



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:20 AM UTC

PDB ID : 6EPI / pdb_00006epi
Title : Structure of the epsilon_1 / zeta_1 antitoxin / toxin system from *Neisseria gonorrhoeae* in complex with UNAM-4P.
Authors : Rocker, A.; Meinhart, A.
Deposited on : 2017-10-11
Resolution : 2.80 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

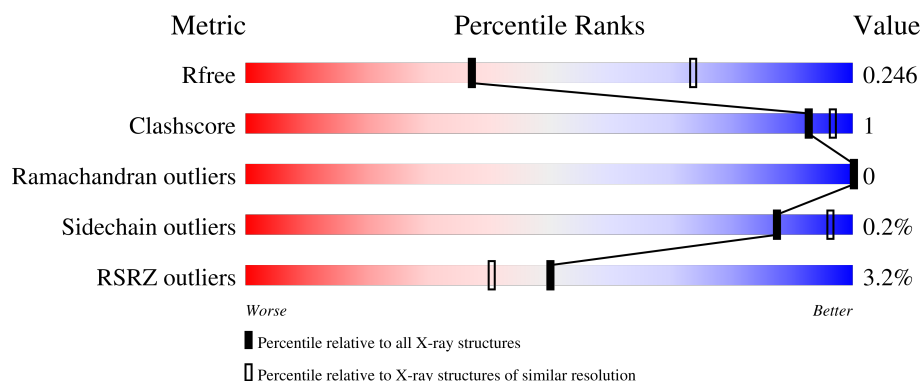
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	61	7% 84% 15%
1	C	61	20% 87% 11%
1	E	61	8% 80% 5% 15%
1	G	61	11% 85% 13%
2	B	401	0% 95% 5%

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Mol	Chain	Length	Quality of chain
2	D	401	2% 95% ..
2	F	401	% 94% ..
2	H	401	3% 95% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14471 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.

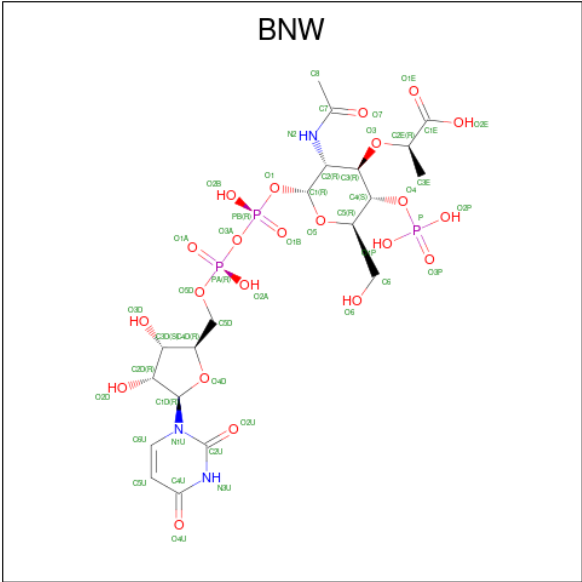
- Molecule 1 is a protein called Epsilon_1 antitoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	52	Total	C	N	O	S	0	0	0
			424	265	80	75	4			
1	C	54	Total	C	N	O	S	0	0	0
			442	275	83	80	4			
1	E	52	Total	C	N	O	S	0	0	0
			424	265	80	75	4			
1	G	53	Total	C	N	O	S	0	0	0
			433	270	82	77	4			

- Molecule 2 is a protein called Zeta_1 toxin.

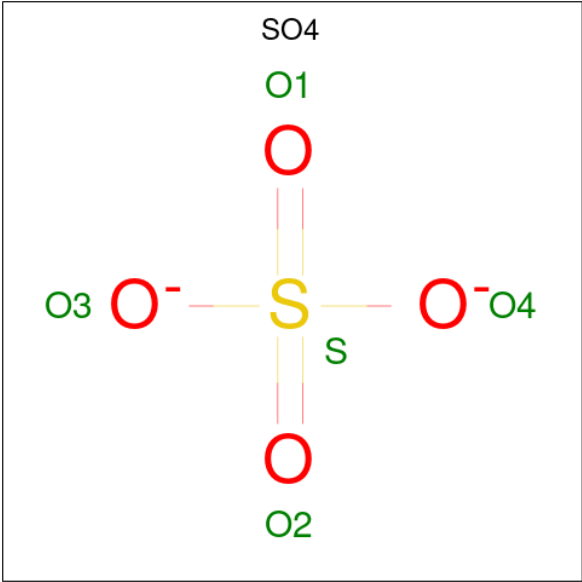
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			3079	1917	539	612	11			
2	D	394	Total	C	N	O	S	0	0	0
			3079	1917	539	612	11			
2	F	395	Total	C	N	O	S	0	0	0
			3087	1922	540	613	12			
2	H	395	Total	C	N	O	S	0	0	0
			3087	1922	540	613	12			

- Molecule 3 is UDP-N-acetyl-muramic acid-4'phosphate (CCD ID: BNW) (formula: $C_{20}H_{32}N_3O_{22}P_3$).



