



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 12:38 pm GMT

PDB ID : 6QTK
Title : 2.31A structure of gepotidacin with S.aureus DNA gyrase and doubly nicked DNA
Authors : Bax, B.D.
Deposited on : 2019-02-25
Resolution : 2.31 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

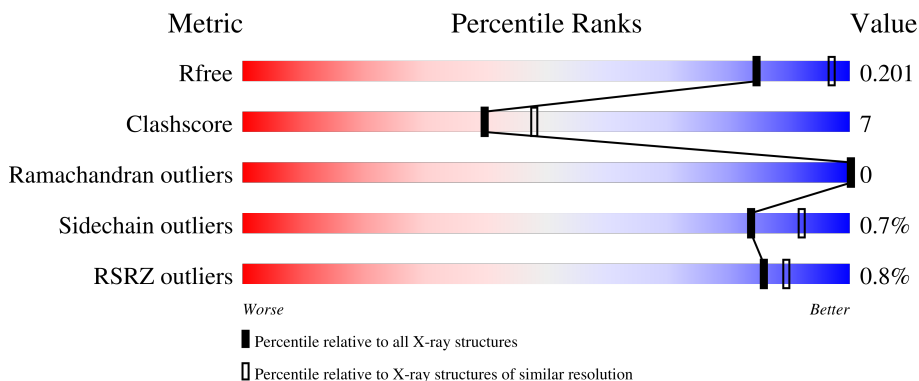
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	B	202	
1	D	202	
2	A	490	
2	C	490	
3	E	20	

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Mol	Chain	Length	Quality of chain
3	F	20	 55% 30% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	501	-	-	X	-
5	GOL	E	2101[B]	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 12785 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 DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	192	1567	980	269	309	9	0	10	0
1	D	192	1481	930	255	287	9	0	0	0

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	LEU	conflict	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	GLY	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	VAL	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	ARG	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TRP	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	ILE	deletion	UNP P66937
B	544	THR	ALA	conflict	UNP P66937
B	545	GLY	ARG	conflict	UNP P66937
D	409	MET	LEU	conflict	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	THR	deletion	UNP P66937
D	?	-	GLN	deletion	UNP P66937
D	?	-	GLY	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	GLN	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	VAL	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	ASN	deletion	UNP P66937
D	?	-	ASP	deletion	UNP P66937
D	?	-	ARG	deletion	UNP P66937
D	?	-	GLU	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	ASP	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	SER	deletion	UNP P66937
D	?	-	GLU	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	ASN	deletion	UNP P66937
D	?	-	PRO	deletion	UNP P66937
D	?	-	THR	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	TRP	deletion	UNP P66937
D	?	-	SER	deletion	UNP P66937
D	?	-	ILE	deletion	UNP P66937
D	544	THR	ALA	conflict	UNP P66937
D	545	GLY	ARG	conflict	UNP P66937

- Molecule 2 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	484	Total	C	N	O	S	0	11	0
			3926	2437	718	754	17			
2	C	482	Total	C	N	O	S	0	17	0
			3966	2461	725	761	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	PHE	TYR	conflict	UNP Q99XG5
C	123	PHE	TYR	conflict	UNP Q99XG5

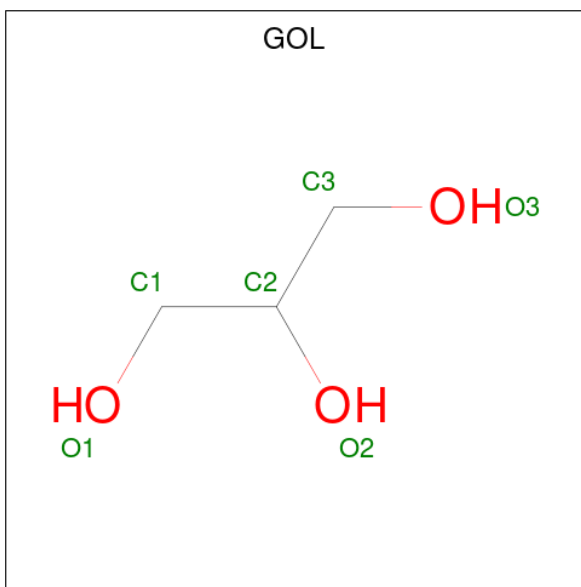
- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G*GP*GP*T
P*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	20	Total	C	N	O	P	0	4	0
			487	232	89	143	23			
3	F	20	Total	C	N	O	P	0	0	0
			398	189	74	116	19			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	1
			2	2		
4	D	1	Total	Mn	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

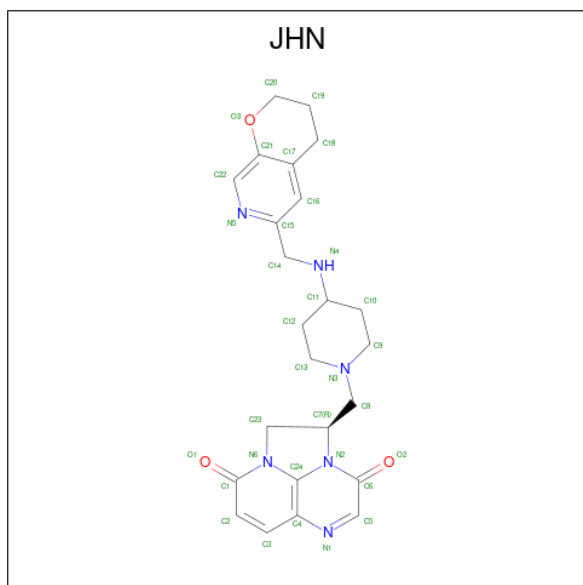


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	E	1	Total C O 12 6 6	0	1
5	E	1	Total C O 6 3 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

- Molecule 7 is (3 {R})-3-[[4-(3,4-dihydro-2 {H}-pyrano[2,3-c]pyridin-6-ylmethylamino) piperidin-1-yl]methyl]-1,4,7-triazatricyclo[6.3.1.0^{4,12}]dodeca-6,8(12),9-triene-5,11-dione (three-letter code: JHN) (formula: C₂₄H₂₈N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	F	1	66	48	12	6	0	1

