

Full wwPDB X-ray Structure Validation Report (i)

Jan 29, 2024 – 04:41 PM EST

PDB ID : 8FV2

Title: Bromodomain of CBP liganded with CCS-1477

Authors: Schonbrunn, E.; Bikowitz, M.

Deposited on : 2023-01-18

Resolution : 1.87 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) : 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)

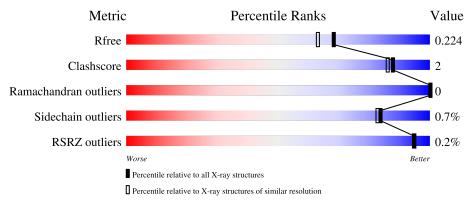
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.87 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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% 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	116	93%	6% •
1	В	116	94%	5% •
1	С	116	97%	
1	D	116	97%	••



2 Entry composition (i)

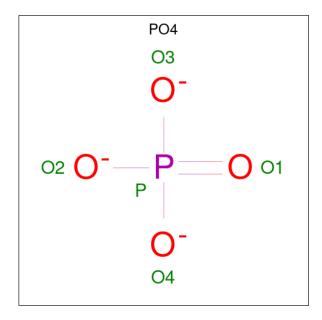
There are 5 unique types of molecules in this entry. The entry contains 4673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CREB-binding protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	116	Total	С	N	О	S	0	3	0
1	A	110	995	646	163	181	5	0	3	0
1	В	115	Total	С	N	О	S	0	3	0
1	Ъ	110	983	637	159	182	5	0	3	
1	С	115	Total	С	N	О	S	0	3	0
1		110	984	639	160	180	5	0	3	
1	D	115	Total	С	N	О	S	0	2	0
1	ע	110	981	637	160	179	5	0	<u> </u>	U

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



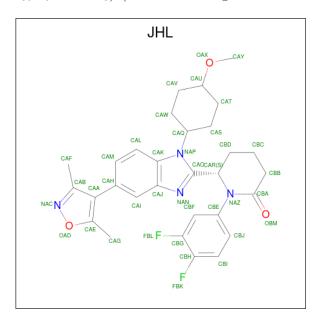
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P	0	0
_	11	_	5 4 1	Ü	0
9	Λ.	1	Total O P	0	0
	Α	1	5 4 1		U



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	В	1	Total O P 5 4 1	0	0
2	В	1	Total O P 5 4 1	0	0

• Molecule 3 is (6S)-1-[3,4-bis(fluoranyl)phenyl]-6-[5-(3,5-dimethyl-1,2-oxazol-4-yl)-1-(4-methoxycyclohexyl)benzimidazol-2-yl]piperidin-2-one (three-letter code: JHL) (formula: $C_{30}H_{32}F_2N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	С	F	N	О	0	0
3	Λ	1	39	30	2	4	3	0	0
3	В	1	Total	С	F	N	О	0	0
3	Ъ	1	39	30	2	4	3	U	U
3	В	1	Total	С	F	N	Ο	0	0
	D	1	39	30	2	4	3	U	0
3	С	1	Total	С	F	N	Ο	0	0
		1	39	30	2	4	3	U	U
3	\mathbf{C}	1	Total	С	F	N	Ο	0	0
		1	39	30	2	4	3	U	U
3	D	1	Total	С	F	N	Ο	0	0
	D	1	39	30	2	4	3		

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





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

• Molecule 5 is water.

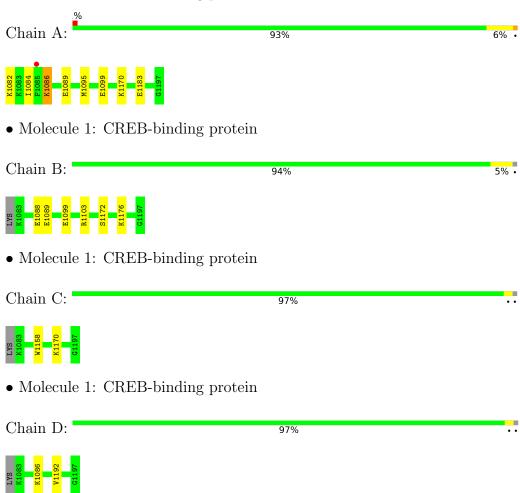
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	110	Total O 110 110	0	0
5	В	120	Total O 120 120	0	0
5	С	129	Total O 129 129	0	0
5	D	104	Total O 104 104	0	0



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: CREB-binding protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants	79.45Å 79.45Å 97.13Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.44 - 1.87	Depositor
Resolution (A)	41.44 - 1.87	EDS
% Data completeness	99.3 (41.44-1.87)	Depositor
(in resolution range)	91.1 (41.44-1.87)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.79 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
D D.	0.190 , 0.226	Depositor
R, R_{free}	0.186 , 0.224	DCC
R_{free} test set	1492 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 32.3	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4673	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 21.10 % 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 7.5416e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

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: PO4, JHL, EDO

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		
IVIOI	Chain	RMSZ $ \# Z > 5$		RMSZ	# Z > 5	
1	A	0.41	0/1025	0.61	0/1390	
1	В	0.42	0/1016	0.61	0/1381	
1	С	0.42	0/1020	0.59	0/1385	
1	D	0.43	0/1011	0.64	0/1372	
All	All	0.42	0/4072	0.61	0/5528	

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	995	0	987	8	0
1	В	983	0	963	3	0
1	С	984	0	977	2	0
1	D	981	0	973	1	0
2	A	15	0	0	1	0
2	В	10	0	0	1	0
3	A	39	0	0	0	0
3	В	78	0	0	0	0
3	С	78	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	39	0	0	0	0
4	В	4	0	6	0	0
4	D	4	0	6	1	0
5	A	110	0	0	4	0
5	В	120	0	0	1	0
5	С	129	0	0	1	0
5	D	104	0	0	1	0
All	All	4673	0	3912	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 2.

