



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:19 am BST

PDB ID : 3G5K
Title : Structure and activity of human mitochondrial peptide deformylase, a novel cancer target
Authors : Escobar-Alvarez, S.; Goldgur, Y.; Yang, G.; Ouerfelli, O.; Li, Y.; Scheinberg, D.A.
Deposited on : 2009-02-05
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

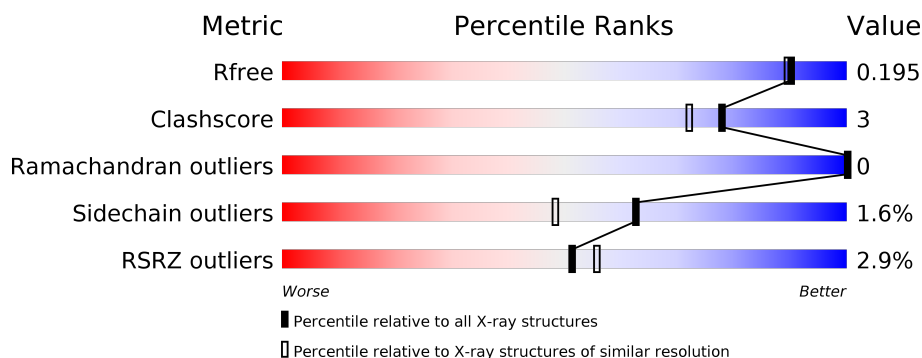
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	183	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	183	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	183	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	183	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>15%</div> <div>.</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6445 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.

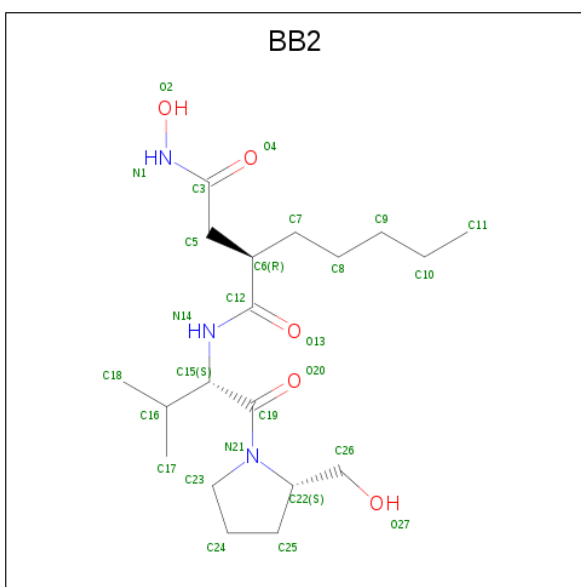
- Molecule 1 is a protein called Peptide deformylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1445	909	272	251	13			
1	B	183	Total	C	N	O	S	0	0	0
			1445	909	272	251	13			
1	C	183	Total	C	N	O	S	0	0	0
			1445	909	272	251	13			
1	D	183	Total	C	N	O	S	0	0	0
			1445	909	272	251	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	HIS	-	EXPRESSION TAG	UNP Q9HBH1
A	4	MET	-	EXPRESSION TAG	UNP Q9HBH1
A	5	SER	-	EXPRESSION TAG	UNP Q9HBH1
B	3	HIS	-	EXPRESSION TAG	UNP Q9HBH1
B	4	MET	-	EXPRESSION TAG	UNP Q9HBH1
B	5	SER	-	EXPRESSION TAG	UNP Q9HBH1
C	3	HIS	-	EXPRESSION TAG	UNP Q9HBH1
C	4	MET	-	EXPRESSION TAG	UNP Q9HBH1
C	5	SER	-	EXPRESSION TAG	UNP Q9HBH1
D	3	HIS	-	EXPRESSION TAG	UNP Q9HBH1
D	4	MET	-	EXPRESSION TAG	UNP Q9HBH1
D	5	SER	-	EXPRESSION TAG	UNP Q9HBH1

- Molecule 2 is ACTINONIN (three-letter code: BB2) (formula: $C_{19}H_{35}N_3O_5$).



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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Co	0	0
			1	1		
3	A	1	Total	Co	0	0
			1	1		
3	D	1	Total	Co	0	0
			1	1		
3	C	1	Total	Co	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		

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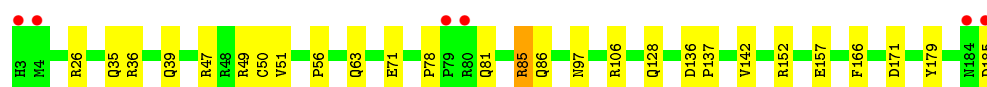
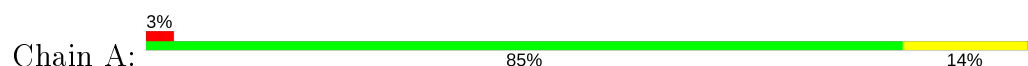
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	129	Total 129	O 129	0	0
4	C	138	Total 138	O 138	0	0
4	D	133	Total 133	O 133	0	0

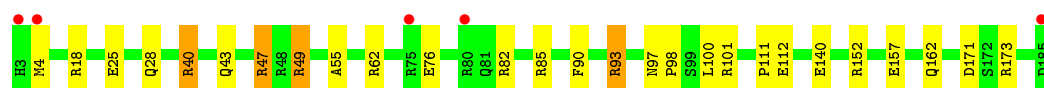
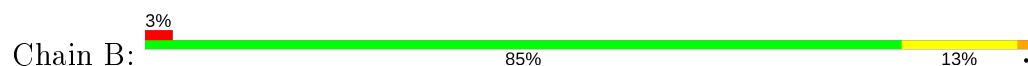
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

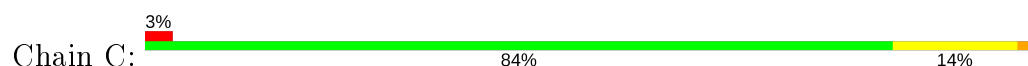
- Molecule 1: Peptide deformylase, mitochondrial