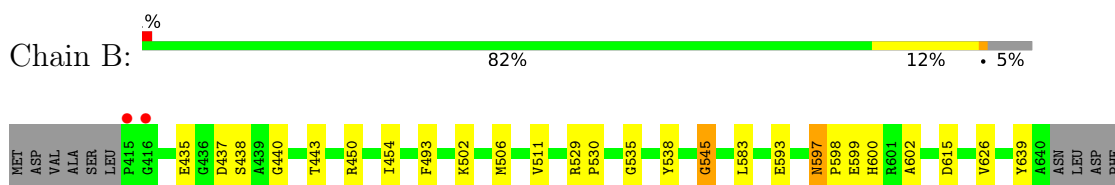
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	77	Total	O	0	5
			79	79		
8	A	285	Total	O	0	3
			287	287		
8	D	50	Total	O	0	0
			50	50		
8	C	312	Total	O	0	4
			316	316		
8	E	55	Total	O	0	5
			58	58		
8	F	44	Total	O	0	3
			46	46		

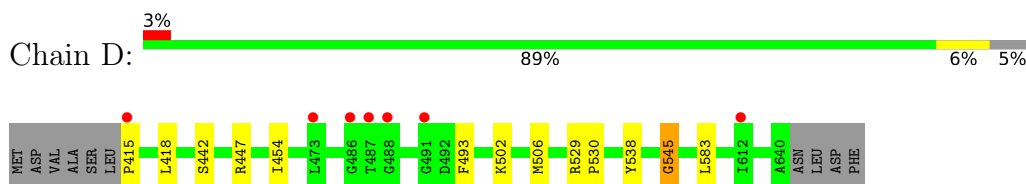
3 Residue-property plots [i](#)

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.

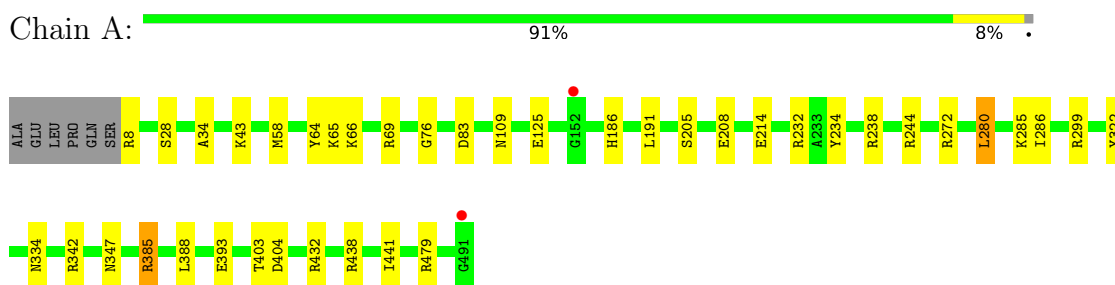
- Molecule 1: DNA gyrase subunit B



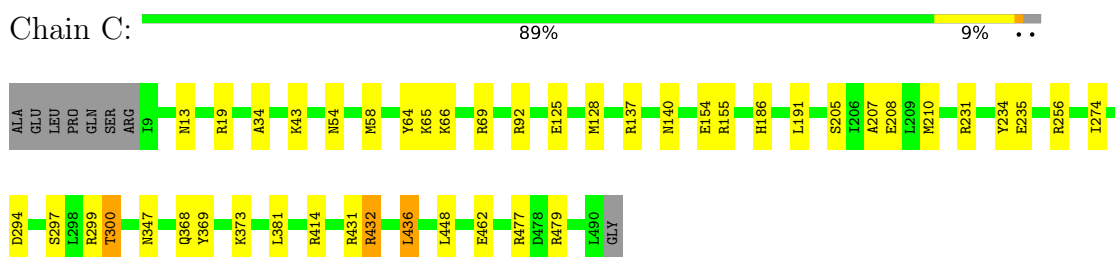
- Molecule 1: DNA gyrase subunit B



- Molecule 2: DNA gyrase subunit A

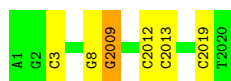


- Molecule 2: DNA gyrase subunit A



- Molecule 3: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

Chain E:  70% 25% 5%



• Molecule 3: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

Chain F:  55% 30% 15%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.73Å 92.73Å 408.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.99 – 2.31 39.96 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.99-2.31) 99.8 (39.96-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.163 , 0.203 0.161 , 0.201	Depositor DCC
R_{free} test set	3426 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.075 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: JHN, MN, GOL, 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	B	0.43	1/1592 (0.1%)	0.79	2/2151 (0.1%)
1	D	0.45	1/1506 (0.1%)	0.78	1/2037 (0.0%)
2	A	0.43	0/3974	0.73	0/5348
2	C	0.43	0/4014	0.75	2/5400 (0.0%)
3	E	0.58	0/544	1.03	3/835 (0.4%)
3	F	0.72	0/445	1.08	4/682 (0.6%)
All	All	0.45	2/12075 (0.0%)	0.79	12/16453 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	545	GLY	C-N	8.79	1.54	1.34
1	B	545	GLY	C-N	5.78	1.47	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	545	GLY	O-C-N	-14.53	99.45	122.70
1	B	545	GLY	O-C-N	-12.46	102.77	122.70
3	E	2019	DC	O5'-P-OP1	7.81	120.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	GLY	CA-C-N	6.43	131.35	117.20
3	F	2019	DC	C1'-O4'-C4'	-6.07	104.03	110.10
3	F	1	DA	C1'-O4'-C4'	-5.95	104.15	110.10
3	F	2012	DC	O5'-P-OP1	-5.60	100.66	105.70
3	F	2019	DC	O5'-P-OP2	-5.57	100.69	105.70
3	E	2009[A]	DG	O4'-C4'-C3'	-5.44	102.32	104.50
3	E	2009[B]	DG	O4'-C4'-C3'	-5.44	102.32	104.50
2	C	432	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	C	256	ARG	CG-CD-NE	-5.11	101.06	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	545	GLY	Mainchain
1	D	545	GLY	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1567	0	1522	24	0
1	D	1481	0	1436	10	0
2	A	3926	0	3965	60	0
2	C	3966	0	3993	50	1
3	E	487	0	271	22	0
3	F	398	0	220	12	1
4	B	2	0	0	0	0
4	D	1	0	0	0	0
5	A	12	0	16	10	0
5	C	24	0	32	6	0
5	E	18	0	24	10	0
6	A	1	0	0	0	0
7	F	66	0	0	0	0
8	A	287	0	0	8	1
8	B	79	0	0	5	0
8	C	316	0	0	15	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	50	0	0	2	0
8	E	58	0	0	11	1
8	F	46	0	0	3	0
All	All	12785	0	11479	170	3

