



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2025 – 10:01 PM EST

PDB ID : 9DM6  
Title : Crystal Structure of Danio rerio histone deacetylase 6 catalytic domain 2 complexed with an ethylhydrazide inhibitor  
Authors : Gaynes, M.N.; Watson, P.R.; Konig, B.; Christianson, D.W.  
Deposited on : 2024-09-12  
Resolution : 1.40 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.3

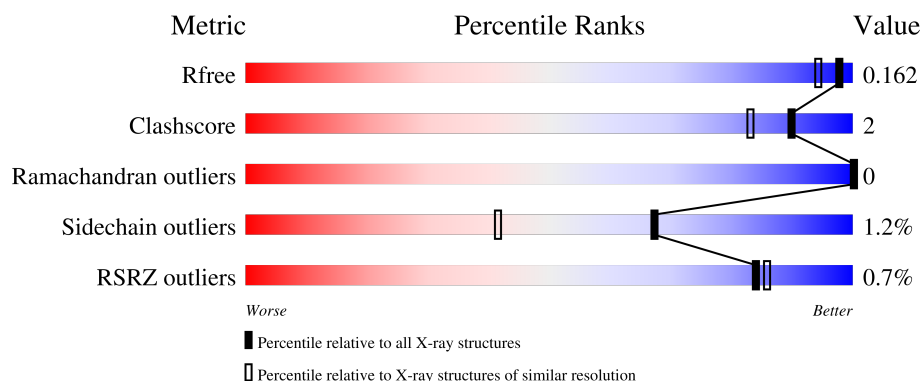
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

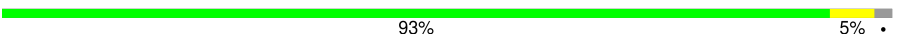


The reported resolution of this entry is 1.40 Å.

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))
$R_{free}$	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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	
1	B	364	
1	C	364	
1	D	364	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12912 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.

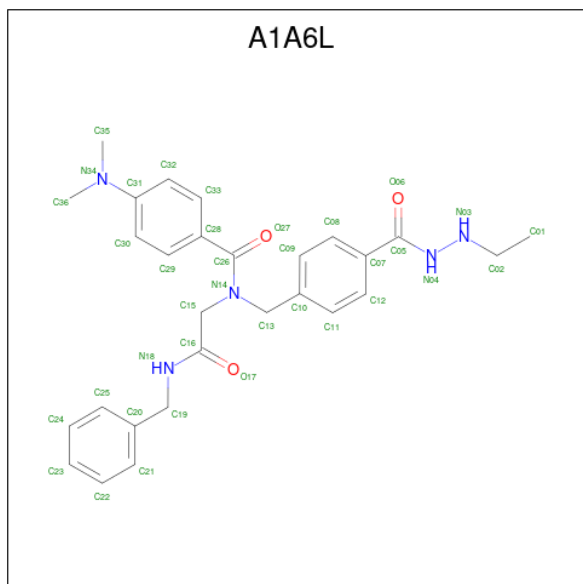
- Molecule 1 is a protein called Hdac6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	357	Total	C	N	O	S	0	13	0
			2850	1798	508	524	20			
1	A	357	Total	C	N	O	S	0	10	0
			2816	1779	497	520	20			
1	C	352	Total	C	N	O	S	0	8	0
			2771	1749	492	511	19			
1	D	356	Total	C	N	O	S	0	6	0
			2791	1759	496	518	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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 N-[2-(benzylamino)-2-oxoethyl]-4-(dimethylamino)-N-{[4-(2-ethylhydrazine-1-carbonyl)phenyl]methyl}benzamide (three-letter code: A1A6L) (formula:  $C_{28}H_{33}N_5O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			36	28	5	3		
2	A	1	Total	C	N	O	0	0
			36	28	5	3		
2	C	1	Total	C	N	O	0	0
			36	28	5	3		
2	D	1	Total	C	N	O	0	0
			36	28	5	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	383	Total O 383 383	0	0
6	A	418	Total O 418 418	0	0
6	C	319	Total O 319 319	0	0
6	D	356	Total O 356 356	0	0

### 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

Chain B: 




- Molecule 1: Hdac6 protein

Chain A: 



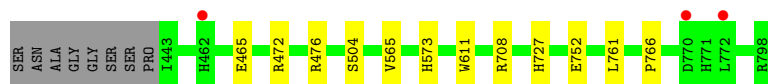
- Molecule 1: Hdac6 protein

Chain C: 



- Molecule 1: Hdac6 protein

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.42Å 95.59Å 98.08Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	65.55 – 1.40 65.55 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (65.55-1.40) 98.5 (65.55-1.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.144 , 0.163 0.145 , 0.162	Depositor DCC
$R_{free}$ test set	278431 reflections (0.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.1	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	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 31.09 % 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 1.1733e-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: ZN, EDO, A1A6L, K

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	0.31	0/2917	0.59	0/3959
1	B	0.31	0/2951	0.59	0/4001
1	C	0.31	0/2863	0.58	0/3881
1	D	0.31	0/2872	0.59	0/3898
All	All	0.31	0/11603	0.59	0/15739

There are no bond length outliers.

There are no bond angle outliers.