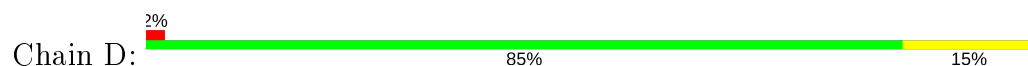
- Molecule 1: Peptide deformylase, mitochondrial



- Molecule 1: Peptide deformylase, mitochondrial



- Molecule 1: Peptide deformylase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.14Å 77.83Å 110.53Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	35.00 – 1.70 33.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.00-1.70) 99.5 (33.37-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.164 , 0.193 0.165 , 0.195	Depositor DCC
R_{free} test set	5160 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6445	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: CO, 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	1.47	6/1477 (0.4%)	1.38	15/2002 (0.7%)
1	B	1.54	11/1477 (0.7%)	1.41	15/2002 (0.7%)
1	C	1.51	11/1477 (0.7%)	1.34	14/2002 (0.7%)
1	D	1.54	14/1477 (0.9%)	1.33	18/2002 (0.9%)
All	All	1.52	42/5908 (0.7%)	1.36	62/8008 (0.8%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	GLU	CB-CG	-14.40	1.24	1.52
1	C	74	CYS	CB-SG	-10.53	1.64	1.82
1	D	157	GLU	CD-OE2	-10.01	1.14	1.25
1	D	50	CYS	CB-SG	-9.09	1.66	1.82
1	B	93	ARG	CZ-NH2	8.88	1.44	1.33
1	A	50	CYS	CB-SG	-8.02	1.68	1.82
1	D	76	GLU	CG-CD	7.77	1.63	1.51
1	A	157	GLU	CG-CD	7.41	1.63	1.51
1	D	74	CYS	CB-SG	-7.30	1.69	1.82
1	D	112	GLU	CD-OE1	7.29	1.33	1.25
1	B	157	GLU	CD-OE2	-6.99	1.18	1.25
1	D	157	GLU	CG-CD	6.95	1.62	1.51
1	C	126	ARG	CZ-NH1	6.92	1.42	1.33
1	B	76	GLU	CD-OE1	6.88	1.33	1.25
1	D	88	GLU	CG-CD	6.81	1.62	1.51
1	B	157	GLU	CG-CD	6.77	1.62	1.51
1	D	157	GLU	CD-OE1	6.68	1.32	1.25
1	A	71	GLU	CG-CD	6.64	1.61	1.51
1	D	112	GLU	CB-CG	-6.60	1.39	1.52
1	C	112	GLU	CB-CG	-6.49	1.39	1.52
1	D	112	GLU	CD-OE2	-6.49	1.18	1.25
1	D	157	GLU	CB-CG	-6.25	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLU	CD-OE1	6.21	1.32	1.25
1	B	55	ALA	CA-CB	6.16	1.65	1.52
1	D	88	GLU	CB-CG	6.13	1.63	1.52
1	C	50	CYS	CB-SG	-6.02	1.72	1.82
1	A	166	PHE	CD2-CE2	6.02	1.51	1.39
1	A	157	GLU	CD-OE2	-5.91	1.19	1.25
1	B	162	GLN	CG-CD	-5.82	1.37	1.51
1	B	140	GLU	CG-CD	5.68	1.60	1.51
1	C	96	VAL	CB-CG1	5.54	1.64	1.52
1	C	157	GLU	CD-OE2	-5.54	1.19	1.25
1	C	106	ARG	CG-CD	5.52	1.65	1.51
1	B	140	GLU	CB-CG	5.45	1.62	1.52
1	C	102	VAL	CB-CG2	5.45	1.64	1.52
1	B	93	ARG	CZ-NH1	5.38	1.40	1.33
1	C	171	ASP	CG-OD1	5.38	1.37	1.25
1	C	112	GLU	CG-CD	5.37	1.60	1.51
1	D	108	VAL	CB-CG2	5.36	1.64	1.52
1	C	110	PHE	CE2-CZ	5.31	1.47	1.37
1	D	124	VAL	CB-CG2	5.04	1.63	1.52
1	B	157	GLU	CB-CG	-5.01	1.42	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ARG	NE-CZ-NH1	-18.71	110.94	120.30
1	A	26	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	C	93	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	B	40	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	A	85	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	D	152	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	B	152	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	85	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	47	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	B	93	ARG	NH1-CZ-NH2	7.89	128.08	119.40
1	D	85	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	B	62	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	82	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	85	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	D	157	GLU	CG-CD-OE2	-7.39	103.53	118.30
1	D	152	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	D	85	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	D	26	ARG	NE-CZ-NH2	-7.09	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	GLU	OE1-CD-OE2	6.96	131.66	123.30
1	C	62	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	D	173	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	D	48	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	36	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	D	171	ASP	CB-CG-OD1	6.35	124.01	118.30
1	C	171	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	40	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	18	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	26	ARG	CG-CD-NE	-5.98	99.23	111.80
1	A	142	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	D	157	GLU	CG-CD-OE1	5.93	130.15	118.30
1	C	171	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	106	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	D	171	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	152	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	49	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	47	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	D	49	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	49	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	85	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	51	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	B	171	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	108	VAL	CG1-CB-CG2	-5.54	102.04	110.90
1	D	85	ARG	CD-NE-CZ	5.39	131.14	123.60
1	C	126	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	142	VAL	N-CA-C	-5.30	96.69	111.00
1	C	62	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	48	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	49	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	18	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	48	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	179	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	B	173	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	D	49	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	101	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	D	136	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	B	112	GLU	N-CA-CB	-5.13	101.36	110.60
1	A	171	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	D	50	CYS	CA-CB-SG	5.05	123.08	114.00
1	B	47	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	C	152	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	B	82	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	1445	0	1456	7	1
1	B	1445	0	1456	11	0
1	C	1445	0	1456	8	1
1	D	1445	0	1456	8	0
2	A	27	0	34	0	0
2	B	27	0	35	0	0
2	C	27	0	34	0	0
2	D	27	0	34	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	153	0	0	0	0
4	B	129	0	0	5	0
4	C	138	0	0	3	0
4	D	133	0	0	2	0
All	All	6445	0	5961	34	1