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

Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap (Å)
1:A:1183:GLU:OE1	5:A:1301:HOH:O	2.05	0.74
2:A:1203:PO4:O1	5:A:1302:HOH:O	2.06	0.74
2:B:1202:PO4:O2	5:B:1301:HOH:O	2.13	0.66
1:A:1095:MET:O	1:A:1099:GLU:HG3	2.01	0.59
1:A:1086:LYS:HG3	1:A:1089:GLU:HB3	1.88	0.56
1:A:1086:LYS:HE3	1:A:1089:GLU:H	1.72	0.54
1:A:1086:LYS:HE3	1:A:1089:GLU:N	2.22	0.54
1:C:1158:TRP:HE3	5:C:1302:HOH:O	1.92	0.53
1:A:1082:LYS:N	5:A:1305:HOH:O	2.46	0.47
1:A:1089:GLU:HA	4:D:1202:EDO:H21	1.97	0.46
1:B:1088:GLU:HG2	1:B:1089:GLU:N	2.31	0.45
1:B:1172:SER:O	1:B:1176:LYS:HG3	2.16	0.45
1:C:1170:LYS:NZ	1:C:1170:LYS:HB2	2.32	0.45
1:D:1192:VAL:HG23	5:D:1310:HOH:O	2.18	0.43
1:B:1099[B]:GLU:O	1:B:1103:ARG:HG3	2.19	0.41
1:A:1084:ILE:HG23	5:A:1371:HOH:O	2.20	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 r	number of residu	ies for which	the backbone	conformation	was
analysed, and the total number of	residues.				

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	A	117/116 (101%)	116 (99%)	1 (1%)	0	100	100
1	В	116/116 (100%)	116 (100%)	0	0	100	100
1	C	116/116 (100%)	116 (100%)	0	0	100	100
1	D	115/116~(99%)	113 (98%)	2 (2%)	0	100	100
All	All	464/464 (100%)	461 (99%)	3 (1%)	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	111/109 (102%)	109 (98%)	2 (2%)	59 52		
1	В	110/109 (101%)	110 (100%)	0	100 100		
1	С	111/109 (102%)	111 (100%)	0	100 100		
1	D	110/109 (101%)	109 (99%)	1 (1%)	78 76		
All	All	442/436 (101%)	439 (99%)	3 (1%)	84 83		

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

Mol	Chain	Res	Type
1	A	1086	LYS
1	A	1170	LYS
1	D	1086	LYS

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)

13 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).

Mal	Т	Clasica	Das	T 21-	В	ond leng	gths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2$
3	JHL	С	1202	-	37,44,44	2.17	9 (24%)	46,65,65	1.03	4 (8%)
4	EDO	D	1202	-	3,3,3	0.49	0	2,2,2	0.28	0
2	PO4	A	1203	-	4,4,4	0.83	0	6,6,6	0.27	0
2	PO4	В	1202	_	4,4,4	0.83	0	6,6,6	0.62	0
2	PO4	В	1201	-	4,4,4	0.98	0	6,6,6	0.65	0
3	JHL	D	1201	-	37,44,44	2.19	9 (24%)	46,65,65	1.02	3 (6%)
3	JHL	С	1201	-	37,44,44	2.22	10 (27%)	46,65,65	1.18	4 (8%)
3	JHL	В	1205	-	37,44,44	2.22	9 (24%)	46,65,65	1.06	4 (8%)
4	EDO	В	1203	-	3,3,3	0.48	0	2,2,2	0.25	0
2	PO4	A	1204	-	4,4,4	1.01	0	6,6,6	0.39	0
2	PO4	A	1201	-	4,4,4	1.00	0	6,6,6	0.76	0
3	JHL	A	1202	-	37,44,44	2.18	9 (24%)	46,65,65	0.99	4 (8%)
3	JHL	В	1204	-	37,44,44	2.24	8 (21%)	46,65,65	1.00	2 (4%)

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	JHL	С	1202	-	-	0/10/42/42	0/6/6/6
4	EDO	D	1202	-	-	0/1/1/1	-
3	JHL	D	1201	-	-	1/10/42/42	0/6/6/6
3	JHL	С	1201	-	-	0/10/42/42	0/6/6/6
3	JHL	В	1205	-	-	0/10/42/42	0/6/6/6
4	EDO	В	1203	-	-	1/1/1/1	-
3	JHL	A	1202	-	-	1/10/42/42	0/6/6/6
3	JHL	В	1204	-	-	0/10/42/42	0/6/6/6

All (54) bond length outliers are listed below:

3 C 1201 JHL CBA-NAZ 7.90 1.52 1.36 3 B 1205 JHL CBA-NAZ 7.88 1.52 1.36 3 B 1204 JHL CBA-NAZ 7.87 1.52 1.36 3 D 1201 JHL CBA-NAZ 7.73 1.51 1.36 3 C 1202 JHL CBA-NAZ 7.72 1.51 1.36 3 A 1202 JHL CBA-NAZ 7.50 1.51 1.36 3 B 1204 JHL CAR-NAZ 7.00 1.59 1.48 3 C 1201 JHL CAR-NAZ 6.77 1.58 1.48 3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.73 1.58 1.48 3 B 1201 JHL CAR-NAZ 6.36 <th>Mol</th> <th>Chain</th> <th>Res</th> <th>Type</th> <th>Atoms</th> <th>Z</th> <th>$\operatorname{Observed}(\text{\AA})$</th> <th>$Ideal(\AA)$</th>	Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3 B 1204 JHL CBA-NAZ 7.87 1.52 1.36 3 D 1201 JHL CBA-NAZ 7.73 1.51 1.36 3 C 1202 JHL CBA-NAZ 7.72 1.51 1.36 3 A 1202 JHL CBA-NAZ 7.50 1.51 1.36 3 B 1204 JHL CAR-NAZ 7.00 1.59 1.48 3 C 1201 JHL CAR-NAZ 6.77 1.58 1.48 3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.62 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 <td>3</td> <td>С</td> <td>1201</td> <td>JHL</td> <td>CBA-NAZ</td> <td>7.90</td> <td>1.52</td> <td>1.36</td>	3	С	1201	JHL	CBA-NAZ	7.90	1.52	1.36
3 D 1201 JHL CBA-NAZ 7.73 1.51 1.36 3 C 1202 JHL CBA-NAZ 7.72 1.51 1.36 3 A 1202 JHL CBA-NAZ 7.50 1.51 1.36 3 B 1204 JHL CAR-NAZ 7.00 1.59 1.48 3 C 1201 JHL CAR-NAZ 6.77 1.58 1.48 3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 C 1202 JHL CAA-CAH 3.62 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 <td>3</td> <td>В</td> <td>1205</td> <td>JHL</td> <td>CBA-NAZ</td> <td>7.88</td> <td>1.52</td> <td>1.36</td>	3	В	1205	JHL	CBA-NAZ	7.88	1.52	1.36
3 C 1202 JHL CBA-NAZ 7.72 1.51 1.36 3 A 1202 JHL CBA-NAZ 7.50 1.51 1.36 3 B 1204 JHL CAR-NAZ 7.00 1.59 1.48 3 C 1201 JHL CAR-NAZ 6.77 1.58 1.48 3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.62 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 C 1202 JHL CAA-CAH 3.62 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 <td>3</td> <td>В</td> <td>1204</td> <td>JHL</td> <td>CBA-NAZ</td> <td>7.87</td> <td>1.52</td> <td>1.36</td>	3	В	1204	JHL	CBA-NAZ	7.87	1.52	1.36
3 A 1202 JHL CBA-NAZ 7.50 1.51 1.36 3 B 1204 JHL CAR-NAZ 7.00 1.59 1.48 3 C 1201 JHL CAR-NAZ 6.77 1.58 1.48 3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.62 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-CAH 3.62 1.56 1.50 3 B 1201 JHL CAG-CAE 3.48 <td>3</td> <td>D</td> <td>1201</td> <td>JHL</td> <td>CBA-NAZ</td> <td>7.73</td> <td>1.51</td> <td>1.36</td>	3	D	1201	JHL	CBA-NAZ	7.73	1.51	1.36
3 B 1204 JHL CAR-NAZ 7.00 1.59 1.48 3 C 1201 JHL CAR-NAZ 6.77 1.58 1.48 3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 D 1201 JHL CAA-CAH 3.62 1.56 1.50 3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAG-CAE 3.20 <td>3</td> <td>С</td> <td>1202</td> <td>JHL</td> <td>CBA-NAZ</td> <td>7.72</td> <td>1.51</td> <td>1.36</td>	3	С	1202	JHL	CBA-NAZ	7.72	1.51	1.36
3 C 1201 JHL CAR-NAZ 6.77 1.58 1.48 3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 D 1201 JHL CAR-CAH 3.62 1.56 1.50 3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 B 1205 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAG-CAE 3.20 <td>3</td> <td>A</td> <td>1202</td> <td>JHL</td> <td>CBA-NAZ</td> <td>7.50</td> <td>1.51</td> <td>1.36</td>	3	A	1202	JHL	CBA-NAZ	7.50	1.51	1.36
3 D 1201 JHL CAR-NAZ 6.73 1.58 1.48 3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 D 1201 JHL CAR-CAH 3.62 1.56 1.50 3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 <td>3</td> <td>В</td> <td>1204</td> <td>JHL</td> <td>CAR-NAZ</td> <td>7.00</td> <td>1.59</td> <td>1.48</td>	3	В	1204	JHL	CAR-NAZ	7.00	1.59	1.48
3 A 1202 JHL CAR-NAZ 6.62 1.58 1.48 3 B 1205 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 D 1201 JHL CAA-CAH 3.62 1.56 1.50 3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAA-CAH 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 <td>3</td> <td>С</td> <td>1201</td> <td>JHL</td> <td>CAR-NAZ</td> <td>6.77</td> <td>1.58</td> <td>1.48</td>	3	С	1201	JHL	CAR-NAZ	6.77	1.58	1.48
