



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 08:57 PM EST

PDB ID : 6DVM  
Title : Crystal structure of Danio rerio histone deacetylase 6 catalytic domain 2 in complex with DDK-122  
Authors : Porter, N.J.; Christianson, D.W.  
Deposited on : 2018-06-24  
Resolution : 1.47 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](mailto: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>.

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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 : 2.36  
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

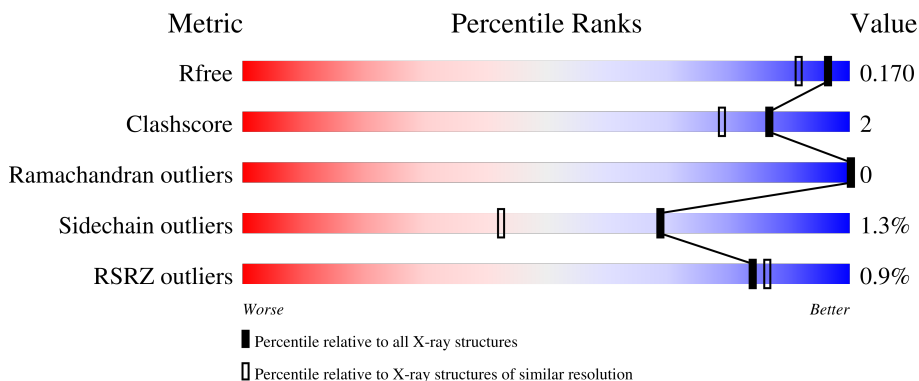
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.47 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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  $\geq 3$ , 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	364	 95%
1	B	364	 94%
1	C	364	 93% 5%
1	D	364	 94%

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	EDO	D	805	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 13430 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 Hdac6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2802	1760	502	522	18	0	6	0
1	B	357	2822	1774	499	531	18	0	8	0
1	C	357	2868	1800	513	536	19	0	12	0
1	D	357	2829	1776	509	525	19	0	6	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	SER	-	expression tag	UNP A7YT55
A	436	ASN	-	expression tag	UNP A7YT55
A	437	ALA	-	expression tag	UNP A7YT55
A	438	GLY	-	expression tag	UNP A7YT55
A	439	GLY	-	expression tag	UNP A7YT55
B	435	SER	-	expression tag	UNP A7YT55
B	436	ASN	-	expression tag	UNP A7YT55
B	437	ALA	-	expression tag	UNP A7YT55
B	438	GLY	-	expression tag	UNP A7YT55
B	439	GLY	-	expression tag	UNP A7YT55
C	435	SER	-	expression tag	UNP A7YT55
C	436	ASN	-	expression tag	UNP A7YT55
C	437	ALA	-	expression tag	UNP A7YT55
C	438	GLY	-	expression tag	UNP A7YT55
C	439	GLY	-	expression tag	UNP A7YT55
D	435	SER	-	expression tag	UNP A7YT55
D	436	ASN	-	expression tag	UNP A7YT55
D	437	ALA	-	expression tag	UNP A7YT55
D	438	GLY	-	expression tag	UNP A7YT55
D	439	GLY	-	expression tag	UNP A7YT55

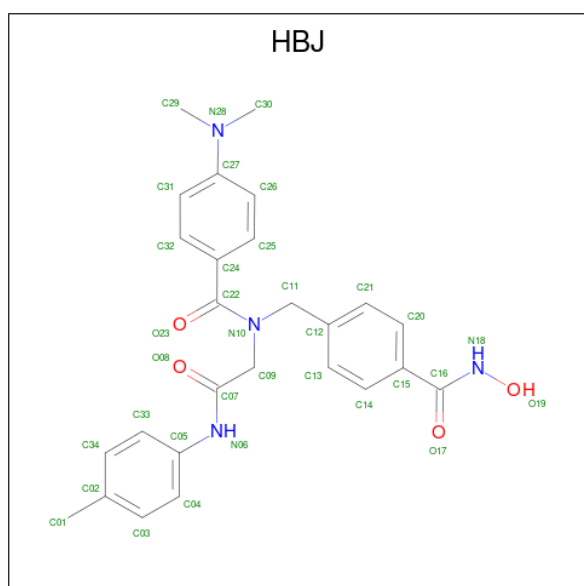
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

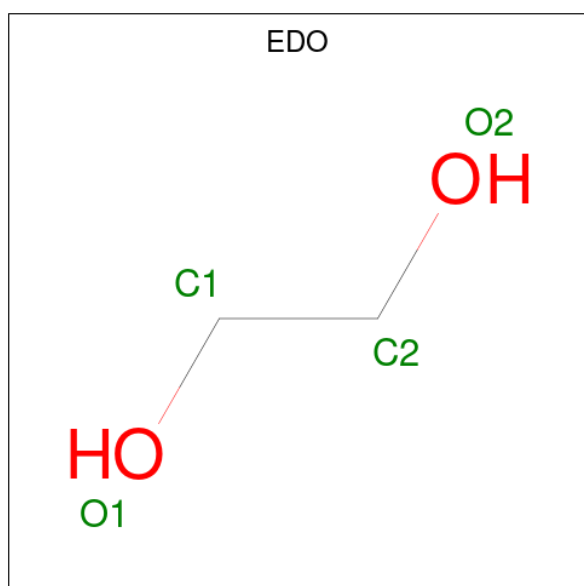
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is 4-(dimethylamino)-N-[[4-(hydroxycarbonyl)phenyl]methyl]-N-[2-[(4-methylphenyl)amino]-2-oxoethyl]benzamide (three-letter code: HBJ) (formula: C<sub>26</sub>H<sub>28</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			34	26	4	4		
4	B	1	Total	C	N	O	0	1
			68	52	8	8		
4	C	1	Total	C	N	O	0	0
			34	26	4	4		
4	D	1	Total	C	N	O	0	0
			34	26	4	4		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



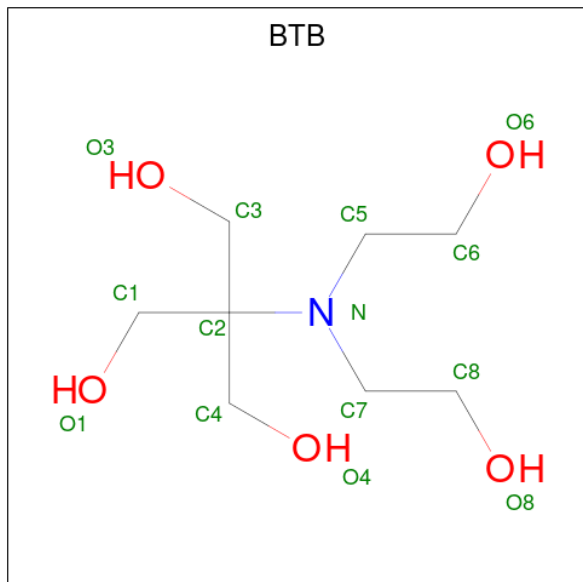
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	406	Total	O	0	0
			406	406		
7	B	463	Total	O	0	0
			463	463		
7	C	483	Total	O	0	0
			483	483		

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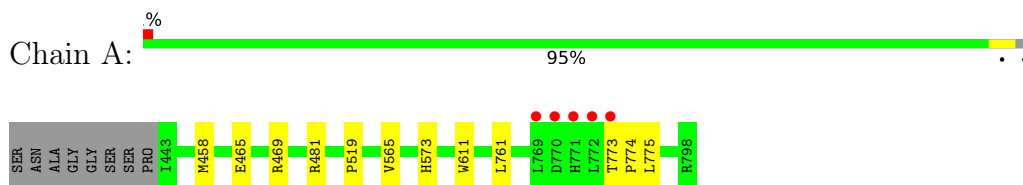
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	D	507	Total 509	O 509	0	2