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	2816	0	2752	9	0
1	B	2850	0	2795	13	0
1	C	2771	0	2700	10	0
1	D	2791	0	2705	7	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
2	D	36	0	0	0	0
3	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	24	5	0
3	C	16	0	24	3	0
3	D	12	0	18	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	418	0	0	1	0
6	B	383	0	0	1	0
6	C	319	0	0	0	0
6	D	356	0	0	1	0
All	All	12912	0	11030	39	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 (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:ALA:HB2	1:B:756[A]:MET:HG2	1.45	0.98
3:B:802:EDO:H21	1:A:600:THR:HG22	1.72	0.70
1:B:776[A]:LYS:NZ	6:B:901:HOH:O	2.28	0.67
1:D:504:SER:HB2	3:D:804:EDO:H11	1.78	0.66
1:C:533:PHE:HB3	3:C:805:EDO:H11	1.77	0.66
1:A:565[A]:VAL:HG13	1:A:761:LEU:HD12	1.80	0.63
1:C:458[B]:MET:HE1	1:C:519:PRO:HB3	1.82	0.60
1:D:708:ARG:NH1	6:D:901:HOH:O	2.35	0.60
1:A:458[A]:MET:HE1	1:A:519:PRO:HB3	1.83	0.58
1:B:672:LYS:O	1:B:776[B]:LYS:NZ	2.33	0.57
1:C:515:GLU:O	1:C:536[B]:ASN:ND2	2.38	0.56
1:B:458[B]:MET:HE1	1:B:519:PRO:HB3	1.87	0.56
1:C:468:GLN:HG2	3:C:803:EDO:H21	1.89	0.54
1:B:565[A]:VAL:HG13	1:B:761:LEU:HD12	1.89	0.53
1:B:679:MET:HG2	1:B:724:HIS:CD2	2.44	0.51
1:A:672:LYS:NZ	1:A:716:GLN:HB3	2.25	0.51
1:A:459:TRP:CZ2	1:A:523:ASN:HB2	2.45	0.51
1:B:536:ASN:OD1	3:B:804:EDO:H21	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565[A]:VAL:HG13	1:D:761:LEU:HD12	1.92	0.51
1:D:472:ARG:HG2	3:D:803:EDO:H11	1.93	0.50
1:B:457:ASN:HD21	3:B:805:EDO:H11	1.78	0.49
1:B:456:HIS:HE1	3:B:804:EDO:H22	1.79	0.47
1:B:459:TRP:CZ2	1:B:523:ASN:HB2	2.50	0.47
1:C:756:MET:CE	1:C:767:PRO:HG3	2.47	0.45
1:A:476:ARG:NE	1:A:752:GLU:OE2	2.50	0.45
1:D:476:ARG:NE	1:D:752:GLU:OE2	2.45	0.45
1:A:682:PHE:HA	1:A:686:VAL:HB	1.99	0.44
1:C:625:GLU:HG2	1:C:656:LEU:HB2	1.98	0.44
1:C:777:THR:H	3:C:804:EDO:H21	1.83	0.44
1:B:457:ASN:HD21	3:B:805:EDO:C1	2.31	0.44
1:C:756:MET:HE1	1:C:767:PRO:HG3	2.00	0.43
1:D:727:HIS:CD2	1:D:766:PRO:HG3	2.53	0.43
1:B:723:ALA:HB2	1:B:756[A]:MET:CG	2.32	0.43
1:C:458[B]:MET:HE1	1:C:519:PRO:CB	2.49	0.42
1:A:458[A]:MET:HB2	1:A:458[A]:MET:HE2	1.75	0.42
1:C:565[A]:VAL:HG13	1:C:761:LEU:HD12	2.01	0.41
1:A:788:ARG:NH2	6:A:907:HOH:O	2.48	0.41
1:D:472:ARG:CG	3:D:803:EDO:H11	2.51	0.40
1:B:682:PHE:HA	1:B:686:VAL:HB	2.02	0.40

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	365/364 (100%)	358 (98%)	7 (2%)	0	100	100
1	B	368/364 (101%)	360 (98%)	8 (2%)	0	100	100
1	C	356/364 (98%)	350 (98%)	6 (2%)	0	100	100
1	D	360/364 (99%)	354 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1449/1456 (100%)	1422 (98%)	27 (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	307/305 (101%)	302 (98%)	5 (2%)	58	29
1	B	311/305 (102%)	308 (99%)	3 (1%)	73	49
1	C	299/305 (98%)	295 (99%)	4 (1%)	65	38
1	D	300/305 (98%)	297 (99%)	3 (1%)	73	49
All	All	1217/1220 (100%)	1202 (99%)	15 (1%)	67	41

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

Mol	Chain	Res	Type
1	B	465	GLU
1	B	573	HIS
1	B	611	TRP
1	A	465	GLU
1	A	573	HIS
1	A	611	TRP
1	A	756[A]	MET
1	A	756[B]	MET
1	C	465	GLU
1	C	527	ASP
1	C	573	HIS
1	C	611	TRP
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 ⓘ

