



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2020 – 11:17 AM GMT

PDB ID : 6TCY
Title : X-ray structure of Danio rerio histone deacetylase 6 (HDAC6) CD2 in complex with a inhibitor SS555
Authors : Stransky, J.; Barinka, C.
Deposited on : 2019-11-06
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

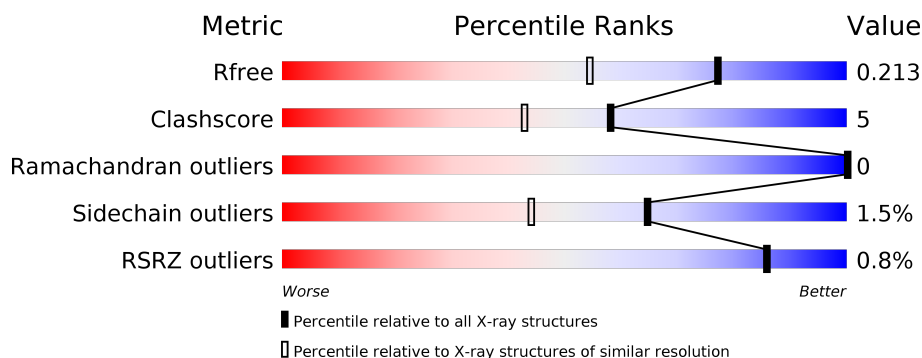
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	359	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	BBB	359	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>

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	AAA	909	-	-	X	-
8	CL	AAA	912	-	-	X	-
9	MXE	BBB	907	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6560 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 Histone deacetylase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	357	Total	C	N	O	S	0	1	0
			2796	1757	502	519	18			
1	BBB	357	Total	C	N	O	S	0	5	0
			2825	1775	510	522	18			

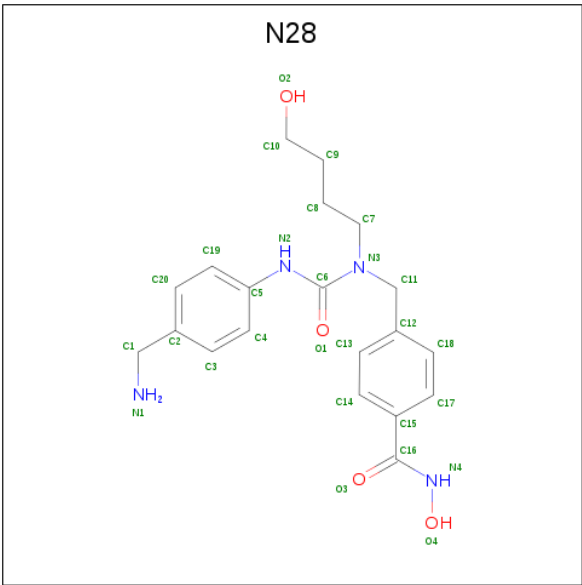
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BBB	1	Total	Zn	0	0
			1	1		
2	AAA	1	Total	Zn	0	0
			1	1		

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

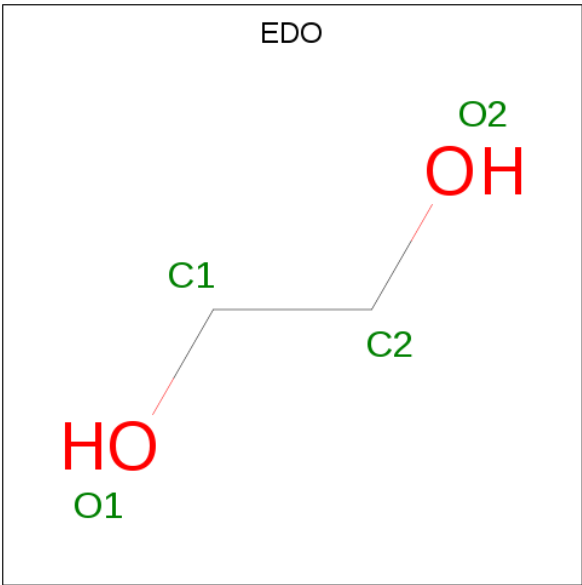
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	2	Total	K	0	0
			2	2		
3	AAA	2	Total	K	0	0
			2	2		

- Molecule 4 is 4-[[[4-(aminomethyl)phenyl]carbamoyl-(4-oxidanylbutyl)amino]methyl]- {N}-oxidanyl-benzamide (three-letter code: N28) (formula: C₂₀H₂₆N₄O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	N	O	0	1
			56	40	8	8		
4	BBB	1	Total	C	N	O	0	1
			56	40	8	8		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



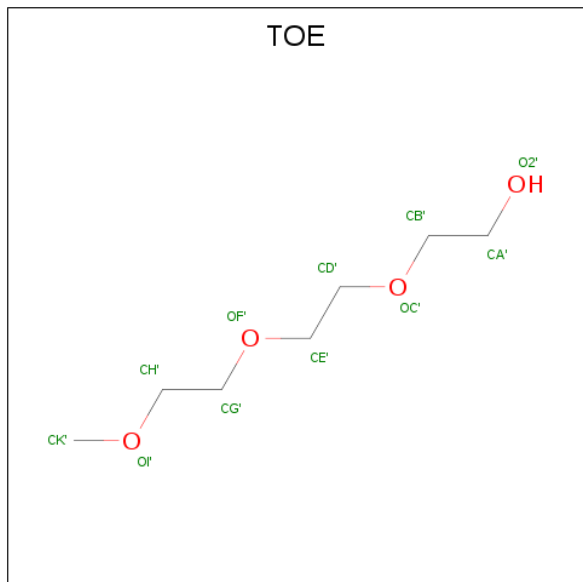
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	1
			8	4	4		
5	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: C₇H₁₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