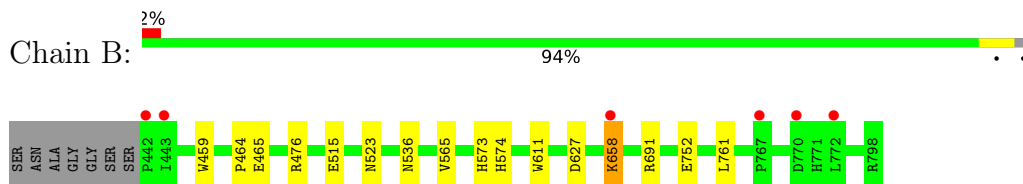
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

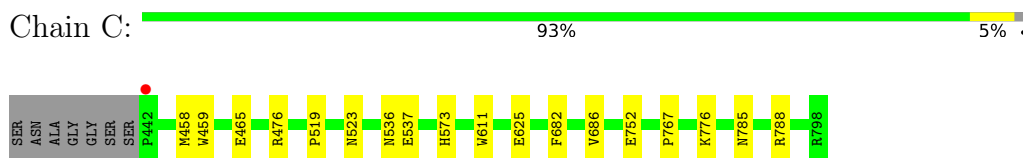
- Molecule 1: Hdac6 protein



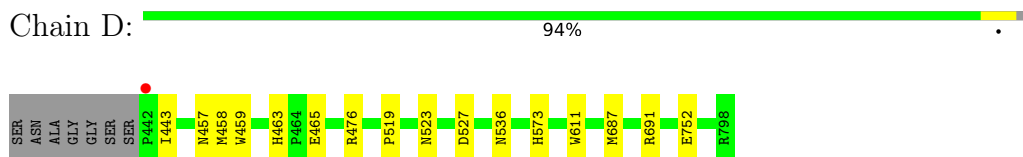
- Molecule 1: Hdac6 protein



- Molecule 1: Hdac6 protein



- Molecule 1: Hdac6 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.45Å 95.18Å 98.03Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	56.42 – 1.47 60.10 – 1.47	Depositor EDS
% Data completeness (in resolution range)	98.8 (56.42-1.47) 98.9 (60.10-1.47)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 1.47Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.148 , 0.170 0.149 , 0.170	Depositor DCC
$R_{free}$ test set	11896 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.2	Xtrriage
Anisotropy	0.736	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.25 % 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 1.3500e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BTB, K, EDO, ZN, HBJ

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	0.44	0/2881	0.63	2/3911 (0.1%)
1	B	0.44	0/2902	0.65	0/3938
1	C	0.47	0/2945	0.65	0/3995
1	D	0.44	0/2903	0.64	0/3938
All	All	0.45	0/11631	0.64	2/15782 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	469	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	2802	0	2702	4	0
1	B	2822	0	2718	11	0
1	C	2868	0	2762	13	0
1	D	2829	0	2733	12	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	34	0	0	0	0
4	B	68	0	0	7	0
4	C	34	0	0	0	0
4	D	34	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	20	0	30	1	0
5	D	24	0	36	9	0
6	C	14	0	19	0	0
7	A	406	0	0	1	0
7	B	463	0	0	2	0
7	C	483	0	0	8	0
7	D	509	0	0	8	0
All	All	13430	0	11012	48	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 2.

All (48) 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)
5:D:805:EDO:H11	7:D:1237:HOH:O	1.74	0.88
5:D:805:EDO:O1	7:D:901:HOH:O	1.92	0.87
5:D:805:EDO:C1	7:D:1237:HOH:O	2.27	0.82
1:C:785:ASN:OD1	1:C:788[A]:ARG:NH1	2.15	0.79
1:A:458:MET:HE1	1:A:519:PRO:HB3	1.64	0.79
1:C:536[A]:ASN:OD1	7:C:901:HOH:O	2.01	0.78
1:D:536[A]:ASN:ND2	7:D:903:HOH:O	2.18	0.76
1:C:776:LYS:NZ	7:C:903:HOH:O	2.20	0.74
1:D:536[A]:ASN:OD1	7:D:902:HOH:O	2.05	0.72
1:B:574:HIS:NE2	4:B:804[B]:HBJ:N18	2.40	0.70
1:B:464:PRO:HD3	4:B:804[B]:HBJ:C29	2.29	0.63
1:D:458:MET:HE1	1:D:519:PRO:HB3	1.81	0.61
1:C:536[A]:ASN:ND2	7:C:906:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:MET:HE1	1:C:519:PRO:HB3	1.85	0.57
1:C:537[A]:GLU:OE2	7:C:902:HOH:O	2.18	0.53
1:C:523:ASN:OD1	5:C:805:EDO:H11	2.09	0.53
4:B:804[B]:HBJ:O23	4:B:804[B]:HBJ:N06	2.42	0.53
1:B:565[B]:VAL:HG23	1:B:761:LEU:HD12	1.92	0.52
1:B:476:ARG:NE	1:B:752[A]:GLU:OE1	2.43	0.51
1:C:752[B]:GLU:HG2	7:C:922:HOH:O	2.09	0.51
1:A:565[B]:VAL:HG13	1:A:761:LEU:HD12	1.92	0.51
1:B:752[A]:GLU:HG2	7:B:1127:HOH:O	2.11	0.50
1:D:463:HIS:HE2	5:D:805:EDO:C2	2.26	0.49
1:B:627:ASP:OD2	1:B:658:LYS:HD3	2.13	0.48
1:D:752:GLU:HG2	7:D:1039[A]:HOH:O	2.13	0.48
4:B:804[B]:HBJ:C01	7:C:1366:HOH:O	2.62	0.48
1:C:767:PRO:HD3	7:C:923:HOH:O	2.13	0.48
5:D:805:EDO:C2	7:D:1237:HOH:O	2.62	0.47
1:D:459:TRP:CZ2	1:D:523:ASN:HB2	2.50	0.47
1:D:687:MET:O	1:D:691[A]:ARG:HG3	2.15	0.47
1:D:476:ARG:NE	1:D:752:GLU:OE1	2.46	0.47
1:B:515:GLU:O	1:B:536[B]:ASN:ND2	2.49	0.46
1:A:773:THR:HA	1:A:774:PRO:HD3	1.88	0.45
4:B:804[B]:HBJ:N06	4:B:804[B]:HBJ:C22	2.80	0.45
1:D:457:ASN:HD21	5:D:806:EDO:C2	2.29	0.45
1:D:527:ASP:CG	5:D:807:EDO:H22	2.37	0.45
1:B:691:ARG:HD3	7:B:1031:HOH:O	2.18	0.44
1:B:464:PRO:CD	4:B:804[B]:HBJ:C29	2.96	0.43
1:B:464:PRO:HD3	4:B:804[B]:HBJ:C30	2.48	0.43
1:C:625:GLU:OE2	7:C:905:HOH:O	2.20	0.43
1:C:459:TRP:CZ2	1:C:523:ASN:HB2	2.53	0.43
1:C:476:ARG:NE	1:C:752[B]:GLU:OE2	2.50	0.42
1:D:463:HIS:HE2	5:D:805:EDO:H22	1.85	0.42
1:D:458:MET:HB2	1:D:458:MET:HE2	1.68	0.41
1:B:459:TRP:CZ2	1:B:523:ASN:HB2	2.55	0.41
1:C:682:PHE:HA	1:C:686:VAL:HB	2.01	0.41
5:D:808:EDO:H22	7:D:1060:HOH:O	2.20	0.41
1:A:481:ARG:NH1	7:A:906:HOH:O	2.54	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/364 (99%)	351 (98%)	9 (2%)	0	100	100
1	B	363/364 (100%)	357 (98%)	6 (2%)	0	100	100
1	C	367/364 (101%)	362 (99%)	5 (1%)	0	100	100
1	D	361/364 (99%)	354 (98%)	7 (2%)	0	100	100
All	All	1451/1456 (100%)	1424 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/305 (99%)	298 (99%)	4 (1%)	69	42
1	B	305/305 (100%)	301 (99%)	4 (1%)	69	42
1	C	310/305 (102%)	307 (99%)	3 (1%)	76	54
1	D	305/305 (100%)	301 (99%)	4 (1%)	69	42
All	All	1222/1220 (100%)	1207 (99%)	15 (1%)	69	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	GLU
1	A	573	HIS