3 B 1205 JHL CAR-NAZ 6.36 1.58 1.48 3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 D 1201 JHL CAA-CAH 3.62 1.56 1.50 3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAA-CAH 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 C 1202 JHL CAB-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 <td>3</td> <td>D</td> <td>1201</td> <td>JHL</td> <td>CAR-NAZ</td> <td>6.73</td> <td>1.58</td> <td>1.48</td>	3	D	1201	JHL	CAR-NAZ	6.73	1.58	1.48
3 C 1202 JHL CAR-NAZ 6.12 1.57 1.48 3 D 1201 JHL CAA-CAH 3.62 1.56 1.50 3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAG-CAE 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CBB-CBA 3.00 <td>3</td> <td>A</td> <td>1202</td> <td>JHL</td> <td>CAR-NAZ</td> <td>6.62</td> <td>1.58</td> <td>1.48</td>	3	A	1202	JHL	CAR-NAZ	6.62	1.58	1.48
3 D 1201 JHL CAA-CAH 3.62 1.56 1.50 3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAA-CAH 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CBB-CBA 3.00 1.57 1.51 3 B 1205 JHL CBB-CBA 2.97 <td>3</td> <td>В</td> <td>1205</td> <td>JHL</td> <td>CAR-NAZ</td> <td>6.36</td> <td>1.58</td> <td>1.48</td>	3	В	1205	JHL	CAR-NAZ	6.36	1.58	1.48
3 C 1202 JHL CAA-CAH 3.58 1.56 1.50 3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAA-CAH 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBC-CBD -2.87 </td <td>3</td> <td>С</td> <td>1202</td> <td>JHL</td> <td>CAR-NAZ</td> <td>6.12</td> <td>1.57</td> <td>1.48</td>	3	С	1202	JHL	CAR-NAZ	6.12	1.57	1.48
3 B 1204 JHL CAG-CAE 3.48 1.53 1.48 3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 A 1202 JHL CAB-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 </td <td>3</td> <td>D</td> <td>1201</td> <td>JHL</td> <td>CAA-CAH</td> <td>3.62</td> <td>1.56</td> <td>1.50</td>	3	D	1201	JHL	CAA-CAH	3.62	1.56	1.50
3 A 1202 JHL CAA-CAH 3.39 1.56 1.50 3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAA-CAH 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 </td <td>3</td> <td>С</td> <td>1202</td> <td>JHL</td> <td>CAA-CAH</td> <td>3.58</td> <td>1.56</td> <td>1.50</td>	3	С	1202	JHL	CAA-CAH	3.58	1.56	1.50
3 C 1201 JHL CAG-CAE 3.35 1.53 1.48 3 B 1205 JHL CAA-CAH 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 </td <td>3</td> <td>В</td> <td>1204</td> <td>JHL</td> <td>CAG-CAE</td> <td>3.48</td> <td>1.53</td> <td>1.48</td>	3	В	1204	JHL	CAG-CAE	3.48	1.53	1.48
3 B 1205 JHL CAA-CAH 3.31 1.56 1.50 3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1204 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 </td <td>3</td> <td>A</td> <td>1202</td> <td>JHL</td> <td>CAA-CAH</td> <td>3.39</td> <td>1.56</td> <td>1.50</td>	3	A	1202	JHL	CAA-CAH	3.39	1.56	1.50
3 B 1205 JHL CAG-CAE 3.20 1.52 1.48 3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	С	1201	JHL	CAG-CAE	3.35	1.53	1.48
3 A 1202 JHL CAG-CAE 3.12 1.52 1.48 3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	В	1205	JHL	CAA-CAH	3.31	1.56	1.50
3 C 1202 JHL CBB-CBA 3.11 1.58 1.51 3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	В	1205	JHL	CAG-CAE	3.20	1.52	1.48
3 B 1204 JHL CAA-CAH 3.11 1.55 1.50 3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	A	1202	JHL	CAG-CAE	3.12	1.52	1.48
3 B 1205 JHL CBB-CBA 3.00 1.57 1.51 3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	С	1202	JHL	CBB-CBA	3.11	1.58	1.51
3 B 1204 JHL CBB-CBA 2.97 1.57 1.51 3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	В	1204	JHL	CAA-CAH	3.11	1.55	1.50
3 B 1205 JHL CBC-CBD -2.87 1.45 1.53 3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	В	1205	JHL	CBB-CBA	3.00	1.57	1.51
3 A 1202 JHL CBB-CBA 2.86 1.57 1.51 3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	В	1204	JHL	CBB-CBA	2.97	1.57	1.51
3 C 1201 JHL CAA-CAH 2.85 1.55 1.50 3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	В	1205	JHL	CBC-CBD	-2.87	1.45	1.53
3 D 1201 JHL CAG-CAE 2.82 1.52 1.48	3	A	1202	JHL	CBB-CBA	2.86	1.57	1.51
	3	С	1201	JHL	CAA-CAH	2.85	1.55	1.50
3 D 1201 JHL CBB-CBA 2.81 1.57 1.51	3	D	1201	JHL	CAG-CAE	2.82	1.52	1.48
	3	D	1201	JHL	CBB-CBA	2.81	1.57	1.51