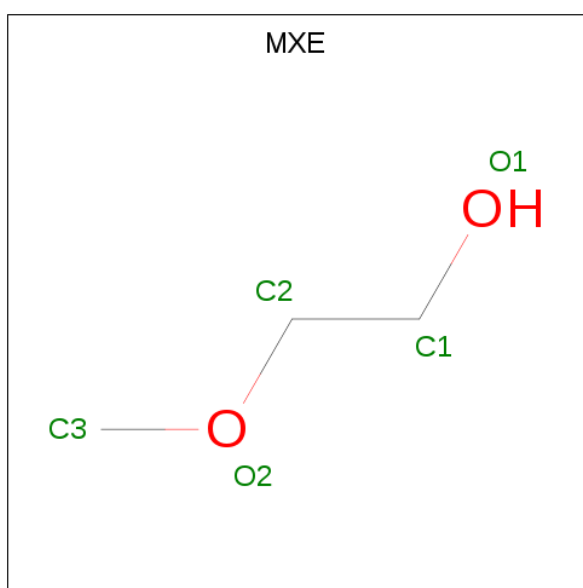


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

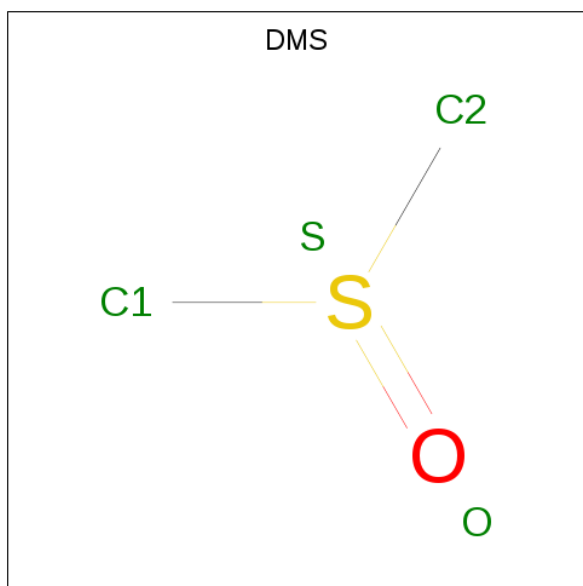
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 2-METHOXYETHANOL (three-letter code: MXE) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	BBB	1	Total	C	O	0	0
			5	3	2		

- Molecule 10 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	BBB	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AAA	399	Total	O	0	2
			401	401		
11	BBB	359	Total	O	0	2
			361	361		

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: Histone deacetylase 6



- Molecule 1: Histone deacetylase 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.81Å 83.81Å 86.09Å 90.00° 97.97° 90.00°	Depositor
Resolution (Å)	54.34 – 1.60 54.28 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (54.34-1.60) 98.7 (54.28-1.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.191 , 0.230 0.203 , 0.213	Depositor DCC
R_{free} test set	4981 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, DMS, CL, K, EDO, N28, MXE, TOE

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	AAA	0.83	0/2867	0.89	0/3888
1	BBB	0.81	1/2902 (0.0%)	0.90	2/3934 (0.1%)
All	All	0.82	1/5769 (0.0%)	0.90	2/7822 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	752	GLU	CD-OE2	-5.05	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	469	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	BBB	469	ARG	NE-CZ-NH2	-5.23	117.69	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	AAA	2796	0	2712	22	0
1	BBB	2825	0	2750	29	0
2	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	1	0	0	0	0
3	AAA	2	0	0	0	0
3	BBB	2	0	0	0	0
4	AAA	56	0	0	2	0
4	BBB	56	0	0	1	0
5	AAA	20	0	29	8	0
5	BBB	12	0	18	2	0
6	AAA	11	0	16	2	0
7	AAA	6	0	8	0	0
8	AAA	1	0	0	2	0
9	BBB	5	0	8	4	0
10	BBB	4	0	6	0	0
11	AAA	401	0	0	7	0
11	BBB	361	0	0	13	0
All	All	6560	0	5547	54	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 5.