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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	B	804	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	A	803	-	3,3,3	0.42	0	2,2,2	0.55	0
3	EDO	C	803	-	3,3,3	0.42	0	2,2,2	0.30	0
3	EDO	D	804	-	3,3,3	0.50	0	2,2,2	0.18	0
3	EDO	B	803	-	3,3,3	0.44	0	2,2,2	0.53	0
2	A1A6L	C	801	4	37,38,38	2.21	7 (18%)	48,50,50	1.61	6 (12%)
3	EDO	C	805	-	3,3,3	0.44	0	2,2,2	0.44	0
3	EDO	A	802	-	3,3,3	0.46	0	2,2,2	0.55	0
2	A1A6L	A	801	4	37,38,38	2.22	9 (24%)	48,50,50	1.66	8 (16%)
3	EDO	C	802	-	3,3,3	0.47	0	2,2,2	0.17	0
3	EDO	D	803	-	3,3,3	0.44	0	2,2,2	0.41	0
3	EDO	B	805	-	3,3,3	0.41	0	2,2,2	0.54	0
2	A1A6L	D	801	4	37,38,38	2.23	8 (21%)	48,50,50	1.63	5 (10%)
2	A1A6L	B	801	4	37,38,38	2.21	7 (18%)	48,50,50	1.60	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	C	804	-	3,3,3	0.45	0	2,2,2	0.67	0
3	EDO	D	802	-	3,3,3	0.45	0	2,2,2	0.52	0
3	EDO	B	802	-	3,3,3	0.49	0	2,2,2	0.41	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	EDO	B	804	-	-	1/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	C	803	-	-	1/1/1/1	-
3	EDO	D	804	-	-	1/1/1/1	-
3	EDO	B	803	-	-	0/1/1/1	-
2	A1A6L	C	801	4	-	0/32/33/33	0/3/3/3
3	EDO	C	805	-	-	1/1/1/1	-
3	EDO	A	802	-	-	1/1/1/1	-
2	A1A6L	A	801	4	-	0/32/33/33	0/3/3/3
3	EDO	C	802	-	-	0/1/1/1	-
3	EDO	D	803	-	-	1/1/1/1	-
3	EDO	B	805	-	-	1/1/1/1	-
2	A1A6L	D	801	4	-	0/32/33/33	0/3/3/3
2	A1A6L	B	801	4	-	0/32/33/33	0/3/3/3
3	EDO	C	804	-	-	0/1/1/1	-
3	EDO	D	802	-	-	0/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1A6L	C16-N18	6.64	1.49	1.33
2	D	801	A1A6L	C16-N18	6.62	1.49	1.33
2	B	801	A1A6L	C16-N18	6.60	1.49	1.33
2	C	801	A1A6L	C16-N18	6.53	1.48	1.33
2	A	801	A1A6L	C26-N14	6.16	1.47	1.34
2	D	801	A1A6L	C26-N14	6.03	1.47	1.34
2	C	801	A1A6L	C26-N14	6.03	1.47	1.34
2	B	801	A1A6L	C26-N14	5.89	1.47	1.34
2	C	801	A1A6L	C05-N04	5.26	1.43	1.35
2	D	801	A1A6L	C05-N04	4.83	1.43	1.35
2	A	801	A1A6L	C05-N04	4.71	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1A6L	C05-N04	4.45	1.42	1.35
2	C	801	A1A6L	C31-N34	4.07	1.47	1.37
2	D	801	A1A6L	C31-N34	4.03	1.46	1.37
2	B	801	A1A6L	C31-N34	4.01	1.46	1.37
2	B	801	A1A6L	N04-N03	3.93	1.44	1.41
2	A	801	A1A6L	C31-N34	3.84	1.46	1.37
2	A	801	A1A6L	N04-N03	3.49	1.44	1.41
2	D	801	A1A6L	N04-N03	3.21	1.43	1.41
2	D	801	A1A6L	O06-C05	-2.51	1.17	1.23
2	D	801	A1A6L	C28-C26	2.50	1.54	1.50
2	C	801	A1A6L	N04-N03	2.34	1.43	1.41
2	A	801	A1A6L	C28-C26	2.33	1.53	1.50
2	C	801	A1A6L	C28-C26	2.31	1.53	1.50
2	C	801	A1A6L	O06-C05	-2.23	1.18	1.23
2	A	801	A1A6L	C08-C07	-2.12	1.36	1.39
2	D	801	A1A6L	C13-C10	2.10	1.55	1.51
2	A	801	A1A6L	C13-C10	2.08	1.55	1.51
2	A	801	A1A6L	O06-C05	-2.06	1.18	1.23
2	B	801	A1A6L	O27-C26	-2.00	1.18	1.22
2	B	801	A1A6L	C12-C07	2.00	1.42	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1A6L	C28-C26-N14	5.58	125.63	118.66
2	B	801	A1A6L	C28-C26-N14	5.07	124.99	118.66
2	C	801	A1A6L	C28-C26-N14	4.91	124.80	118.66
2	A	801	A1A6L	C28-C26-N14	4.77	124.61	118.66
2	A	801	A1A6L	C10-C13-N14	-4.72	105.73	113.15
2	C	801	A1A6L	C10-C13-N14	-4.49	106.10	113.15
2	B	801	A1A6L	C10-C13-N14	-4.37	106.28	113.15
2	D	801	A1A6L	O27-C26-N14	-4.30	115.58	122.35
2	A	801	A1A6L	O27-C26-N14	-4.10	115.90	122.35
2	D	801	A1A6L	C10-C13-N14	-4.06	106.77	113.15
2	B	801	A1A6L	O27-C26-N14	-3.81	116.35	122.35
2	C	801	A1A6L	O27-C26-N14	-3.80	116.37	122.35
2	A	801	A1A6L	C07-C05-N04	2.92	119.33	115.98
2	C	801	A1A6L	C32-C31-N34	-2.90	117.78	121.65
2	D	801	A1A6L	C30-C31-N34	-2.43	118.40	121.65
2	A	801	A1A6L	C19-N18-C16	-2.33	118.64	122.42
2	C	801	A1A6L	C33-C28-C29	2.32	121.52	118.57
2	A	801	A1A6L	C32-C31-N34	-2.18	118.74	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1A6L	C02-N03-N04	-2.17	109.10	111.32
2	A	801	A1A6L	C11-C12-C07	-2.16	118.49	120.80
2	B	801	A1A6L	C07-C05-N04	2.12	118.40	115.98
2	A	801	A1A6L	C02-N03-N04	-2.11	109.16	111.32
2	C	801	A1A6L	C19-N18-C16	-2.07	119.06	122.42
2	B	801	A1A6L	C02-N03-N04	-2.03	109.24	111.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	803	EDO	O1-C1-C2-O2
3	D	804	EDO	O1-C1-C2-O2
3	B	804	EDO	O1-C1-C2-O2
3	C	805	EDO	O1-C1-C2-O2
3	B	805	EDO	O1-C1-C2-O2
3	A	802	EDO	O1-C1-C2-O2
3	C	803	EDO	O1-C1-C2-O2