 $Continued\ from\ previous\ page...$

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
3	С	1202	JHL	CBC-CBD	-2.79	1.45	1.53
3	D	1201	JHL	CBC-CBD	-2.75	1.46	1.53
3	В	1205	JHL	CBE-NAZ	2.74	1.47	1.43
3	С	1202	JHL	CAG-CAE	2.73	1.52	1.48
3	A	1202	JHL	CBC-CBD	-2.72	1.46	1.53
3	С	1201	JHL	CBC-CBD	-2.72	1.46	1.53
3	В	1204	JHL	CBC-CBD	-2.71	1.46	1.53
3	С	1201	JHL	CBB-CBA	2.67	1.57	1.51
3	С	1202	JHL	CBD-CAR	-2.41	1.46	1.53
3	С	1202	JHL	CBE-NAZ	2.40	1.47	1.43
3	В	1204	JHL	CBE-NAZ	2.37	1.47	1.43
3	D	1201	JHL	CBE-NAZ	2.34	1.47	1.43
3	В	1204	JHL	CBD-CAR	-2.32	1.46	1.53
3	С	1201	JHL	CBD-CAR	-2.32	1.46	1.53
3	D	1201	JHL	CBD-CAR	-2.28	1.46	1.53
3	A	1202	JHL	CBD-CAR	-2.27	1.46	1.53
3	С	1202	JHL	OBM-CBA	-2.27	1.18	1.23
3	В	1205	JHL	CBD-CAR	-2.25	1.46	1.53
3	С	1201	JHL	CAO-CAR	2.24	1.54	1.50
3	A	1202	JHL	CBE-NAZ	2.22	1.46	1.43
3	В	1205	JHL	OBM-CBA	-2.19	1.18	1.23
3	С	1201	JHL	CAL-CAM	2.14	1.41	1.36
3	С	1201	JHL	CBE-NAZ	2.14	1.46	1.43
3	A	1202	JHL	OBM-CBA	-2.10	1.18	1.23
3	D	1201	JHL	OBM-CBA	-2.02	1.18	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	1201	JHL	CAO-NAP-CAQ	-3.43	122.74	125.50
3	В	1204	JHL	CBE-NAZ-CBA	-3.28	115.38	118.60
3	С	1201	JHL	CBE-NAZ-CBA	-3.10	115.55	118.60
3	D	1201	JHL	CBE-NAZ-CBA	-2.57	116.07	118.60
3	В	1205	JHL	CBJ-CBE-NAZ	2.56	122.96	120.13
3	В	1205	JHL	CAH-CAI-CAJ	-2.55	119.20	121.44
3	С	1202	JHL	CAH-CAI-CAJ	-2.46	119.28	121.44
3	D	1201	JHL	CBJ-CBE-NAZ	2.39	122.77	120.13
3	A	1202	JHL	CBE-NAZ-CBA	-2.37	116.27	118.60
3	С	1201	JHL	OBM-CBA-NAZ	-2.35	119.38	122.52
3	В	1204	JHL	CAO-NAP-CAQ	-2.33	123.63	125.50
3	В	1205	JHL	CBF-CBE-NAZ	-2.32	116.97	119.47
3	В	1205	JHL	CBD-CBC-CBB	2.19	116.83	111.20