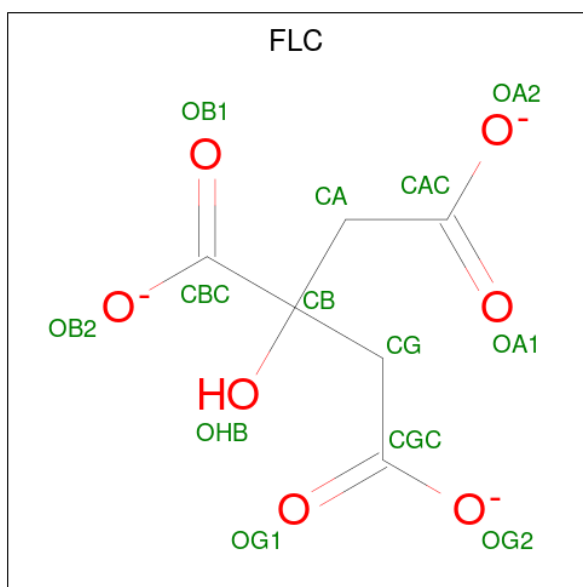
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	20	3	22	3		
3	D	1	Total	C	N	O	P	0	0
			48	20	3	22	3		
3	F	1	Total	C	N	O	P	0	0
			48	20	3	22	3		
3	H	1	Total	C	N	O	P	0	0
			48	20	3	22	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	6	7		

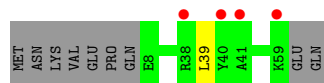
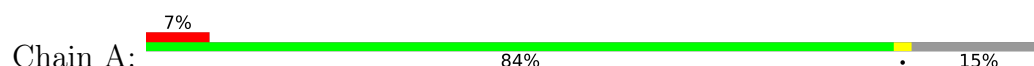
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	31	Total	O	0	0
			31	31		
6	C	5	Total	O	0	0
			5	5		
6	D	35	Total	O	0	0
			35	35		
6	F	36	Total	O	0	0
			36	36		
6	G	3	Total	O	0	0
			3	3		
6	H	31	Total	O	0	0
			31	31		

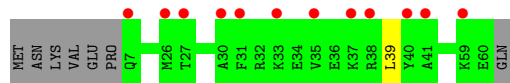
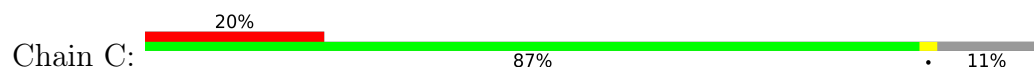
3 Residue-property plots [i](#)

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.

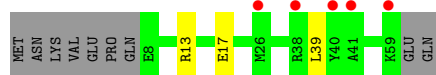
- Molecule 1: Epsilon_1 antitoxin



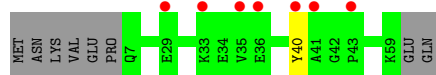
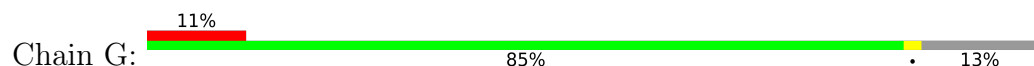
- Molecule 1: Epsilon_1 antitoxin



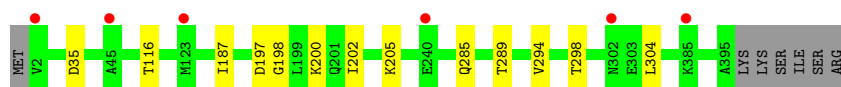
- Molecule 1: Epsilon_1 antitoxin



- Molecule 1: Epsilon_1 antitoxin



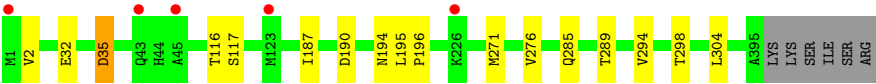
- Molecule 2: Zeta_1 toxin



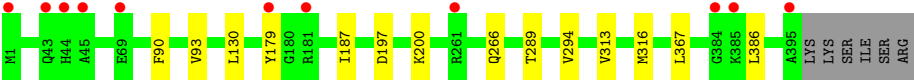
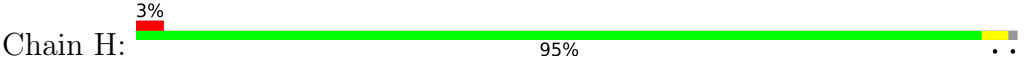
- Molecule 2: Zeta_1 toxin



• Molecule 2: Zeta_1 toxin



• Molecule 2: Zeta_1 toxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.51Å 149.32Å 125.44Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	49.17 – 2.80 49.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.17-2.80) 98.6 (49.17-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.219 , 0.244 0.222 , 0.246	Depositor DCC
R_{free} test set	3688 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14471	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9902e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, BNW, FLC