There are no ring outliers.

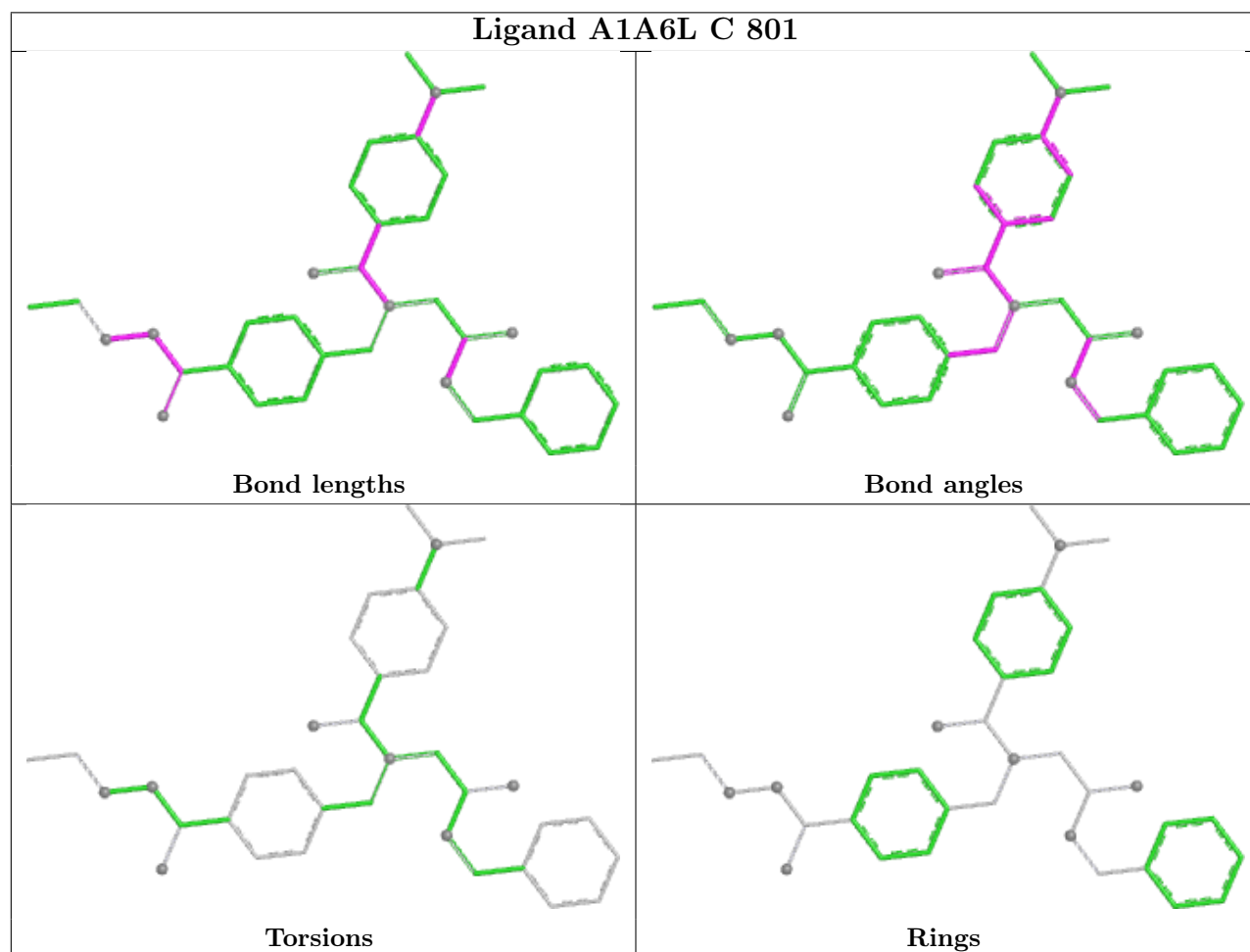
8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	EDO	2	0
3	C	803	EDO	1	0
3	D	804	EDO	1	0
3	C	805	EDO	1	0
3	D	803	EDO	2	0
3	B	805	EDO	2	0
3	C	804	EDO	1	0
3	B	802	EDO	1	0

