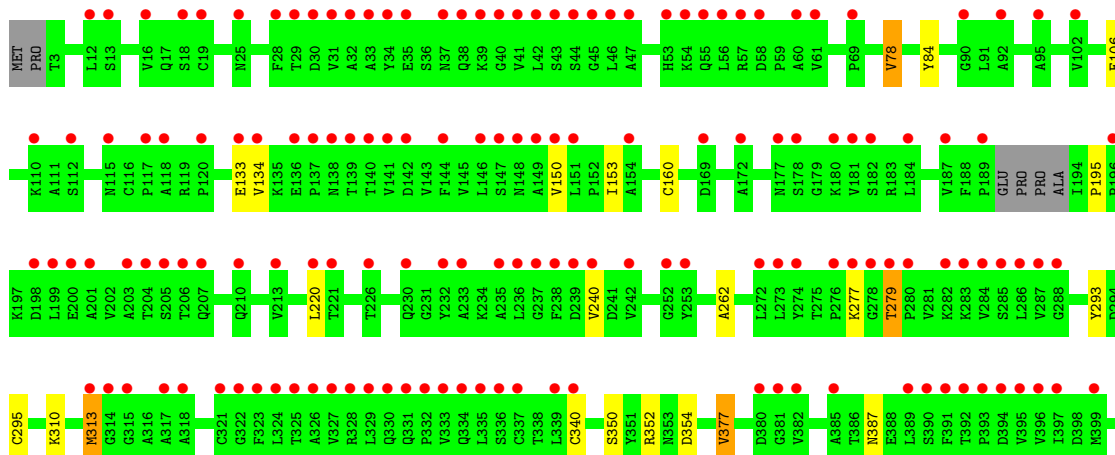


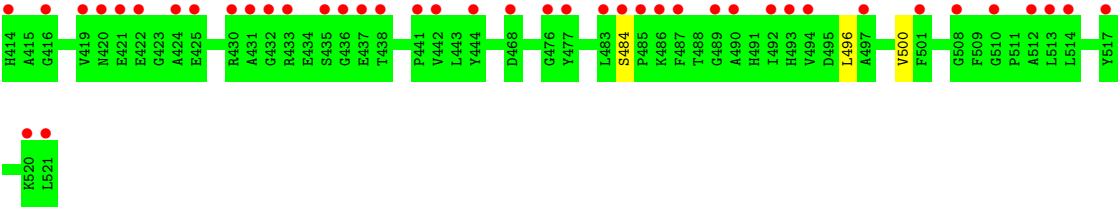


- Molecule 1: Aminopeptidase, putative



- Molecule 1: Aminopeptidase, putative





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.91Å 165.73Å 121.98Å 90.00° 112.45° 90.00°	Depositor
Resolution (Å)	41.50 – 3.00 41.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.50-3.00) 87.0 (41.50-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.265 , 0.296 (Not available) , 0.280	Depositor DCC
R_{free} test set	3327 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	22720	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: MN, BB2

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	0.78	0/3847	0.99	2/5254 (0.0%)
1	B	0.79	1/3864 (0.0%)	0.99	5/5279 (0.1%)
1	C	0.77	0/3870	0.98	3/5282 (0.1%)
1	D	0.76	2/3809 (0.1%)	0.98	7/5208 (0.1%)
1	E	0.79	1/3844 (0.0%)	1.00	6/5255 (0.1%)
1	F	0.77	1/3713 (0.0%)	0.98	5/5082 (0.1%)
All	All	0.78	5/22947 (0.0%)	0.99	28/31360 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	467	ARG	CA-C	8.87	1.64	1.52
1	D	193	ALA	N-CA	6.08	1.54	1.46
1	E	279	THR	CA-C	5.61	1.58	1.52
1	D	195	PRO	CA-C	5.31	1.54	1.51
1	F	279	THR	CA-C	5.07	1.58	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	ALA	N-CA-CB	7.76	123.60	110.49
1	B	467	ARG	N-CA-C	-7.22	98.84	110.32
1	D	488	THR	CB-CA-C	-6.78	98.00	109.38
1	E	88	VAL	CB-CA-C	6.68	120.08	110.33
1	A	150	VAL	N-CA-C	6.09	116.83	110.62
1	D	195	PRO	N-CA-C	5.96	116.19	110.47
1	D	150	VAL	N-CA-C	5.75	116.48	110.62
1	B	313	MET	CG-SD-CE	-5.70	88.36	100.90
1	E	277	LYS	N-CA-C	5.64	118.16	111.33
1	C	313	MET	CG-SD-CE	-5.56	88.67	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	277	LYS	N-CA-C	5.55	118.05	111.33
1	E	331	GLN	N-CA-C	-5.54	102.80	109.83
1	B	277	LYS	N-CA-C	5.53	118.03	111.33
1	B	50	VAL	N-CA-C	5.41	115.77	107.77
1	F	313	MET	CG-SD-CE	5.39	112.77	100.90
1	D	192	PRO	N-CA-C	5.38	123.56	112.47
1	F	195	PRO	N-CA-C	5.37	115.62	110.47
1	E	313	MET	CG-SD-CE	5.33	112.62	100.90
1	D	313	MET	CG-SD-CE	5.33	112.62	100.90
1	F	150	VAL	N-CA-C	5.28	116.01	110.62
1	A	313	MET	CG-SD-CE	5.27	112.50	100.90
1	C	91	LEU	CA-CB-CG	5.27	134.74	116.30
1	E	195	PRO	N-CA-C	5.27	115.53	110.47
1	F	279	THR	CB-CA-C	5.22	117.86	109.51
1	E	63	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	C	150	VAL	N-CA-C	5.09	115.81	110.62
1	B	150	VAL	N-CA-C	5.08	115.81	110.62
1	D	50	VAL	N-CA-C	5.05	115.25	107.77

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	3775	0	3629	9	0
1	B	3789	0	3658	7	0
1	C	3795	0	3690	8	0
1	D	3738	0	3594	10	0
1	E	3769	0	3641	7	0
1	F	3646	0	3418	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
3	A	27	0	34	0	0
3	B	27	0	34	1	0
3	C	27	0	34	0	0
3	D	27	0	34	0	0
3	E	27	0	34	0	0
3	F	27	0	34	0	0
4	A	8	0	0	1	0
4	B	6	0	0	0	0
4	C	8	0	0	0	0
4	D	1	0	0	0	0
4	E	9	0	0	0	0
4	F	2	0	0	0	0
All	All	22720	0	21834	50	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 1.

All (50) 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:F:78:VAL:HG23	1:F:84:TYR:HB2	1.50	0.92
1:F:78:VAL:CG2	1:F:84:TYR:HB2	2.14	0.76
1:F:78:VAL:HG23	1:F:84:TYR:CB	2.16	0.75
1:F:340:CYS:HB3	1:F:377:VAL:HG13	1.77	0.67
1:C:340:CYS:HB3	1:C:377:VAL:HG13	1.78	0.65
1:A:340:CYS:HB3	1:A:377:VAL:HG13	1.78	0.65
1:B:340:CYS:HB3	1:B:377:VAL:HG13	1.79	0.65
1:E:340:CYS:HB3	1:E:377:VAL:HG13	1.79	0.64
1:B:467:ARG:O	1:B:468:ASP:HB2	2.00	0.61
1:A:119:ARG:NH1	1:A:121:ASP:OD2	2.37	0.58
1:F:310:LYS:O	1:F:313:MET:HE3	2.05	0.57
1:D:310:LYS:O	1:D:313:MET:HE3	2.04	0.57
1:B:212:LEU:HB3	1:B:313:MET:HE1	1.86	0.57
1:E:310:LYS:O	1:E:313:MET:HE3	2.05	0.56
1:A:310:LYS:O	1:A:313:MET:HE3	2.04	0.56
1:C:212:LEU:HB3	1:C:313:MET:HE1	1.88	0.55
1:D:496:LEU:HD13	1:D:500:VAL:CG1	2.40	0.51
1:F:496:LEU:HD13	1:F:500:VAL:CG1	2.41	0.51
1:A:496:LEU:HD13	1:A:500:VAL:CG1	2.41	0.51
1:C:262:ALA:HB2	1:C:350:SER:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ALA:HB2	1:E:350:SER:HA	1.91	0.50
1:E:496:LEU:HD13	1:E:500:VAL:CG1	2.40	0.50
1:A:262:ALA:HB2	1:A:350:SER:HA	1.94	0.49
1:A:352:ARG:HD3	1:D:293:TYR:CD2	2.47	0.49
1:F:262:ALA:HB2	1:F:350:SER:HA	1.93	0.49
1:B:262:ALA:HB2	1:B:350:SER:HA	1.93	0.49
1:B:496:LEU:HD13	1:B:500:VAL:CG1	2.42	0.49
1:D:192:PRO:HB2	1:D:194:ILE:O	2.13	0.49
1:D:262:ALA:HB2	1:D:350:SER:HA	1.94	0.48
1:C:496:LEU:HD13	1:C:500:VAL:CG1	2.43	0.48
4:A:707:HOH:O	1:D:170:GLY:HA2	2.15	0.47
1:B:293:TYR:CD2	1:D:352:ARG:HD3	2.51	0.46
1:C:352:ARG:HD3	1:F:293:TYR:CD2	2.52	0.44
1:C:387:ASN:HB2	1:C:484:SER:HB2	1.99	0.44
1:A:37:ASN:C	1:A:37:ASN:OD1	2.60	0.44
1:F:387:ASN:HB2	1:F:484:SER:HB2	1.98	0.44
1:E:293:TYR:CD2	1:F:352:ARG:HD3	2.52	0.44
1:A:387:ASN:HB2	1:A:484:SER:HB2	2.00	0.43
1:B:387:ASN:HB2	1:B:484:SER:HB2	2.00	0.43
1:D:373:GLU:O	1:D:377:VAL:HG13	2.18	0.43
1:F:220:LEU:HD23	1:F:313:MET:CE	2.49	0.43
1:D:387:ASN:HB2	1:D:484:SER:HB2	1.99	0.42
3:B:603:BB2:O13	3:B:603:BB2:H16	2.20	0.42
1:D:220:LEU:HD23	1:D:313:MET:CE	2.49	0.42
1:E:387:ASN:HB2	1:E:484:SER:HB2	2.01	0.41
1:C:20:VAL:HA	1:C:232:TYR:CE2	2.55	0.41
1:E:220:LEU:HD23	1:E:313:MET:CE	2.50	0.41
1:F:78:VAL:CG1	1:F:106:GLU:HB2	2.50	0.41
1:A:220:LEU:HD23	1:A:313:MET:CE	2.51	0.41
1:C:517:TYR:CZ	1:C:521:LEU:HD21	2.56	0.41

