

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2024 - 02:06 PM JST

:	8WY3
:	Crystal Structure of the first bromodomain of human BRD4 in complex with
	the inhibitor 21
:	Xu, H.; Zhao, X.; Shen, H.; Xu, Y.; Wu, X.
:	2023-10-30
:	2.78 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

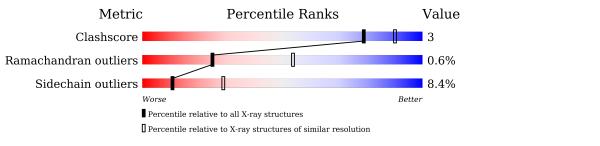
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.78 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	141	67%	8% •	24%
1	В	141	69%	9%	22%
1	С	141	67%	12%	• 18%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2941 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	107	Total	С	Ν	0	S	0	0	0
	A	107	903	592	145	160	6	0	0	0
1	В	110	Total	С	Ν	0	S	0	1	0
	D	110	940	612	153	169	6	0	1	0
1	С	115	Total	С	Ν	0	S	0	0	0
	I U	110	971	633	161	171	6	0	0	U

• Molecule 1 is a protein called Bromodomain-containing protein 4.

Chain	Residue	Modelled	Actual	Comment	Reference
А	28	MET	- initiating methionine		UNP O60885
А	29	LYS	-	expression tag	UNP O60885
А	30	LYS	-	expression tag	UNP O60885
А	31	GLY	-	expression tag	UNP O60885
А	32	HIS	-	expression tag	UNP O60885
А	33	HIS	-	expression tag	UNP O60885
А	34	HIS	-	expression tag	UNP O60885
А	35	HIS	-	expression tag	UNP O60885
А	36	HIS	-	expression tag	UNP O60885
А	37	HIS	-	expression tag	UNP O60885
А	38	LEU	-	expression tag	UNP O60885
А	39	VAL	-	expression tag	UNP O60885
А	40	PRO	-	expression tag	UNP O60885
А	41	ARG	-	expression tag	UNP O60885
А	42	GLY	-	expression tag	UNP O60885
А	43	SER	-	expression tag	UNP O60885
В	28	MET	-	initiating methionine	UNP O60885
В	29	LYS	-	expression tag	UNP O60885
В	30	LYS	-	expression tag	UNP O60885
В	31	GLY	-	expression tag	UNP O60885
В	32	HIS	- expression tag		UNP O60885
В	33	HIS	-	expression tag	UNP O60885
В	34	HIS	-	expression tag	UNP O60885
				Continued	on nert nage

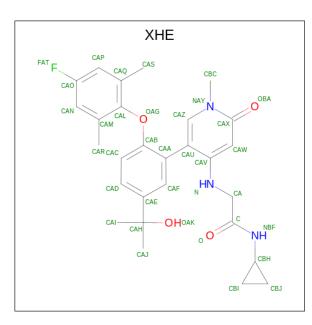
There are 48 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	35	HIS	-	expression tag	UNP O60885
В	36	HIS	-	expression tag	UNP O60885
В	37	HIS	-	expression tag	UNP O60885
В	38	LEU	-	expression tag	UNP O60885
В	39	VAL	-	expression tag	UNP O60885
В	40	PRO	-	expression tag	UNP O60885
В	41	ARG	-	expression tag	UNP O60885
В	42	GLY	-	expression tag	UNP O60885
В	43	SER	-	expression tag	UNP O60885
С	28	MET	-	initiating methionine	UNP O60885
С	29	LYS	-	expression tag	UNP O60885
С	30	LYS	-	expression tag	UNP O60885
С	31	GLY	-	expression tag	UNP O60885
С	32	HIS	-	expression tag	UNP O60885
С	33	HIS	-	expression tag	UNP O60885
С	34	HIS	-	expression tag	UNP O60885
С	35	HIS	-	expression tag	UNP O60885
С	36	HIS	-	expression tag	UNP O60885
С	37	HIS	-	expression tag	UNP O60885
С	38	LEU	-	expression tag	UNP O60885
С	39	VAL	-	expression tag	UNP O60885
С	40	PRO	- expression tag		UNP O60885
С	41	ARG	- expression tag		UNP O60885
С	42	GLY	-	expression tag	UNP O60885
С	43	SER	-	expression tag	UNP O60885