All (54) 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:AAA:909:EDO:H22	1:BBB:746:ASN:HD21	1.38	0.88
8:AAA:912:CL:CL	11:AAA:1375:HOH:O	2.37	0.79
1:AAA:671:GLY:HA2	11:AAA:1007:HOH:O	1.82	0.78
1:AAA:655:GLY:H	5:AAA:906:EDO:H12	1.49	0.76
1:BBB:560:GLN:HG3	11:BBB:1033:HOH:O	1.88	0.74
1:BBB:481[B]:ARG:CG	1:BBB:481[B]:ARG:HH21	2.03	0.70
1:AAA:520:ARG:HD3	1:AAA:524:ARG:NH2	2.08	0.67
1:AAA:533:PHE:HB3	6:AAA:910:TOE:H9	1.77	0.67
1:BBB:515:GLU:OE1	11:BBB:1002:HOH:O	2.13	0.66
1:BBB:788:ARG:NH1	11:BBB:1005:HOH:O	2.21	0.66
1:BBB:537:GLU:OE2	11:BBB:1003:HOH:O	2.15	0.64
1:AAA:520:ARG:HD3	1:AAA:524:ARG:HH22	1.62	0.62
1:BBB:442:PRO:N	11:BBB:1007:HOH:O	2.33	0.61
4:AAA:904[A]:N28:C4	4:AAA:904[A]:N28:O1	2.45	0.61
1:BBB:613:VAL:N	11:BBB:1001:HOH:O	2.34	0.61
1:BBB:481[B]:ARG:CG	1:BBB:481[B]:ARG:NH2	2.64	0.58
5:AAA:909:EDO:H22	1:BBB:746:ASN:ND2	2.14	0.58
1:AAA:442:PRO:N	11:AAA:1006:HOH:O	2.36	0.58
1:BBB:531:SER:HA	9:BBB:907:MXE:H12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:481[B]:ARG:HG3	1:BBB:481[B]:ARG:HH21	1.67	0.57
1:BBB:520:ARG:O	1:BBB:524:ARG:HG3	2.04	0.57
1:AAA:613:VAL:N	11:AAA:1001:HOH:O	2.37	0.56
5:AAA:909:EDO:H12	1:BBB:709:GLY:HA3	1.88	0.54
1:AAA:655:GLY:N	5:AAA:906:EDO:H12	2.21	0.53
1:BBB:583:PHE:HE1	9:BBB:907:MXE:H21	1.74	0.52
1:BBB:756:MET:HG2	11:BBB:1016:HOH:O	2.10	0.52
1:AAA:476:ARG:HH12	5:AAA:909:EDO:H21	1.76	0.51
1:BBB:655:GLY:H	5:BBB:906:EDO:H12	1.74	0.51
1:AAA:653:LYS:HB3	5:AAA:906:EDO:H11	1.91	0.51
1:AAA:712:LEU:N	1:AAA:712:LEU:HD12	2.26	0.51
1:AAA:481:ARG:HA	8:AAA:912:CL:CL	2.49	0.50
1:BBB:481[B]:ARG:NH2	1:BBB:481[B]:ARG:HG2	2.26	0.50
1:AAA:480:LEU:O	11:AAA:1002:HOH:O	2.19	0.49
1:BBB:624:GLU:OE1	11:BBB:1004:HOH:O	2.20	0.47
1:AAA:442:PRO:CA	11:AAA:1006:HOH:O	2.61	0.47
1:BBB:463:HIS:HE2	9:BBB:907:MXE:C2	2.27	0.47
9:BBB:907:MXE:H32	11:BBB:1180:HOH:O	2.14	0.47
1:AAA:476:ARG:HH12	5:AAA:909:EDO:C2	2.28	0.47
1:BBB:655:GLY:H	5:BBB:906:EDO:C1	2.28	0.47
1:AAA:691:ARG:HD3	11:AAA:1081:HOH:O	2.15	0.46
1:BBB:773:THR:HG23	11:BBB:1166:HOH:O	2.14	0.46
1:AAA:459:TRP:CZ2	1:AAA:523:ASN:HB2	2.51	0.46
1:AAA:739:ILE:HD12	1:AAA:761:LEU:HD11	1.98	0.45
1:BBB:791:ALA:N	1:BBB:792:PRO:CD	2.80	0.45
1:BBB:481[B]:ARG:NH1	11:BBB:1017:HOH:O	2.50	0.44
1:AAA:473:ILE:HD11	1:AAA:750:ILE:HD12	1.99	0.43
1:BBB:613:VAL:HG12	11:BBB:1001:HOH:O	2.18	0.42
1:AAA:614:HIS:CE1	4:AAA:904[A]:N28:C14	3.03	0.42
1:AAA:463:HIS:HE2	6:AAA:910:TOE:CH'	2.33	0.41
1:BBB:560:GLN:CG	11:BBB:1033:HOH:O	2.59	0.41
1:BBB:574:HIS:NE2	4:BBB:904[B]:N28:N4	2.68	0.41
1:BBB:626:ASP:OD1	1:BBB:628:SER:OG	2.32	0.40
1:AAA:458:MET:HG3	1:AAA:459:TRP:CE2	2.56	0.40
1:BBB:520:ARG:HH21	1:BBB:524:ARG:HE	1.70	0.40

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	AAA	356/359 (99%)	348 (98%)	8 (2%)	0	100	100
1	BBB	360/359 (100%)	348 (97%)	12 (3%)	0	100	100
All	All	716/718 (100%)	696 (97%)	20 (3%)	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	AAA	302/303 (100%)	298 (99%)	4 (1%)	69	50
1	BBB	306/303 (101%)	301 (98%)	5 (2%)	62	41
All	All	608/606 (100%)	599 (98%)	9 (2%)	65	44

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

Mol	Chain	Res	Type
1	AAA	465	GLU
1	AAA	573	HIS
1	AAA	611	TRP
1	AAA	701	SER
1	BBB	465	GLU
1	BBB	573	HIS
1	BBB	579	THR
1	BBB	611	TRP

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Mol	Chain	Res	Type
1	BBB	770	ASP

Some 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 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	$\# Z > 2$
4	N28	BBB	904[B]	2	29,29,29	0.23	0	36,37,37	0.53	0
10	DMS	BBB	908	-	3,3,3	0.23	0	3,3,3	0.11	0
6	TOE	AAA	910	-	10,10,10	0.44	0	9,9,9	0.23	0
5	EDO	AAA	909	-	3,3,3	0.46	0	2,2,2	1.09	0
5	EDO	BBB	905[B]	-	3,3,3	0.09	0	2,2,2	0.18	0
5	EDO	BBB	905[A]	-	3,3,3	0.15	0	2,2,2	0.05	0
5	EDO	BBB	906	-	3,3,3	0.58	0	2,2,2	0.55	0
9	MXE	BBB	907	-	4,4,4	0.16	0	3,3,3	0.43	0
5	EDO	AAA	906	-	3,3,3	1.08	0	2,2,2	0.60	0
5	EDO	AAA	907	-	3,3,3	0.11	0	2,2,2	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	AAA	908	-	3,3,3	0.09	0	2,2,2	0.18	0
4	N28	AAA	904[A]	2	29,29,29	0.27	0	36,37,37	1.02	2 (5%)
7	GOL	AAA	911	-	5,5,5	0.11	0	5,5,5	0.28	0
4	N28	BBB	904[A]	2	29,29,29	0.28	0	36,37,37	0.99	3 (8%)
5	EDO	AAA	905	-	3,3,3	0.05	0	2,2,2	0.02	0
4	N28	AAA	904[B]	2	29,29,29	0.25	0	36,37,37	1.23	6 (16%)