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	517/521 (99%)	500 (97%)	16 (3%)	1 (0%)	43	76
1	B	518/521 (99%)	503 (97%)	13 (2%)	2 (0%)	30	65
1	C	516/521 (99%)	502 (97%)	13 (2%)	1 (0%)	43	76
1	D	516/521 (99%)	499 (97%)	14 (3%)	3 (1%)	21	56
1	E	517/521 (99%)	502 (97%)	14 (3%)	1 (0%)	43	76
1	F	510/521 (98%)	495 (97%)	14 (3%)	1 (0%)	43	76
All	All	3094/3126 (99%)	3001 (97%)	84 (3%)	9 (0%)	36	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP
1	B	354	ASP
1	B	468	ASP
1	C	354	ASP
1	D	192	PRO
1	D	193	ALA
1	D	354	ASP
1	E	354	ASP
1	F	354	ASP

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	380/411 (92%)	370 (97%)	10 (3%)	40	72
1	B	386/411 (94%)	377 (98%)	9 (2%)	44	74
1	C	389/411 (95%)	377 (97%)	12 (3%)	35	68
1	D	375/411 (91%)	366 (98%)	9 (2%)	43	73
1	E	383/411 (93%)	372 (97%)	11 (3%)	37	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	349/411 (85%)	340 (97%)	9 (3%)	40 72
All	All	2262/2466 (92%)	2202 (97%)	60 (3%)	39 71

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	78	VAL
1	A	133	GLU
1	A	134	VAL
1	A	153	ILE
1	A	160	CYS
1	A	240	VAL
1	A	295	CYS
1	A	336	SER
1	A	377	VAL
1	B	133	GLU
1	B	134	VAL
1	B	153	ILE
1	B	162	LYS
1	B	240	VAL
1	B	282	LYS
1	B	295	CYS
1	B	336	SER
1	B	377	VAL
1	C	35	GLU
1	C	78	VAL
1	C	79	LYS
1	C	91	LEU
1	C	133	GLU
1	C	153	ILE
1	C	160	CYS
1	C	240	VAL
1	C	282	LYS
1	C	295	CYS
1	C	336	SER
1	C	377	VAL
1	D	78	VAL
1	D	134	VAL
1	D	153	ILE
1	D	160	CYS
1	D	240	VAL

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Mol	Chain	Res	Type
1	D	295	CYS
1	D	336	SER
1	D	419	VAL
1	D	488	THR
1	E	78	VAL
1	E	88	VAL
1	E	134	VAL
1	E	153	ILE
1	E	160	CYS
1	E	240	VAL
1	E	279	THR
1	E	282	LYS
1	E	295	CYS
1	E	336	SER
1	E	377	VAL
1	F	78	VAL
1	F	133	GLU
1	F	134	VAL
1	F	153	ILE
1	F	160	CYS
1	F	240	VAL
1	F	279	THR
1	F	295	CYS
1	F	377	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	114	ASN
1	E	114	ASN
1	E	413	HIS
1	F	210	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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$
3	BB2	F	603	2	27,27,27	0.43	0	34,35,35	2.39	6 (17%)
3	BB2	B	603	2	27,27,27	0.64	0	34,35,35	2.41	12 (35%)
3	BB2	D	603	2	27,27,27	0.53	0	34,35,35	1.74	6 (17%)
3	BB2	A	603	2	27,27,27	0.84	1 (3%)	34,35,35	1.45	6 (17%)
3	BB2	E	603	2	27,27,27	0.49	0	34,35,35	1.52	5 (14%)
3	BB2	C	603	2	27,27,27	0.63	0	34,35,35	1.29	3 (8%)

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
3	BB2	F	603	2	-	7/33/43/43	0/1/1/1
3	BB2	B	603	2	-	16/33/43/43	0/1/1/1
3	BB2	D	603	2	-	18/33/43/43	0/1/1/1
3	BB2	A	603	2	-	10/33/43/43	0/1/1/1
3	BB2	E	603	2	-	7/33/43/43	0/1/1/1
3	BB2	C	603	2	-	15/33/43/43	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	BB2	C3-N1	3.56	1.36	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	603	BB2	O4-C3-N1	-9.14	112.05	123.27
3	F	603	BB2	O2-N1-C3	-6.63	110.00	119.79
3	B	603	BB2	O4-C3-N1	-6.55	115.22	123.27
3	D	603	BB2	O4-C3-N1	-5.86	116.08	123.27
3	E	603	BB2	O4-C3-N1	-5.59	116.40	123.27
3	B	603	BB2	O13-C12-C6	-5.21	114.16	122.19
3	B	603	BB2	C6-C12-N14	5.01	124.82	116.19
3	B	603	BB2	O4-C3-C5	4.72	128.44	121.54
3	F	603	BB2	C5-C3-N1	4.64	122.17	115.14
3	D	603	BB2	O2-N1-C3	-4.58	113.02	119.79
3	C	603	BB2	O4-C3-N1	-4.33	117.95	123.27
3	A	603	BB2	C5-C3-N1	3.75	120.82	115.14
3	A	603	BB2	O4-C3-C5	-3.72	116.10	121.54
3	C	603	BB2	C5-C6-C12	3.66	114.92	109.71
3	F	603	BB2	C5-C6-C12	3.45	114.63	109.71
3	B	603	BB2	C16-C15-N14	3.41	119.69	111.44
3	B	603	BB2	O20-C19-C15	-3.28	113.78	119.96
3	B	603	BB2	C7-C6-C12	3.21	114.84	109.63
3	F	603	BB2	O4-C3-C5	2.90	125.77	121.54
3	E	603	BB2	O2-N1-C3	-2.86	115.57	119.79
3	D	603	BB2	C5-C3-N1	2.77	119.34	115.14
3	E	603	BB2	C5-C6-C12	2.71	113.57	109.71
3	B	603	BB2	C23-N21-C22	-2.70	106.69	111.44
3	B	603	BB2	O2-N1-C3	-2.52	116.08	119.79
3	E	603	BB2	O4-C3-C5	2.50	125.19	121.54
3	F	603	BB2	C16-C15-C19	2.45	115.50	110.71
3	B	603	BB2	C15-C19-N21	2.34	124.38	118.65
3	A	603	BB2	C15-C19-N21	2.34	124.37	118.65
3	D	603	BB2	C15-N14-C12	2.31	127.61	121.90
3	A	603	BB2	O20-C19-C15	-2.26	115.70	119.96
3	A	603	BB2	C18-C16-C15	2.19	117.16	111.16
3	A	603	BB2	O13-C12-C6	-2.13	118.90	122.19
3	C	603	BB2	C5-C3-N1	2.12	118.35	115.14
3	B	603	BB2	C18-C16-C15	2.08	116.86	111.16
3	D	603	BB2	O4-C3-C5	2.05	124.54	121.54
3	E	603	BB2	C5-C3-N1	2.04	118.23	115.14
3	B	603	BB2	C26-C22-N21	-2.03	103.75	112.51
3	D	603	BB2	C15-C19-N21	2.02	123.59	118.65