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 7.

All (170) 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:A:385[B]:ARG:CD	2:A:385[B]:ARG:CG	1.75	1.56
3:E:2009[B]:DG:H5''	3:E:2009[B]:DG:C8	1.53	1.42
3:E:2009[B]:DG:C8	3:E:2009[B]:DG:C5'	2.21	1.22
3:E:2009[B]:DG:C5'	3:E:2009[B]:DG:H8	1.56	1.17
3:E:2009[B]:DG:OP2	5:E:2101[B]:GOL:H12	1.47	1.14
2:C:65[B]:LYS:HG3	8:C:865[B]:HOH:O	1.54	1.05
2:C:155:ARG:HG2	5:C:503:GOL:H31	1.36	1.05
3:F:2019:DC:H3'	3:F:2020:DT:C5'	1.92	1.00
3:F:2019:DC:H3'	3:F:2020:DT:H5''	1.00	0.99
2:C:69[B]:ARG:HD3	8:C:792[B]:HOH:O	1.63	0.98
3:F:2019:DC:C3'	3:F:2020:DT:H5''	1.94	0.98
3:F:5:DG:OP2	8:F:2201:HOH:O	1.82	0.97
1:B:438[B]:SER:HB3	8:E:2204[B]:HOH:O	1.73	0.89
3:E:2009[B]:DG:N7	5:E:2101[B]:GOL:H11	1.89	0.88
3:E:8:DG:O6	5:E:2101[B]:GOL:H32	1.76	0.86
3:E:2009[B]:DG:H4'	8:E:2231[B]:HOH:O	1.76	0.86
3:E:2009[B]:DG:OP2	5:E:2101[B]:GOL:C1	2.23	0.86
2:A:65[B]:LYS:HD3	2:A:69:ARG:NH1	1.93	0.83
2:A:69:ARG:HB2	5:A:501:GOL:O2	1.79	0.83
1:B:437[B]:ASP:O	1:B:440:GLY:N	2.11	0.83
3:E:2009[B]:DG:C4'	8:E:2231[B]:HOH:O	2.27	0.83
2:C:208[A]:GLU:OE1	8:C:601:HOH:O	1.97	0.82
3:F:2013:DC:OP2	8:F:2202:HOH:O	1.96	0.81
2:A:58[B]:MET:SD	2:A:65[B]:LYS:HB2	2.20	0.81
3:E:2009[B]:DG:O6	3:F:2012:DC:N4	2.14	0.81
2:C:205:SER:OG	2:C:208[B]:GLU:HG3	1.82	0.79
5:E:2102:GOL:O2	8:E:2201:HOH:O	2.00	0.79
3:E:2009[B]:DG:O5'	8:E:2231[B]:HOH:O	2.00	0.79
2:A:65[B]:LYS:HD3	2:A:69:ARG:HD3	1.66	0.77
2:A:65[B]:LYS:CD	2:A:69:ARG:HD3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2009[B]:DG:C8	5:E:2101[B]:GOL:H11	2.21	0.76
2:A:69:ARG:HD2	5:A:501:GOL:C3	2.16	0.76
2:C:58[B]:MET:SD	2:C:65[B]:LYS:HB2	2.26	0.75
3:E:2013[A]:DC:H5''	8:E:2238[A]:HOH:O	1.85	0.74
2:A:69:ARG:HD2	5:A:501:GOL:H31	1.68	0.74
3:E:2009[B]:DG:C8	3:E:2009[B]:DG:H5'	2.24	0.73
3:E:2009[B]:DG:H5''	3:E:2009[B]:DG:H8	0.67	0.72
2:A:238:ARG:HH21	2:A:334:ASN:HD21	1.38	0.71
1:D:502:LYS:NZ	8:D:801:HOH:O	2.21	0.71
2:C:297:SER:OG	2:C:300:THR:HG23	1.90	0.70
2:A:65[B]:LYS:CE	5:A:501:GOL:H12	2.22	0.70
2:A:83[A]:ASP:OD1	8:A:601[A]:HOH:O	2.10	0.69
2:A:65[B]:LYS:HD3	2:A:69:ARG:CZ	2.21	0.69
3:E:2009[B]:DG:OP1	8:E:2202:HOH:O	2.10	0.69
8:A:687:HOH:O	2:C:431:ARG:HD2	1.94	0.68
2:A:385[B]:ARG:CG	2:A:385[B]:ARG:NE	2.52	0.66
3:F:2011:DA:H2''	3:F:2012:DC:H5''	1.78	0.66
1:B:615:ASP:HB3	8:B:839:HOH:O	1.96	0.64
2:C:207:ALA:HB2	2:C:231[B]:ARG:HH22	1.62	0.64
3:F:1:DA:H2'	3:F:2:DG:C8	2.34	0.63
2:C:208[A]:GLU:HG2	8:C:601:HOH:O	1.98	0.63
3:E:2009[B]:DG:C5'	8:E:2231[B]:HOH:O	2.44	0.63
5:E:2102:GOL:H12	8:E:2228:HOH:O	1.99	0.62
2:A:65[B]:LYS:HE2	5:A:501:GOL:H31	1.81	0.62