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Mol	Chain	Res	Type
1	A	611	TRP
1	A	775	LEU
1	B	465	GLU
1	B	573	HIS
1	B	611	TRP
1	B	658	LYS
1	C	465	GLU
1	C	573	HIS
1	C	611	TRP
1	D	443	ILE
1	D	465	GLU
1	D	573	HIS
1	D	611	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 31 ligands modelled in this entry, 12 are monoatomic - leaving 19 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	EDO	C	808	-	3,3,3	0.40	0	2,2,2	0.29	0
5	EDO	C	809	-	3,3,3	0.50	0	2,2,2	0.27	0
5	EDO	D	805	-	3,3,3	0.29	0	2,2,2	0.35	0
5	EDO	D	809	-	3,3,3	0.37	0	2,2,2	0.61	0
4	HBJ	C	804	2	36,36,36	1.70	6 (16%)	48,49,49	1.33	3 (6%)
5	EDO	A	805	-	3,3,3	0.56	0	2,2,2	0.21	0
4	HBJ	B	804[A]	2	36,36,36	2.06	8 (22%)	48,49,49	1.62	7 (14%)
5	EDO	C	807	-	3,3,3	0.53	0	2,2,2	0.38	0
5	EDO	D	808	-	3,3,3	0.41	0	2,2,2	0.28	0
5	EDO	B	805	-	3,3,3	0.49	0	2,2,2	0.41	0
5	EDO	D	810	-	3,3,3	0.45	0	2,2,2	0.60	0
5	EDO	D	806	-	3,3,3	0.38	0	2,2,2	0.65	0
5	EDO	C	805	-	3,3,3	0.44	0	2,2,2	0.16	0
4	HBJ	A	804	2	36,36,36	1.71	6 (16%)	48,49,49	1.35	5 (10%)
4	HBJ	D	804	2	36,36,36	1.91	9 (25%)	48,49,49	1.32	3 (6%)
5	EDO	C	806	-	3,3,3	0.46	0	2,2,2	0.64	0
6	BTB	C	810	-	13,13,13	2.03	6 (46%)	7,16,16	0.99	0
5	EDO	D	807	-	3,3,3	0.45	0	2,2,2	0.47	0
4	HBJ	B	804[B]	2	36,36,36	2.41	9 (25%)	48,49,49	1.39	10 (20%)

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	EDO	C	808	-	-	1/1/1/1	-
5	EDO	C	809	-	-	0/1/1/1	-
5	EDO	D	805	-	-	1/1/1/1	-
5	EDO	D	809	-	-	1/1/1/1	-
4	HBJ	C	804	2	-	1/30/30/30	0/3/3/3
5	EDO	A	805	-	-	0/1/1/1	-
4	HBJ	B	804[A]	2	-	3/30/30/30	0/3/3/3
5	EDO	C	807	-	-	0/1/1/1	-
5	EDO	D	808	-	-	1/1/1/1	-
5	EDO	B	805	-	-	0/1/1/1	-
5	EDO	D	810	-	-	0/1/1/1	-
5	EDO	D	806	-	-	1/1/1/1	-
5	EDO	C	805	-	-	0/1/1/1	-
4	HBJ	A	804	2	-	2/30/30/30	0/3/3/3
4	HBJ	D	804	2	-	2/30/30/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	806	-	-	0/1/1/1	-
6	BTB	C	810	-	-	2/21/21/21	-
5	EDO	D	807	-	-	0/1/1/1	-
4	HBJ	B	804[B]	2	-	4/30/30/30	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	804[B]	HBJ	C16-N18	8.13	1.43	1.32
4	B	804[A]	HBJ	C16-N18	6.29	1.40	1.32
4	B	804[B]	HBJ	C22-N10	5.99	1.48	1.34
4	A	804	HBJ	C16-N18	5.85	1.40	1.32
4	B	804[B]	HBJ	C07-N06	5.23	1.47	1.35
4	B	804[A]	HBJ	C22-N10	5.15	1.46	1.34
4	B	804[A]	HBJ	C07-N06	5.05	1.46	1.35
4	D	804	HBJ	C11-N10	-4.79	1.39	1.46
4	D	804	HBJ	C22-N10	4.59	1.45	1.34
4	D	804	HBJ	C07-N06	4.57	1.45	1.35
4	C	804	HBJ	C07-N06	4.54	1.45	1.35
4	C	804	HBJ	C22-N10	4.41	1.44	1.34
4	B	804[A]	HBJ	C11-N10	-4.29	1.40	1.46
4	A	804	HBJ	C07-N06	3.88	1.44	1.35
4	C	804	HBJ	C11-N10	-3.78	1.41	1.46
4	A	804	HBJ	C22-N10	3.67	1.42	1.34
4	B	804[B]	HBJ	C27-N28	3.57	1.45	1.37
4	D	804	HBJ	C16-N18	3.54	1.37	1.32
6	C	810	BTB	C4-C2	3.14	1.57	1.53
6	C	810	BTB	C3-C2	3.08	1.57	1.53
6	C	810	BTB	C5-N	2.98	1.52	1.48
6	C	810	BTB	C7-N	2.85	1.52	1.48
6	C	810	BTB	C1-C2	2.83	1.57	1.53
4	A	804	HBJ	O08-C07	-2.63	1.17	1.23
4	B	804[B]	HBJ	O08-C07	-2.63	1.17	1.23
4	D	804	HBJ	O08-C07	-2.58	1.18	1.23
4	B	804[B]	HBJ	C09-C07	2.56	1.56	1.52
4	D	804	HBJ	O19-N18	-2.55	1.33	1.40
4	C	804	HBJ	O08-C07	-2.55	1.18	1.23
6	C	810	BTB	C2-N	2.51	1.53	1.48
4	B	804[B]	HBJ	C24-C22	2.50	1.54	1.50
4	B	804[B]	HBJ	O23-C22	-2.41	1.17	1.22
4	A	804	HBJ	C11-N10	-2.38	1.43	1.46
4	B	804[A]	HBJ	O08-C07	-2.33	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	804[B]	HBJ	O19-N18	-2.31	1.34	1.40
4	D	804	HBJ	C09-C07	2.27	1.55	1.52
4	B	804[A]	HBJ	C04-C05	2.24	1.43	1.39
4	D	804	HBJ	C32-C24	2.21	1.43	1.39
4	B	804[A]	HBJ	O23-C22	-2.19	1.18	1.22
4	D	804	HBJ	O23-C22	-2.19	1.18	1.22
4	C	804	HBJ	O19-N18	-2.17	1.34	1.40
4	C	804	HBJ	O23-C22	-2.13	1.18	1.22
4	B	804[A]	HBJ	C09-C07	2.11	1.55	1.52
4	A	804	HBJ	O23-C22	-2.10	1.18	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804[A]	HBJ	C24-C22-N10	4.98	125.04	118.72
4	D	804	HBJ	C24-C22-N10	4.90	124.94	118.72
4	A	804	HBJ	C24-C22-N10	4.79	124.80	118.72
4	C	804	HBJ	C24-C22-N10	4.33	124.22	118.72
4	A	804	HBJ	O23-C22-N10	-3.77	116.11	122.34
4	B	804[A]	HBJ	O17-C16-N18	-3.74	115.96	122.94
4	B	804[A]	HBJ	C15-C16-N18	3.58	121.90	116.16
4	D	804	HBJ	O23-C22-N10	-3.55	116.46	122.34
4	B	804[A]	HBJ	O23-C22-N10	-3.14	117.14	122.34
4	C	804	HBJ	O23-C22-N10	-2.88	117.58	122.34
4	C	804	HBJ	O17-C16-N18	-2.82	117.67	122.94
4	B	804[A]	HBJ	C12-C11-N10	-2.80	108.63	113.13
4	B	804[B]	HBJ	O17-C16-N18	-2.68	117.94	122.94
4	B	804[B]	HBJ	C33-C05-C04	-2.53	115.58	119.03
4	A	804	HBJ	C15-C16-N18	2.48	120.14	116.16
4	B	804[B]	HBJ	C31-C27-C26	-2.44	114.20	119.16
4	B	804[B]	HBJ	C20-C15-C14	-2.43	115.12	118.59
4	B	804[B]	HBJ	C09-C07-N06	2.43	118.68	114.12
4	A	804	HBJ	O17-C16-N18	-2.38	118.50	122.94
4	B	804[A]	HBJ	C33-C05-C04	-2.33	115.84	119.03
4	B	804[B]	HBJ	O23-C22-N10	-2.32	118.50	122.34
4	B	804[B]	HBJ	C15-C16-N18	2.31	119.87	116.16
4	B	804[B]	HBJ	C11-C12-C13	2.24	124.97	120.77
4	A	804	HBJ	C33-C05-C04	-2.15	116.09	119.03
4	B	804[A]	HBJ	C07-C09-N10	-2.11	108.57	113.60
4	B	804[B]	HBJ	C21-C12-C13	-2.10	114.86	118.17
4	D	804	HBJ	C12-C11-N10	-2.06	109.82	113.13
4	B	804[B]	HBJ	C25-C26-C27	2.01	122.97	120.32