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
4	N28	BBB	904[B]	2	-	3/25/25/25	0/2/2/2
5	EDO	BBB	905[A]	-	-	1/1/1/1	-
6	TOE	AAA	910	-	-	5/8/8/8	-
5	EDO	AAA	909	-	-	0/1/1/1	-
5	EDO	BBB	905[B]	-	-	1/1/1/1	-
7	GOL	AAA	911	-	-	4/4/4/4	-
5	EDO	BBB	906	-	-	1/1/1/1	-
9	MXE	BBB	907	-	-	2/2/2/2	-
5	EDO	AAA	906	-	-	1/1/1/1	-
5	EDO	AAA	907	-	-	1/1/1/1	-
5	EDO	AAA	908	-	-	1/1/1/1	-
4	N28	AAA	904[A]	2	-	13/25/25/25	0/2/2/2
4	N28	BBB	904[A]	2	-	3/25/25/25	0/2/2/2
5	EDO	AAA	905	-	-	0/1/1/1	-
4	N28	AAA	904[B]	2	-	5/25/25/25	0/2/2/2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	904[A]	N28	N2-C6-N3	3.99	120.45	115.89
4	AAA	904[B]	N28	C15-C16-N4	3.72	122.12	116.16
4	AAA	904[B]	N28	O3-C16-N4	-2.97	117.41	122.94
4	BBB	904[A]	N28	N2-C6-N3	2.95	119.27	115.89
4	AAA	904[B]	N28	C14-C15-C16	2.63	129.12	120.62
4	AAA	904[B]	N28	O1-C6-N3	-2.42	118.38	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	904[A]	N28	O4-N4-C16	2.40	125.56	119.64
4	AAA	904[B]	N28	C17-C15-C16	-2.34	113.04	120.62
4	BBB	904[A]	N28	C17-C15-C16	2.22	127.80	120.62
4	AAA	904[B]	N28	O4-N4-C16	-2.17	114.28	119.64
4	BBB	904[A]	N28	C14-C15-C16	-2.01	114.09	120.62

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	904[B]	N28	C15-C16-N4-O4
4	BBB	904[B]	N28	O3-C16-N4-O4
7	AAA	911	GOL	C1-C2-C3-O3
4	AAA	904[A]	N28	N2-C6-N3-C7
4	AAA	904[A]	N28	N2-C6-N3-C11
4	AAA	904[A]	N28	O1-C6-N3-C7
4	AAA	904[A]	N28	O1-C6-N3-C11
4	AAA	904[A]	N28	C14-C15-C16-N4
4	AAA	904[A]	N28	C17-C15-C16-N4
4	AAA	904[A]	N28	O3-C16-N4-O4
4	BBB	904[A]	N28	C15-C16-N4-O4
4	BBB	904[A]	N28	O3-C16-N4-O4
6	AAA	910	TOE	O2'-CA'-CB'-OC'
6	AAA	910	TOE	OC'-CD'-CE'-OF'
4	BBB	904[A]	N28	N3-C7-C8-C9
4	BBB	904[B]	N28	N3-C7-C8-C9
6	AAA	910	TOE	OF'-CG'-CH'-OI'
7	AAA	911	GOL	O1-C1-C2-C3
4	AAA	904[B]	N28	N3-C7-C8-C9
7	AAA	911	GOL	O2-C2-C3-O3
5	AAA	908	EDO	O1-C1-C2-O2
5	AAA	906	EDO	O1-C1-C2-O2
9	BBB	907	MXE	O1-C1-C2-O2
4	AAA	904[B]	N28	O2-C10-C9-C8
7	AAA	911	GOL	O1-C1-C2-O2
6	AAA	910	TOE	CG'-CH'-OI'-CK'
5	AAA	907	EDO	O1-C1-C2-O2
5	BBB	905[B]	EDO	O1-C1-C2-O2
4	AAA	904[A]	N28	C14-C15-C16-O3
6	AAA	910	TOE	CA'-CB'-OC'-CD'
5	BBB	906	EDO	O1-C1-C2-O2
5	BBB	905[A]	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	AAA	904[A]	N28	C17-C15-C16-O3
4	AAA	904[B]	N28	C14-C15-C16-O3
4	AAA	904[A]	N28	C15-C16-N4-O4
4	AAA	904[A]	N28	N3-C11-C12-C13
4	AAA	904[A]	N28	N3-C11-C12-C18
4	AAA	904[B]	N28	C19-C5-N2-C6
4	AAA	904[B]	N28	C4-C5-N2-C6
9	BBB	907	MXE	C1-C2-O2-C3
4	AAA	904[A]	N28	O2-C10-C9-C8