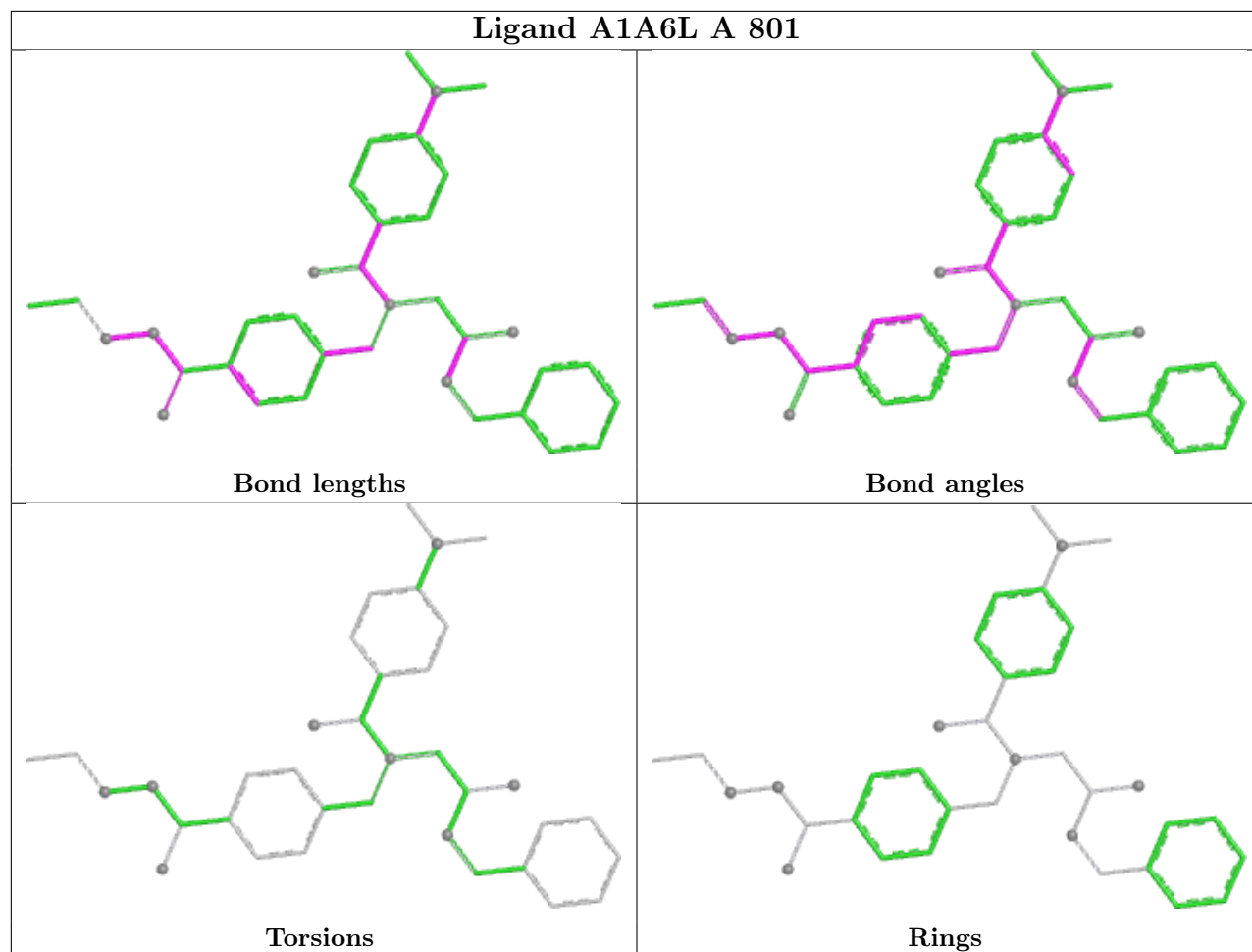
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