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	804[B]	HBJ	C07-C09-N10-C11
4	B	804[B]	HBJ	C07-C09-N10-C22
4	B	804[B]	HBJ	C04-C05-N06-C07
4	B	804[B]	HBJ	C33-C05-N06-C07
4	A	804	HBJ	C07-C09-N10-C11
4	B	804[A]	HBJ	C07-C09-N10-C11
4	C	804	HBJ	C07-C09-N10-C11
4	D	804	HBJ	C07-C09-N10-C11
6	C	810	BTB	N-C7-C8-O8
5	D	805	EDO	O1-C1-C2-O2
6	C	810	BTB	N-C2-C3-O3
5	D	808	EDO	O1-C1-C2-O2
4	A	804	HBJ	C07-C09-N10-C22
4	B	804[A]	HBJ	C07-C09-N10-C22
4	D	804	HBJ	C07-C09-N10-C22
4	B	804[A]	HBJ	O08-C07-C09-N10
5	C	808	EDO	O1-C1-C2-O2
5	D	806	EDO	O1-C1-C2-O2
5	D	809	EDO	O1-C1-C2-O2

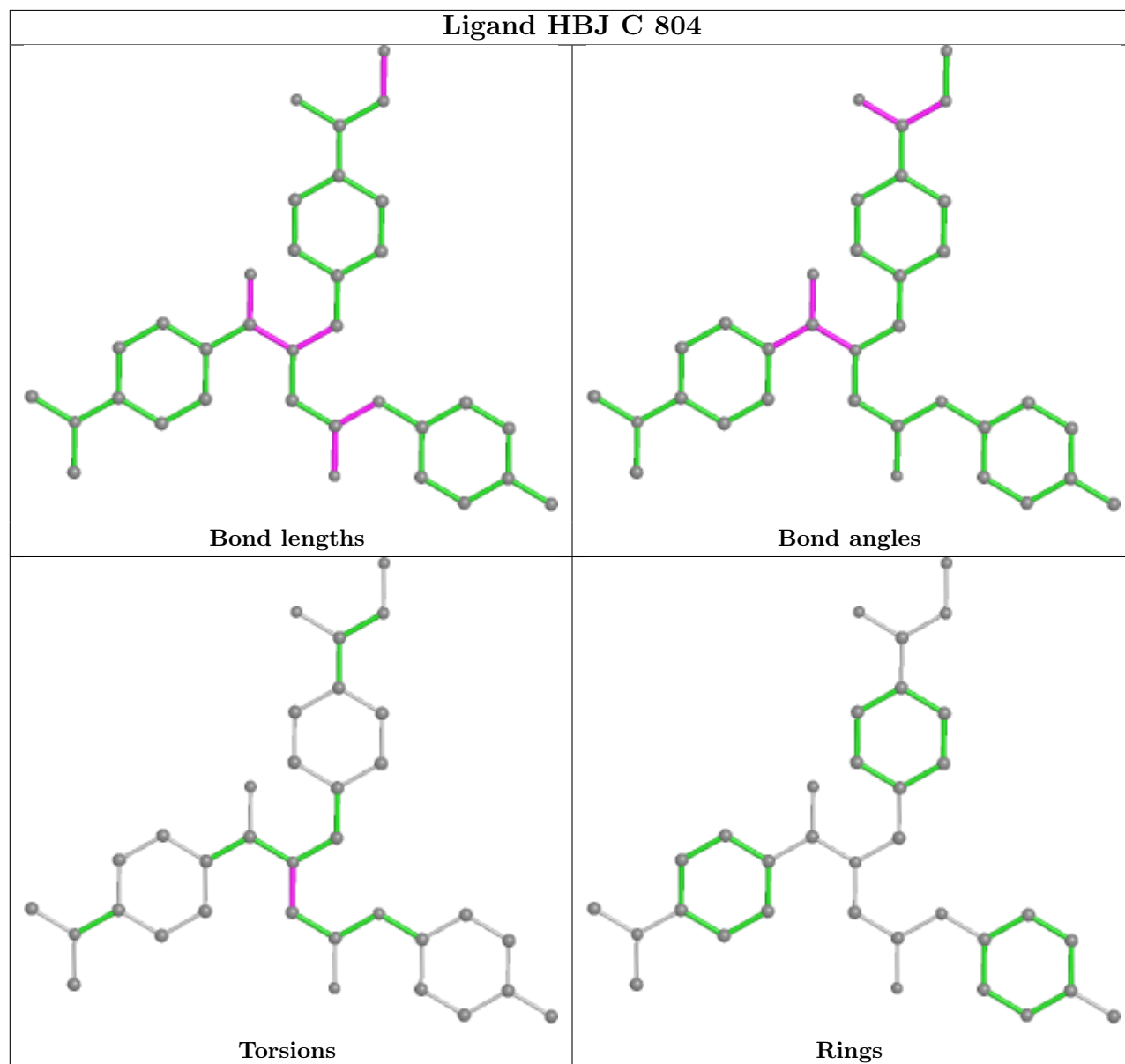
There are no ring outliers.