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	0.55	0/429	0.88	0/571
1	C	0.55	0/447	0.86	0/595
1	E	0.53	0/429	0.84	0/571
1	G	0.56	0/438	0.89	0/583
2	B	0.54	0/3117	0.77	1/4186 (0.0%)
2	D	0.54	0/3117	0.76	0/4186
2	F	0.53	0/3125	0.78	1/4196 (0.0%)
2	H	0.55	0/3125	0.77	0/4196
All	All	0.54	0/14227	0.78	2/19084 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	32	GLU	N-CA-C	5.91	117.80	111.36
2	B	205	LYS	N-CA-C	5.76	117.64	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	424	0	443	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	442	0	457	2	0
1	E	424	0	443	3	0
1	G	433	0	451	1	0
2	B	3079	0	3080	10	0
2	D	3079	0	3080	12	0
2	F	3087	0	3092	15	0
2	H	3087	0	3092	12	0
3	B	48	0	0	1	0
3	D	48	0	0	1	0
3	F	48	0	0	1	0
3	H	48	0	0	1	0
4	B	15	0	0	0	0
4	D	20	0	0	0	0
4	F	15	0	0	0	0
4	H	20	0	0	0	0
5	D	13	0	5	0	0
6	B	31	0	0	0	0
6	C	5	0	0	0	0
6	D	35	0	0	0	0
6	F	36	0	0	0	0
6	G	3	0	0	0	0
6	H	31	0	0	0	0
All	All	14471	0	14143	42	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 (42) 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:B:200:LYS:HD3	2:D:304:LEU:HD22	1.27	1.10
2:H:294:VAL:HG13	2:H:316:MET:HE1	1.45	0.99
2:D:30:ALA:O	2:D:34:THR:OG1	1.94	0.83
2:B:200:LYS:CD	2:D:304:LEU:HD22	2.08	0.83
2:H:289:THR:HG22	2:H:294:VAL:HG12	1.70	0.74
1:E:13:ARG:NH1	1:E:17:GLU:OE2	2.20	0.73
2:F:190:ASP:O	2:F:194:ASN:ND2	2.24	0.69
2:D:289:THR:HG22	2:D:294:VAL:HG12	1.75	0.69
2:F:304:LEU:HD22	2:H:200:LYS:HD2	1.77	0.66
2:F:2:VAL:N	2:F:35:ASP:OD1	2.26	0.61
2:H:367:LEU:HD13	2:H:386:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:LYS:HD3	2:D:304:LEU:CD2	2.19	0.58
2:F:304:LEU:HD22	2:H:200:LYS:CD	2.35	0.56
2:F:195:LEU:HB3	2:F:196:PRO:HD3	1.88	0.56
2:B:197:ASP:HA	2:D:304:LEU:HD21	1.88	0.55
2:D:187:ILE:HD11	3:D:501:BNW:C7	2.36	0.54
2:F:289:THR:HG22	2:F:294:VAL:HG12	1.92	0.52
1:E:39:LEU:HD11	2:F:117:SER:HA	1.92	0.52
2:F:187:ILE:HD11	3:F:501:BNW:C7	2.40	0.51
2:H:93:VAL:HG11	2:H:130:LEU:HD13	1.91	0.51
2:F:190:ASP:OD1	2:F:194:ASN:ND2	2.44	0.50
2:B:198:GLY:O	2:B:202:ILE:HG13	2.15	0.47
1:G:40:TYR:HB3	2:H:179:TYR:HB2	1.96	0.47
1:A:39:LEU:HD22	2:B:116:THR:HG22	1.97	0.47
2:B:285:GLN:CG	2:B:298:THR:HG22	2.45	0.47
2:H:187:ILE:HD11	3:H:501:BNW:C7	2.45	0.47
2:H:313:VAL:HB	2:H:316:MET:HE2	1.96	0.47
2:B:289:THR:HG22	2:B:294:VAL:HG12	1.98	0.46
2:H:90:PHE:CD2	2:H:130:LEU:HD21	2.50	0.46
2:F:285:GLN:CG	2:F:298:THR:HG22	2.46	0.46
2:D:285:GLN:CG	2:D:298:THR:HG22	2.46	0.45
2:H:294:VAL:CG1	2:H:316:MET:HE1	2.31	0.44
2:F:304:LEU:HD21	2:H:197:ASP:HA	1.99	0.43
2:F:271:MET:HE2	2:F:276:VAL:CG2	2.48	0.43
1:C:39:LEU:HD22	2:D:116:THR:HG22	2.01	0.43
2:B:304:LEU:HD21	2:D:197:ASP:HA	2.01	0.42
2:D:90:PHE:CD2	2:D:130:LEU:HD21	2.55	0.42
2:B:187:ILE:HD11	3:B:501:BNW:C7	2.50	0.41
2:F:271:MET:HE2	2:F:276:VAL:HG23	2.03	0.41
2:F:285:GLN:HG3	2:F:298:THR:HG22	2.02	0.41
1:C:39:LEU:HD11	2:D:117:SER:HA	2.03	0.41
1:E:39:LEU:HD22	2:F:116:THR:HG22	2.02	0.41

There are no symmetry-related clashes.

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	50/61 (82%)	49 (98%)	1 (2%)	0	100	100
1	C	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
1	E	50/61 (82%)	49 (98%)	1 (2%)	0	100	100
1	G	51/61 (84%)	50 (98%)	1 (2%)	0	100	100
2	B	392/401 (98%)	385 (98%)	7 (2%)	0	100	100
2	D	392/401 (98%)	386 (98%)	6 (2%)	0	100	100
2	F	393/401 (98%)	388 (99%)	5 (1%)	0	100	100
2	H	393/401 (98%)	387 (98%)	6 (2%)	0	100	100
All	All	1773/1848 (96%)	1744 (98%)	29 (2%)	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	44/53 (83%)	44 (100%)	0	100	100
1	C	46/53 (87%)	46 (100%)	0	100	100
1	E	44/53 (83%)	44 (100%)	0	100	100
1	G	45/53 (85%)	45 (100%)	0	100	100
2	B	336/343 (98%)	335 (100%)	1 (0%)	86	95
2	D	336/343 (98%)	336 (100%)	0	100	100
2	F	337/343 (98%)	336 (100%)	1 (0%)	86	95
2	H	337/343 (98%)	336 (100%)	1 (0%)	86	95
All	All	1525/1584 (96%)	1522 (100%)	3 (0%)	87	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	35	ASP
2	F	35	ASP
2	H	266	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	201	GLN
2	B	251	GLN
2	B	284	GLN
2	B	325	GLN
2	B	376	ASN
2	D	43	GLN
2	D	44	HIS
2	D	220	ASN
2	D	325	GLN
2	D	376	ASN
2	F	33	GLN
2	F	44	HIS
2	F	241	GLN
2	F	251	GLN
2	F	325	GLN
2	F	362	HIS
2	H	100	GLN
2	H	201	GLN
2	H	220	ASN
2	H	284	GLN
2	H	333	GLN
2	H	362	HIS
2	H	376	ASN