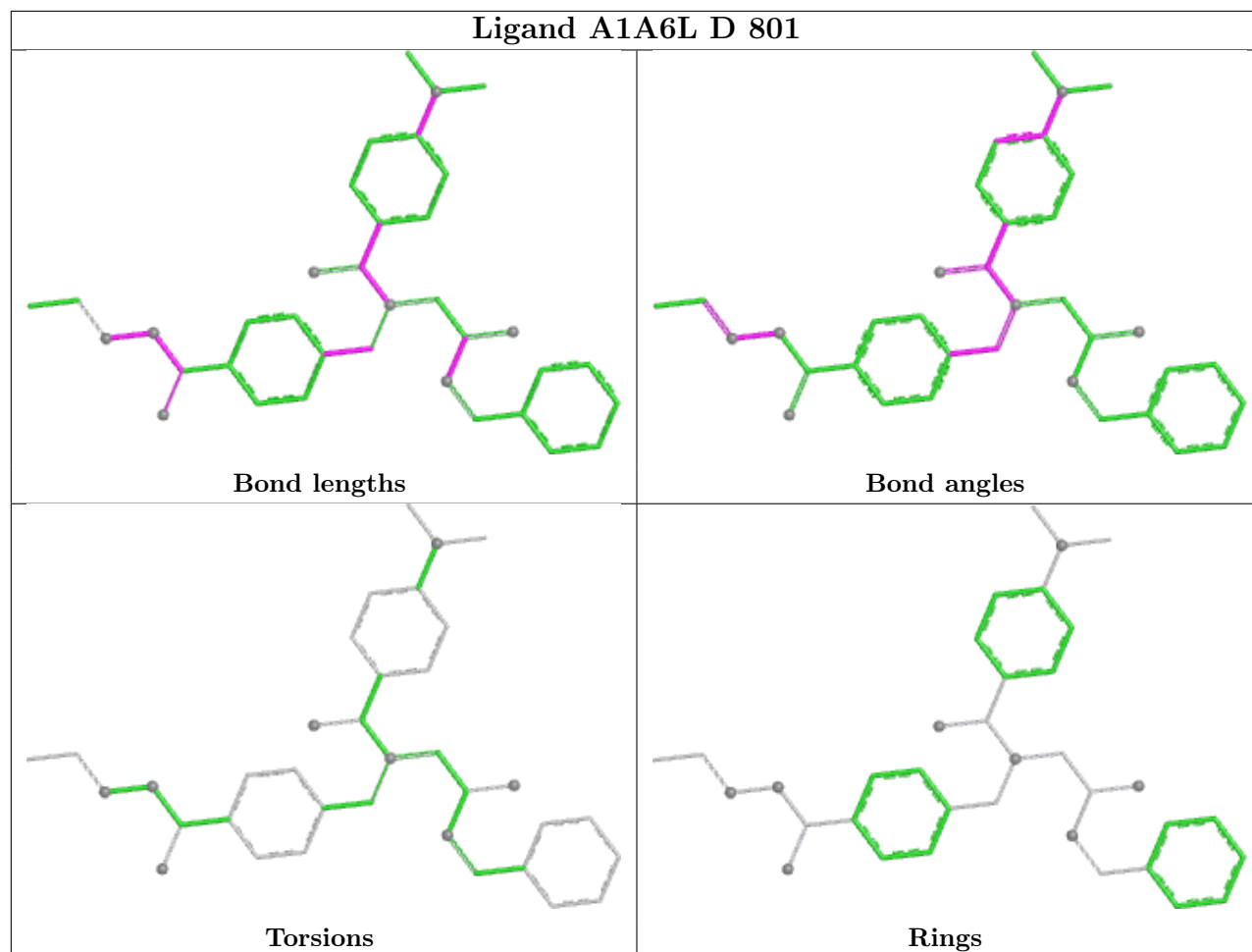
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