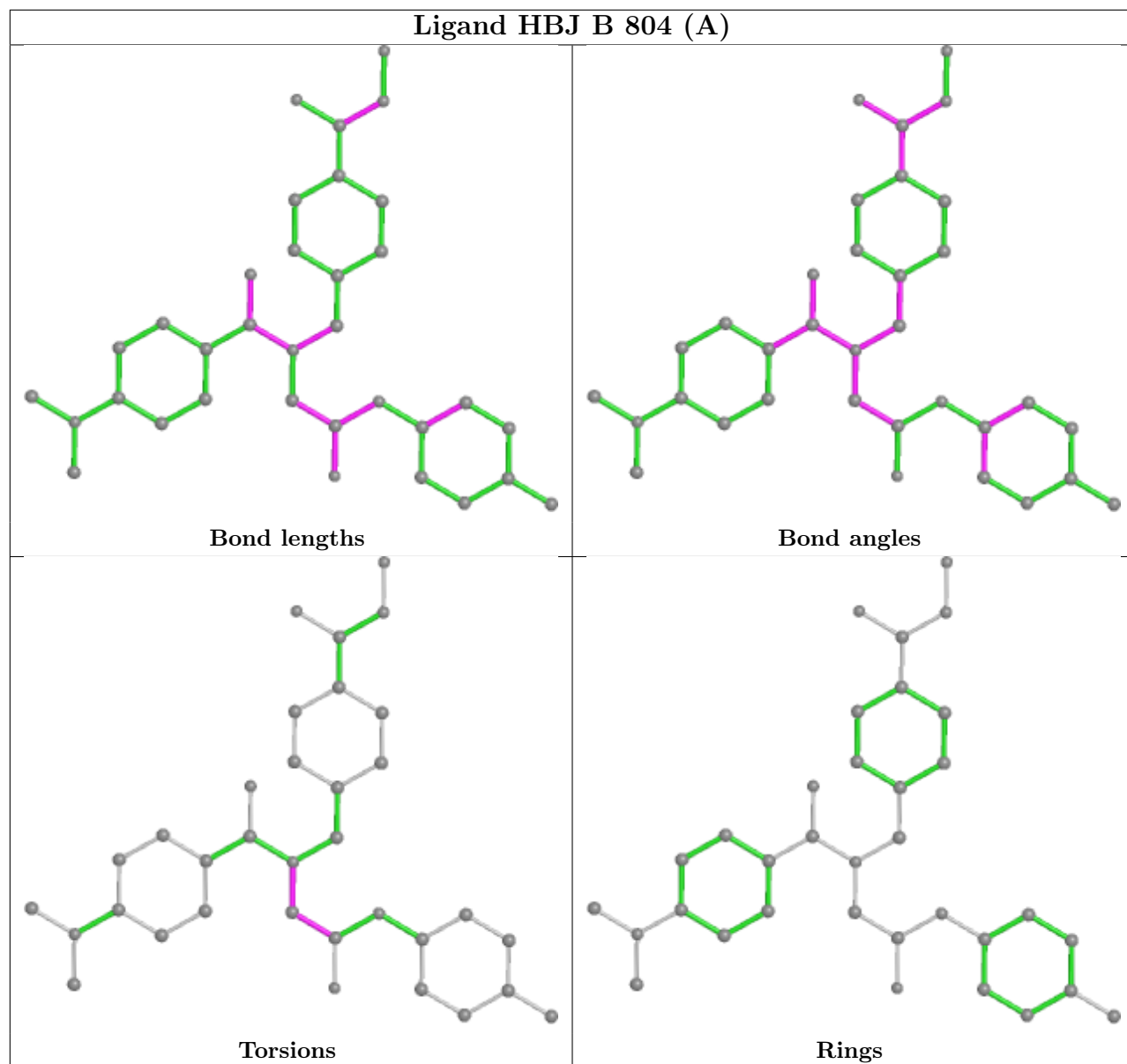
6 monomers are involved in 17 short contacts:

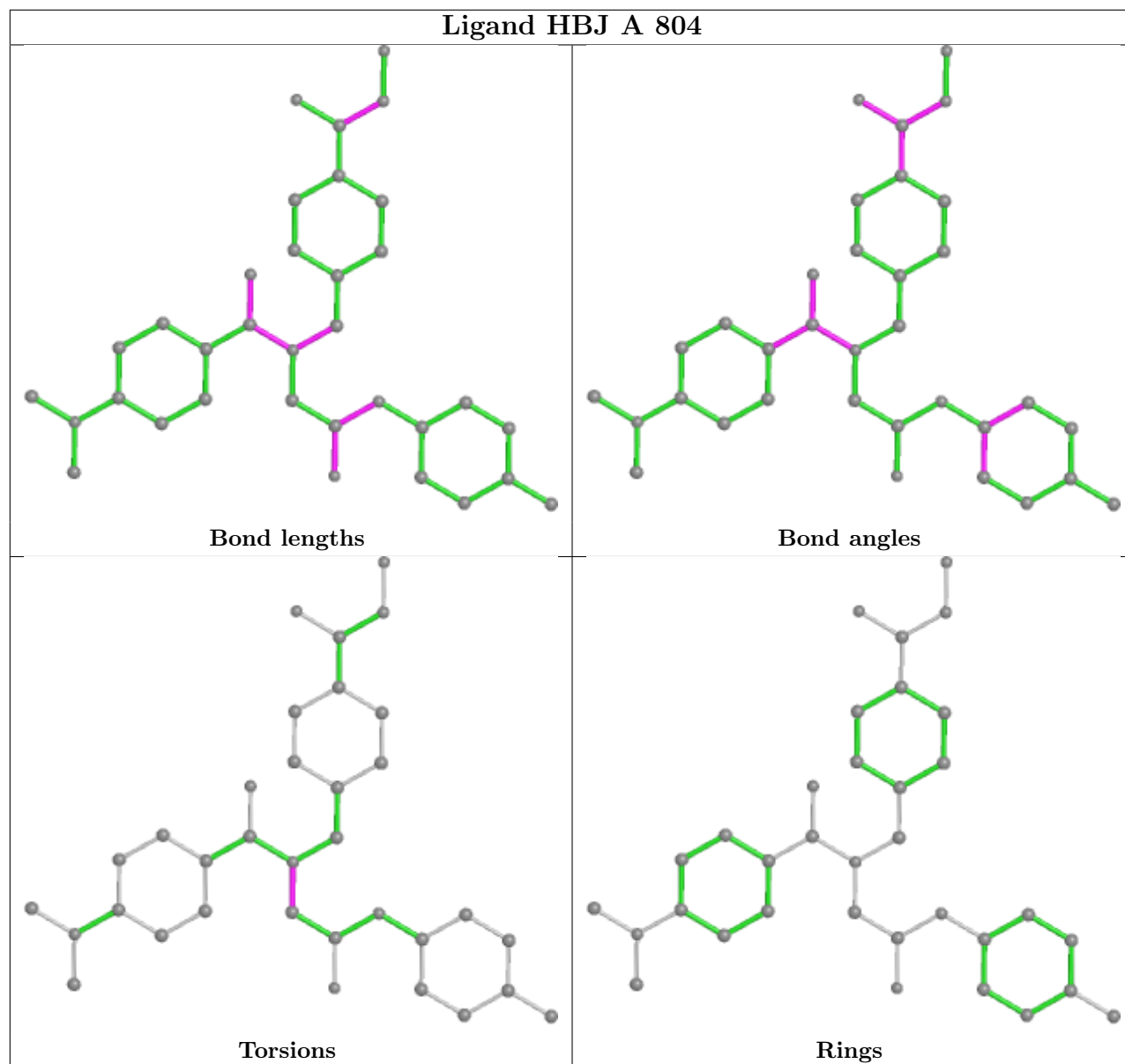
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	805	EDO	6	0
5	D	808	EDO	1	0
5	D	806	EDO	1	0
5	C	805	EDO	1	0
5	D	807	EDO	1	0
4	B	804[B]	HBJ	7	0