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](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	H	504	-	4,4,4	0.43	0	6,6,6	0.13	0
5	FLC	D	506	-	12,12,12	1.69	1 (8%)	17,17,17	5.46	8 (47%)
4	SO4	B	504	-	4,4,4	0.43	0	6,6,6	0.20	0
3	BNW	H	501	-	49,50,50	1.14	4 (8%)	70,76,76	0.76	1 (1%)
3	BNW	D	501	-	49,50,50	1.09	4 (8%)	70,76,76	0.78	3 (4%)
4	SO4	H	503	-	4,4,4	0.42	0	6,6,6	0.14	0
4	SO4	D	502	-	4,4,4	0.41	0	6,6,6	0.15	0
3	BNW	F	501	-	49,50,50	1.08	4 (8%)	70,76,76	0.75	1 (1%)
3	BNW	B	501	-	49,50,50	1.19	4 (8%)	70,76,76	0.73	1 (1%)
4	SO4	B	503	-	4,4,4	0.41	0	6,6,6	0.17	0
4	SO4	D	504	-	4,4,4	0.41	0	6,6,6	0.11	0
4	SO4	F	502	-	4,4,4	0.43	0	6,6,6	0.15	0
4	SO4	B	502	-	4,4,4	0.42	0	6,6,6	0.14	0
4	SO4	D	505	-	4,4,4	0.42	0	6,6,6	0.20	0
4	SO4	H	502	-	4,4,4	0.43	0	6,6,6	0.12	0
4	SO4	F	503	-	4,4,4	0.43	0	6,6,6	0.11	0
4	SO4	D	503	-	4,4,4	0.42	0	6,6,6	0.14	0
4	SO4	H	505	-	4,4,4	0.48	0	6,6,6	0.11	0
4	SO4	F	504	-	4,4,4	0.44	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BNW	F	501	-	-	4/39/76/76	0/3/3/3
3	BNW	B	501	-	-	5/39/76/76	0/3/3/3
5	FLC	D	506	-	-	8/16/16/16	-
3	BNW	H	501	-	-	4/39/76/76	0/3/3/3
3	BNW	D	501	-	-	8/39/76/76	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	BNW	PA-O3A	-4.59	1.54	1.59
5	D	506	FLC	CG-CB	4.37	1.59	1.54
3	B	501	BNW	PB-O3A	-4.36	1.54	1.59
3	H	501	BNW	PB-O3A	-4.27	1.54	1.59
3	D	501	BNW	PB-O3A	-4.09	1.55	1.59
3	H	501	BNW	PA-O3A	-4.03	1.55	1.59
3	F	501	BNW	PA-O3A	-3.87	1.55	1.59
3	F	501	BNW	PB-O3A	-3.57	1.55	1.59
3	D	501	BNW	PA-O3A	-3.25	1.56	1.59
3	B	501	BNW	O1E-C1E	3.11	1.31	1.22
3	F	501	BNW	O1E-C1E	3.06	1.31	1.22
3	D	501	BNW	O1E-C1E	3.04	1.31	1.22
3	H	501	BNW	O1E-C1E	3.01	1.31	1.22
3	D	501	BNW	O2E-C1E	-2.80	1.21	1.30
3	H	501	BNW	O2E-C1E	-2.76	1.21	1.30
3	B	501	BNW	O2E-C1E	-2.71	1.22	1.30
3	F	501	BNW	O2E-C1E	-2.68	1.22	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	506	FLC	OHB-CB-CBC	-15.53	86.94	108.96
5	D	506	FLC	OHB-CB-CA	-9.85	86.92	109.38
5	D	506	FLC	OHB-CB-CG	-9.19	88.42	109.38
5	D	506	FLC	CA-CB-CBC	5.62	122.46	110.03
5	D	506	FLC	CG-CB-CA	3.93	119.41	109.31
5	D	506	FLC	CG-CB-CBC	3.39	117.53	110.03
5	D	506	FLC	OB2-CBC-CB	3.14	119.16	113.14
3	D	501	BNW	C2-N2-C7	2.62	129.23	123.11
3	B	501	BNW	C2-N2-C7	2.50	128.96	123.11
3	F	501	BNW	C2-N2-C7	2.47	128.90	123.11
3	H	501	BNW	C2-N2-C7	2.43	128.79	123.11
5	D	506	FLC	CB-CA-CAC	2.25	120.08	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	BNW	O2B-PB-O3A	2.04	112.78	107.27
3	D	501	BNW	O2E-C1E-C2E	2.02	121.34	113.96

There are no chirality outliers.