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 (34) 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:40:ARG:NH2	4:B:1047:HOH:O	2.01	0.93
1:D:81:GLN:HG3	1:D:85:ARG:NH1	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:OE1	1:A:39:GLN:NE2	2.23	0.71
1:C:80:ARG:O	1:C:80:ARG:HD2	1.90	0.71
1:B:100:LEU:HD23	1:B:101:ARG:N	2.06	0.71
1:D:7:SER:OG	1:D:40:ARG:HD2	1.92	0.69
1:A:86:GLN:HE22	1:A:128:GLN:HE22	1.41	0.69
1:C:48:ARG:NH1	4:C:1061:HOH:O	2.28	0.66
1:B:85:ARG:CZ	4:B:1069:HOH:O	2.44	0.65
1:D:131:GLN:HE21	1:D:145:GLN:HE21	1.44	0.64
1:D:131:GLN:NE2	1:D:145:GLN:HE21	1.96	0.62
1:C:4:MET:HA	4:C:1102:HOH:O	2.00	0.62
1:B:100:LEU:C	1:B:100:LEU:HD23	2.23	0.59
1:B:85:ARG:NH1	4:B:1069:HOH:O	2.35	0.59
1:B:43:GLN:HE21	1:B:47:ARG:HE	1.52	0.58
1:B:85:ARG:NH2	4:B:1069:HOH:O	2.36	0.58
1:C:131:GLN:HB3	1:C:145:GLN:HG2	1.87	0.57
1:A:63:GLN:HE21	1:A:97:ASN:HA	1.72	0.55
1:C:43:GLN:HE21	1:C:47:ARG:HE	1.55	0.55
1:B:90:PHE:HB2	1:B:93:ARG:HH12	1.73	0.53
1:A:81:GLN:HG3	1:A:85:ARG:NH1	2.24	0.53
1:D:47:ARG:HD3	4:D:1088:HOH:O	2.08	0.52
1:A:86:GLN:NE2	1:A:128:GLN:HE22	2.09	0.47
1:D:140:GLU:HB3	4:D:1039:HOH:O	2.15	0.47
1:A:136:ASP:HB2	1:A:137:PRO:CD	2.46	0.46
1:D:43:GLN:HE21	1:D:47:ARG:HH21	1.64	0.44
1:C:65:LEU:HD12	1:C:65:LEU:C	2.38	0.44
1:C:171:ASP:HB2	4:C:1117:HOH:O	2.18	0.43
1:D:63:GLN:HE21	1:D:97:ASN:HA	1.83	0.42
1:B:25:GLU:HB2	1:B:28:GLN:OE1	2.18	0.42
1:A:136:ASP:HB2	1:A:137:PRO:HD2	2.02	0.42
1:B:111:PRO:HD2	4:B:1069:HOH:O	2.21	0.41
1:C:7:SER:OG	1:C:40:ARG:HD2	2.21	0.41
1:B:97:ASN:N	1:B:98:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:OD2	1:C:3:HIS:O[4_555]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
1	B	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
1	C	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
1	D	181/183 (99%)	180 (99%)	1 (1%)	0	100	100
All	All	724/732 (99%)	720 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	158/158 (100%)	155 (98%)	3 (2%)	57	41
1	B	158/158 (100%)	156 (99%)	2 (1%)	69	56
1	C	158/158 (100%)	154 (98%)	4 (2%)	47	29
1	D	158/158 (100%)	157 (99%)	1 (1%)	86	80
All	All	632/632 (100%)	622 (98%)	10 (2%)	62	48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	56	PRO

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Mol	Chain	Res	Type
1	A	78	PRO
1	B	4	MET
1	B	49	ARG
1	C	18	ARG
1	C	73	LEU
1	C	136	ASP
1	C	157	GLU
1	D	18	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	63	GLN
1	A	86	GLN
1	A	138	ASN
1	B	43	GLN
1	B	63	GLN
1	C	81	GLN
1	D	43	GLN
1	D	63	GLN
1	D	81	GLN
1	D	131	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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$
2	BB2	C	1003	3	27,27,27	1.94	6 (22%)	34,35,35	1.99	8 (23%)
2	BB2	D	1004	3	27,27,27	1.87	5 (18%)	34,35,35	1.97	11 (32%)
2	BB2	A	1001	3	27,27,27	1.93	7 (25%)	34,35,35	3.10	10 (29%)
2	BB2	B	1002	3	27,27,27	2.29	9 (33%)	34,35,35	2.90	12 (35%)