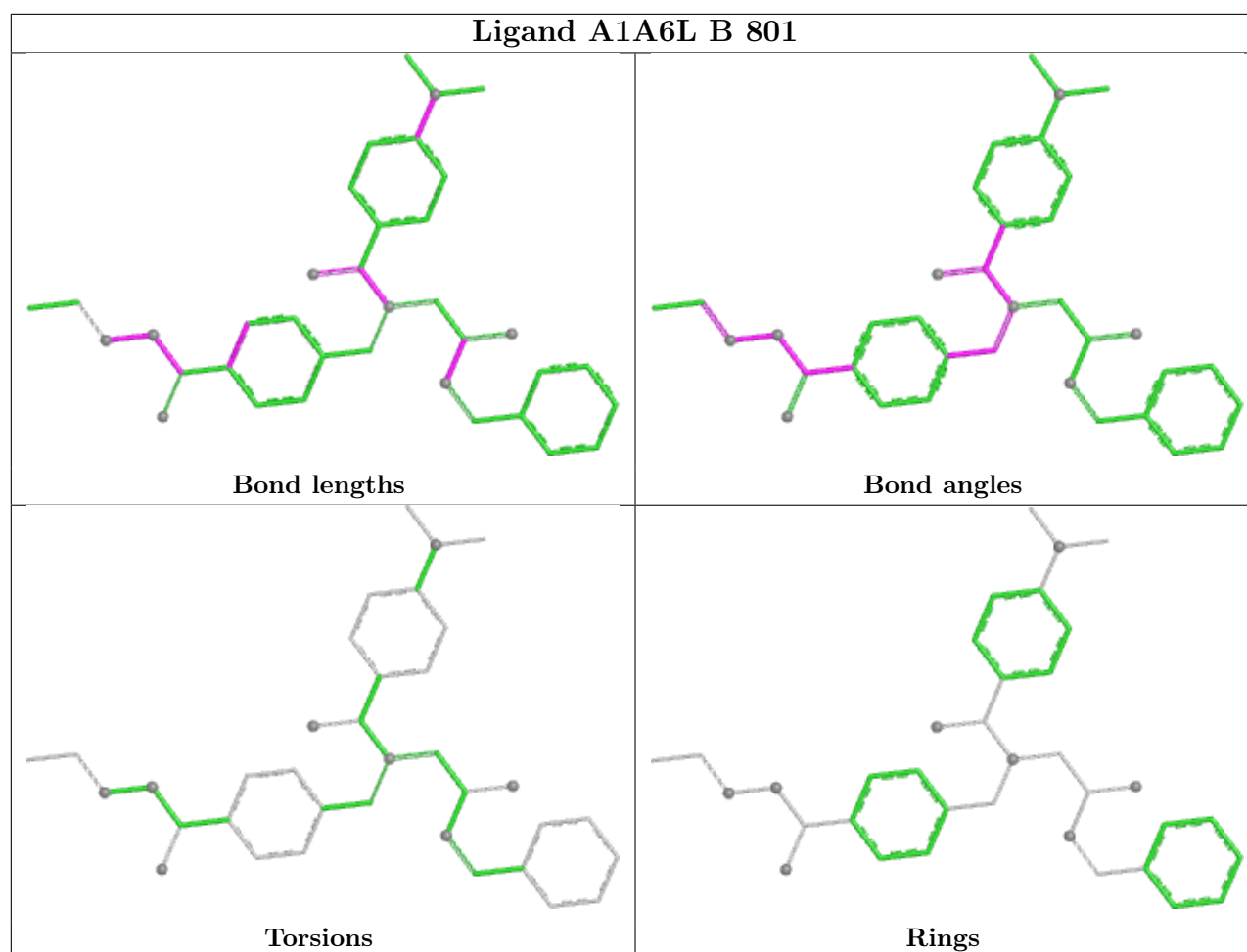


## Ligand A1A6L A 801



## Ligand A1A6L D 801





## 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	357/364 (98%)	-0.54	1 (0%) 90 92	5, 9, 17, 30	10 (2%)
1	B	357/364 (98%)	-0.51	1 (0%) 90 92	3, 9, 17, 29	13 (3%)
1	C	352/364 (96%)	-0.28	5 (1%) 73 75	6, 11, 23, 46	8 (2%)
1	D	356/364 (97%)	-0.44	3 (0%) 82 84	4, 10, 19, 39	6 (1%)
All	All	1422/1456 (97%)	-0.44	10 (0%) 84 86	3, 10, 19, 46	37 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	775	LEU	5.1
1	C	774	PRO	4.9
1	B	442	PRO	3.7
1	A	442	PRO	3.5
1	C	769	LEU	3.4
1	D	770	ASP	2.6
1	D	772	LEU	2.3
1	C	797	LEU	2.2
1	C	798	ARG	2.1
1	D	462	HIS	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 ⓘ

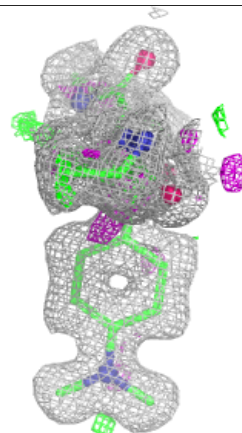
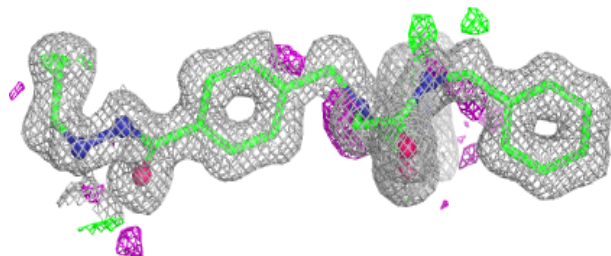
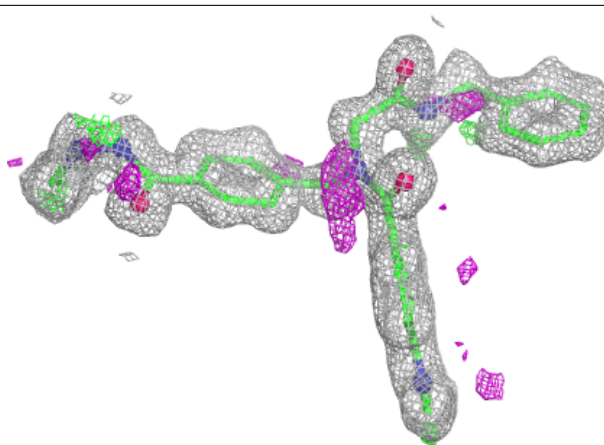
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	EDO	C	804	4/4	0.67	0.19	35,37,38,45	0
3	EDO	C	805	4/4	0.68	0.27	34,39,39,52	0
3	EDO	D	803	4/4	0.74	0.22	29,33,41,49	0
3	EDO	D	802	4/4	0.79	0.20	30,33,38,53	0
3	EDO	C	803	4/4	0.80	0.21	26,27,38,49	0
3	EDO	A	803	4/4	0.85	0.18	21,34,34,52	0
3	EDO	B	803	4/4	0.86	0.14	25,33,36,43	0
3	EDO	D	804	4/4	0.86	0.18	20,20,30,47	0
3	EDO	B	802	4/4	0.87	0.20	16,25,27,42	0
3	EDO	B	805	4/4	0.89	0.14	19,29,31,38	0
3	EDO	A	802	4/4	0.90	0.15	25,30,32,49	0
3	EDO	B	804	4/4	0.91	0.14	13,28,32,39	0
2	A1A6L	A	801	36/36	0.95	0.06	4,8,12,13	0
2	A1A6L	C	801	36/36	0.95	0.07	5,9,12,13	0
2	A1A6L	B	801	36/36	0.96	0.06	5,7,12,13	0
2	A1A6L	D	801	36/36	0.96	0.06	5,8,13,15	0
3	EDO	C	802	4/4	0.97	0.06	9,10,10,12	0
5	K	C	808	1/1	0.97	0.06	12,12,12,12	0
5	K	C	807	1/1	0.98	0.04	8,8,8,8	0
5	K	D	806	1/1	0.99	0.03	5,5,5,5	0
5	K	D	807	1/1	0.99	0.03	8,8,8,8	1
5	K	B	807	1/1	1.00	0.03	6,6,6,6	0
5	K	B	808	1/1	1.00	0.03	7,7,7,7	1
5	K	A	805	1/1	1.00	0.04	6,6,6,6	0
5	K	A	806	1/1	1.00	0.02	7,7,7,7	1
4	ZN	B	806	1/1	1.00	0.01	6,6,6,6	0
4	ZN	A	804	1/1	1.00	0.01	6,6,6,6	0
4	ZN	C	806	1/1	1.00	0.02	7,7,7,7	0
4	ZN	D	805	1/1	1.00	0.01	6,6,6,6	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.