1:D:418:LEU:C	1:D:418:LEU:HD23	2.20	0.62
2:A:65[B]:LYS:HD3	2:A:69:ARG:CD	2.29	0.61
3:E:2012[A]:DC:H2''	8:E:2238[A]:HOH:O	2.00	0.61
2:C:414[A]:ARG:HD3	8:C:754[A]:HOH:O	1.99	0.60
8:D:806:HOH:O	2:C:19:ARG:HD2	2.01	0.60
2:C:58[A]:MET:HG2	2:C:65[A]:LYS:HG3	1.82	0.60
2:C:369:TYR:CE2	2:C:373:LYS:HE3	2.36	0.60
1:B:435[B]:GLU:HG3	8:B:805:HOH:O	2.02	0.60
2:A:403:THR:HG22	2:C:436:LEU:HD22	1.83	0.60
2:A:280:LEU:HD22	2:A:285:LYS:HB2	1.84	0.59
2:C:207:ALA:HB2	2:C:231[B]:ARG:NH2	2.16	0.59
2:A:385[A]:ARG:CG	2:A:385[A]:ARG:HH11	2.15	0.59
1:B:443:THR:HG22	1:B:454:ILE:HD12	1.84	0.59
2:C:479:ARG:HD2	8:C:806:HOH:O	2.01	0.59
2:A:432:ARG:HG3	2:A:432:ARG:HH11	1.68	0.59
2:A:65[B]:LYS:HD3	2:A:69:ARG:HH11	1.68	0.58
2:A:214[B]:GLU:CG	8:A:603:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ARG:HD2	8:B:806:HOH:O	2.02	0.57
2:A:69:ARG:HB2	5:A:501:GOL:HO2	1.67	0.57
2:A:205:SER:OG	2:A:208[B]:GLU:HG3	2.03	0.57
2:A:232:ARG:NH1	8:A:607:HOH:O	2.37	0.57
2:C:58[B]:MET:SD	2:C:65[B]:LYS:CB	2.92	0.57
1:D:506:MET:HG2	1:D:583:LEU:HD11	1.87	0.56
2:C:140:ASN:HB2	8:C:682:HOH:O	2.05	0.56
2:A:272:ARG:CZ	3:E:3:DC:H5''	2.35	0.56
2:C:368:GLN:NE2	8:C:605:HOH:O	2.38	0.56
1:B:506:MET:HG2	1:B:583:LEU:HD11	1.88	0.55
1:B:597:ASN:HD22	1:B:598:PRO:HD2	1.70	0.55
2:A:58[A]:MET:HG2	2:A:65[A]:LYS:HG3	1.89	0.55
2:A:76:GLY:HA3	2:C:69[B]:ARG:HE	1.69	0.55
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.42	0.55
5:E:2102:GOL:H11	8:E:2247:HOH:O	2.07	0.55
2:C:34:ALA:O	2:C:43:LYS:HE2	2.07	0.54
2:A:34:ALA:O	2:A:43:LYS:HE2	2.07	0.54
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.37	0.54
2:A:65[B]:LYS:CD	2:A:69:ARG:NH1	2.68	0.54
1:D:415:PRO:HG2	1:D:418:LEU:HB2	1.90	0.53
2:C:137:ARG:HD2	8:C:872:HOH:O	2.08	0.53
2:A:385[B]:ARG:HG3	2:A:438:ARG:CZ	2.38	0.53
2:A:238:ARG:HE	2:A:334:ASN:ND2	2.05	0.53
3:E:2009[B]:DG:N7	5:E:2101[B]:GOL:C1	2.69	0.53
1:B:443:THR:CG2	1:B:454:ILE:HD12	2.39	0.52
2:A:66:LYS:HD2	8:A:793:HOH:O	2.09	0.52
2:C:58[B]:MET:HE3	8:C:645:HOH:O	2.08	0.52
2:C:58[B]:MET:CE	2:C:65[B]:LYS:HB2	2.39	0.52
2:C:125:GLU:OE2	5:C:504:GOL:H12	2.09	0.52
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.45	0.52
1:B:602:ALA:HB2	2:A:8:ARG:HH21	1.73	0.52
2:C:125:GLU:CD	5:C:504:GOL:H12	2.30	0.52
1:D:493:PHE:CE1	1:D:530:PRO:HB2	2.45	0.51
2:A:58[B]:MET:SD	2:A:65[B]:LYS:CB	2.95	0.51
2:C:154:GLU:HA	5:C:503:GOL:H32	1.93	0.51
2:C:231[B]:ARG:NE	2:C:235:GLU:OE2	2.30	0.51
1:B:502:LYS:HG2	1:B:538:TYR:CE1	2.46	0.51
3:E:2009[B]:DG:C8	3:E:2009[B]:DG:C4'	2.89	0.50
2:A:65[B]:LYS:HE2	5:A:501:GOL:H12	1.93	0.50
2:A:69:ARG:HH11	5:A:501:GOL:H31	1.77	0.50