All (29) torsion outliers are listed below:

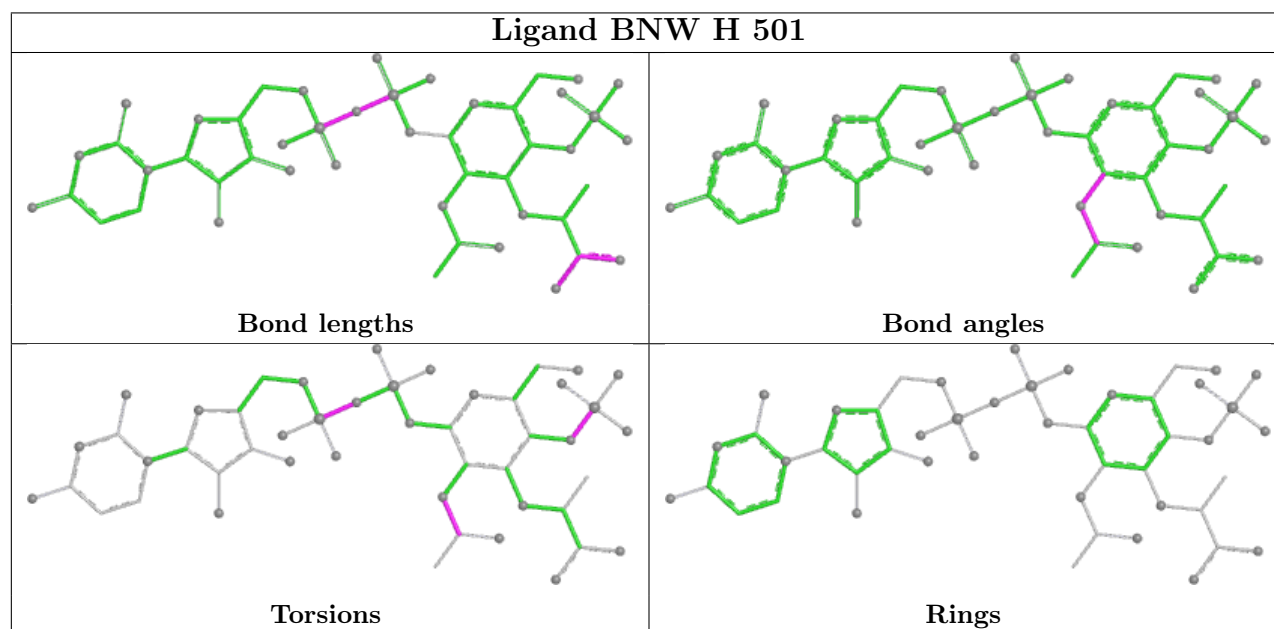
Mol	Chain	Res	Type	Atoms
3	B	501	BNW	PB-O3A-PA-O5D
3	D	501	BNW	C5D-O5D-PA-O1A
3	D	501	BNW	O4D-C4D-C5D-O5D
3	F	501	BNW	PB-O3A-PA-O5D
5	D	506	FLC	CG-CB-CBC-OB1
5	D	506	FLC	CG-CB-CBC-OB2
5	D	506	FLC	OHB-CB-CBC-OB1
5	D	506	FLC	OHB-CB-CBC-OB2
5	D	506	FLC	CA-CB-CG-CGC
3	D	501	BNW	C3D-C4D-C5D-O5D
5	D	506	FLC	CAC-CA-CB-CBC
3	B	501	BNW	O7-C7-N2-C2
3	B	501	BNW	C8-C7-N2-C2
3	D	501	BNW	O7-C7-N2-C2
3	D	501	BNW	C8-C7-N2-C2
3	F	501	BNW	O7-C7-N2-C2
3	F	501	BNW	C8-C7-N2-C2
3	H	501	BNW	O7-C7-N2-C2
3	H	501	BNW	C8-C7-N2-C2
5	D	506	FLC	CBC-CB-CG-CGC
3	D	501	BNW	PB-O3A-PA-O5D
3	H	501	BNW	PB-O3A-PA-O5D
3	B	501	BNW	O1E-C1E-C2E-C3E
3	D	501	BNW	PB-O3A-PA-O1A
5	D	506	FLC	CA-CB-CBC-OB2
3	D	501	BNW	C1-O1-PB-O1B
3	B	501	BNW	PB-O3A-PA-O1A
3	H	501	BNW	C4-O4-P-O3P
3	F	501	BNW	PB-O3A-PA-O2A