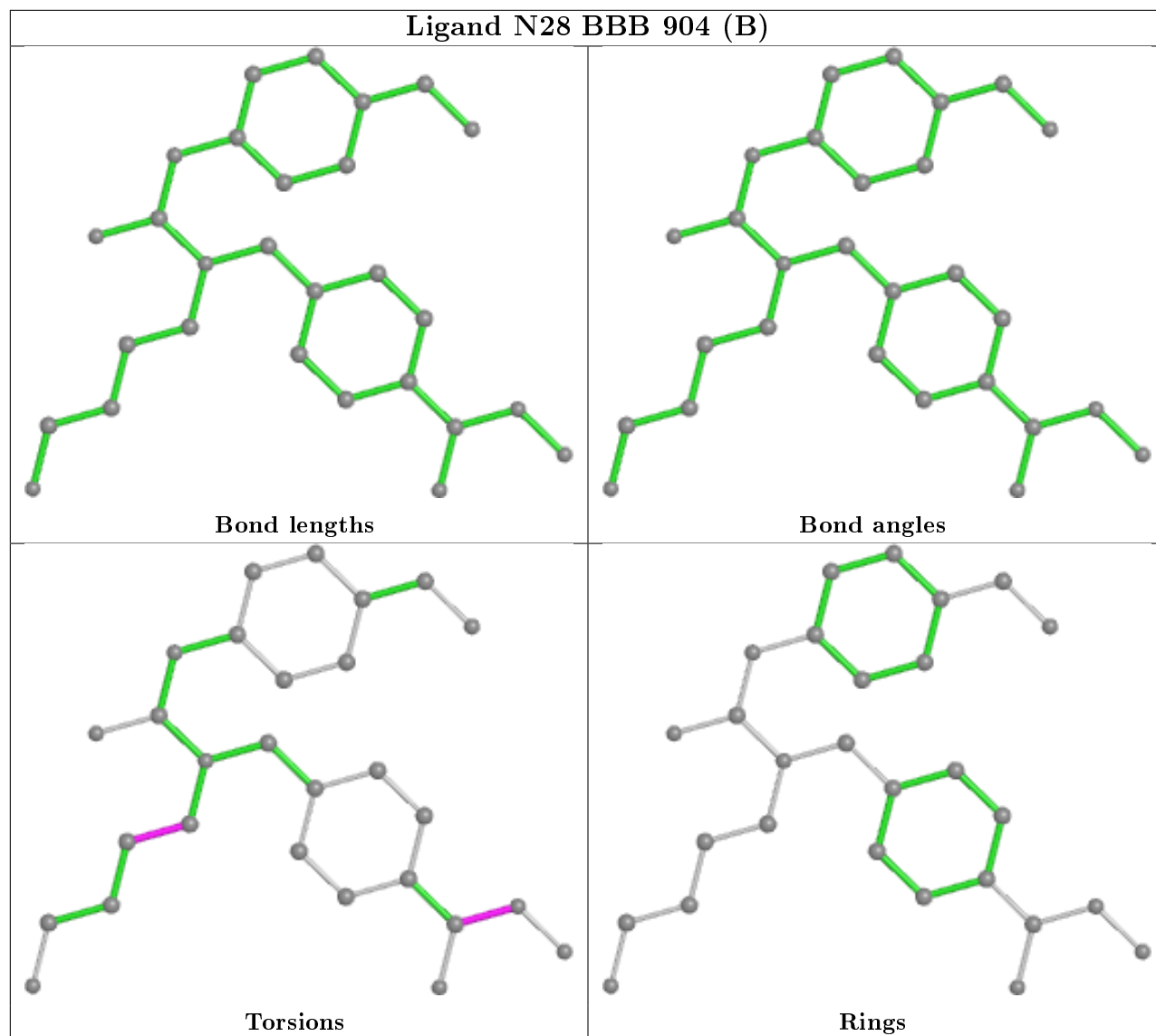
There are no ring outliers.

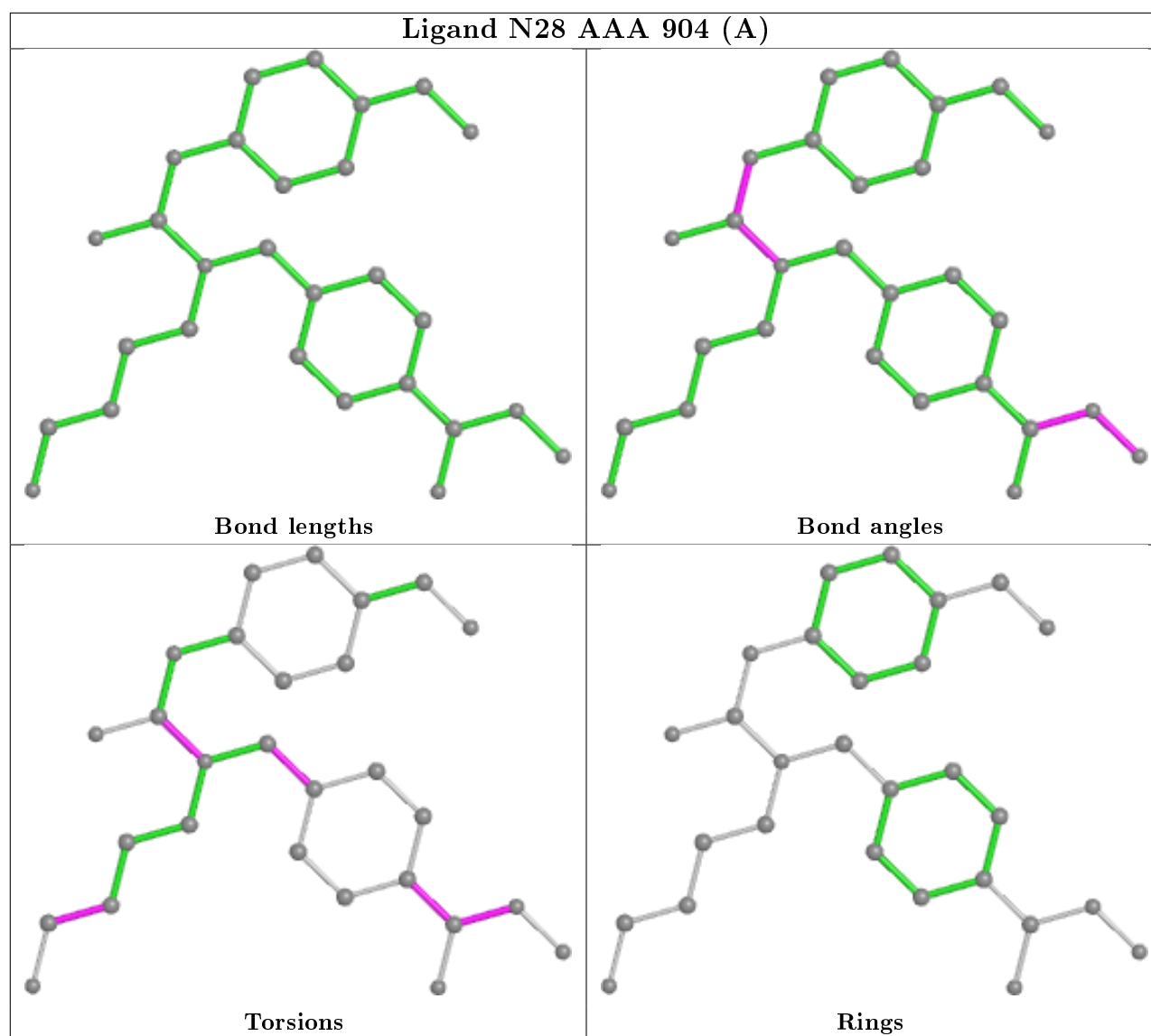
7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	904[B]	N28	1	0
6	AAA	910	TOE	2	0
5	AAA	909	EDO	5	0
5	BBB	906	EDO	2	0
9	BBB	907	MXE	4	0
5	AAA	906	EDO	3	0
4	AAA	904[A]	N28	2	0