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	1202	JHL	CBJ-CBE-NAZ	2.13	122.49	120.13
3	A	1202	JHL	CAH-CAI-CAJ	-2.13	119.58	121.44
3	С	1202	JHL	OBM-CBA-NAZ	-2.12	119.68	122.52
3	С	1202	JHL	CBF-CBE-NAZ	-2.11	117.19	119.47
3	D	1201	JHL	CBF-CBE-NAZ	-2.07	117.24	119.47
3	С	1201	JHL	CAF-CAB-NAC	2.07	125.55	119.19
3	С	1202	JHL	CAO-NAP-CAQ	-2.03	123.86	125.50
3	A	1202	JHL	CBF-CBE-NAZ	-2.02	117.30	119.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	1203	EDO	O1-C1-C2-O2
3	A	1202	JHL	CAT-CAU-OAX-CAY
3	D	1201	JHL	CAT-CAU-OAX-CAY

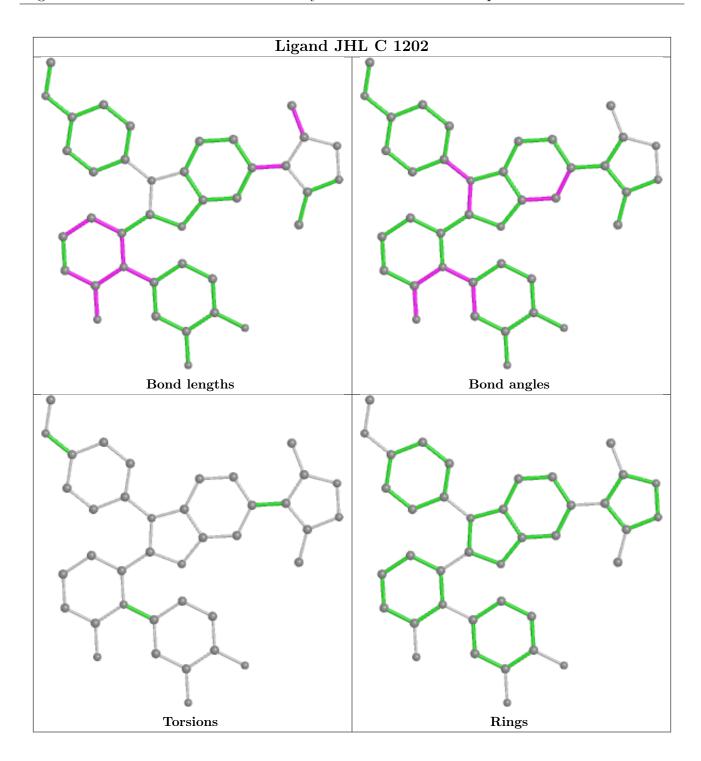
There are no ring outliers.

3 monomers are involved in 3 short contacts:

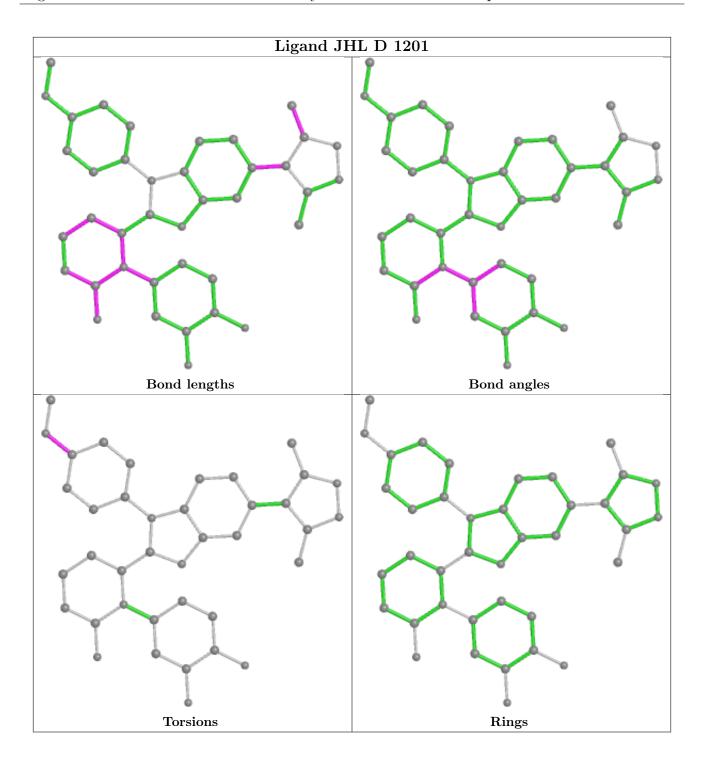
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1202	EDO	1	0
2	A	1203	PO4	1	0
2	В	1202	PO4	1	0

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.