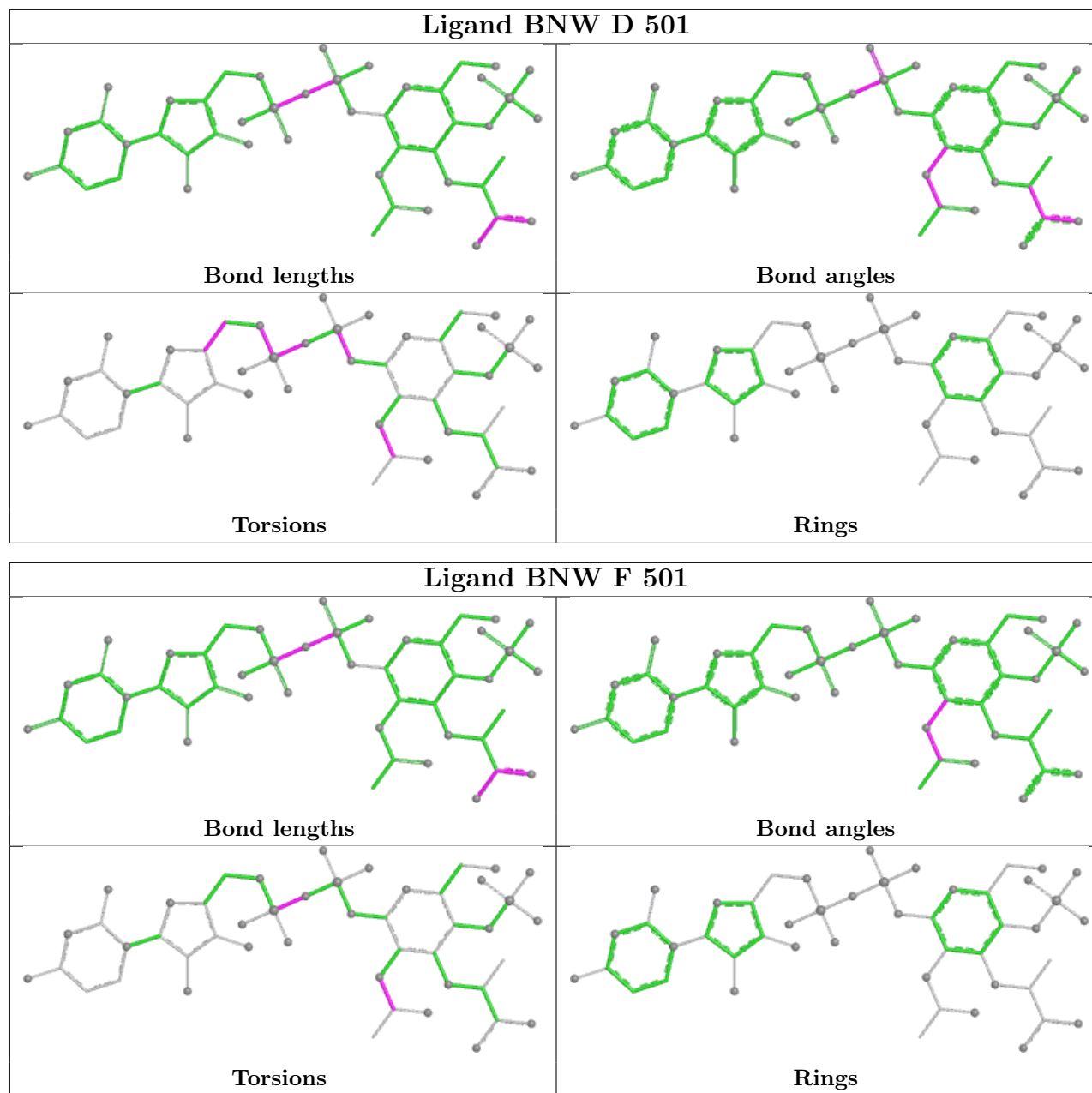
There are no ring outliers.

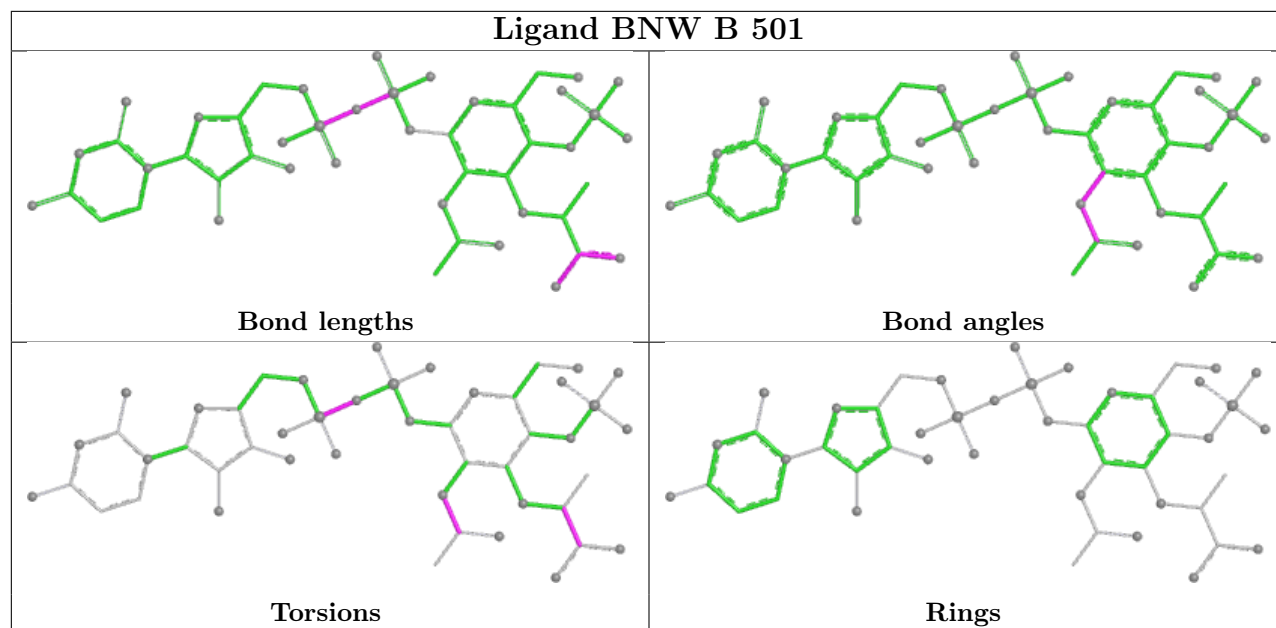
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	501	BNW	1	0
3	D	501	BNW	1	0
3	F	501	BNW	1	0
3	B	501	BNW	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	52/61 (85%)	0.86	4 (7%) 19 14	43, 75, 121, 132	0
1	C	54/61 (88%)	0.93	12 (22%) 2 1	45, 76, 141, 148	0
1	E	52/61 (85%)	0.82	5 (9%) 13 10	44, 77, 97, 111	0
1	G	53/61 (86%)	0.91	7 (13%) 7 6	50, 83, 131, 138	0
2	B	394/401 (98%)	0.11	6 (1%) 72 63	38, 55, 80, 114	0
2	D	394/401 (98%)	0.13	8 (2%) 65 56	35, 56, 83, 102	0
2	F	395/401 (98%)	0.15	5 (1%) 75 66	37, 56, 85, 104	0
2	H	395/401 (98%)	0.14	11 (2%) 55 45	37, 56, 81, 113	0
All	All	1789/1848 (96%)	0.22	58 (3%) 50 40	35, 58, 93, 148	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	TYR	5.7
1	A	41	ALA	4.5
1	C	40	TYR	3.8
1	A	40	TYR	3.5
1	C	41	ALA	3.3
2	F	45	ALA	3.3
2	F	1	MET	3.2
1	G	41	ALA	3.2
2	H	179	TYR	3.1
1	C	26	MET	3.1
2	B	45	ALA	3.1
2	B	123	MET	3.1
1	G	40	TYR	3.0
2	D	179	TYR	3.0
2	D	45	ALA	3.0
2	H	44	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	384	GLY	2.9
2	H	1	MET	2.8
2	B	2	VAL	2.8
1	E	26	MET	2.7
1	C	27	THR	2.6
2	D	123	MET	2.6
2	F	43	GLN	2.6
2	H	181	ARG	2.6
1	C	30	ALA	2.6
1	C	31	PHE	2.6
1	E	38	ARG	2.5
2	B	302	ASN	2.5
1	C	33	LYS	2.5
2	H	69	GLU	2.5
1	E	59	LYS	2.5
2	H	261	ARG	2.4
2	H	43	GLN	2.4
2	F	123	MET	2.4
2	B	385	LYS	2.4
2	D	35	ASP	2.4
2	H	395	ALA	2.4
2	D	100	GLN	2.4
1	A	59	LYS	2.3
1	C	35	VAL	2.3
1	G	35	VAL	2.3
2	B	240	GLU	2.3
1	E	41	ALA	2.3
2	H	385	LYS	2.3
1	G	36	GLU	2.2
2	H	45	ALA	2.2
2	D	2	VAL	2.2
1	C	37	LYS	2.2
1	C	7	GLN	2.2
2	D	44	HIS	2.1
2	F	226	LYS	2.1
1	G	43	PRO	2.1
1	C	38	ARG	2.1
1	C	59	LYS	2.0
2	D	302	ASN	2.0
1	G	29	GLU	2.0
1	G	33	LYS	2.0
1	A	38	ARG	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](#)