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	BB2	C3-C5-C6-C7
3	A	603	BB2	C12-C6-C7-C8
3	A	603	BB2	C15-C19-N21-C22
3	A	603	BB2	C15-C19-N21-C23
3	A	603	BB2	O20-C19-N21-C22
3	A	603	BB2	O20-C19-N21-C23
3	A	603	BB2	N21-C22-C26-O27
3	A	603	BB2	C25-C22-C26-O27
3	B	603	BB2	C3-C5-C6-C12
3	B	603	BB2	C3-C5-C6-C7
3	B	603	BB2	O13-C12-C6-C7
3	B	603	BB2	N14-C12-C6-C7
3	B	603	BB2	C12-C6-C7-C8
3	B	603	BB2	C16-C15-N14-C12
3	B	603	BB2	N21-C22-C26-O27
3	B	603	BB2	C25-C22-C26-O27
3	C	603	BB2	C5-C6-C7-C8
3	C	603	BB2	C12-C6-C7-C8
3	C	603	BB2	C15-C19-N21-C22
3	C	603	BB2	C15-C19-N21-C23
3	C	603	BB2	O20-C19-N21-C22
3	C	603	BB2	O20-C19-N21-C23
3	C	603	BB2	N21-C22-C26-O27
3	C	603	BB2	C25-C22-C26-O27
3	D	603	BB2	O13-C12-C6-C5
3	D	603	BB2	N14-C12-C6-C5
3	D	603	BB2	C12-C6-C7-C8
3	D	603	BB2	C15-C19-N21-C22
3	D	603	BB2	C15-C19-N21-C23
3	D	603	BB2	O20-C19-N21-C22
3	D	603	BB2	O20-C19-N21-C23
3	D	603	BB2	N21-C22-C26-O27
3	D	603	BB2	C25-C22-C26-O27
3	E	603	BB2	C15-C19-N21-C22
3	E	603	BB2	C15-C19-N21-C23
3	E	603	BB2	O20-C19-N21-C22
3	E	603	BB2	O20-C19-N21-C23
3	F	603	BB2	C12-C6-C7-C8
3	F	603	BB2	C15-C19-N21-C22
3	F	603	BB2	C15-C19-N21-C23
3	F	603	BB2	O20-C19-N21-C22
3	F	603	BB2	O20-C19-N21-C23
3	C	603	BB2	N14-C15-C16-C18

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Mol	Chain	Res	Type	Atoms
3	C	603	BB2	N14-C15-C16-C17
3	B	603	BB2	O20-C19-N21-C23
3	C	603	BB2	C19-C15-C16-C18
3	C	603	BB2	C19-C15-C16-C17
3	D	603	BB2	N14-C15-C16-C18
3	D	603	BB2	N14-C15-C16-C17
3	B	603	BB2	C6-C7-C8-C9
3	B	603	BB2	C5-C6-C7-C8
3	B	603	BB2	O20-C19-N21-C22
3	C	603	BB2	C6-C7-C8-C9
3	D	603	BB2	C19-C15-C16-C17
3	D	603	BB2	C19-C15-C16-C18
3	C	603	BB2	C7-C8-C9-C10
3	A	603	BB2	C5-C6-C7-C8
3	D	603	BB2	C5-C6-C7-C8
3	F	603	BB2	C5-C6-C7-C8
3	D	603	BB2	O13-C12-C6-C7
3	D	603	BB2	N14-C12-C6-C7
3	D	603	BB2	C7-C8-C9-C10
3	E	603	BB2	C6-C7-C8-C9
3	B	603	BB2	C15-C19-N21-C23
3	E	603	BB2	C11-C10-C9-C8
3	B	603	BB2	C15-C19-N21-C22
3	F	603	BB2	C7-C8-C9-C10
3	A	603	BB2	C11-C10-C9-C8
3	B	603	BB2	N14-C15-C16-C18
3	E	603	BB2	O13-C12-C6-C5
3	C	603	BB2	C11-C10-C9-C8
3	B	603	BB2	C19-C15-C16-C18
3	D	603	BB2	C6-C7-C8-C9

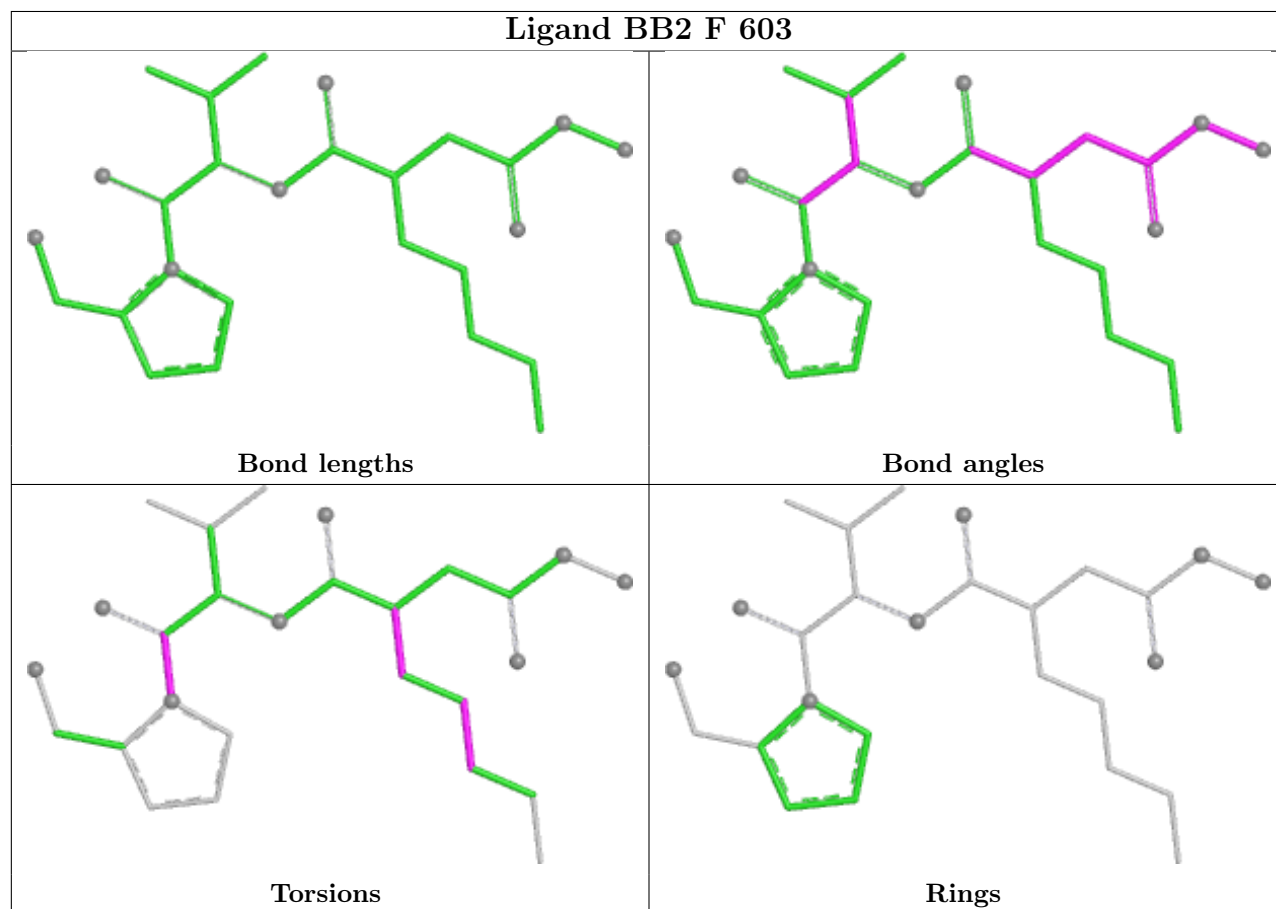
There are no ring outliers.

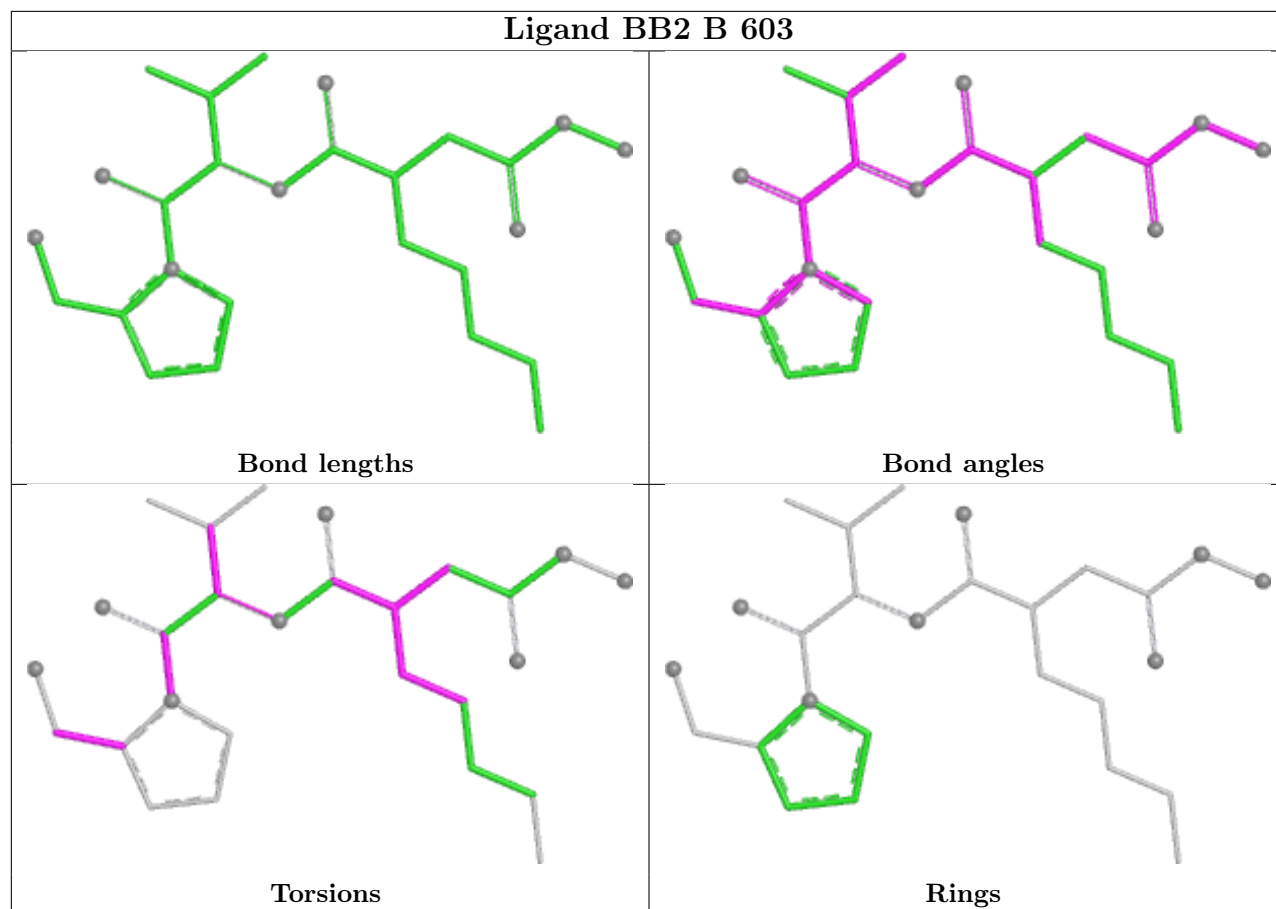
1 monomer is involved in 1 short contact:

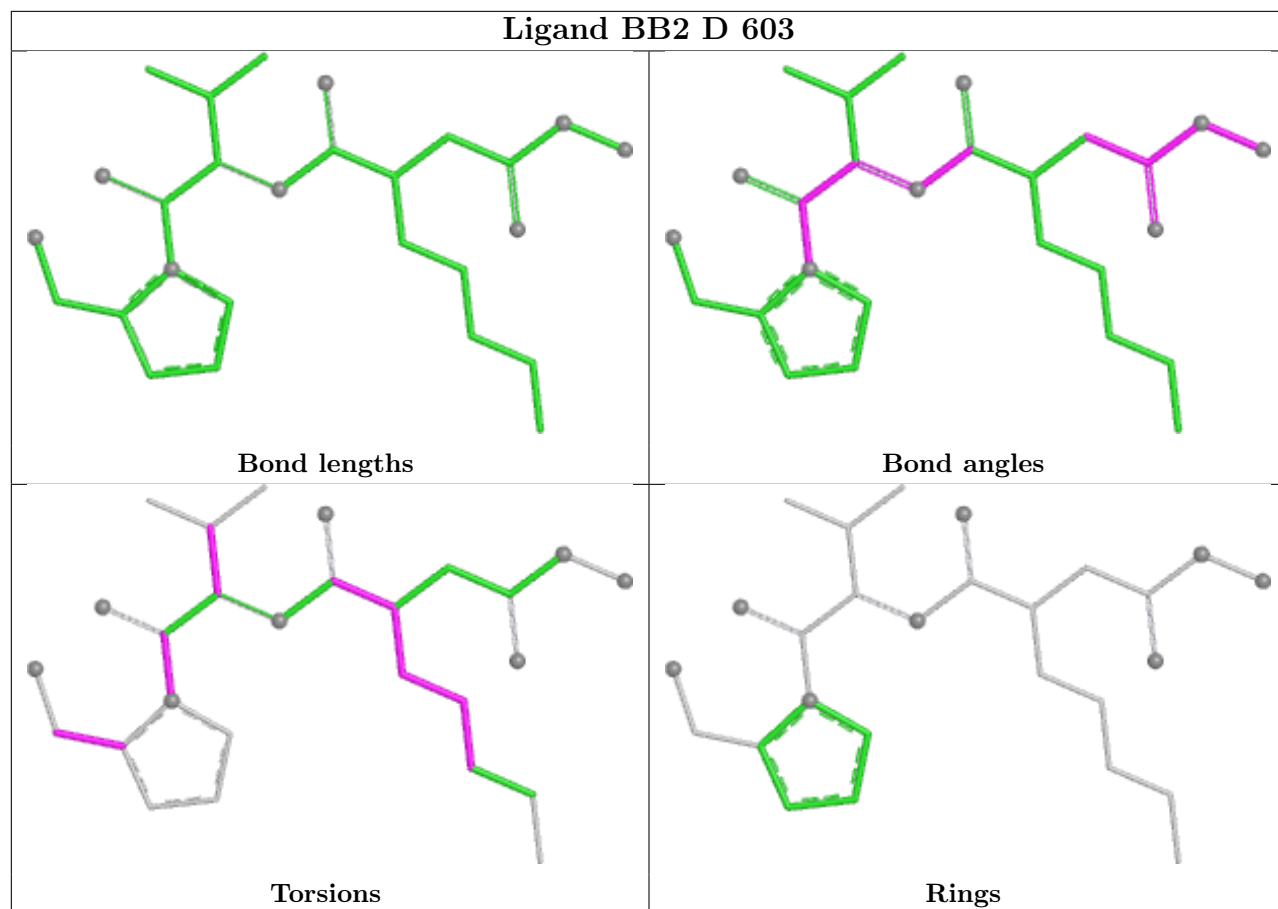
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	BB2	1	0

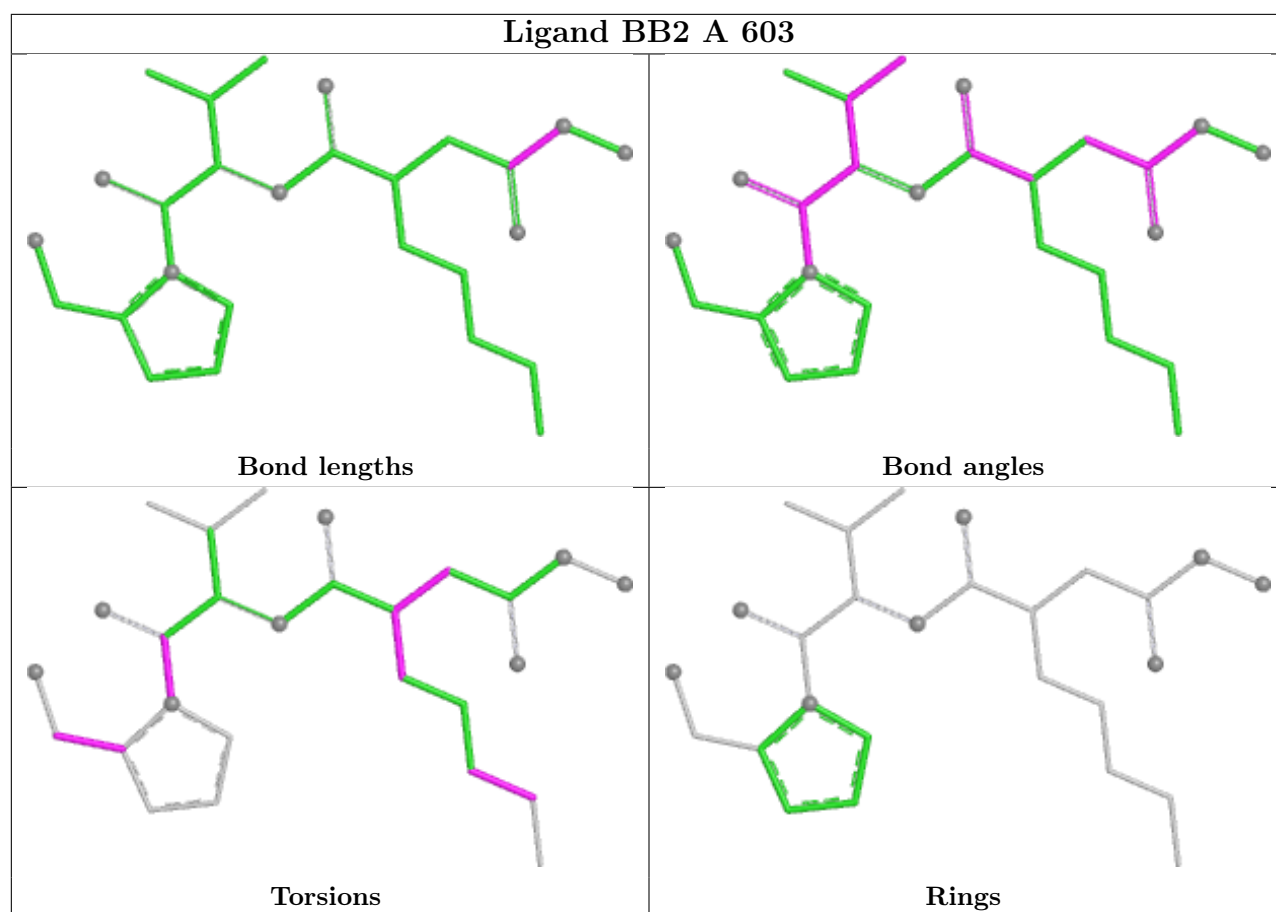
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