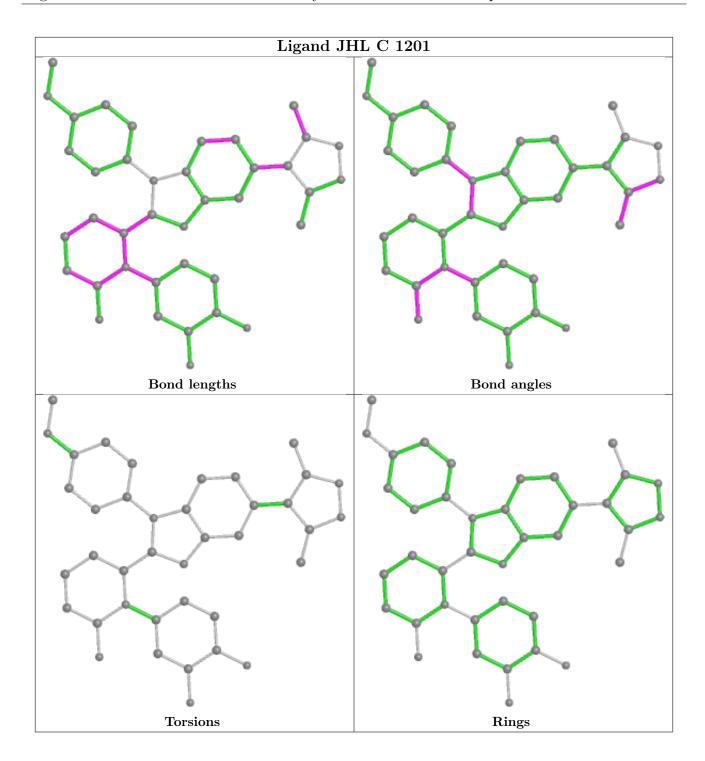




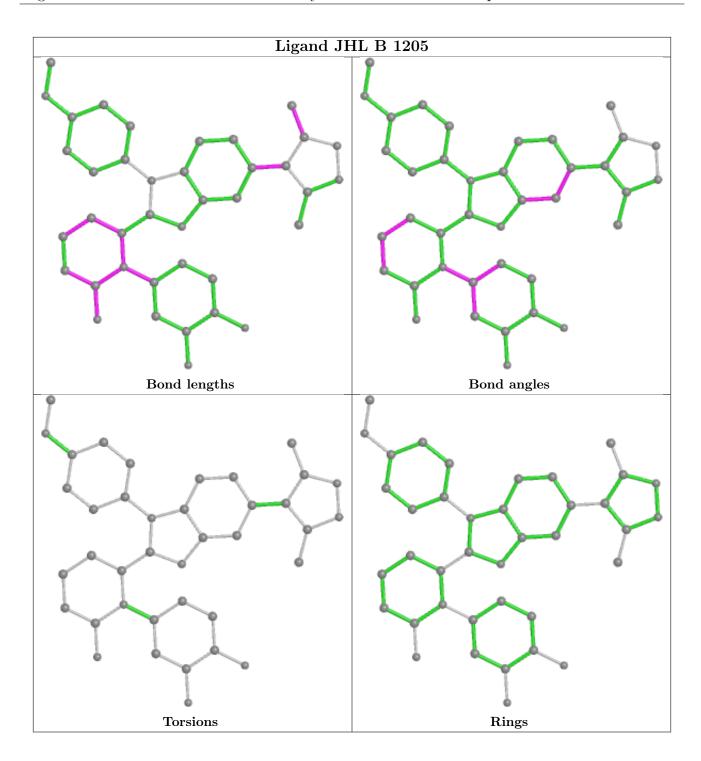




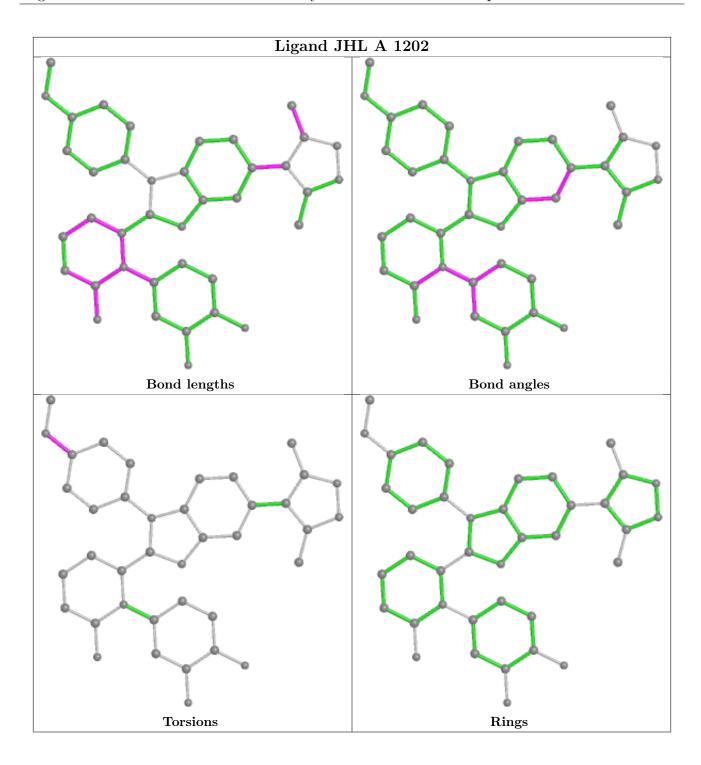




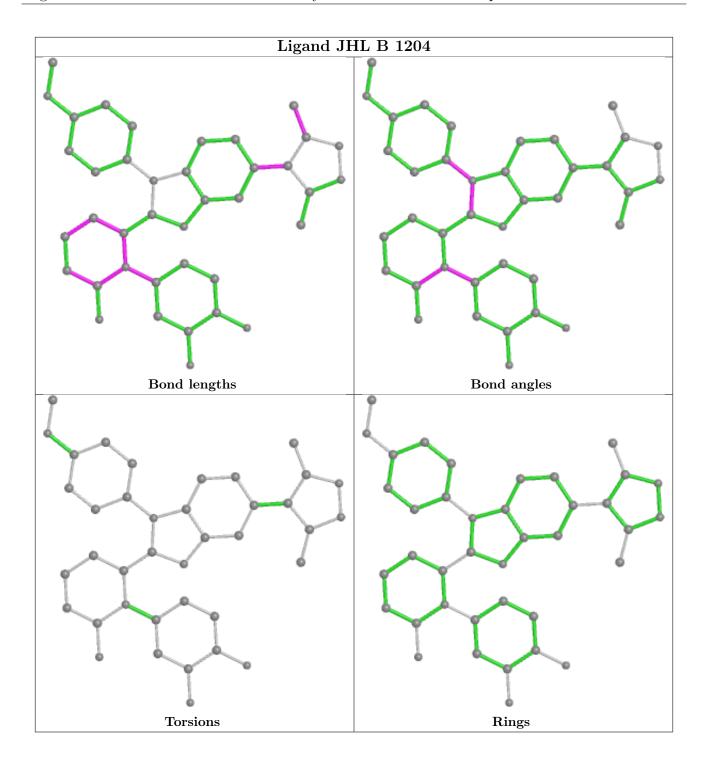












5.7 Other polymers (i)

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)

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^{th} 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>	# RSRZ > 2	$OWAB(A^2)$	Q < 0.9
1	A	116/116 (100%)	-0.48	1 (0%) 84 85	13, 19, 40, 64	0
1	В	115/116 (99%)	-0.65	0 100 100	14, 17, 29, 42	0
1	С	115/116 (99%)	-0.58	0 100 100	14, 17, 28, 44	0
1	D	115/116 (99%)	-0.51	0 100 100	13, 19, 38, 45	0
All	All	461/464 (99%)	-0.56	1 (0%) 95 95	13, 19, 35, 64	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	A	1085	PHE	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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	EDO	В	1203	4/4	0.84	0.15	33,36,40,41	0