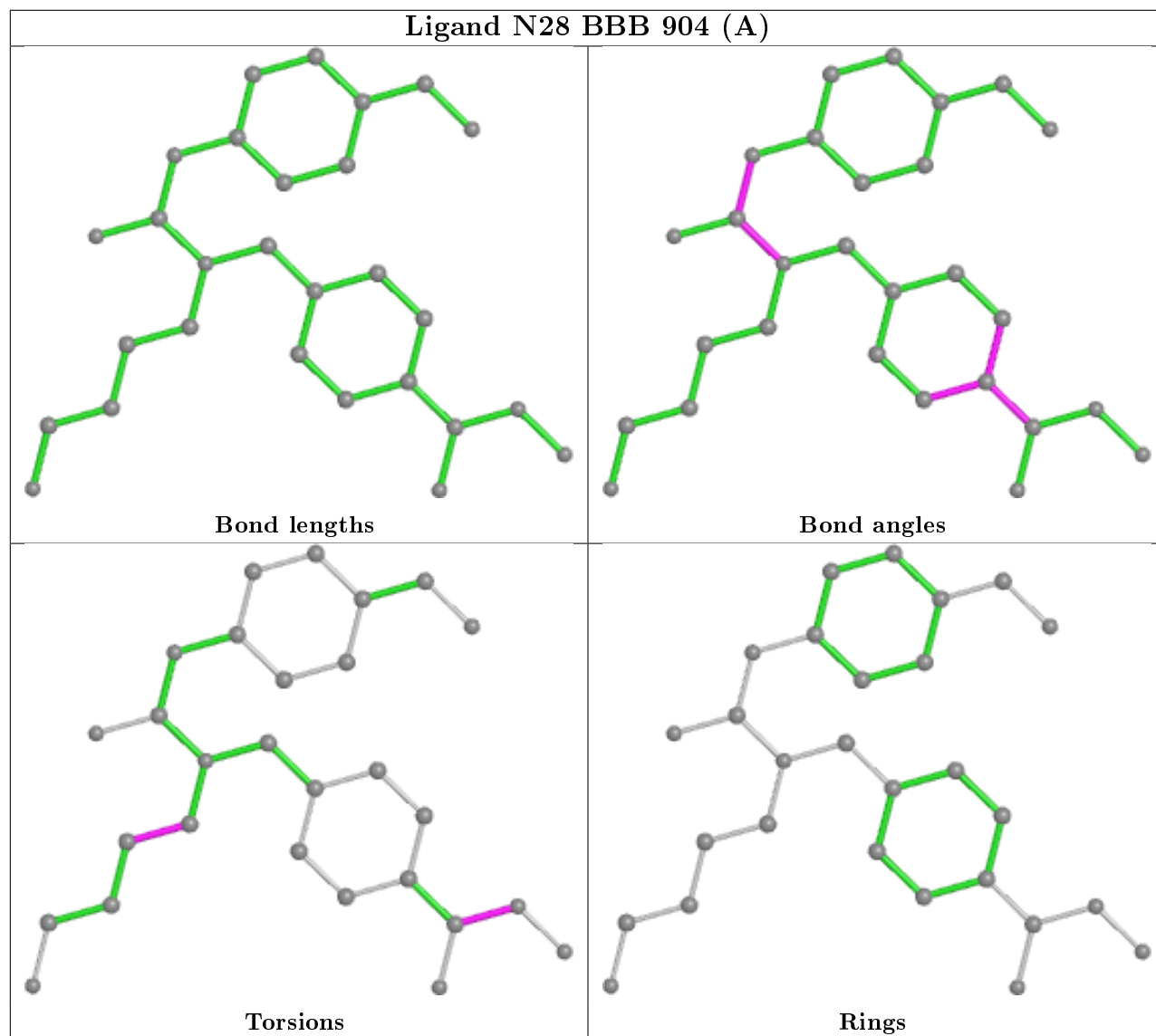
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