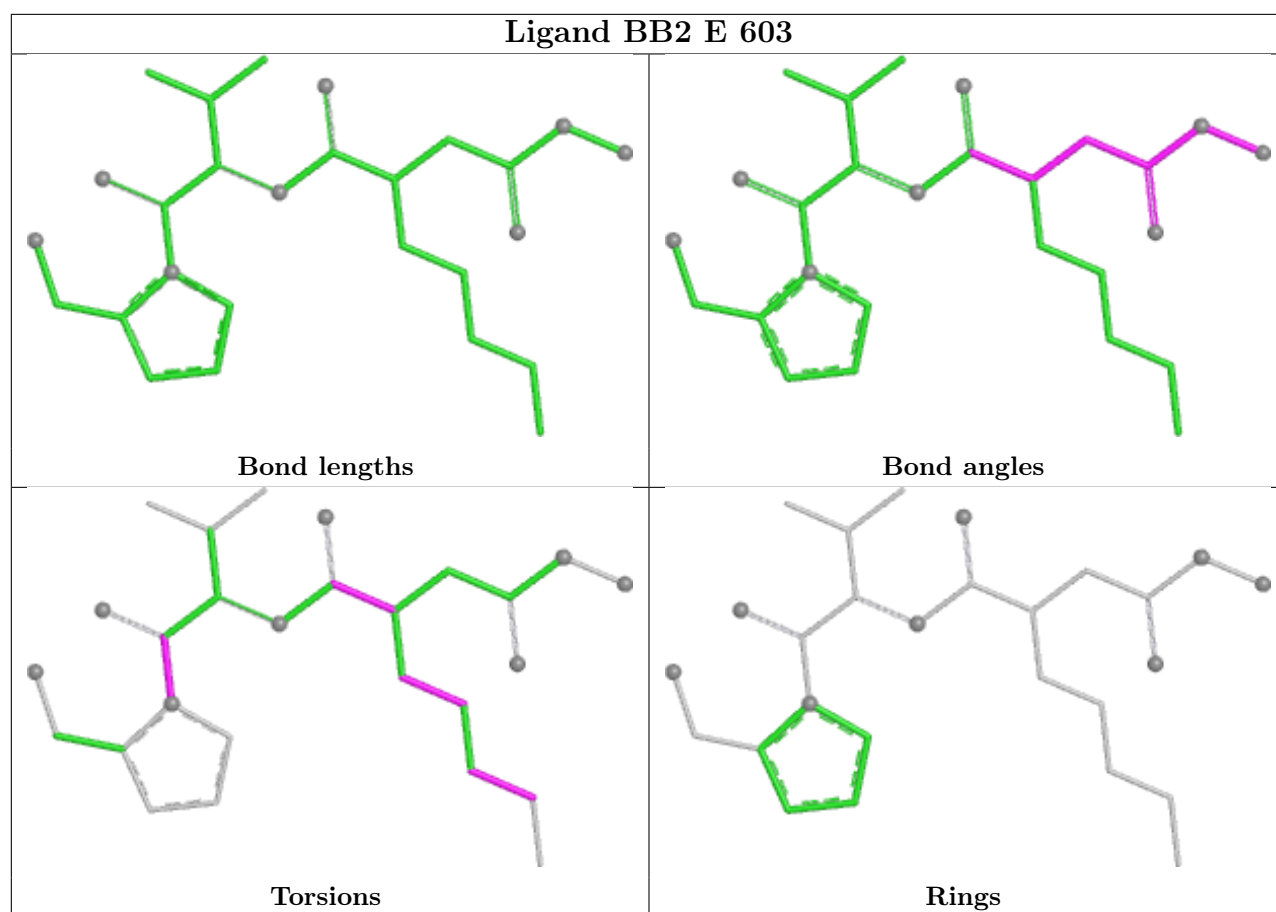
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

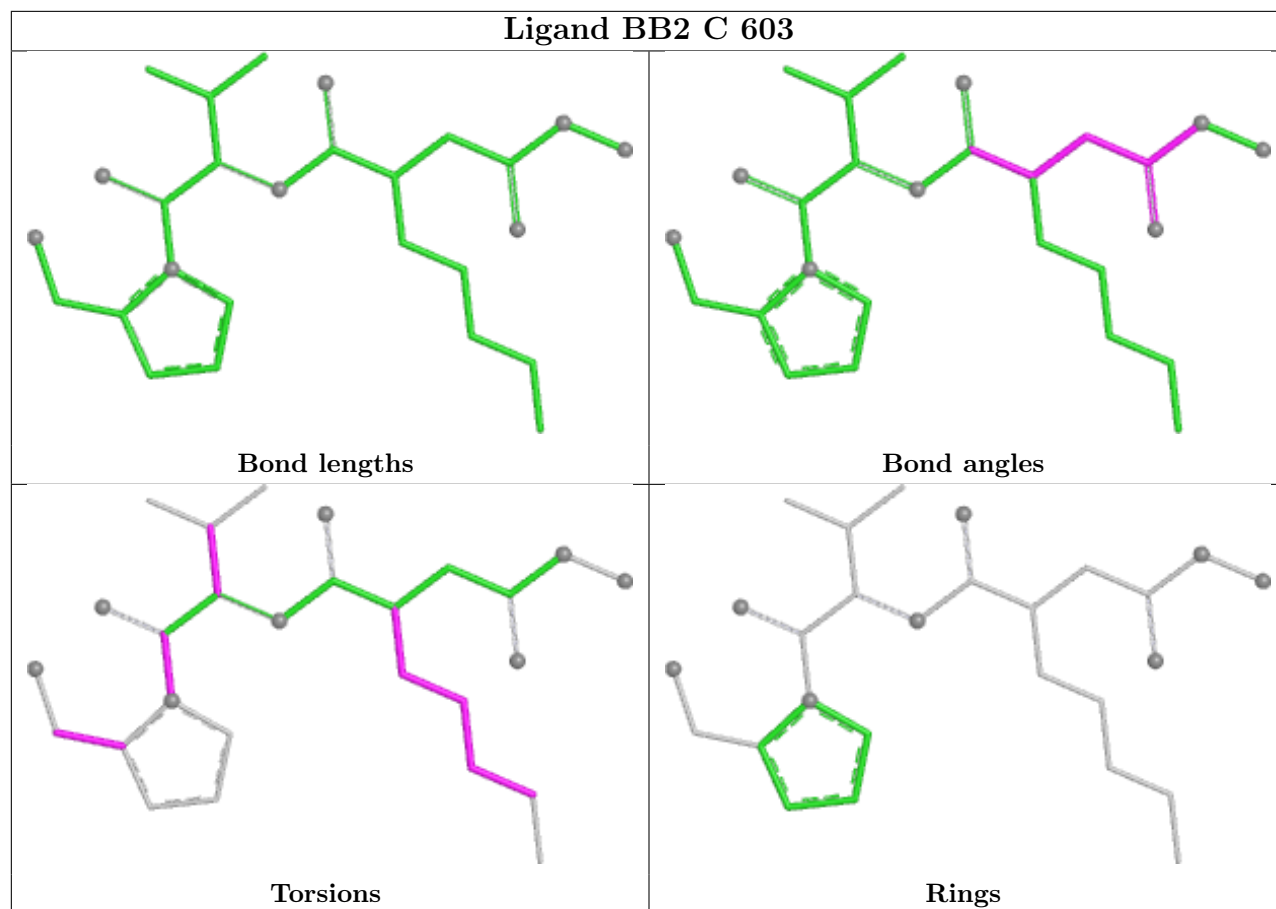












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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	518/521 (99%)	0.61	16 (3%)	51 30	10, 29, 53, 67	2 (0%)
1	B	518/521 (99%)	0.50	18 (3%)	47 27	9, 24, 55, 96	2 (0%)
1	C	517/521 (99%)	0.42	14 (2%)	56 33	7, 24, 46, 78	1 (0%)
1	D	518/521 (99%)	1.76	198 (38%)	1 1	24, 56, 91, 117	0
1	E	518/521 (99%)	0.40	22 (4%)	40 22	9, 23, 60, 85	1 (0%)
1	F	514/521 (98%)	1.75	193 (37%)	1 1	20, 52, 85, 109	0
All	All	3103/3126 (99%)	0.91	461 (14%)	5 3	7, 32, 77, 117	6 (0%)