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	BB2	C	1003	3	-	1/33/43/43	0/1/1/1
2	BB2	D	1004	3	-	0/33/43/43	0/1/1/1
2	BB2	A	1001	3	-	2/33/43/43	0/1/1/1
2	BB2	B	1002	3	-	0/33/43/43	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1003	BB2	C3-N1	-7.57	1.24	1.32
2	D	1004	BB2	C3-N1	-7.15	1.24	1.32
2	B	1002	BB2	C3-N1	-6.45	1.25	1.32
2	A	1001	BB2	C6-C12	-4.96	1.42	1.51
2	B	1002	BB2	C6-C12	-4.95	1.43	1.51
2	A	1001	BB2	C3-N1	-4.21	1.27	1.32
2	B	1002	BB2	O20-C19	3.49	1.28	1.22
2	A	1001	BB2	C12-N14	3.17	1.41	1.34
2	D	1004	BB2	O20-C19	3.01	1.27	1.22
2	A	1001	BB2	O20-C19	2.96	1.27	1.22
2	B	1002	BB2	C5-C6	2.91	1.59	1.53
2	B	1002	BB2	C25-C22	2.84	1.60	1.53
2	B	1002	BB2	C24-C23	2.75	1.61	1.51
2	C	1003	BB2	C23-N21	2.69	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	BB2	O2-N1	2.54	1.46	1.40
2	B	1002	BB2	C23-N21	2.53	1.52	1.47
2	D	1004	BB2	C23-N21	2.44	1.52	1.47
2	C	1003	BB2	C8-C7	2.29	1.62	1.52
2	A	1001	BB2	O4-C3	2.27	1.27	1.23
2	C	1003	BB2	O2-N1	2.25	1.45	1.40
2	A	1001	BB2	C23-N21	2.24	1.51	1.47
2	C	1003	BB2	C25-C22	2.22	1.59	1.53
2	D	1004	BB2	C5-C3	-2.21	1.46	1.51
2	C	1003	BB2	C15-N14	2.21	1.50	1.45
2	B	1002	BB2	C15-N14	2.20	1.50	1.45
2	D	1004	BB2	O4-C3	2.17	1.27	1.23
2	A	1001	BB2	C25-C22	2.13	1.58	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	BB2	O4-C3-N1	-13.31	106.93	123.27
2	B	1002	BB2	O4-C3-N1	-12.45	107.99	123.27
2	C	1003	BB2	O2-N1-C3	-5.94	111.02	119.79
2	C	1003	BB2	O4-C3-N1	-5.61	116.39	123.27
2	A	1001	BB2	C5-C3-N1	5.33	123.22	115.14
2	A	1001	BB2	O4-C3-C5	5.27	129.22	121.50
2	D	1004	BB2	O4-C3-N1	-5.16	116.93	123.27
2	D	1004	BB2	O2-N1-C3	-4.75	112.77	119.79
2	B	1002	BB2	C5-C3-N1	4.69	122.24	115.14
2	A	1001	BB2	C17-C16-C18	4.52	123.23	110.59
2	B	1002	BB2	O27-C26-C22	-4.01	95.52	111.50
2	B	1002	BB2	C24-C23-N21	-3.87	96.46	103.25
2	C	1003	BB2	C23-N21-C22	3.59	117.53	111.52
2	A	1001	BB2	C6-C12-N14	3.46	122.20	116.21
2	A	1001	BB2	O13-C12-N14	-3.41	116.61	122.93
2	C	1003	BB2	O27-C26-C22	-3.40	97.98	111.50
2	B	1002	BB2	O13-C12-C6	3.36	126.49	122.12
2	B	1002	BB2	O4-C3-C5	3.36	126.41	121.50
2	D	1004	BB2	C18-C16-C15	-3.19	102.14	111.16
2	C	1003	BB2	C5-C3-N1	3.14	119.90	115.14
2	B	1002	BB2	O13-C12-N14	-3.14	117.12	122.93
2	D	1004	BB2	O20-C19-N21	-3.01	116.01	121.38
2	D	1004	BB2	C5-C3-N1	2.86	119.47	115.14
2	B	1002	BB2	C7-C6-C12	-2.81	104.74	109.53
2	A	1001	BB2	O2-N1-C3	-2.53	116.05	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1004	BB2	C6-C5-C3	-2.49	107.38	112.10
2	D	1004	BB2	C25-C22-C26	-2.48	105.85	112.95
2	A	1001	BB2	O27-C26-C22	-2.45	101.75	111.50
2	C	1003	BB2	C5-C6-C12	-2.44	106.24	109.77
2	B	1002	BB2	O20-C19-C15	2.42	124.71	119.99
2	B	1002	BB2	O2-N1-C3	-2.39	116.25	119.79
2	D	1004	BB2	O27-C26-C22	-2.38	102.03	111.50
2	A	1001	BB2	C7-C6-C5	2.36	118.00	109.85
2	C	1003	BB2	O20-C19-N21	-2.36	117.17	121.38
2	D	1004	BB2	O13-C12-N14	-2.27	118.72	122.93
2	D	1004	BB2	C16-C15-C19	-2.23	106.21	110.73
2	B	1002	BB2	C25-C22-C26	-2.22	106.58	112.95
2	C	1003	BB2	O20-C19-C15	2.17	124.22	119.99
2	D	1004	BB2	O20-C19-C15	2.15	124.18	119.99
2	B	1002	BB2	C26-C22-N21	-2.04	103.18	112.53
2	A	1001	BB2	C24-C23-N21	2.04	106.82	103.25

There are no chirality outliers.