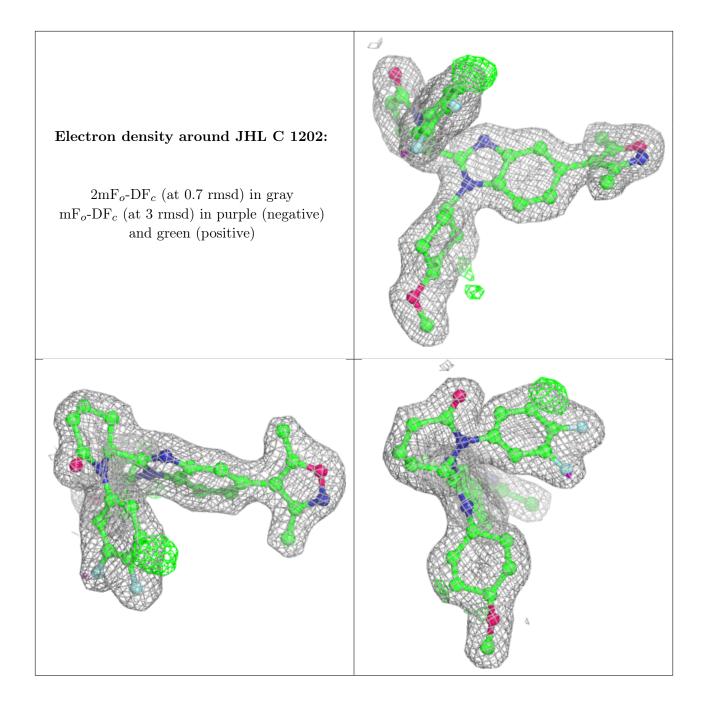


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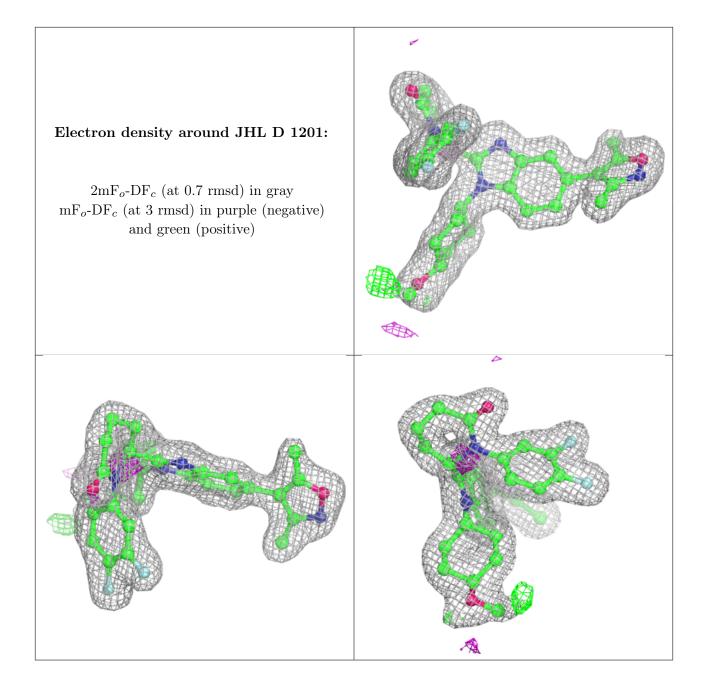
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	PO4	В	1202	5/5	0.91	0.20	31,40,46,47	0
2	PO4	A	1203	5/5	0.91	0.16	30,38,44,52	0
4	EDO	D	1202	4/4	0.92	0.10	39,43,43,44	0
3	JHL	С	1202	39/39	0.95	0.08	13,19,25,30	0
3	JHL	D	1201	39/39	0.95	0.09	15,21,28,31	0
3	JHL	A	1202	39/39	0.95	0.09	15,20,26,28	0
3	JHL	В	1204	39/39	0.95	0.09	14,20,26,27	0
3	JHL	В	1205	39/39	0.96	0.08	14,19,25,33	0
3	JHL	С	1201	39/39	0.96	0.08	14,20,27,28	0
2	PO4	A	1204	5/5	0.97	0.14	31,41,53,58	0
2	PO4	В	1201	5/5	0.98	0.11	30,36,40,50	0
2	PO4	A	1201	5/5	0.98	0.10	30,36,39,45	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.

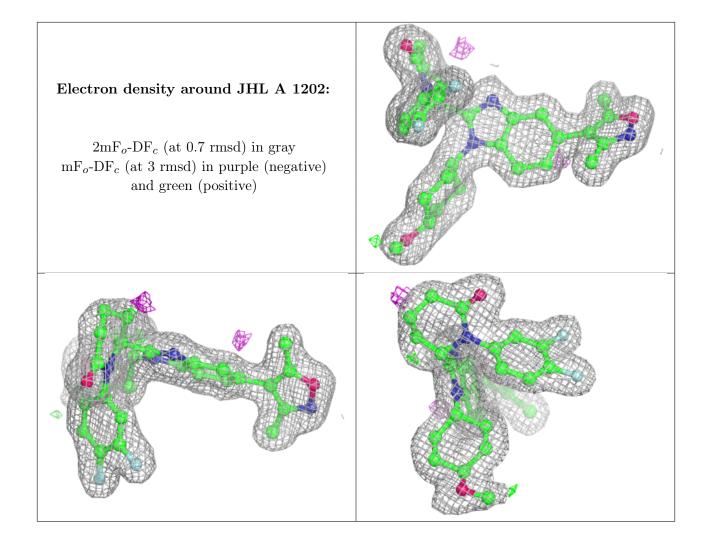








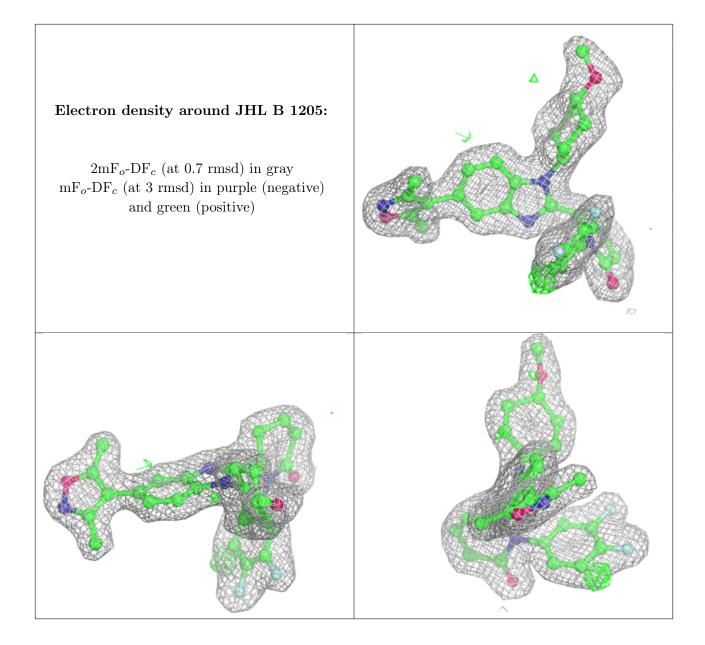




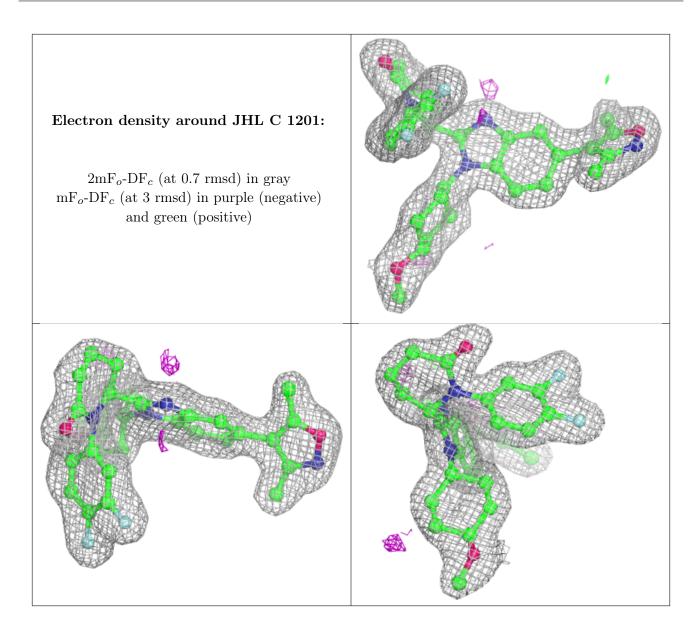


Electron density around JHL B 1204: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