All (461) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	239	ASP	6.6
1	F	285	SER	5.6
1	D	95	ALA	5.6
1	F	136	GLU	5.2
1	F	336	SER	5.1
1	C	40	GLY	5.1
1	D	196	PRO	5.1
1	D	149	ALA	5.0
1	F	30	ASP	4.9
1	D	25	ASN	4.7
1	F	521	LEU	4.7
1	F	395	VAL	4.7
1	F	332	PRO	4.6
1	F	335	LEU	4.6
1	D	333	VAL	4.6
1	D	44	SER	4.5
1	D	198	ASP	4.4
1	F	32	ALA	4.4
1	D	205	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	42	LEU	4.3
1	D	335	LEU	4.3
1	D	521	LEU	4.3
1	F	420	ASN	4.3
1	A	138	ASN	4.3
1	B	91	LEU	4.2
1	A	137	PRO	4.2
1	F	274	TYR	4.2
1	F	323	PHE	4.2
1	D	232	TYR	4.2
1	D	399	MET	4.1
1	D	395	VAL	4.1
1	F	147	SER	4.1
1	F	334	GLN	4.1
1	D	274	TYR	4.0
1	F	25	ASN	4.0
1	D	331	GLN	3.9
1	F	44	SER	3.9
1	D	37	ASN	3.9
1	F	327	VAL	3.8
1	D	40	GLY	3.8
1	D	147	SER	3.8
1	F	40	GLY	3.8
1	F	35	GLU	3.8
1	F	69	PRO	3.8
1	F	199	LEU	3.8
1	F	238	PHE	3.8
1	F	385	ALA	3.7
1	D	273	LEU	3.7
1	E	69	PRO	3.7
1	F	284	VAL	3.7
1	D	238	PHE	3.7
1	D	337	CYS	3.7
1	D	323	PHE	3.7
1	F	288	GLY	3.7
1	F	150	VAL	3.6
1	D	150	VAL	3.6
1	F	424	ALA	3.6
1	D	397	ILE	3.6
1	D	38	GLN	3.6
1	F	92	ALA	3.6
1	F	390	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	138	ASN	3.6
1	F	61	VAL	3.6
1	F	393	PRO	3.5
1	F	28	PHE	3.5
1	D	424	ALA	3.5
1	F	325	THR	3.5
1	F	512	ALA	3.5
1	D	489	GLY	3.5
1	D	245	GLY	3.4
1	F	137	PRO	3.4
1	F	54	LYS	3.4
1	D	394	ASP	3.4
1	F	31	VAL	3.4
1	D	275	THR	3.4
1	D	191	PRO	3.4
1	F	38	GLN	3.4
1	B	138	ASN	3.3
1	B	3	THR	3.3
1	D	206	THR	3.3
1	D	46	LEU	3.3
1	D	318	ALA	3.3
1	D	58	ASP	3.3
1	F	492	ILE	3.3
1	D	31	VAL	3.3
1	F	421	GLU	3.3
1	D	334	GLN	3.3
1	F	55	GLN	3.3
1	F	187	VAL	3.3
1	F	287	VAL	3.3
1	D	389	LEU	3.3
1	F	151	LEU	3.3
1	D	434	GLU	3.3
1	D	20	VAL	3.2
1	F	392	THR	3.2
1	D	201	ALA	3.2
1	F	149	ALA	3.2
1	D	332	PRO	3.2
1	D	233	ALA	3.2
1	F	45	GLY	3.2
1	D	272	LEU	3.2
1	D	34	TYR	3.2
1	D	117	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	41	VAL	3.2
1	D	242	VAL	3.2
1	D	338	THR	3.2
1	D	175	ALA	3.1
1	F	146	LEU	3.1
1	D	88	VAL	3.1
1	F	389	LEU	3.1
1	D	26	VAL	3.1
1	D	102	VAL	3.1
1	B	135	LYS	3.1
1	D	85	GLY	3.1
1	F	517	TYR	3.1
1	F	273	LEU	3.1
1	D	133	GLU	3.1
1	D	30	ASP	3.1
1	D	192	PRO	3.1
1	D	285	SER	3.0
1	F	141	VAL	3.0
1	C	136	GLU	3.0
1	F	399	MET	3.0
1	F	514	LEU	3.0
1	D	45	GLY	3.0
1	D	3	THR	3.0
1	C	63	ARG	3.0
1	F	232	TYR	3.0
1	F	117	PRO	2.9
1	D	111	ALA	2.9
1	A	45	GLY	2.9
1	F	237	GLY	2.9
1	D	492	ILE	2.9
1	F	313	MET	2.9
1	D	279	THR	2.9
1	F	46	LEU	2.9
1	B	137	PRO	2.9
1	D	23	LYS	2.9
1	D	396	VAL	2.9
1	D	430	ARG	2.9
1	D	519	ARG	2.9
1	D	9	ALA	2.9
1	D	200	GLU	2.9
1	F	485	PRO	2.9
1	D	520	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	3	THR	2.9
1	D	158	ALA	2.9
1	D	393	PRO	2.9
1	D	322	GLY	2.9
1	F	397	ILE	2.9
1	D	230	GLN	2.9
1	D	441	PRO	2.9
1	F	140	THR	2.9
1	F	322	GLY	2.9
1	D	151	LEU	2.9
1	F	286	LEU	2.9
1	D	193	ALA	2.8
1	F	394	ASP	2.8
1	F	90	GLY	2.8
1	D	194	ILE	2.8
1	F	112	SER	2.8
1	D	512	ALA	2.8
1	C	138	ASN	2.8
1	D	93	ASN	2.8
1	F	283	LYS	2.8
1	E	85	GLY	2.8
1	E	90	GLY	2.8
1	F	42	LEU	2.8
1	D	414	HIS	2.8
1	B	466[A]	ARG	2.8
1	F	333	VAL	2.8
1	D	190	GLU	2.8
1	D	400	ALA	2.8
1	F	235	ALA	2.8
1	F	41	VAL	2.8
1	F	181	VAL	2.8
1	D	324	LEU	2.8
1	C	304	ASP	2.8
1	F	416	GLY	2.8
1	D	103	VAL	2.8
1	F	134	VAL	2.8
1	D	473	SER	2.8
1	F	184	LEU	2.8
1	D	188	PHE	2.7
1	D	282	LYS	2.7
1	F	490	ALA	2.7
1	D	185	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	240	VAL	2.7
1	B	4	LEU	2.7
1	F	43	SER	2.7
1	F	315	GLY	2.7
1	F	142	ASP	2.7
1	D	284	VAL	2.7
1	F	230	GLN	2.7
1	D	199	LEU	2.7
1	F	340	CYS	2.7
1	D	182	SER	2.7
1	F	414	HIS	2.7
1	F	494	VAL	2.7
1	F	328	ARG	2.7
1	D	36	SER	2.7
1	D	241	ASP	2.7
1	F	329	LEU	2.7
1	F	513	LEU	2.7
1	D	228	ILE	2.7
1	D	57	ARG	2.7
1	F	133	GLU	2.7
1	D	92	ALA	2.7
1	D	4	LEU	2.7
1	F	37	ASN	2.7
1	F	391	PHE	2.6
1	D	278	GLY	2.6
1	D	29	THR	2.6
1	D	336	SER	2.6
1	F	33	ALA	2.6
1	F	382	VAL	2.6
1	D	120	PRO	2.6
1	F	180	LYS	2.6
1	F	276	PRO	2.6
1	D	413	HIS	2.6
1	F	441	PRO	2.6
1	D	169	ASP	2.6
1	F	58	ASP	2.6
1	B	90	GLY	2.6
1	D	429	LEU	2.6
1	B	41	VAL	2.6
1	F	95	ALA	2.6
1	F	226	THR	2.6
1	D	487	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	501	PHE	2.6
1	D	68	ASN	2.6
1	D	315	GLY	2.6
1	F	12	LEU	2.6
1	D	235	ALA	2.6
1	E	467	ARG	2.6
1	F	279	THR	2.6
1	D	189	PRO	2.6
1	D	314	GLY	2.6
1	F	200	GLU	2.6
1	F	422	GLU	2.6
1	B	92	ALA	2.6
1	D	141	VAL	2.6
1	F	60	ALA	2.6
1	D	321	CYS	2.5
1	F	280	PRO	2.5
1	D	97	SER	2.5
1	F	435	SER	2.5
1	C	467	ARG	2.5
1	F	120	PRO	2.5
1	E	231	GLY	2.5
1	F	13	SER	2.5
1	F	182	SER	2.5
1	D	187	VAL	2.5
1	E	86	VAL	2.5
1	D	73	GLU	2.5
1	D	253	TYR	2.5
1	C	41	VAL	2.5
1	F	318	ALA	2.5
1	D	153	ILE	2.5
1	D	518	PHE	2.5
1	F	144	PHE	2.5
1	F	282	LYS	2.5
1	F	444	TYR	2.5
1	F	330	GLN	2.5
1	F	331	GLN	2.5
1	A	387	ASN	2.5
1	D	28	PHE	2.5
1	E	3	THR	2.5
1	C	251	ARG	2.5
1	D	423	GLY	2.5
1	F	489	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	88	VAL	2.5
1	F	419	VAL	2.5
1	F	442	VAL	2.5
1	D	490	ALA	2.4
1	D	497	ALA	2.4
1	D	421	GLU	2.4
1	D	109	THR	2.4
1	D	184	LEU	2.4
1	D	281	VAL	2.4
1	F	508	GLY	2.4
1	D	32	ALA	2.4
1	E	74	ALA	2.4
1	F	203	ALA	2.4
1	D	19	CYS	2.4
1	F	487	PHE	2.4
1	D	433	ARG	2.4
1	D	148	ASN	2.4
1	D	392	THR	2.4
1	F	29	THR	2.4
1	D	240	VAL	2.4
1	F	242	VAL	2.4
1	F	252	GLY	2.4
1	F	205	SER	2.4
1	D	87	LEU	2.4
1	D	146	LEU	2.4
1	F	102	VAL	2.4
1	D	90	GLY	2.4
1	E	84	TYR	2.4
1	F	493	HIS	2.4
1	D	203	ALA	2.4
1	D	234	LYS	2.4
1	E	35	GLU	2.4
1	F	139	THR	2.4
1	D	51	GLY	2.4
1	D	449	HIS	2.4
1	D	72	ALA	2.4
1	D	155	ALA	2.4
1	F	201	ALA	2.4
1	F	57	ARG	2.4
1	E	87	LEU	2.4
1	D	6	LYS	2.3
1	D	504	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	305	TYR	2.3
1	F	56	LEU	2.3
1	D	280	PRO	2.3
1	F	484	SER	2.3
1	D	7	ALA	2.3
1	F	154	ALA	2.3
1	F	321	CYS	2.3
1	F	326	ALA	2.3
1	D	380	ASP	2.3
1	C	250	GLU	2.3
1	D	422	GLU	2.3
1	A	281	VAL	2.3
1	C	134	VAL	2.3
1	D	139	THR	2.3
1	F	18	SER	2.3
1	F	47	ALA	2.3
1	F	172	ALA	2.3
1	F	337	CYS	2.3
1	D	286	LEU	2.3
1	D	35	GLU	2.3
1	F	396	VAL	2.3
1	D	276	PRO	2.3
1	E	65	PRO	2.3
1	F	189	PRO	2.3
1	F	314	GLY	2.3
1	F	476	GLY	2.3
1	F	477	TYR	2.3
1	F	115	ASN	2.3
1	F	148	ASN	2.3
1	D	330	GLN	2.3
1	F	210	GLN	2.3
1	A	136	GLU	2.3
1	F	213	VAL	2.3
1	A	196	PRO	2.3
1	C	137	PRO	2.3
1	D	5	PRO	2.3
1	F	510	GLY	2.3
1	D	136	GLU	2.2
1	A	59	PRO	2.2
1	D	309	MET	2.2
1	F	233	ALA	2.2
1	E	91	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	236	LEU	2.2
1	F	272	LEU	2.2
1	F	324	LEU	2.2
1	D	52	THR	2.2
1	F	204	THR	2.2
1	D	18	SER	2.2
1	E	486	LYS	2.2
1	F	34	TYR	2.2
1	D	183	ARG	2.2
1	D	160	CYS	2.2
1	D	442	VAL	2.2
1	F	177	ASN	2.2
1	D	239	ASP	2.2
1	D	247	ASP	2.2
1	B	139	THR	2.2
1	D	325	THR	2.2
1	F	486	LYS	2.2
1	D	100	VAL	2.2
1	F	19	CYS	2.2
1	D	316	ALA	2.2
1	D	476	GLY	2.2
1	F	520	LYS	2.2
1	F	206	THR	2.2
1	F	438	THR	2.2
1	D	43	SER	2.2
1	D	361	SER	2.2
1	D	64	LEU	2.2
1	D	131	LEU	2.2
1	A	276	PRO	2.2
1	C	266	ALA	2.2
1	D	33	ALA	2.2
1	D	508	GLY	2.2
1	F	497	ALA	2.2
1	B	140	THR	2.2
1	D	493	HIS	2.2
1	B	134	VAL	2.2
1	D	444	TYR	2.2
1	E	88	VAL	2.2
1	D	49	LEU	2.2
1	E	68	ASN	2.2
1	D	137	PRO	2.2
1	A	394	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	16	VAL	2.1
1	B	147	SER	2.1
1	D	39	LYS	2.1
1	E	70	ALA	2.1
1	E	136	GLU	2.1
1	F	118	ALA	2.1
1	D	432	GLY	2.1
1	F	278	GLY	2.1
1	F	198	ASP	2.1
1	E	305	TYR	2.1
1	B	87	LEU	2.1
1	F	220	LEU	2.1
1	D	55	GLN	2.1
1	B	182	SER	2.1
1	F	381	GLY	2.1
1	F	425	GLU	2.1
1	A	41	VAL	2.1
1	E	53	HIS	2.1
1	D	248	LEU	2.1
1	D	277	LYS	2.1
1	D	364	THR	2.1
1	F	39	LYS	2.1
1	F	483	LEU	2.1
1	F	433	ARG	2.1
1	A	388	GLU	2.1
1	F	196	PRO	2.1
1	F	432	GLY	2.1
1	F	436	GLY	2.1
1	F	178	SER	2.1
1	D	138	ASN	2.1
1	F	110	LYS	2.1
1	F	169	ASP	2.1
1	F	277	LYS	2.1
1	C	64	LEU	2.1
1	D	116	CYS	2.1
1	F	380	ASP	2.1
1	F	221	THR	2.1
1	F	253	TYR	2.1
1	F	317	ALA	2.1
1	F	431	ALA	2.1
1	D	207	GLN	2.1
1	B	315	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	48	VAL	2.1
1	D	494	VAL	2.1
1	F	468	ASP	2.1
1	F	207	GLN	2.1
1	D	391	PHE	2.1
1	F	437	GLU	2.1
1	D	419	VAL	2.0
1	A	361	SER	2.0
1	E	42	LEU	2.0
1	F	339	LEU	2.0
1	D	482	HIS	2.0
1	D	307	LYS	2.0
1	A	187	VAL	2.0
1	D	472	VAL	2.0
1	D	467	ARG	2.0
1	D	514	LEU	2.0
1	F	430	ARG	2.0
1	F	53	HIS	2.0
1	D	204	THR	2.0
1	E	67	TYR	2.0
1	D	121	ASP	2.0
1	C	190	GLU	2.0