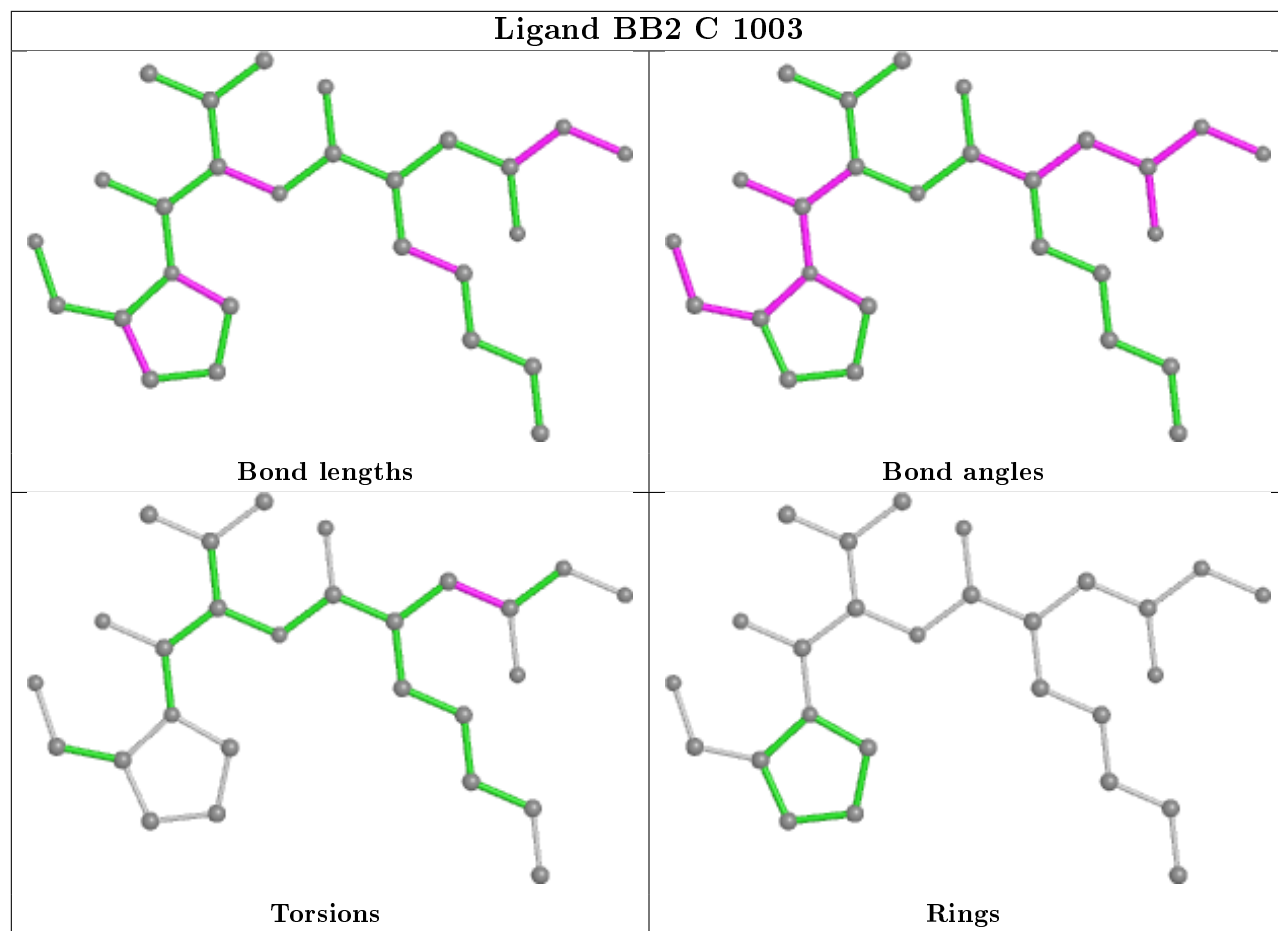
All (3) torsion outliers are listed below:

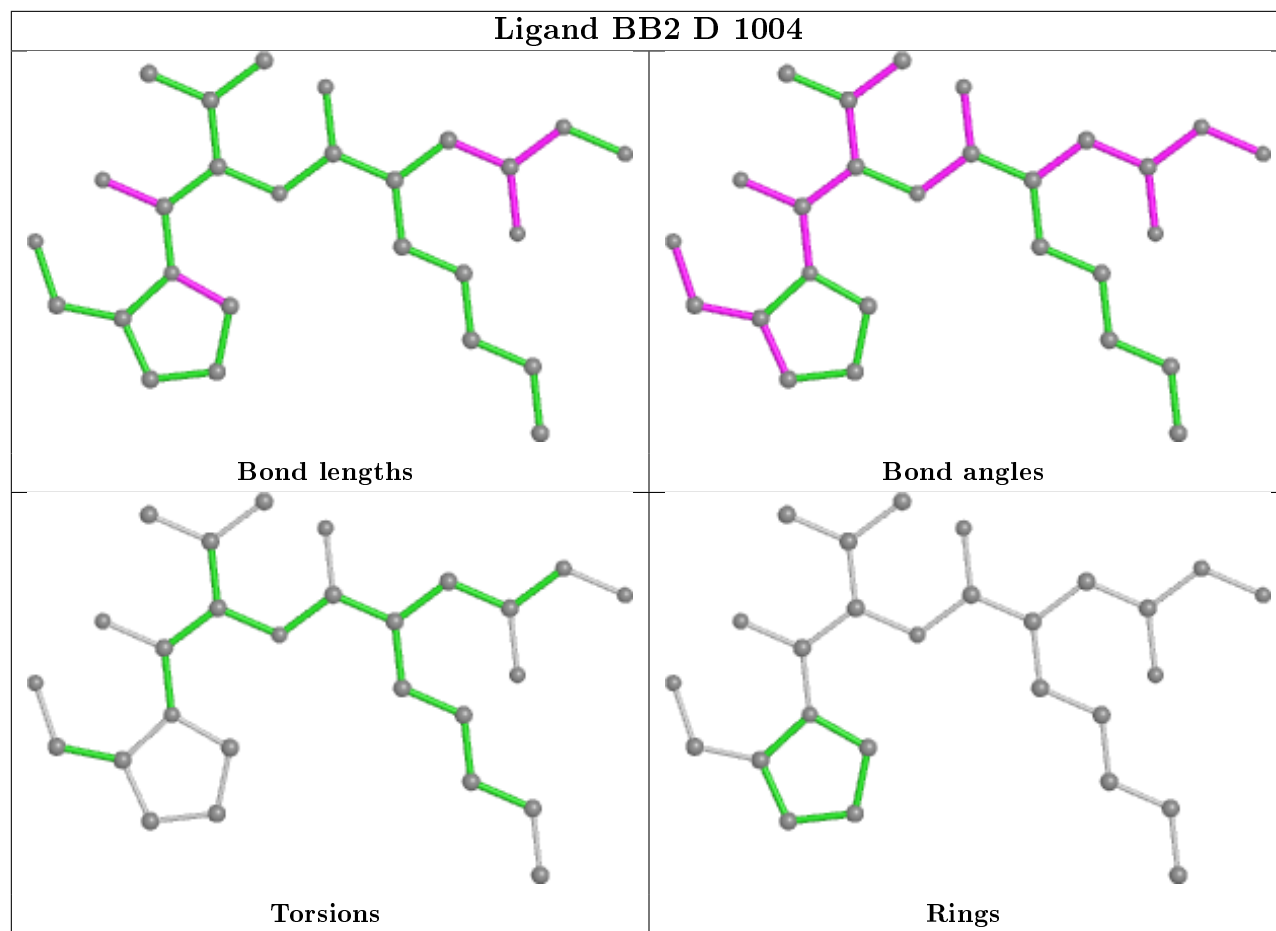
Mol	Chain	Res	Type	Atoms
2	C	1003	BB2	N1-C3-C5-C6
2	A	1001	BB2	N1-C3-C5-C6
2	A	1001	BB2	O4-C3-C5-C6