2:A:385[A]:ARG:HH11	2:A:385[A]:ARG:CB	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:69:ARG:HD2	5:A:501:GOL:O3	2.11	0.49
2:A:234:TYR:O	2:A:347:ASN:HB2	2.12	0.49
2:C:125:GLU:OE1	5:C:504:GOL:H12	2.13	0.48
2:A:385[B]:ARG:CD	2:A:385[B]:ARG:CB	2.80	0.48
2:C:66:LYS:HB2	2:C:69[B]:ARG:HG3	1.96	0.48
1:B:597:ASN:HD22	1:B:598:PRO:CD	2.27	0.48
1:D:447:ARG:HD3	1:D:454:ILE:HD11	1.96	0.48
2:A:388:LEU:HD12	2:A:441:ILE:HD12	1.96	0.47
2:A:65[B]:LYS:CE	2:A:69:ARG:HD3	2.44	0.47
1:B:511[B]:VAL:HG11	2:A:28:SER:HB2	1.96	0.47
2:A:479:ARG:HD2	8:A:665:HOH:O	2.14	0.47
2:A:385[A]:ARG:HH11	2:A:385[A]:ARG:HG2	1.79	0.47
2:C:64:TYR:HB3	2:C:125:GLU:HB3	1.97	0.47
2:C:58[B]:MET:CE	2:C:65[B]:LYS:CB	2.92	0.47
2:C:155:ARG:CG	5:C:503:GOL:H31	2.26	0.46
2:A:244:ARG:HG3	2:A:322:TYR:CE1	2.51	0.46
2:C:69[B]:ARG:CD	8:C:792[B]:HOH:O	2.41	0.45
1:B:435[B]:GLU:N	8:B:805:HOH:O	2.49	0.45
2:C:92[A]:ARG:NH1	3:F:5:DG:OP1	2.50	0.45
2:C:234:TYR:O	2:C:347:ASN:HB2	2.17	0.45
2:A:208[A]:GLU:OE2	8:A:602:HOH:O	2.20	0.44
2:C:210:MET:SD	2:C:231[B]:ARG:HD3	2.56	0.44
1:D:447:ARG:HD3	1:D:454:ILE:CD1	2.47	0.44
2:A:65[B]:LYS:HD3	2:A:69:ARG:NE	2.32	0.44
1:D:529:ARG:N	1:D:530:PRO:CD	2.81	0.44
1:B:535:GLY:HA2	8:B:866:HOH:O	2.18	0.44
1:B:639:TYR:CD2	2:A:342:ARG:HG2	2.52	0.43
3:E:2009[A]:DG:O6	5:E:2101[A]:GOL:H11	2.18	0.43
1:B:593:GLU:OE1	1:B:600:HIS:HD2	2.01	0.43
3:F:2013:DC:H5''	8:F:2202:HOH:O	2.18	0.43
2:A:186:HIS:HB2	2:A:191:LEU:HD11	2.00	0.43
2:A:280:LEU:HD13	2:A:286:ILE:HB	2.01	0.43
2:C:477:ARG:NE	8:C:616:HOH:O	2.48	0.43
1:B:626:VAL:HG11	3:F:2017:DG:H3'	2.01	0.42
2:A:65[B]:LYS:HE2	5:A:501:GOL:C1	2.49	0.42
2:A:385[B]:ARG:HG3	2:A:438:ARG:NH2	2.34	0.42
2:C:432:ARG:HD3	8:C:824:HOH:O	2.18	0.42
2:A:65[B]:LYS:CD	2:A:69:ARG:HH11	2.30	0.42
2:C:414[A]:ARG:CD	8:C:754[A]:HOH:O	2.65	0.42
1:B:597:ASN:ND2	1:B:599:GLU:H	2.17	0.42
2:A:385[A]:ARG:HG2	2:A:385[A]:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:64:TYR:HB3	2:A:125:GLU:HB3	2.01	0.41
2:C:381:LEU:HD12	2:C:448[B]:LEU:HD12	2.02	0.41
2:A:432:ARG:HG3	2:A:432:ARG:NH1	2.34	0.41
1:B:529:ARG:N	1:B:530:PRO:CD	2.83	0.41
2:C:54:ASN:HA	2:C:128:MET:CE	2.50	0.41
2:A:393:GLU:HG3	8:A:613:HOH:O	2.21	0.41
1:B:511[B]:VAL:HG11	2:A:28:SER:CB	2.50	0.41
1:B:597:ASN:HD22	1:B:598:PRO:N	2.19	0.41
2:C:462:GLU:HA	2:C:462:GLU:OE2	2.21	0.41
2:C:65[B]:LYS:HE3	2:C:69[B]:ARG:HB2	2.03	0.40
2:C:186:HIS:HB2	2:C:191:LEU:HD11	2.02	0.40
2:C:297:SER:HG	2:C:300:THR:HG23	1.83	0.40
3:F:1:DA:N3	3:F:1:DA:O4'	2.53	0.40
2:C:274:ILE:HD13	2:C:294:ASP:HB2	2.04	0.40
2:C:13:ASN:ND2	8:C:622:HOH:O	2.54	0.40
2:A:109:ASN:HB2	1:D:442:SER:OG	2.20	0.40