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
3	BB2	A	603	27/27	0.83	0.18	24,38,45,49	0

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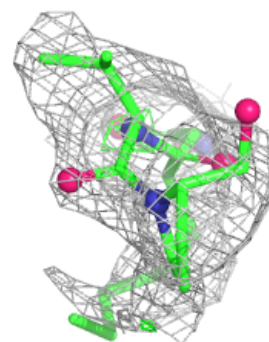
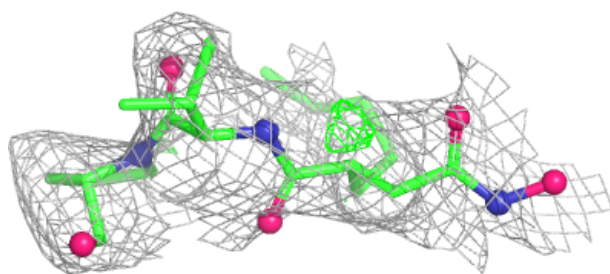
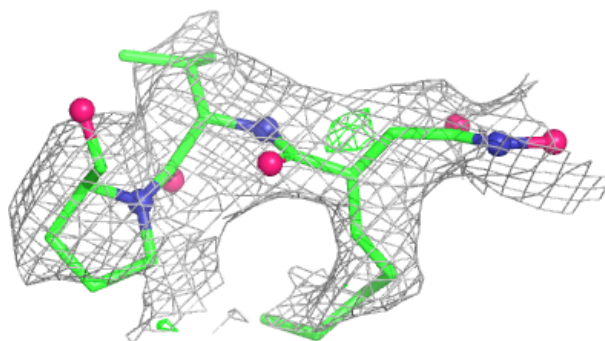
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BB2	D	603	27/27	0.87	0.17	37,49,56,62	0
3	BB2	C	603	27/27	0.88	0.15	18,28,32,33	0
3	BB2	F	603	27/27	0.88	0.18	38,57,68,68	0
3	BB2	B	603	27/27	0.89	0.16	22,35,43,44	0
3	BB2	E	603	27/27	0.94	0.12	22,27,41,42	0
2	MN	F	601	1/1	0.96	0.05	38,38,38,38	0
2	MN	F	602	1/1	0.97	0.05	36,36,36,36	0
2	MN	E	601	1/1	0.98	0.05	20,20,20,20	0
2	MN	B	602	1/1	0.98	0.07	25,25,25,25	0
2	MN	D	602	1/1	0.98	0.04	45,45,45,45	0
2	MN	D	601	1/1	0.99	0.03	42,42,42,42	0
2	MN	A	602	1/1	0.99	0.03	21,21,21,21	0
2	MN	B	601	1/1	0.99	0.04	21,21,21,21	0
2	MN	E	602	1/1	0.99	0.05	22,22,22,22	0
2	MN	A	601	1/1	0.99	0.03	22,22,22,22	0
2	MN	C	601	1/1	0.99	0.06	20,20,20,20	0
2	MN	C	602	1/1	1.00	0.02	17,17,17,17	0

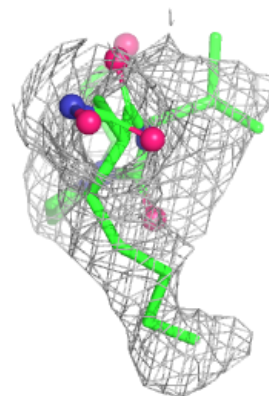
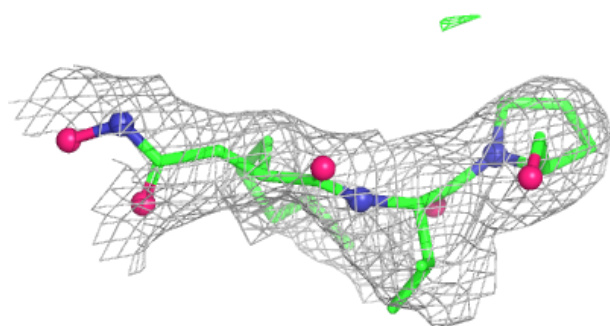
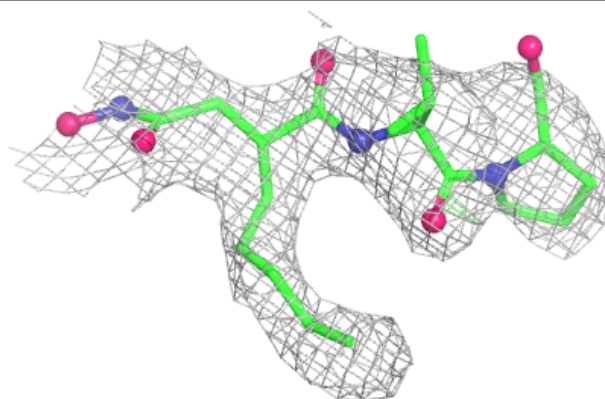
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BB2 A 603:

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

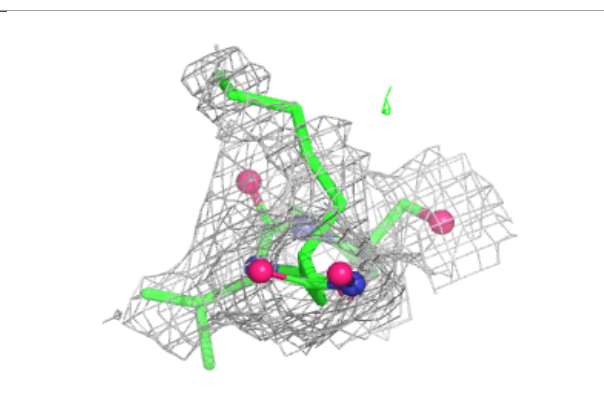
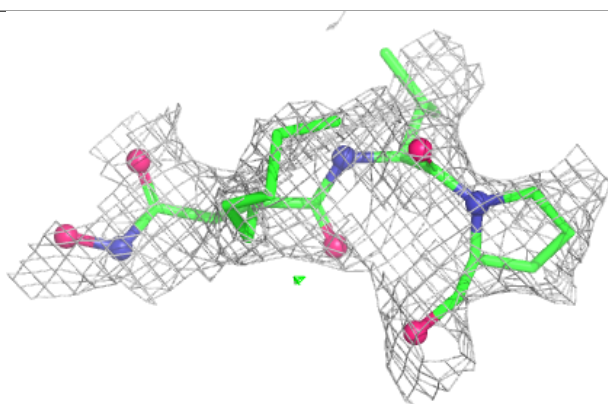
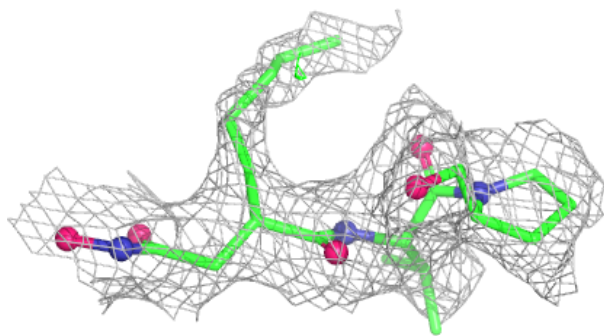
**Electron density around BB2 D 603:**

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

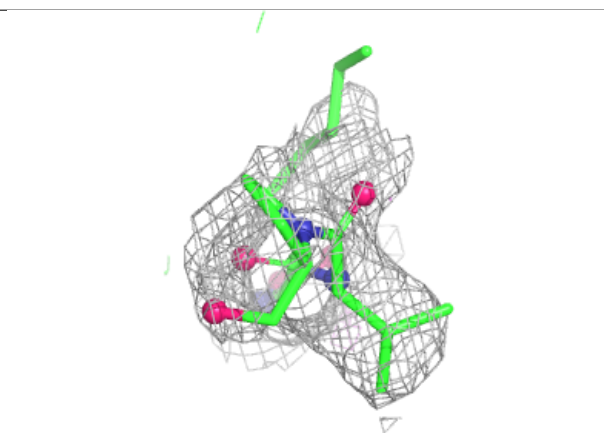
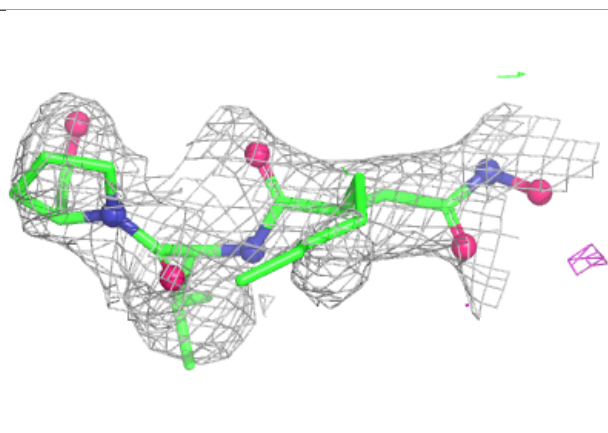
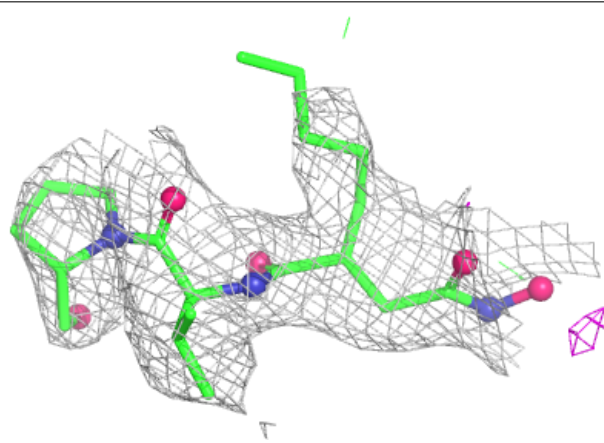


Electron density around BB2 C 603:

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

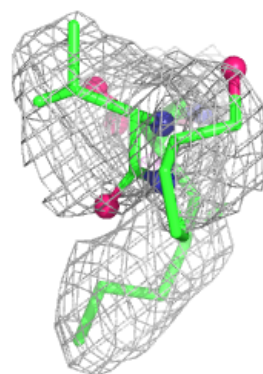
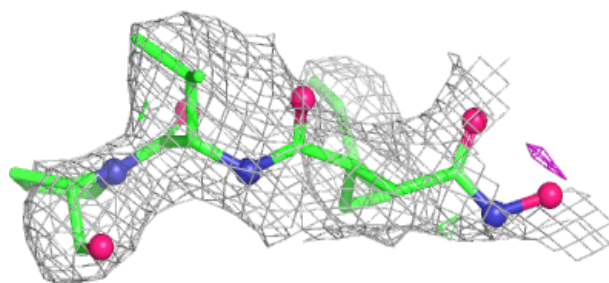
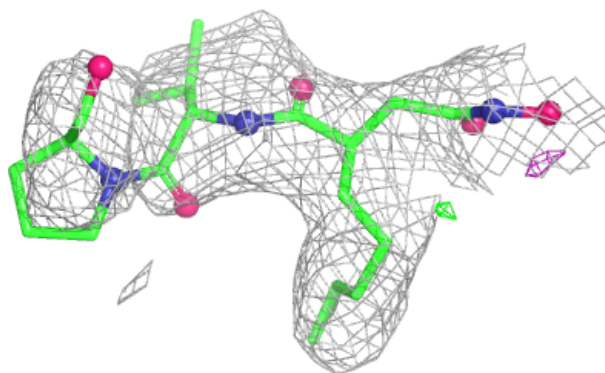
**Electron density around BB2 F 603:**

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



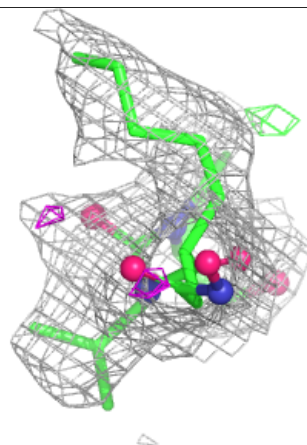
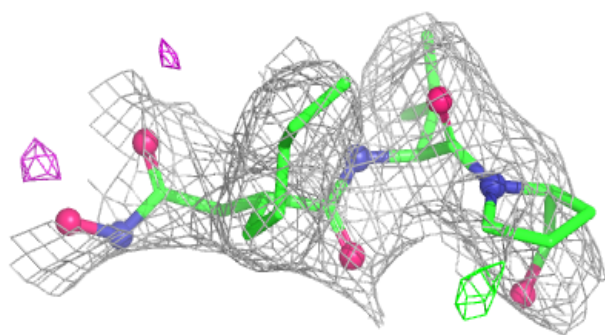
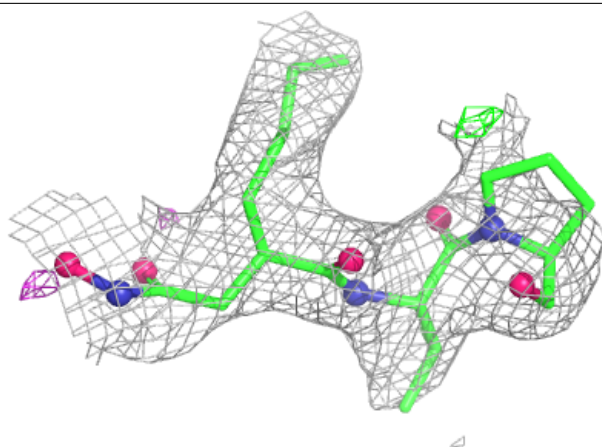
Electron density around BB2 B 603:

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



Electron density around BB2 E 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 [i](#)

There are no such residues in this entry.