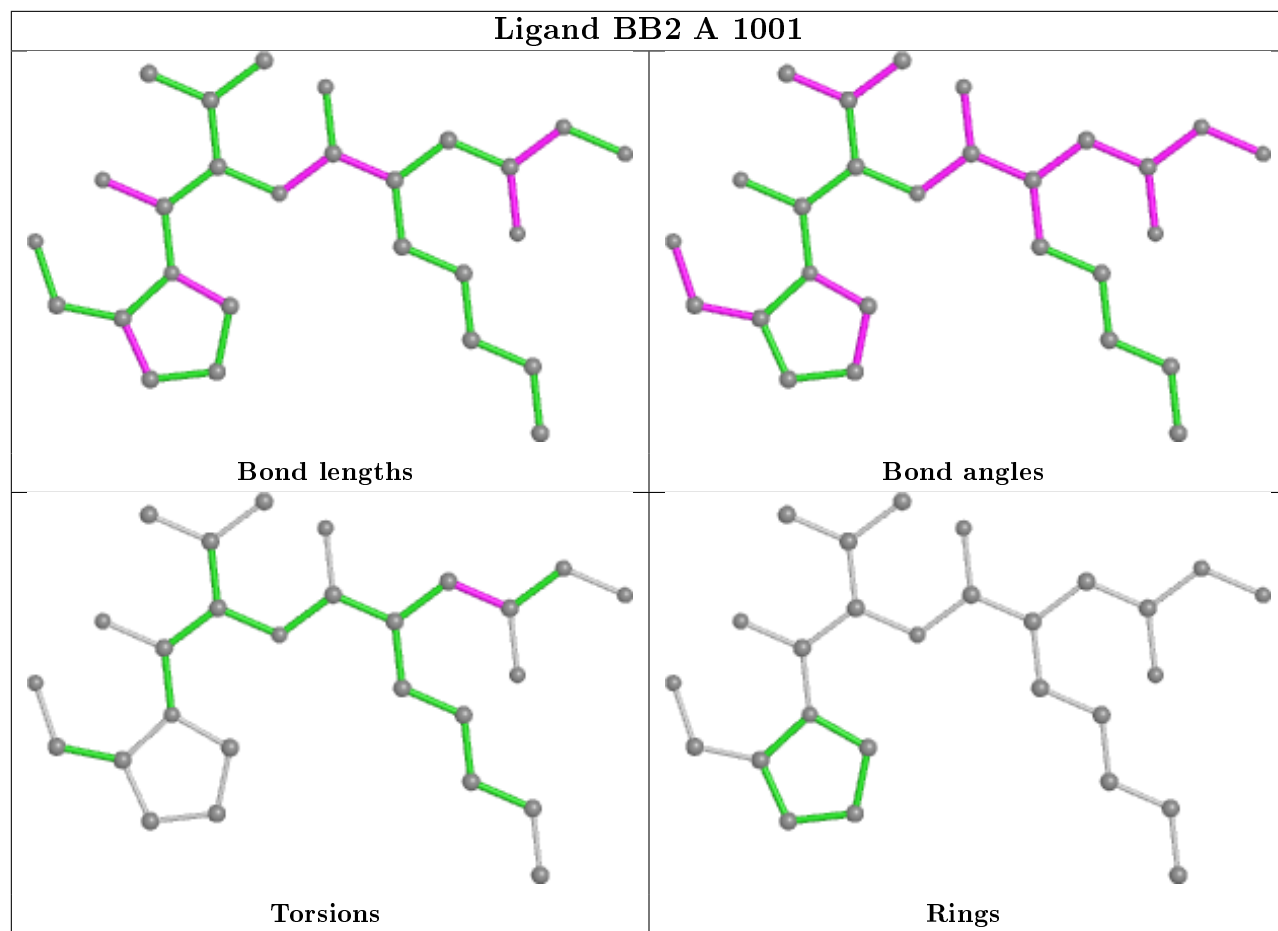
There are no ring outliers.