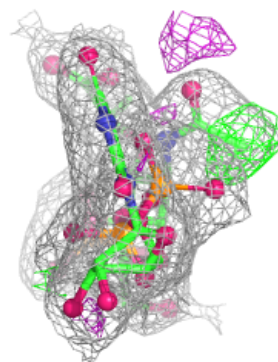
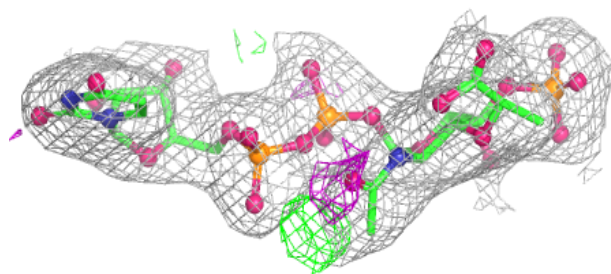
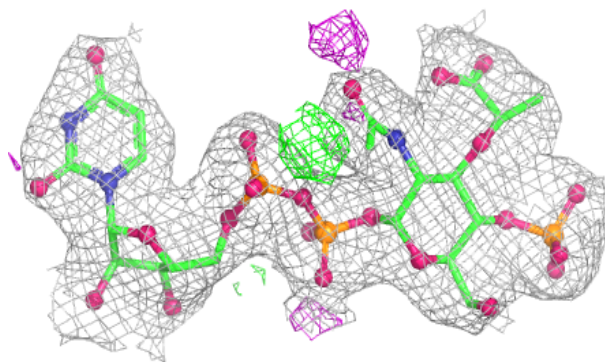
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FLC	D	506	13/13	0.76	0.18	96,105,113,115	0
4	SO4	F	504	5/5	0.84	0.16	96,96,97,97	0
4	SO4	D	505	5/5	0.84	0.16	87,90,92,95	0
4	SO4	H	504	5/5	0.87	0.14	89,90,91,93	0
4	SO4	B	504	5/5	0.87	0.12	87,92,93,93	0
4	SO4	H	505	5/5	0.89	0.15	78,79,81,83	0
4	SO4	D	504	5/5	0.93	0.12	75,77,79,80	0
3	BNW	F	501	48/48	0.96	0.08	39,47,50,54	0
3	BNW	H	501	48/48	0.96	0.08	39,45,55,58	0
4	SO4	H	503	5/5	0.96	0.07	63,64,65,65	0
4	SO4	B	503	5/5	0.96	0.06	67,67,68,70	0
3	BNW	B	501	48/48	0.96	0.08	40,47,55,58	0
3	BNW	D	501	48/48	0.96	0.08	38,42,55,60	0
4	SO4	F	503	5/5	0.97	0.06	64,64,66,66	0
4	SO4	D	503	5/5	0.97	0.10	60,60,61,62	0
4	SO4	D	502	5/5	0.98	0.05	48,49,50,51	0
4	SO4	F	502	5/5	0.98	0.06	44,45,46,47	0
4	SO4	B	502	5/5	0.99	0.05	39,40,40,40	0
4	SO4	H	502	5/5	0.99	0.04	44,45,46,46	0