• Molecule 2 is {N}-cyclopropyl-2-[[5-[2-(4-fluoranyl-2,6-dimethyl-phenoxy)-5-(2-oxidanylp ropan-2-yl)phenyl]-1-methyl-2-oxidanylidene-pyridin-4-yl]amino]ethanamide (three-letter code: XHE) (formula: C₂₈H₃₂FN₃O₄) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Δ	1	Total					0	0
	11	1	36	28	1	3	4	0	0
2	В	1	Total	\mathbf{C}	F	Ν	Ο	0	0
2	D	1	36	28	1	3	4	0	0
2	С	1	Total	Ċ	F	N	O	0	0
	U	1	36	28	1	3	4	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	14	Total O 14 14	0	0
3	В	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	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. 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. 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.

Note EDS was not executed.

• Molecule 1: Bromodomain-containing protein 4

Chain A:	67%	8%	• 2	4%
MET LYS LYS GLY GLY HIS HIS HIS HIS HIS HIS CLEU VAL CLEU SER SER SER PRO	PRO PRO GLU GLU THR SER ASN ASN ASN LYS PRO LYS PRO CYS	GLN 160 192 192 193 193 193 104 103 103 103 103 103	K112 R113 T131 N135	K155 N162 T166 GLU GLU
• Molecule 1: Bromodor	nain-containing pr	otein 4		
Chain B:	69%	g	9% 2	22%
MET LYS LYS GLY GLY HIS HIS HIS HIS HIS HIS HIS ARG CAY SER ARG GLY SER ARG	PRO PRO GLU GLU GLU SER ASN PRO PRO PRO PRO PRO PRO R58 CYS	q59 q62 R68 R68 K72 K12 K111	K112 N116 K141 I146	K155 P165 E167 GLU
• Molecule 1: Bromodor	nain-containing pr	rotein 4		
Chain C:	67%	12	2% •	18%
MET LYS LYS GLY GLY GLY HIS HIS HIS HIS HIS HIS ASC ARC ASC ASC ASS	PRO PRO PRO PRO CLU CLU SER SE FS6 FS6 FS6 FS6 FS6 FS6	N61 164 765 765 769 772 772	N93 L94 K102 R113	N116 D128 1138 1138 1138 1138 1138 1138 1138 1



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 61 2 2	Depositor	
Cell constants	140.41Å 140.41Å 134.48Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	121.60 - 2.78	Depositor	
% Data completeness	97.0 (121.60-2.78)	Depositor	
(in resolution range)	51.0 (121.00 2.10)	Depositor	
R_{merge}	0.22	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC 5.8.0189	Depositor	
R, R_{free}	0.186 , 0.234	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2941	wwPDB-VP	
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP	



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: XHE

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	Mol Chain		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.78	0/927	0.90	2/1259~(0.2%)	
1	В	0.83	0/964	0.89	1/1308~(0.1%)	
1	С	0.76	0/997	0.92	2/1353~(0.1%)	
All	All	0.79	0/2888	0.90	5/3920~(0.1%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	113	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	А	113	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	С	113	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	А	94	LEU	CA-CB-CG	5.30	127.49	115.30
1	В	68	ARG	NE-CZ-NH1	5.27	122.94	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	А	903	0	905	2	0
1	В	940	0	935	5	0
1	С	971	0	978	12	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	А	36	0	0	0	0
2	В	36	0	0	1	0
2	С	36	0	0	0	0
3	А	14	0	0	0	0
3	В	5	0	0	0	0
All	All	2941	0	2818	16	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 3.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:XHE:CAO	2:B:201:XHE:FAT	1.63	1.34
1:C:61:ASN:HD22	1:C:64:GLN:H	1.34	0.74
1:B:62:GLN:NE2	1:B:165:PRO:O	2.29	0.65
1:C:93:ASN:O	1:C:94:LEU:HD23	2.02	0.60
1:B:116:ASN:ND2	1:C:116:ASN:HD21	2.01	0.59
1:C:61:ASN:ND2	1:C:64:GLN:H	2.02	0.57
1:C:65:TYR:CZ	1:C:69:VAL:HG11	2.45	0.52
1:B:58:ARG:HE	1:C:64:GLN:HE21	1.59	0.49
1:C:139:TYR:O	1:C:139:TYR:CD1	2.67	0.48
1:C:155:LYS:HE3	1:C:159:GLN:NE2	2.30	0.47
1:B:116:ASN:ND2	1:C:116:ASN:ND2	2.65	0.44
1:A:92:LEU:O	1:A:94:LEU:HD13	2.18	0.44
1:C:155:LYS:CE	1:C:159:GLN:NE2	2.82	0.43
1:C:139:TYR:CD1	1:C:139:TYR:C	2.93	0.41
1:B:116:ASN:HD21	1:C:116:ASN:HD21	1.67	0.41
1:A:131:THR:HG22	1:A:135:ASN:ND2	2.35	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	105/141~(74%)	100 (95%)	5 (5%)	0	100	100
1	В	109/141~(77%)	106 (97%)	3~(3%)	0	100	100
1	С	113/141 (80%)	104 (92%)	7~(6%)	2(2%)	8	25
All	All	327/423~(77%)	310 (95%)	15~(5%)	2 (1%)	25	54