All (3) 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)
8:A:866:HOH:O	8:C:885:HOH:O[5_554]	1.98	0.22
8:C:618:HOH:O	8:E:2212:HOH:O[1_445]	2.00	0.20
2:C:414[B]:ARG:NH2	3:F:2020:DT:OP1[1_445]	2.10	0.10

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	B	200/202 (99%)	187 (94%)	13 (6%)	0	100 100
1	D	190/202 (94%)	184 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	493/490 (101%)	482 (98%)	11 (2%)	0	100	100
2	C	497/490 (101%)	486 (98%)	11 (2%)	0	100	100
All	All	1380/1384 (100%)	1339 (97%)	41 (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	B	164/168 (98%)	163 (99%)	1 (1%)	86	93
1	D	153/168 (91%)	153 (100%)	0	100	100
2	A	425/423 (100%)	420 (99%)	5 (1%)	71	83
2	C	428/423 (101%)	425 (99%)	3 (1%)	84	92
All	All	1170/1182 (99%)	1161 (99%)	9 (1%)	84	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	597	ASN
2	A	280	LEU
2	A	299	ARG
2	A	385[A]	ARG
2	A	385[B]	ARG
2	A	404	ASP
2	C	299	ARG
2	C	300	THR
2	C	436	LEU

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

Mol	Chain	Res	Type
1	B	597	ASN
1	B	600	HIS
1	B	605	GLN
2	A	54	ASN
2	A	324	GLN
2	A	334	ASN
2	A	368	GLN
2	C	13	ASN
2	C	107	GLN
2	C	324	GLN
2	C	368	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z > 2$
5	GOL	C	504	-	5,5,5	0.17	0	5,5,5	0.58	0
5	GOL	E	2101[B]	-	5,5,5	0.13	0	5,5,5	0.45	0
5	GOL	C	501	-	5,5,5	0.16	0	5,5,5	0.41	0
5	GOL	A	501	-	5,5,5	0.17	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	JHN	F	2101[A]	-	37,38,38	0.91	1 (2%)	34,55,55	0.90	2 (5%)
5	GOL	C	502	-	5,5,5	0.13	0	5,5,5	0.42	0
5	GOL	C	503	-	5,5,5	0.21	0	5,5,5	0.65	0
5	GOL	E	2101[A]	-	5,5,5	0.15	0	5,5,5	0.40	0
5	GOL	A	503	-	5,5,5	0.13	0	5,5,5	0.22	0
5	GOL	E	2102	-	5,5,5	0.13	0	5,5,5	0.23	0
7	JHN	F	2101[B]	-	37,38,38	0.92	2 (5%)	34,55,55	0.97	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
5	GOL	C	504	-	-	4/4/4/4	-
5	GOL	E	2101[B]	-	-	0/4/4/4	-
5	GOL	C	501	-	-	0/4/4/4	-
5	GOL	A	501	-	-	1/4/4/4	-
7	JHN	F	2101[A]	-	-	2/9/34/34	0/6/6/6
5	GOL	C	502	-	-	2/4/4/4	-
5	GOL	C	503	-	-	2/4/4/4	-
5	GOL	E	2101[A]	-	-	3/4/4/4	-
5	GOL	A	503	-	-	2/4/4/4	-
5	GOL	E	2102	-	-	4/4/4/4	-
7	JHN	F	2101[B]	-	-	2/9/34/34	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	2101[A]	JHN	C4-C24	-3.74	1.37	1.43
7	F	2101[B]	JHN	C4-C24	-3.60	1.38	1.43
7	F	2101[B]	JHN	C24-N6	-2.07	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	2101[B]	JHN	C20-O3-C21	2.39	117.77	113.65
7	F	2101[A]	JHN	C20-O3-C21	2.18	117.41	113.65
7	F	2101[A]	JHN	C23-N6-C24	2.14	111.40	108.42
7	F	2101[B]	JHN	C19-C18-C17	-2.04	107.42	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	2101[B]	JHN	O1-C1-N6	-2.01	116.75	119.16

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	504	GOL	O1-C1-C2-O2
5	C	504	GOL	O1-C1-C2-C3
5	E	2101[A]	GOL	O1-C1-C2-C3
5	E	2102	GOL	O1-C1-C2-C3
5	E	2102	GOL	C1-C2-C3-O3
5	E	2101[A]	GOL	O1-C1-C2-O2
5	C	502	GOL	C1-C2-C3-O3
5	C	504	GOL	C1-C2-C3-O3
5	C	502	GOL	O2-C2-C3-O3
5	C	504	GOL	O2-C2-C3-O3
5	E	2102	GOL	O1-C1-C2-O2
5	E	2102	GOL	O2-C2-C3-O3
5	A	503	GOL	O1-C1-C2-C3
7	F	2101[B]	JHN	N4-C14-C15-N5
7	F	2101[B]	JHN	N4-C14-C15-C16
5	C	503	GOL	C1-C2-C3-O3
7	F	2101[A]	JHN	N4-C14-C15-N5
7	F	2101[A]	JHN	N4-C14-C15-C16
5	A	501	GOL	O1-C1-C2-C3
5	A	503	GOL	C1-C2-C3-O3
5	E	2101[A]	GOL	C1-C2-C3-O3
5	C	503	GOL	O2-C2-C3-O3

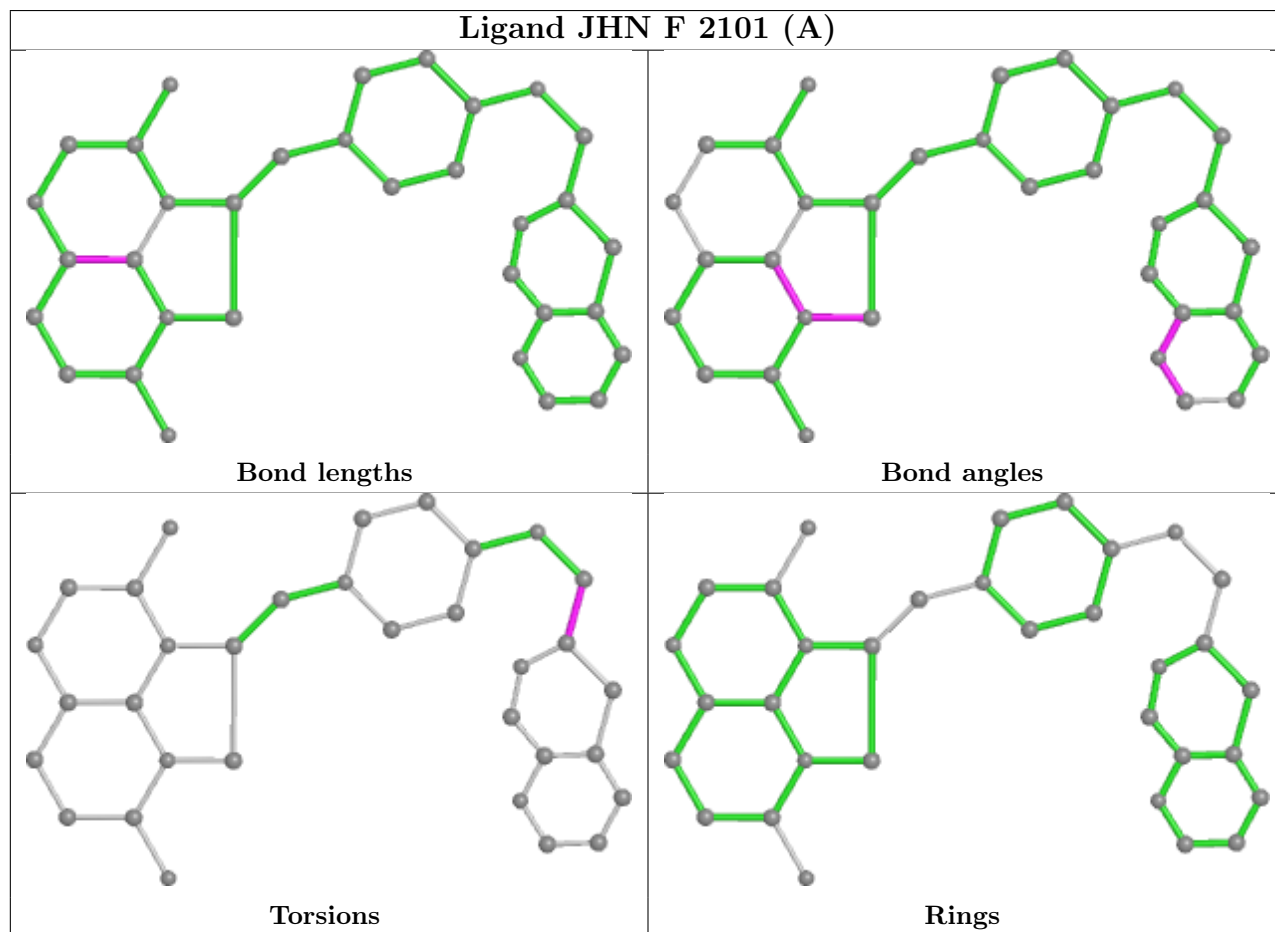
There are no ring outliers.