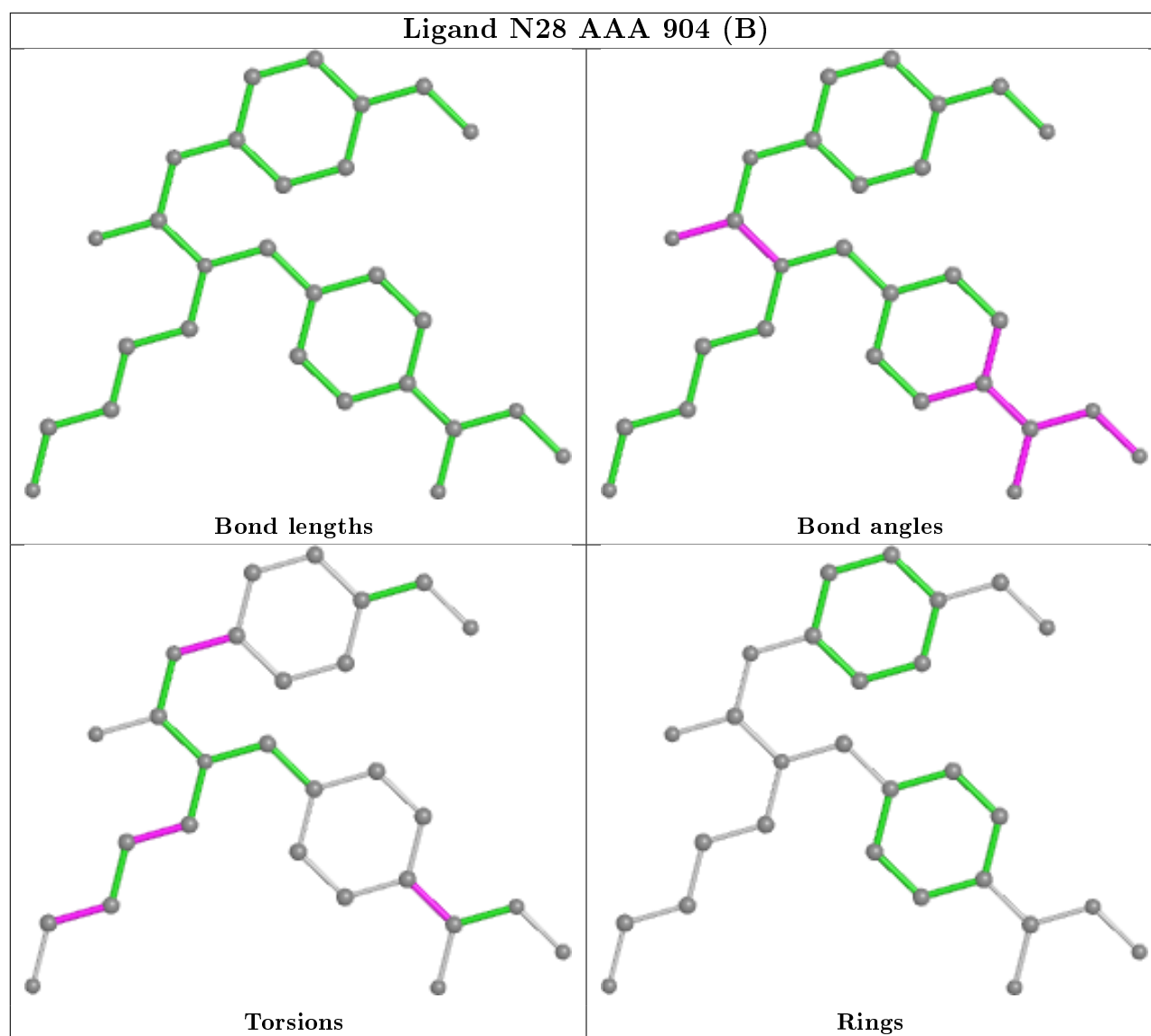
Ligand N28 BBB 904 (B)





Ligand N28 BBB 904 (A)





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, 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	AAA	357/359 (99%)	-0.21	2 (0%) 89 89	9, 14, 23, 37	10 (2%)
1	BBB	357/359 (99%)	-0.08	4 (1%) 80 80	10, 16, 29, 58	13 (3%)
All	All	714/718 (99%)	-0.15	6 (0%) 86 86	9, 15, 26, 58	23 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	442	PRO	3.8
1	BBB	772	LEU	3.6
1	BBB	771	HIS	2.6
1	BBB	442	PRO	2.5
1	BBB	788	ARG	2.3
1	AAA	459	TRP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

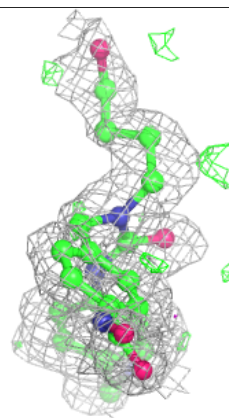
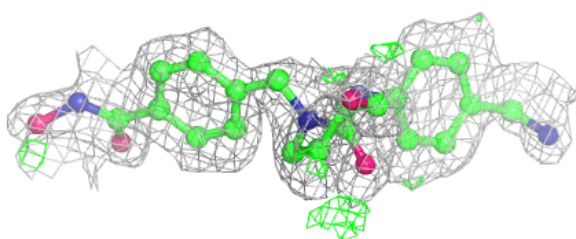
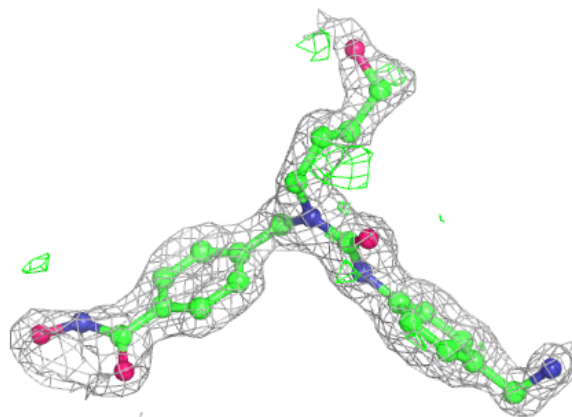
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	DMS	BBB	908	4/4	0.57	0.32	32,34,36,39	4
5	EDO	AAA	909	4/4	0.71	0.19	28,31,33,39	0
7	GOL	AAA	911	6/6	0.76	0.11	40,44,45,47	0
6	TOE	AAA	910	11/11	0.80	0.28	28,41,54,58	0
5	EDO	AAA	905	4/4	0.87	0.14	38,38,40,41	0
5	EDO	AAA	908	4/4	0.88	0.10	38,40,40,43	0
4	N28	BBB	904[B]	28/28	0.89	0.13	15,17,28,33	28
4	N28	AAA	904[A]	28/28	0.89	0.13	14,24,28,30	28
4	N28	BBB	904[A]	28/28	0.89	0.13	16,24,35,41	28
4	N28	AAA	904[B]	28/28	0.89	0.13	12,14,18,19	28
5	EDO	BBB	905[A]	4/4	0.90	0.13	22,23,24,26	4
5	EDO	BBB	905[B]	4/4	0.90	0.13	35,37,38,40	4
5	EDO	BBB	906	4/4	0.90	0.15	21,25,26,36	0
5	EDO	AAA	907	4/4	0.93	0.14	25,28,32,35	0
5	EDO	AAA	906	4/4	0.93	0.15	17,20,24,31	0
9	MXE	BBB	907	5/5	0.94	0.12	17,22,27,28	0
3	K	BBB	903	1/1	0.99	0.05	15,15,15,15	0
3	K	BBB	902	1/1	0.99	0.04	15,15,15,15	0
8	CL	AAA	912	1/1	0.99	0.04	26,26,26,26	0
3	K	AAA	902	1/1	1.00	0.04	14,14,14,14	0
2	ZN	BBB	901	1/1	1.00	0.04	14,14,14,14	0
2	ZN	AAA	901	1/1	1.00	0.03	12,12,12,12	0
3	K	AAA	903	1/1	1.00	0.06	12,12,12,12	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.