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

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	102	LYS
1	С	138	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	100/132~(76%)	92~(92%)	8 (8%)	12 31		
1	В	104/132~(79%)	96~(92%)	8 (8%)	13 32		
1	С	108/132~(82%)	98 (91%)	10 (9%)	9 24		
All	All	312/396~(79%)	286~(92%)	26 (8%)	11 29		

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	60	THR
1	А	94	LEU
1	А	103	THR
1	А	105	MET
1	А	112	LYS
1	А	155	LYS
1	А	162	ASN
1	А	166	THR



\mathbf{Mol}	Chain	Res	Type
1	В	59	GLN
1	В	72	LYS
1	В	102	LYS
1	В	111	LYS
1	В	112	LYS
1	В	141	LYS
1	В	146	ILE
1	В	155	LYS
1	С	55	LYS
1	С	57	LYS
1	C C	60	THR
1	С	72	LYS
1	С	78	GLN
1	С	94	LEU
1	С	102	LYS
1	С	128	ASP
1	С	155	LYS
1	С	163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	162	ASN
1	В	116	ASN
1	В	159	GLN
1	С	52	ASN
1	С	61	ASN
1	С	116	ASN
1	С	159	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol Type C		Chain	Chain Res	Res	Dec	Dec	Dec	Dec	Dec	Dec	Link	B	ond leng	gths	B	Bond angles		
INIOI	Type	Chain			Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2								
2	XHE	С	201	-	39,39,39	3.42	11 (28%)	52,58,58	1.95	8 (15%)								
2	XHE	А	201	-	39,39,39	2.96	12 (30%)	52,58,58	2.20	13 (25%)								
2	XHE	В	201	-	39,39,39	3.65	9 (23%)	52,58,58	2.43	14 (26%)								

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
2	XHE	С	201	-	-	2/23/25/25	0/4/4/4
2	XHE	А	201	-	-	2/23/25/25	0/4/4/4
2	XHE	В	201	-	-	0/23/25/25	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	201	XHE	CAH-CAE	-16.53	1.42	1.53
2	В	201	XHE	CAH-CAE	-15.53	1.42	1.53
2	А	201	XHE	CAH-CAE	-12.70	1.44	1.53
2	В	201	XHE	FAT-CAO	11.23	1.63	1.36
2	С	201	XHE	FAT-CAO	-6.61	1.20	1.36
2	В	201	XHE	CAR-CAM	-6.28	1.38	1.51
2	С	201	XHE	CAR-CAM	-6.18	1.38	1.51
2	А	201	XHE	CAR-CAM	-6.14	1.38	1.51