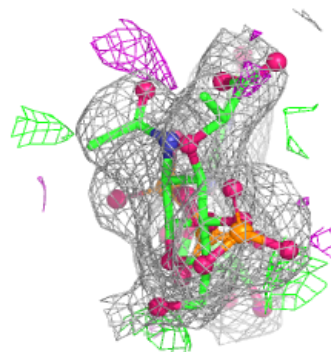
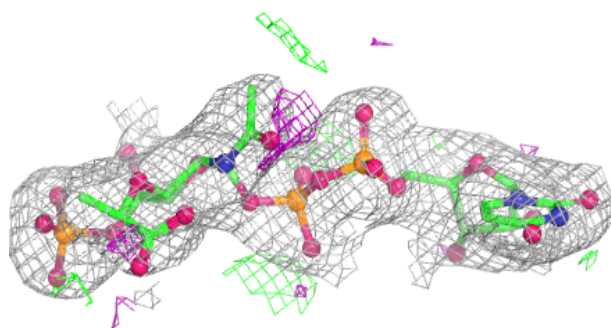
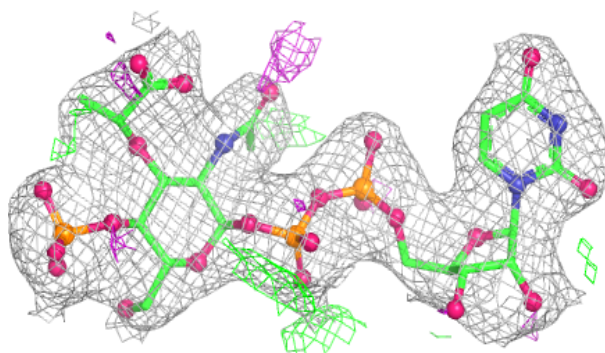
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNW F 501:

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

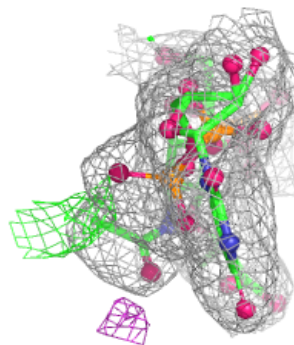
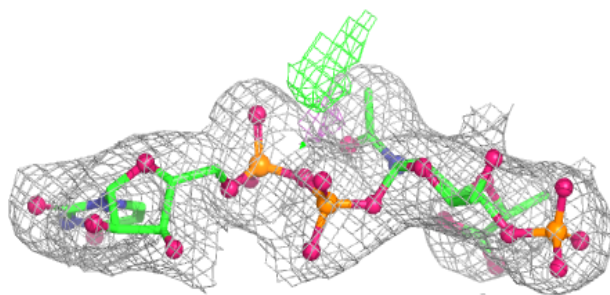
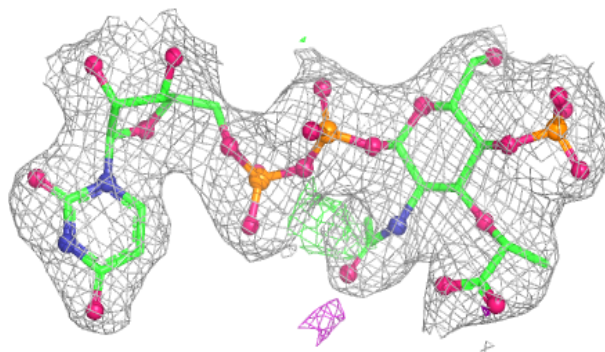
**Electron density around BNW H 501:**

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

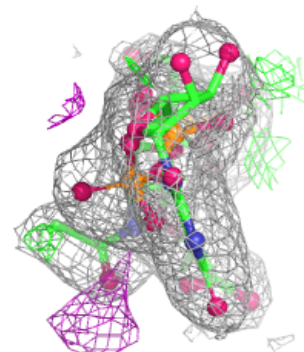
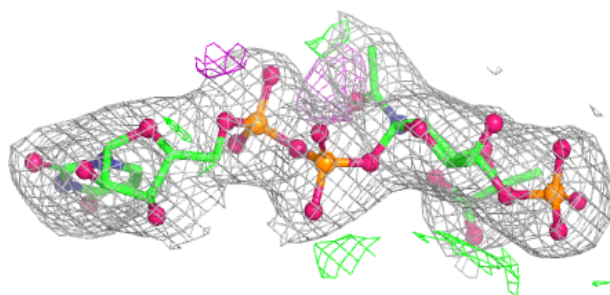
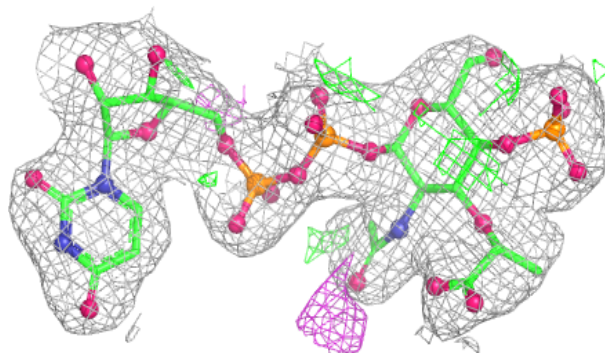


Electron density around BNW B 501:

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

**Electron density around BNW D 501:**

$2mF_o-DF_c$ (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.