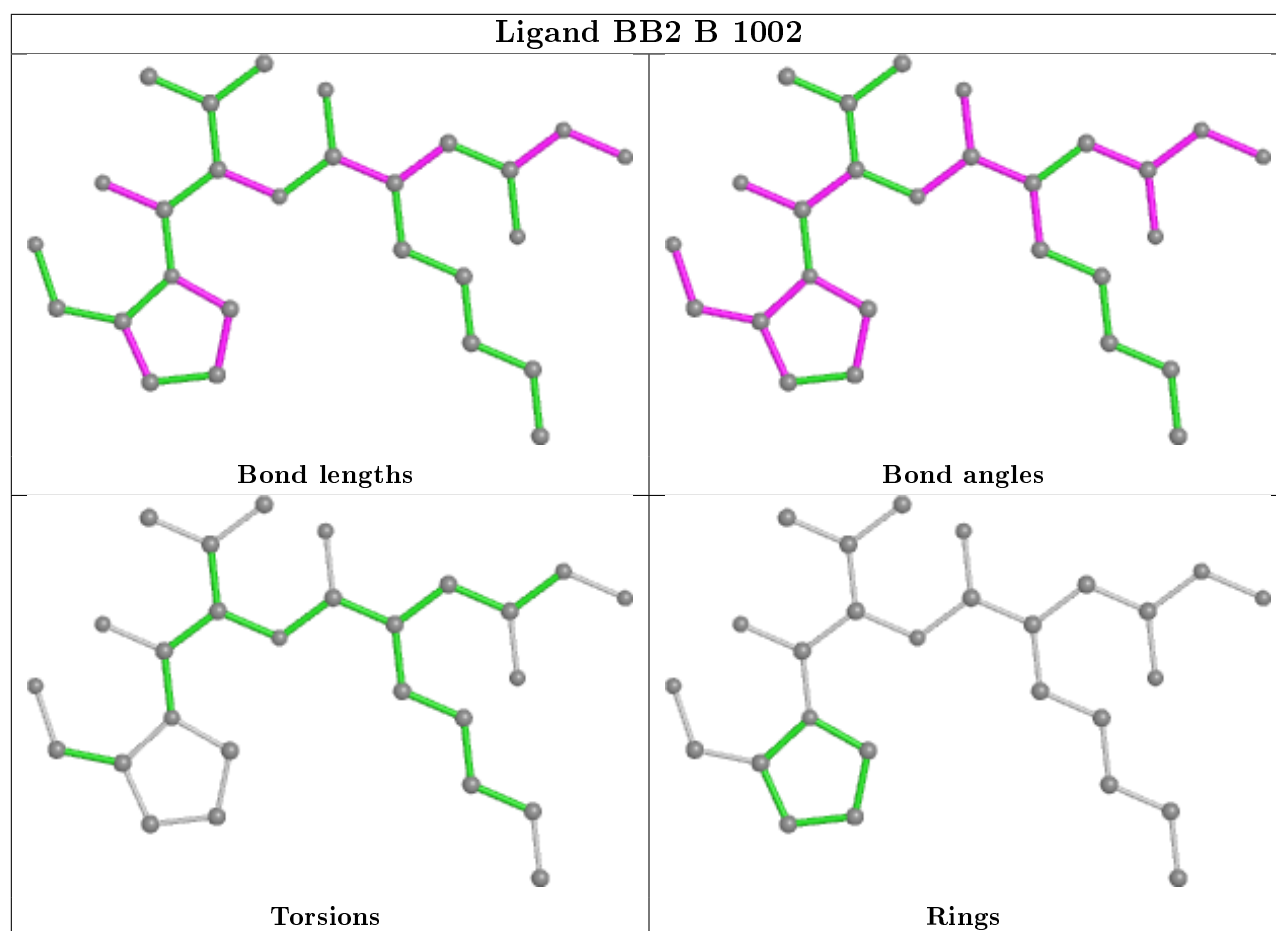
No monomer is involved in short contacts.

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 ⓘ

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	183/183 (100%)	-0.39	6 (3%)	46	51	6, 12, 33, 59	0
1	B	183/183 (100%)	-0.18	5 (2%)	54	58	5, 12, 34, 68	0
1	C	183/183 (100%)	-0.18	6 (3%)	46	51	6, 13, 37, 68	0
1	D	183/183 (100%)	-0.34	4 (2%)	62	66	6, 14, 34, 58	0
All	All	732/732 (100%)	-0.28	21 (2%)	51	56	5, 13, 35, 68	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	HIS	10.3
1	C	3	HIS	9.1
1	A	3	HIS	7.4
1	B	4	MET	6.6
1	D	3	HIS	6.5
1	D	185	ASP	5.8
1	A	185	ASP	5.2
1	B	185	ASP	3.4
1	C	138	ASN	3.2
1	C	185	ASP	3.2
1	A	80	ARG	3.2
1	A	4	MET	3.1
1	B	80	ARG	3.0
1	D	4	MET	2.9
1	C	80	ARG	2.7
1	D	27	ALA	2.6
1	C	4	MET	2.6
1	A	79	PRO	2.3
1	A	184	ASN	2.1
1	B	75	ARG	2.0
1	C	137	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

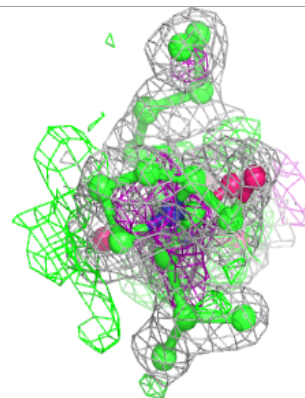
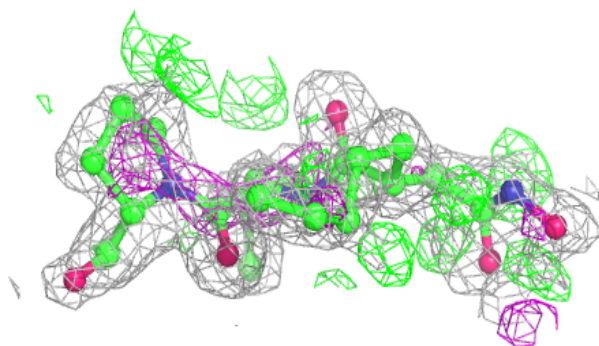
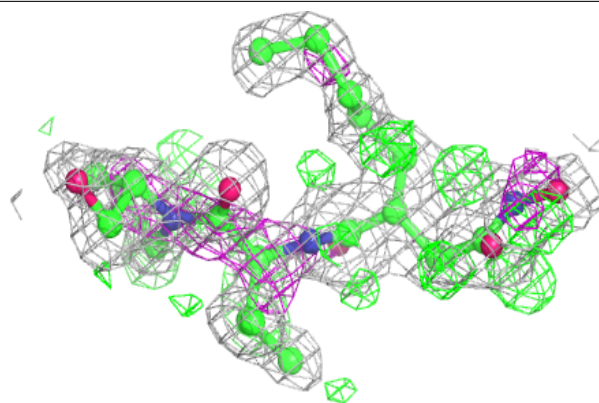
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BB2	B	1002	27/27	0.90	0.14	6,22,33,40	0
2	BB2	A	1001	27/27	0.91	0.13	7,21,28,31	0
2	BB2	C	1003	27/27	0.95	0.09	10,17,25,36	0
2	BB2	D	1004	27/27	0.96	0.08	9,17,27,29	0
3	CO	B	1003	1/1	0.99	0.04	9,9,9,9	0
3	CO	D	2	1/1	0.99	0.04	10,10,10,10	0
3	CO	A	1002	1/1	1.00	0.04	9,9,9,9	0
3	CO	C	1	1/1	1.00	0.03	8,8,8,8	0