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	201	XHE	CAS-CAQ	-6.12	1.38	1.51
2	А	201	XHE	CAS-CAQ	-5.72	1.39	1.51
2	А	201	XHE	CAA-CAU	-5.33	1.42	1.49
2	В	201	XHE	CAA-CAU	-4.80	1.42	1.49
2	С	201	XHE	CAS-CAQ	-4.49	1.42	1.51
2	А	201	XHE	FAT-CAO	3.64	1.45	1.36
2	С	201	XHE	CAA-CAU	-3.60	1.44	1.49
2	А	201	XHE	CAN-CAO	3.02	1.42	1.37
2	С	201	XHE	CAW-CAV	2.62	1.41	1.36
2	В	201	XHE	CA-C	-2.61	1.44	1.52
2	А	201	XHE	CAP-CAO	2.38	1.41	1.37
2	В	201	XHE	CAW-CAV	2.37	1.41	1.36
2	А	201	XHE	OAK-CAH	2.32	1.47	1.44
2	С	201	XHE	CAZ-NAY	2.28	1.42	1.36
2	С	201	XHE	CA-N	2.26	1.51	1.45
2	С	201	XHE	CAF-CAE	2.26	1.43	1.39
2	А	201	XHE	CAW-CAV	2.23	1.41	1.36
2	С	201	XHE	OAK-CAH	2.18	1.47	1.44
2	В	201	XHE	CAJ-CAH	2.16	1.55	1.52
2	А	201	XHE	CAU-CAV	-2.16	1.39	1.43
2	А	201	XHE	CAF-CAA	2.13	1.43	1.39
2	А	201	XHE	CAF-CAE	2.09	1.42	1.39
2	В	201	XHE	CAW-CAX	-2.06	1.38	1.43
2	С	201	XHE	OAG-CAL	-2.02	1.35	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	201	XHE	CBJ-CBH-NBF	-10.83	103.08	118.61
2	С	201	XHE	CAA-CAU-CAV	10.17	129.81	120.00
2	А	201	XHE	CAA-CAU-CAV	10.05	129.70	120.00
2	В	201	XHE	CAA-CAU-CAV	8.64	128.33	120.00
2	А	201	XHE	CAJ-CAH-CAE	-4.47	102.90	110.91
2	В	201	XHE	CBH-NBF-C	-3.89	117.19	122.92
2	А	201	XHE	OAK-CAH-CAE	3.89	115.49	109.13
2	А	201	XHE	CAB-CAA-CAU	3.82	126.05	121.50
2	С	201	XHE	CAB-CAA-CAU	3.57	125.74	121.50
2	А	201	XHE	CBJ-CBH-NBF	-3.54	113.53	118.61
2	В	201	XHE	OAK-CAH-CAE	3.30	114.53	109.13
2	В	201	XHE	OBA-CAX-CAW	-3.09	117.82	125.72
2	С	201	XHE	OAG-CAB-CAA	-2.97	111.93	118.81
2	С	201	XHE	CAW-CAV-N	-2.83	120.28	124.88



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	201	XHE	CAP-CAO-CAN	-2.80	119.98	123.52
2	А	201	XHE	CBI-CBH-NBF	-2.77	114.64	118.61
2	А	201	XHE	CBH-NBF-C	-2.75	118.87	122.92
2	А	201	XHE	CAI-CAH-CAE	2.71	115.78	110.91
2	В	201	XHE	CAF-CAE-CAH	2.71	123.82	120.43
2	В	201	XHE	CAB-CAA-CAU	2.63	124.63	121.50
2	С	201	XHE	CAF-CAA-CAB	-2.61	114.64	118.29
2	С	201	XHE	CBJ-CBH-NBF	-2.43	115.12	118.61
2	В	201	XHE	CAW-CAV-N	-2.41	120.97	124.88
2	С	201	XHE	CAJ-CAH-CAI	-2.30	107.67	110.49
2	С	201	XHE	CAC-CAD-CAE	-2.30	118.14	121.22
2	А	201	XHE	CAZ-NAY-CAX	-2.29	120.24	123.00
2	А	201	XHE	CA-C-NBF	-2.25	110.72	116.10
2	А	201	XHE	CAW-CAV-N	-2.24	121.24	124.88
2	В	201	XHE	CAJ-CAH-CAE	-2.21	106.94	110.91
2	В	201	XHE	CBI-CBJ-CBH	-2.21	57.98	59.84
2	В	201	XHE	CAD-CAE-CAH	-2.20	118.74	121.55
2	В	201	XHE	FAT-CAO-CAN	2.15	121.33	118.25
2	А	201	XHE	O-C-CA	2.15	125.19	120.75
2	В	201	XHE	CAB-OAG-CAL	2.06	122.36	117.79
2	А	201	XHE	OAK-CAH-CAI	-2.05	102.94	107.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	201	XHE	CAW-CAV-N-CA
2	А	201	XHE	CAU-CAV-N-CA
2	С	201	XHE	CAU-CAV-N-CA
2	С	201	XHE	CAW-CAV-N-CA

There are no ring outliers.