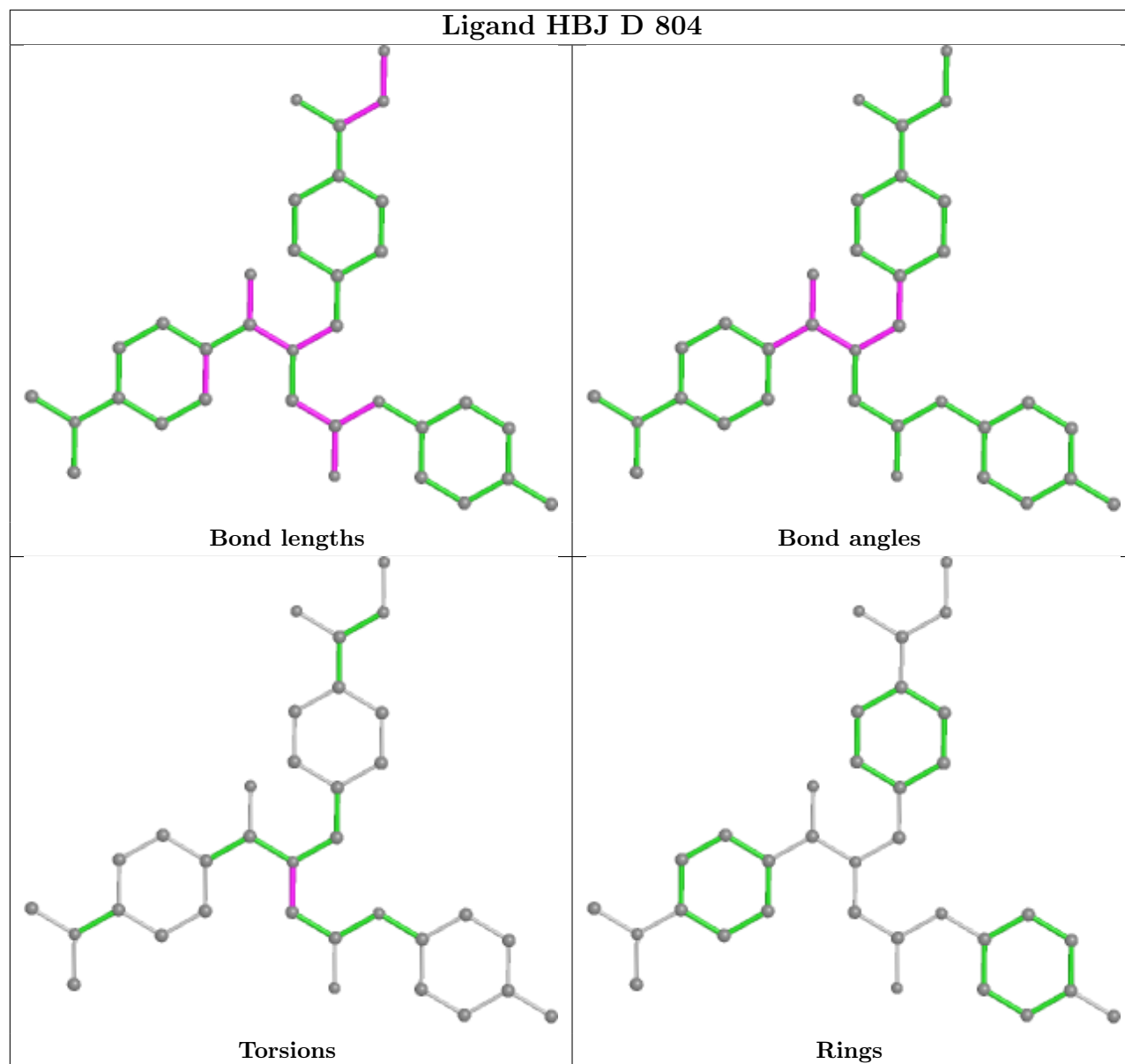
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

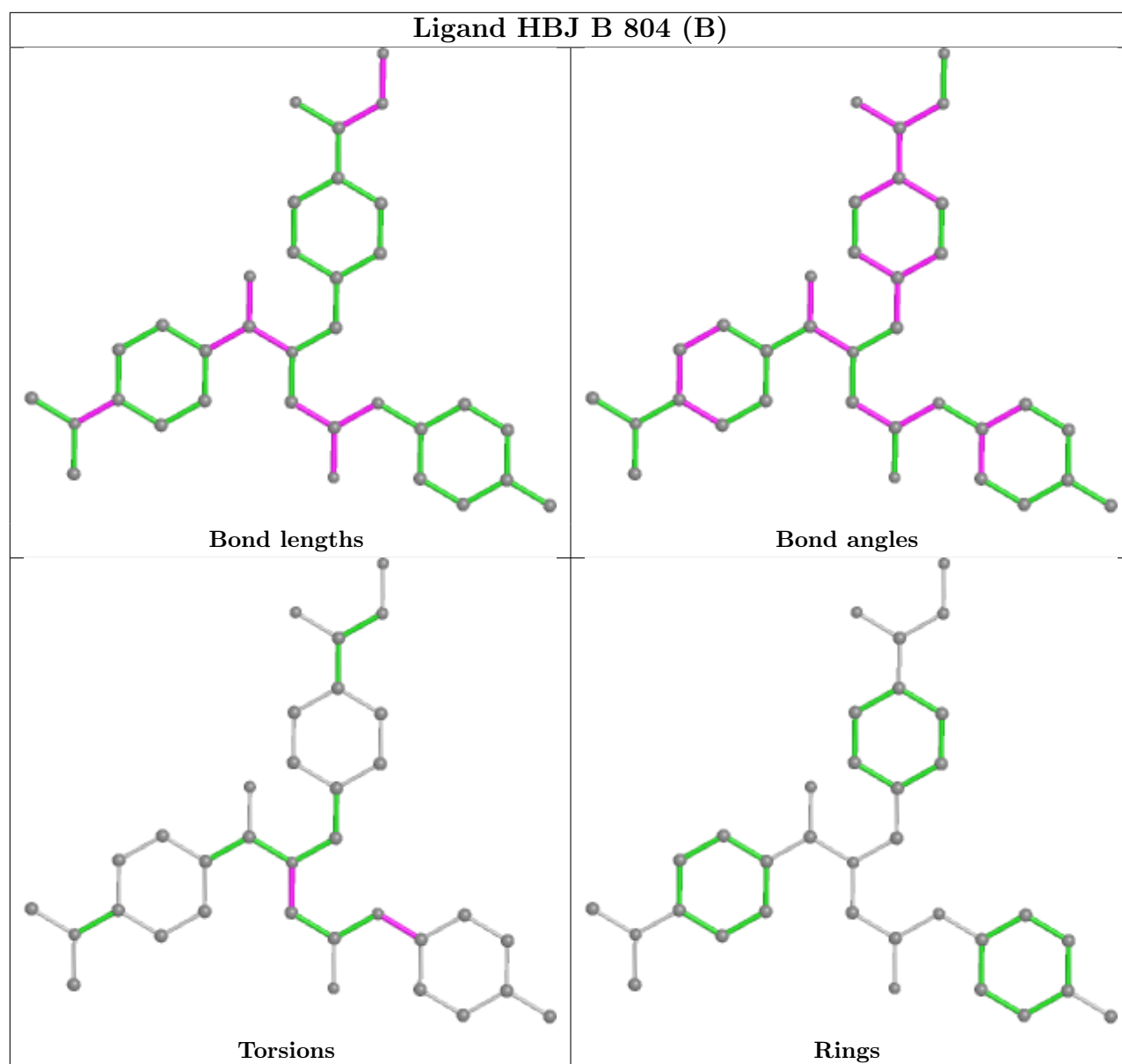
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	356/364 (97%)	-0.04	5 (1%) 75 78	6, 10, 23, 48	0
1	B	357/364 (98%)	-0.17	6 (1%) 70 73	5, 9, 22, 45	0
1	C	357/364 (98%)	-0.23	1 (0%) 94 95	5, 8, 16, 33	0
1	D	357/364 (98%)	-0.18	1 (0%) 94 95	5, 8, 17, 35	0
All	All	1427/1456 (98%)	-0.15	13 (0%) 84 86	5, 9, 19, 48	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	772	LEU	7.5
1	B	442	PRO	6.4
1	A	773	THR	4.9
1	D	442	PRO	4.9
1	B	443	ILE	2.9
1	A	771	HIS	2.9
1	B	772	LEU	2.8
1	C	442	PRO	2.6
1	B	770	ASP	2.5
1	B	658	LYS	2.5
1	A	769	LEU	2.4
1	B	767	PRO	2.3
1	A	770	ASP	2.1