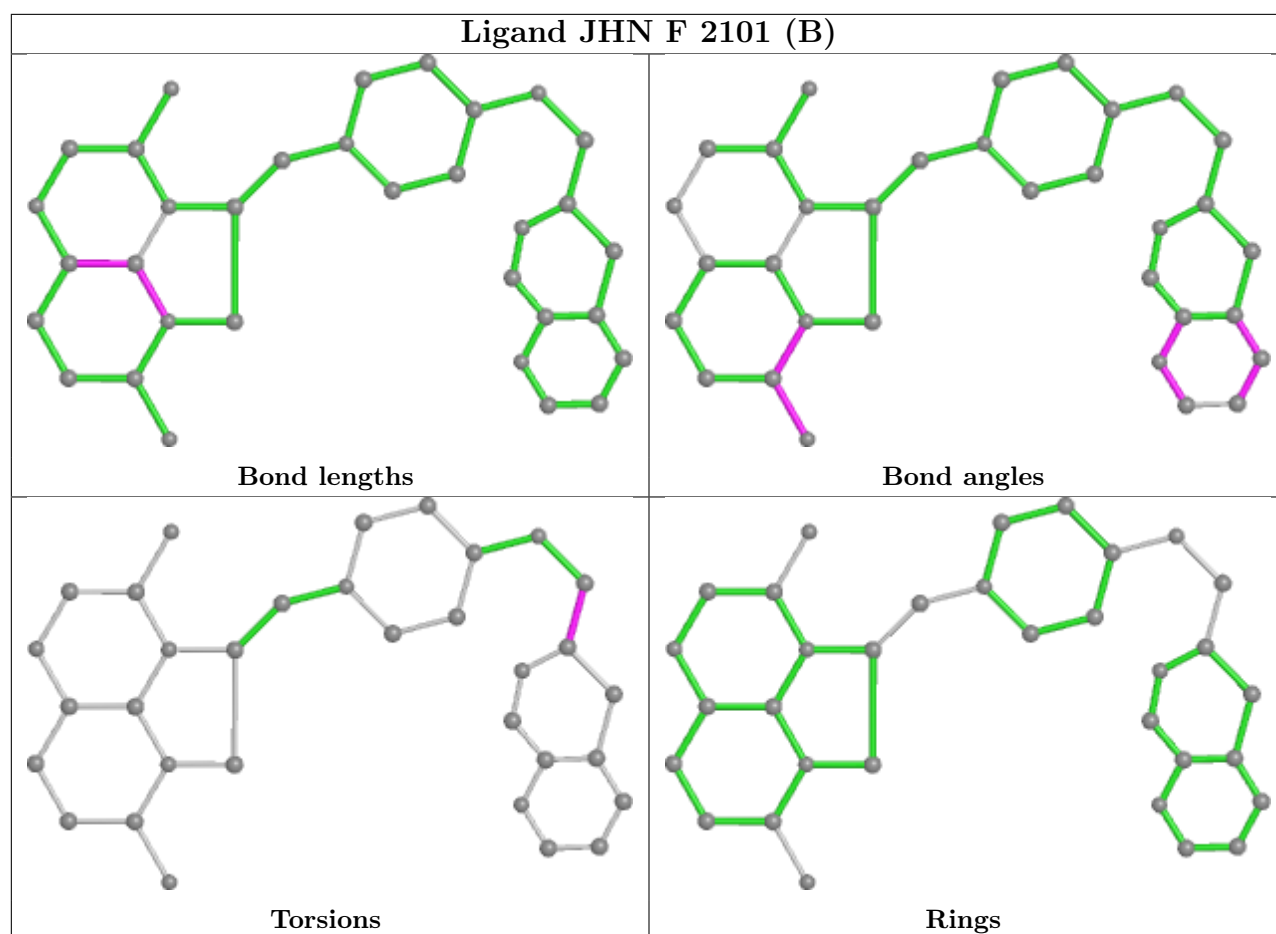
6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	GOL	3	0
5	E	2101[B]	GOL	6	0
5	A	501	GOL	10	0
5	C	503	GOL	3	0
5	E	2101[A]	GOL	1	0
5	E	2102	GOL	3	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	2
3	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	8:DG	O3'	2009[B]:DG	P	5.76
1	E	8:DG	O3'	2009[A]:DG	P	3.23
1	F	8:DG	O3'	2009:DG	P	3.20