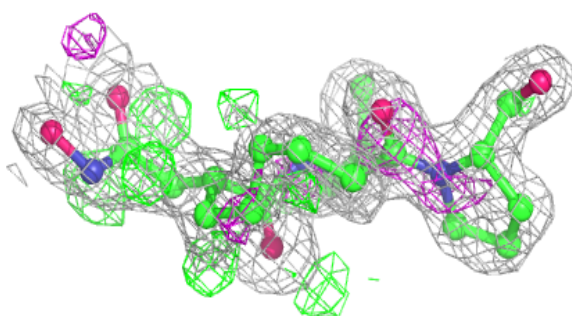
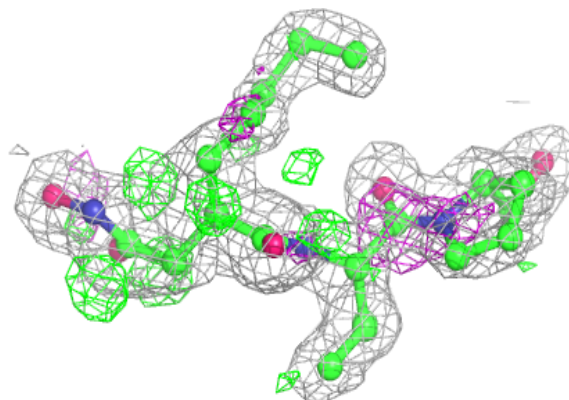
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BB2 B 1002:

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

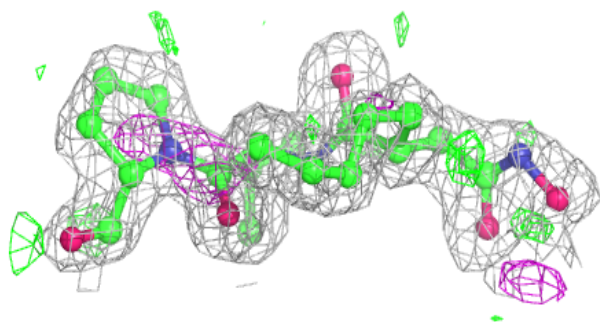
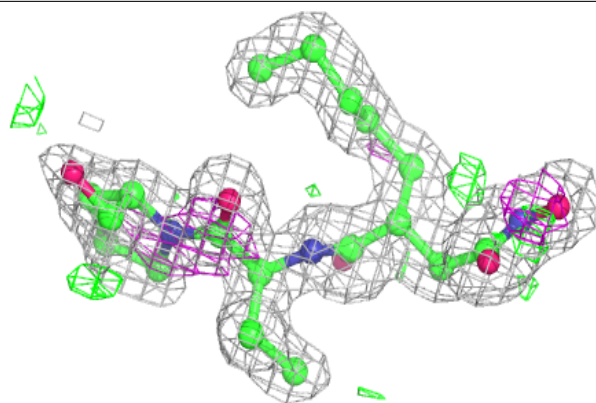
**Electron density around BB2 A 1001:**

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

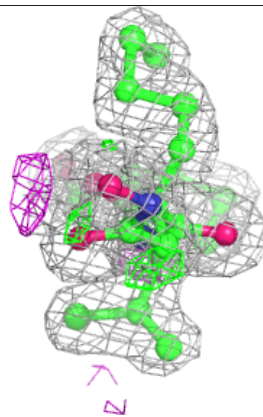
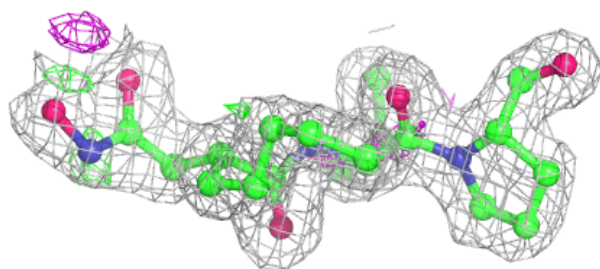
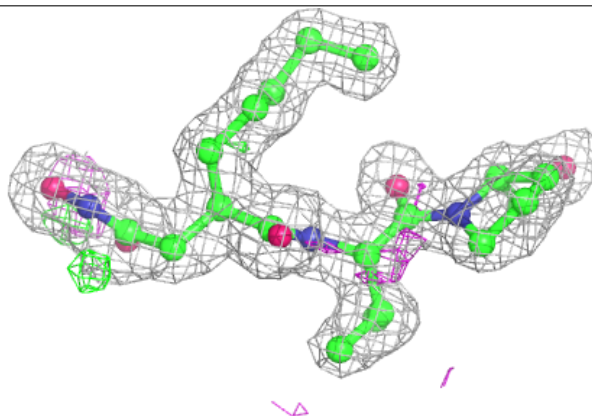


Electron density around BB2 C 1003:

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

**Electron density around BB2 D 1004:**

$2mF_o-DF_c$ (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.