### 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](#)

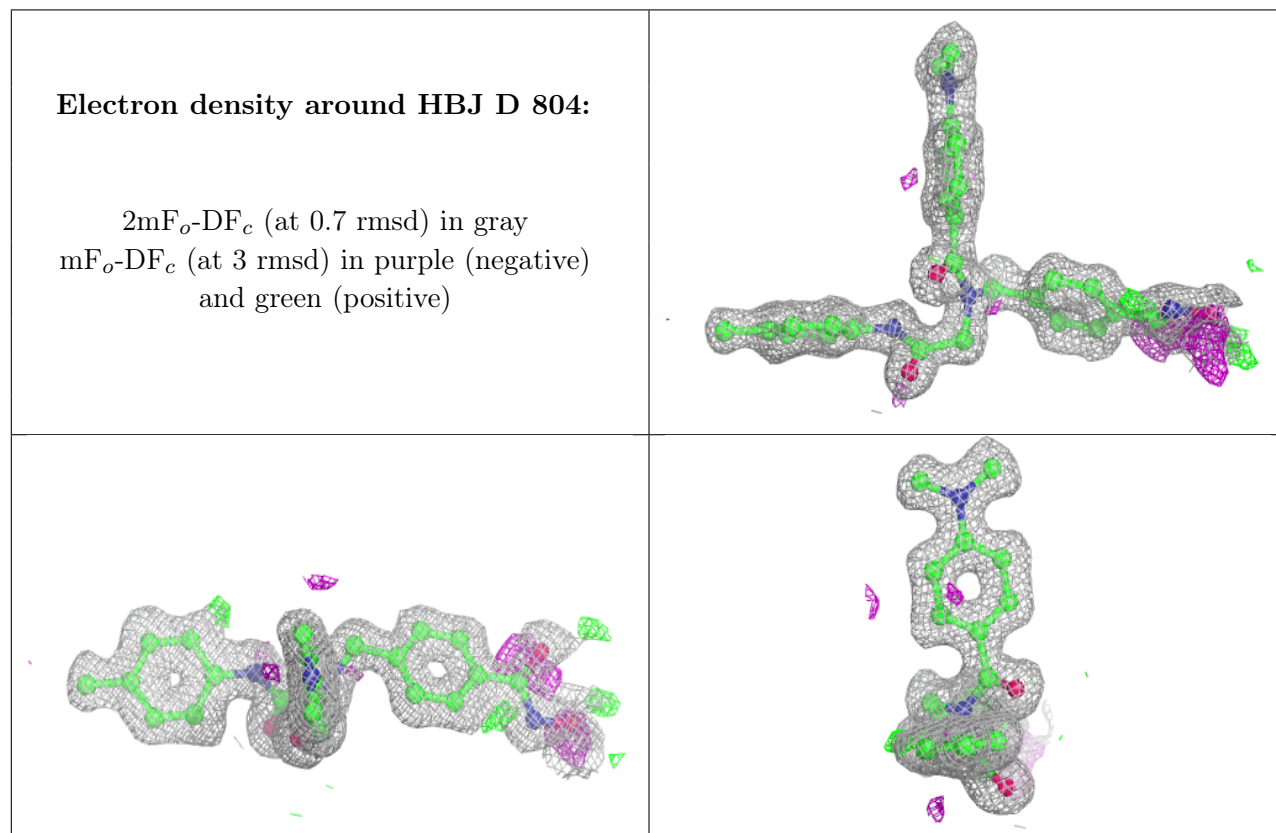
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