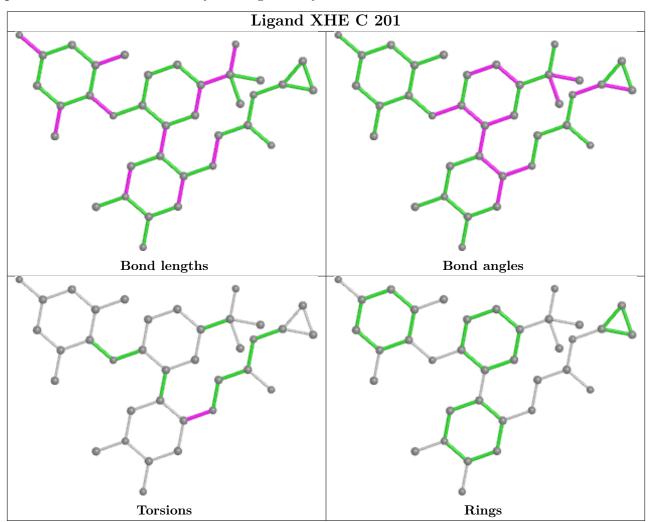
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	201	XHE	1	0

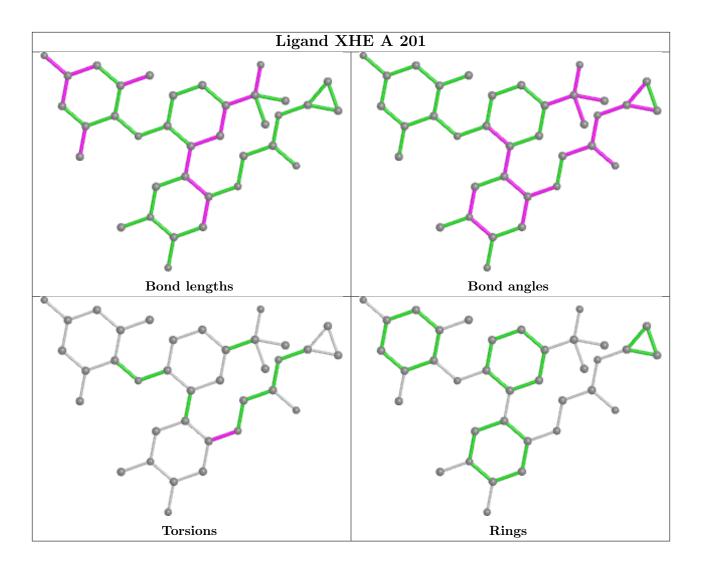
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



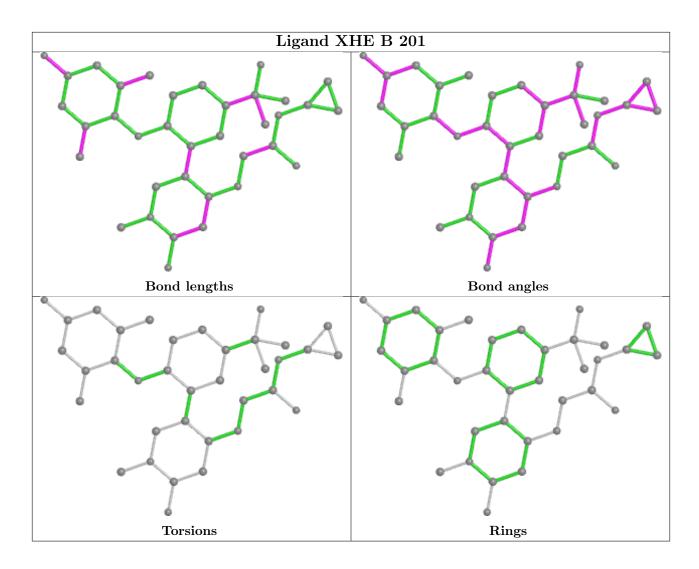
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