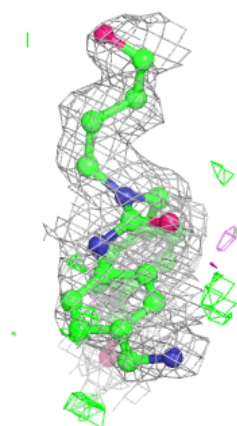
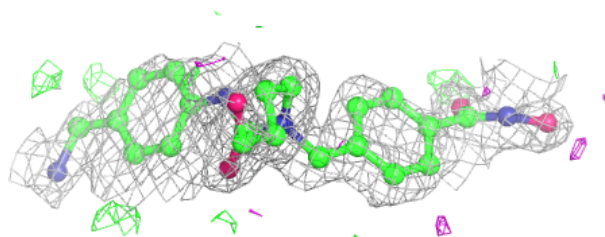
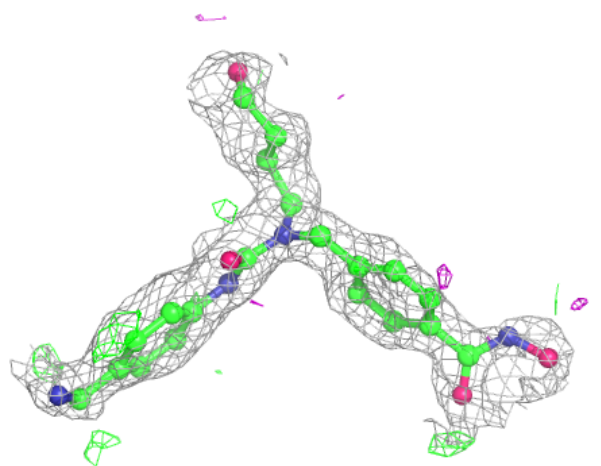
Electron density around N28 BBB 904 (B):

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



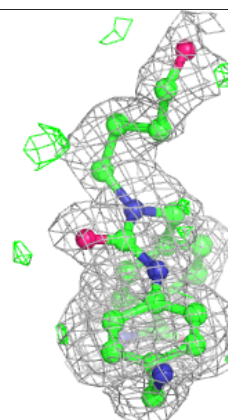
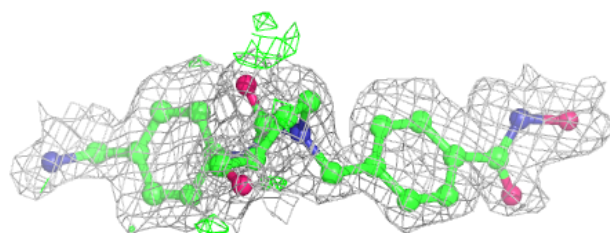
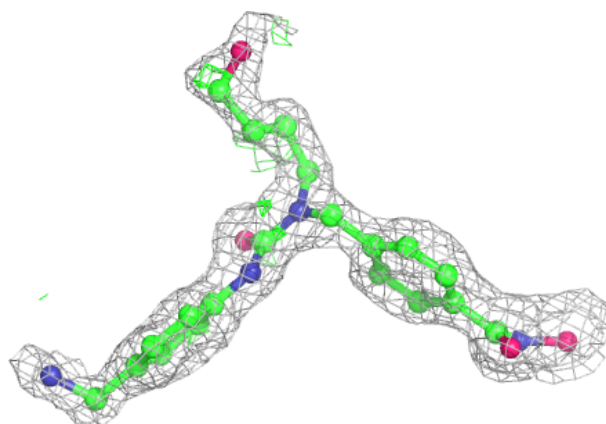
Electron density around N28 AAA 904 (A):

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

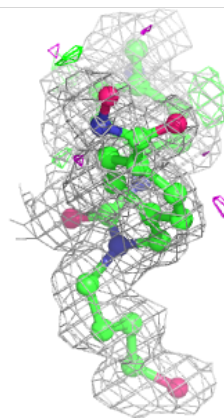
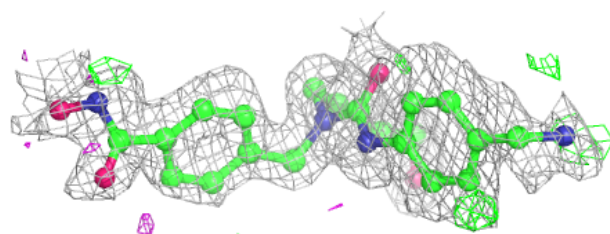
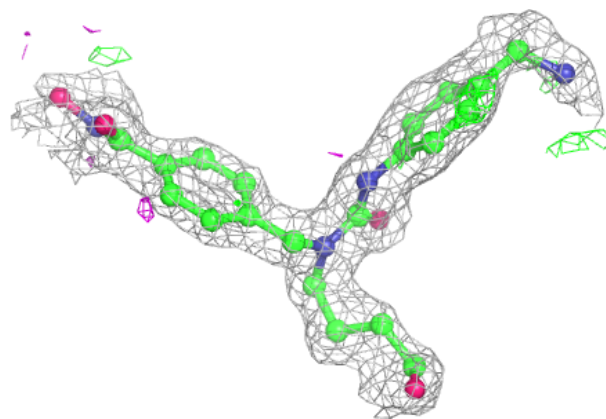


Electron density around N28 BBB 904 (A):

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

**Electron density around N28 AAA 904 (B):**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.