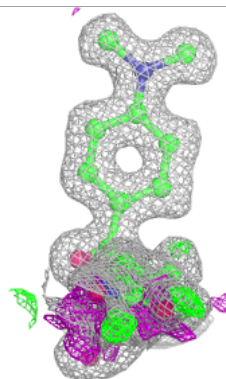
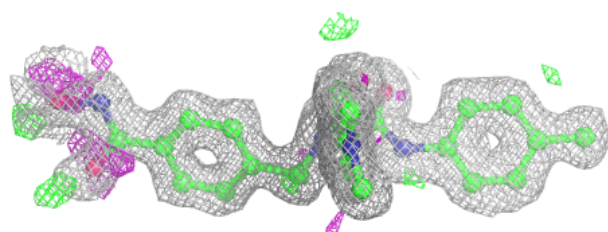
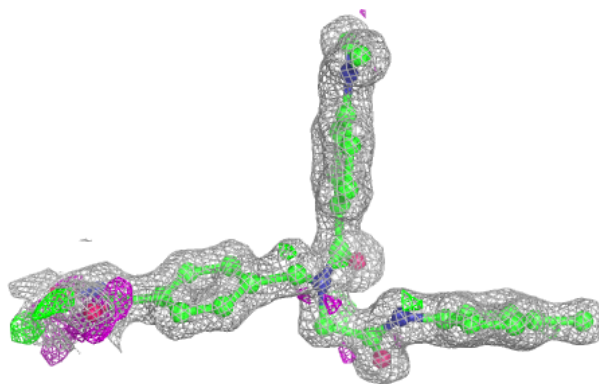
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	D	810	4/4	0.74	0.20	26,32,35,35	0
5	EDO	C	809	4/4	0.79	0.19	30,31,32,35	0
6	BTB	C	810	14/14	0.82	0.18	16,23,32,32	0
5	EDO	D	806	4/4	0.84	0.22	20,24,28,33	0
5	EDO	C	807	4/4	0.87	0.14	22,25,26,36	0
5	EDO	C	806	4/4	0.88	0.14	16,16,20,29	0
5	EDO	D	809	4/4	0.90	0.11	19,23,30,36	0
5	EDO	C	808	4/4	0.91	0.28	19,24,30,37	0
5	EDO	D	807	4/4	0.92	0.10	17,23,24,33	0
5	EDO	C	805	4/4	0.92	0.14	20,22,25,31	0
5	EDO	D	805	4/4	0.92	0.26	21,22,25,32	0
4	HBJ	D	804	34/34	0.92	0.10	6,11,18,32	0
5	EDO	D	808	4/4	0.93	0.17	24,25,31,31	0
5	EDO	B	805	4/4	0.93	0.14	20,26,28,30	0
4	HBJ	C	804	34/34	0.93	0.10	5,10,19,31	0
4	HBJ	A	804	34/34	0.93	0.10	6,11,18,32	0
4	HBJ	B	804[B]	34/34	0.94	0.13	6,9,13,14	34
4	HBJ	B	804[A]	34/34	0.94	0.13	5,8,13,20	34
5	EDO	A	805	4/4	0.97	0.08	7,7,8,8	0
3	K	A	803	1/1	0.99	0.07	11,11,11,11	0
3	K	A	802	1/1	0.99	0.07	7,7,7,7	0
3	K	D	803	1/1	1.00	0.06	6,6,6,6	0
2	ZN	C	801	1/1	1.00	0.06	7,7,7,7	0
2	ZN	D	801	1/1	1.00	0.06	7,7,7,7	0
2	ZN	A	801	1/1	1.00	0.04	9,9,9,9	0
2	ZN	B	801	1/1	1.00	0.07	7,7,7,7	0
3	K	B	802	1/1	1.00	0.05	5,5,5,5	0
3	K	B	803	1/1	1.00	0.06	8,8,8,8	0
3	K	C	802	1/1	1.00	0.06	5,5,5,5	0
3	K	C	803	1/1	1.00	0.05	8,8,8,8	0
3	K	D	802	1/1	1.00	0.07	5,5,5,5	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.

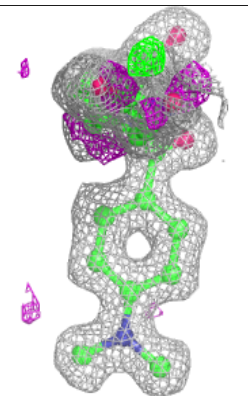
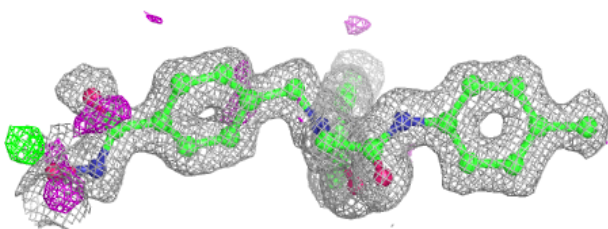
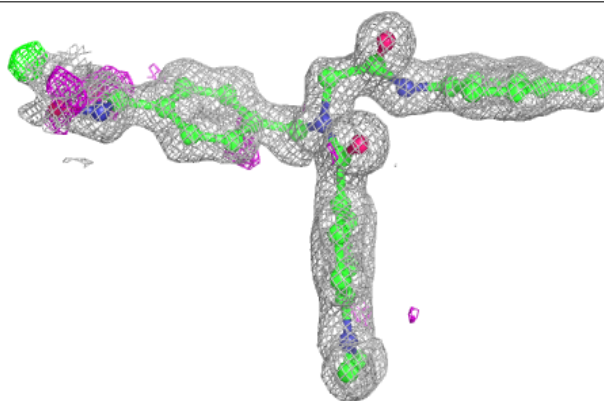


**Electron density around HBJ C 804:**

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

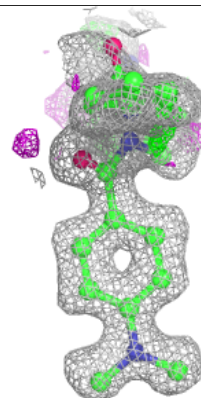
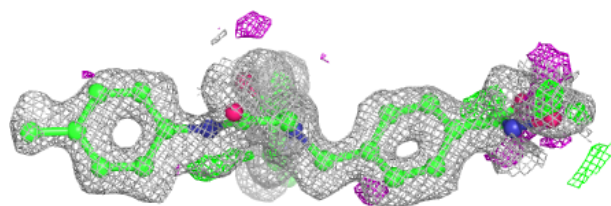
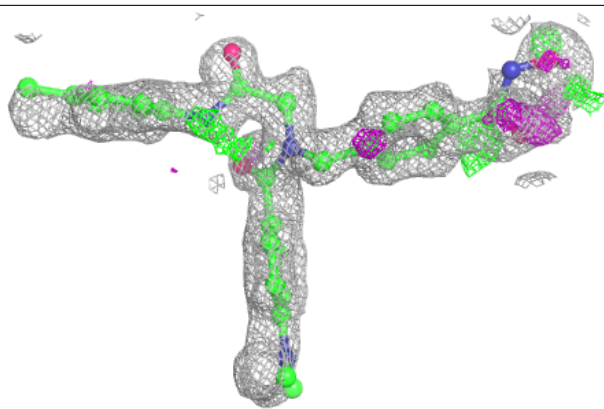
**Electron density around HBJ A 804:**

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

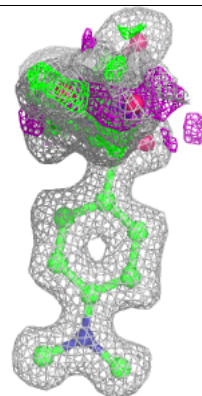
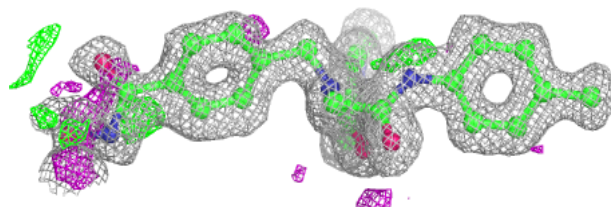
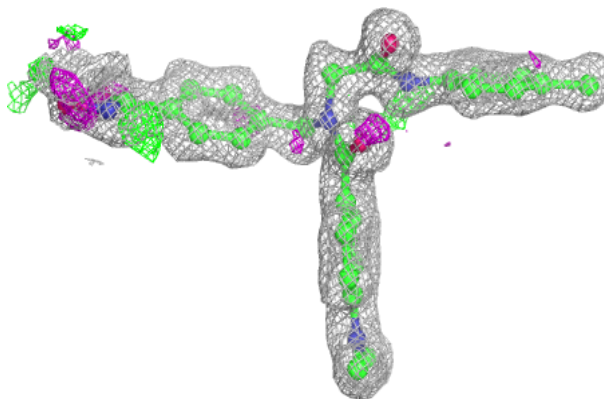


**Electron density around HBJ B 804 (B):**

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

**Electron density around HBJ B 804 (A):**

$2mF_o-DF_c$  (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.