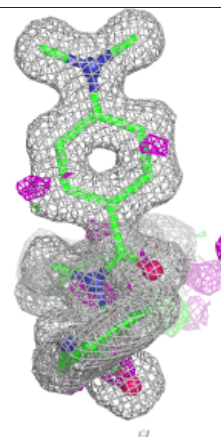
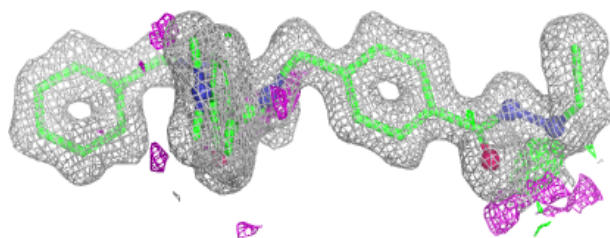
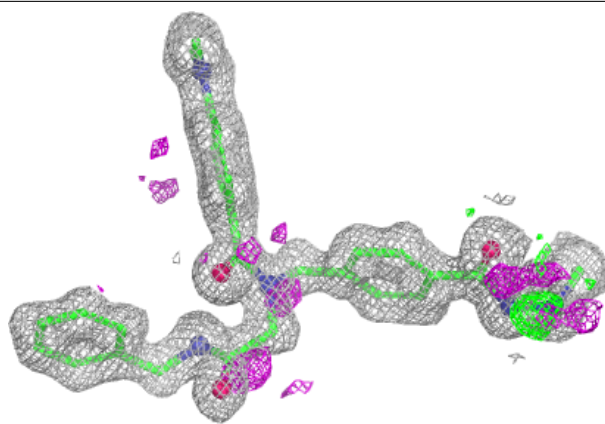
**Electron density around A1A6L A 801:**

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



**Electron density around A1A6L C 801:**

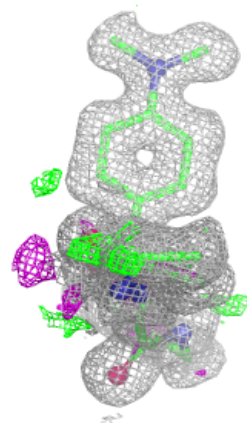
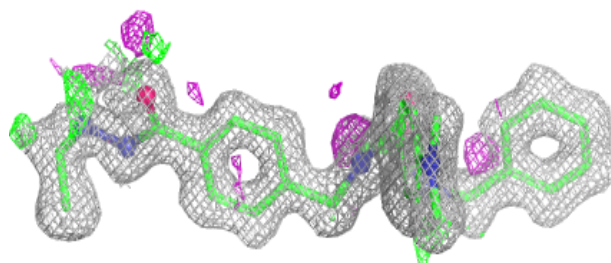
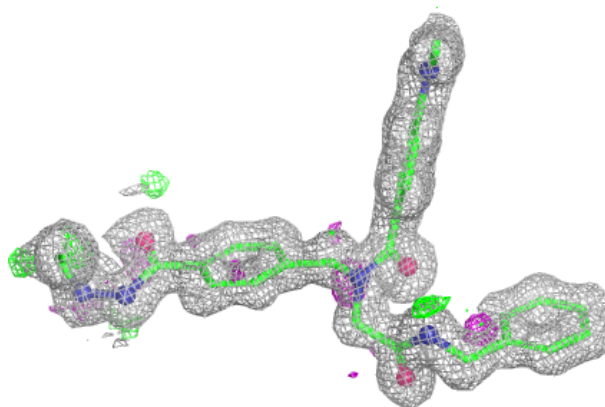
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



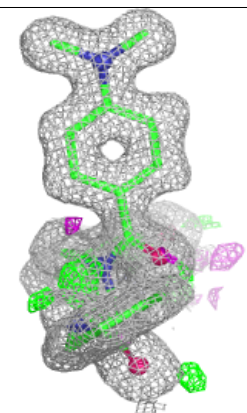
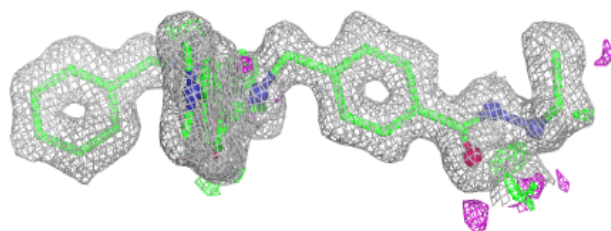
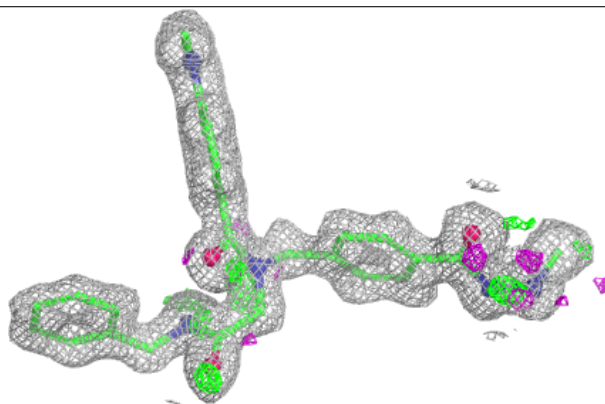


**Electron density around A1A6L B 801:**

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

**Electron density around A1A6L D 801:**

$2mF_o-DF_c$  (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.