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	B	192/202 (95%)	-0.36	2 (1%) 82 86	25, 39, 57, 71	0
1	D	192/202 (95%)	-0.12	7 (3%) 42 49	27, 42, 64, 77	0
2	A	484/490 (98%)	-0.61	2 (0%) 92 95	21, 31, 49, 68	0
2	C	482/490 (98%)	-0.57	0 100 100	21, 30, 46, 70	0
3	E	20/20 (100%)	-0.65	0 100 100	26, 33, 46, 51	0
3	F	20/20 (100%)	-0.45	0 100 100	26, 36, 59, 70	0
All	All	1390/1424 (97%)	-0.49	11 (0%) 86 89	21, 33, 53, 77	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	PRO	3.3
1	D	487	THR	2.6
1	D	491	GLY	2.5
1	D	612	ILE	2.5
1	D	488	GLY	2.3
2	A	491	GLY	2.3
1	B	415	PRO	2.3
2	A	152	GLY	2.2
1	B	416	GLY	2.2
1	D	473	LEU	2.0
1	D	486	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

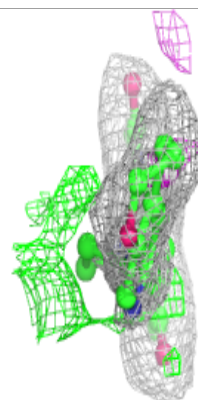
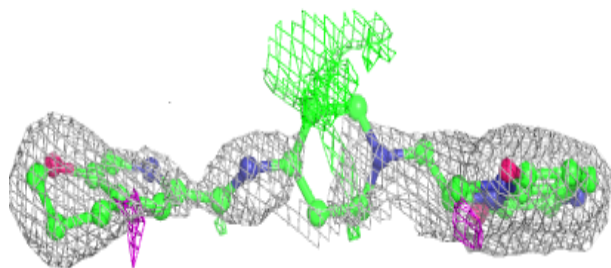
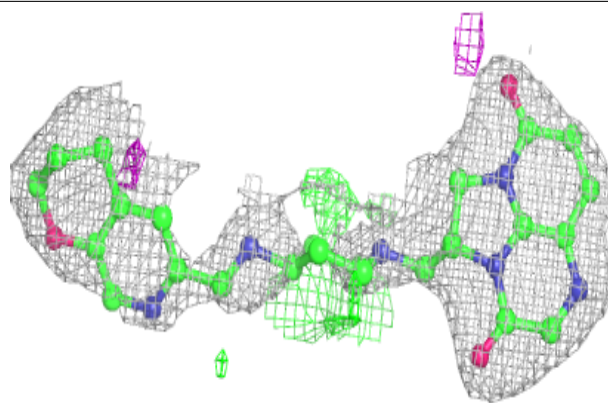
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	C	504	6/6	0.78	0.20	54,60,61,63	0
5	GOL	C	503	6/6	0.85	0.26	52,55,59,69	0
5	GOL	A	501	6/6	0.85	0.20	46,47,55,56	0
5	GOL	E	2101[A]	6/6	0.89	0.19	40,41,46,46	6
5	GOL	E	2101[B]	6/6	0.89	0.19	41,45,47,48	6
5	GOL	E	2102	6/6	0.91	0.15	51,55,56,61	0
5	GOL	A	503	6/6	0.93	0.16	57,58,61,64	0
7	JHN	F	2101[A]	33/33	0.94	0.22	33,40,44,45	33
7	JHN	F	2101[B]	33/33	0.94	0.22	36,40,42,43	33
5	GOL	C	501	6/6	0.95	0.12	41,46,49,52	0
5	GOL	C	502	6/6	0.97	0.15	45,50,53,59	0
6	NA	A	502	1/1	0.97	0.05	33,33,33,33	0
4	MN	B	701[A]	1/1	0.99	0.08	28,28,28,28	1
4	MN	B	701[B]	1/1	0.99	0.08	32,32,32,32	1
4	MN	D	701	1/1	0.99	0.08	35,35,35,35	0

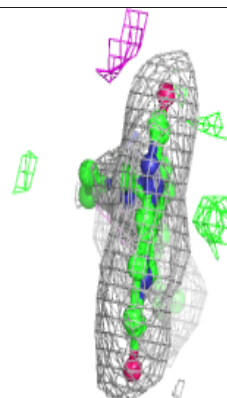
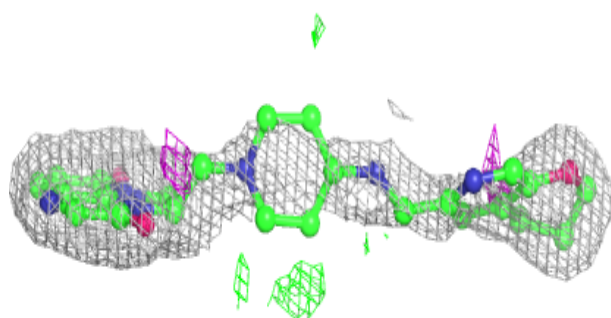
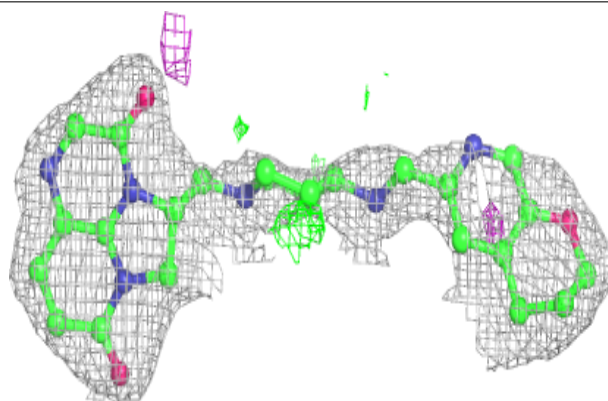
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JHN F 2101 (A):

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

**Electron density around JHN F 2101 (B):**

$2mF_o-DF_c$ (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.