



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:05 AM UTC

PDB ID : 8FV2 / pdb_00008fv2
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

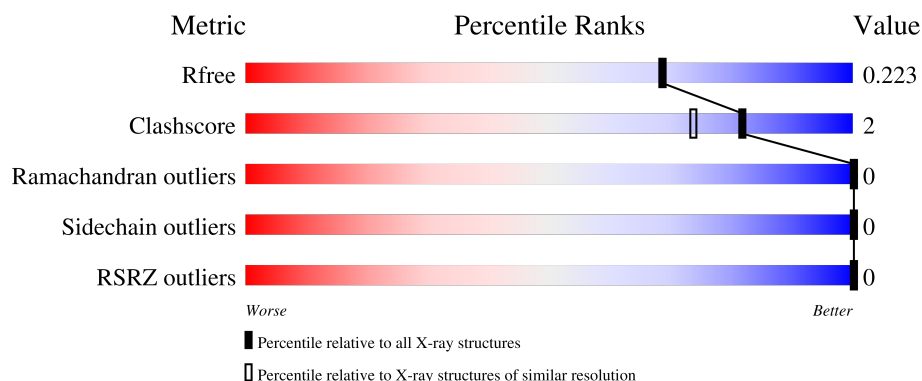
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

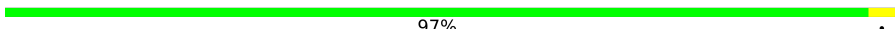
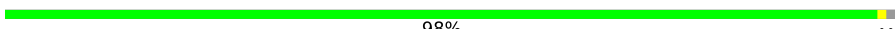
The reported resolution of this entry is 1.87 Å.

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. 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	116	 91% 9%
1	B	116	 92% 7% .
1	C	116	 97% ..
1	D	116	 98% ..

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	A	116	Total	C	N	O	S	0	3	0
			995	646	163	181	5			
1	B	115	Total	C	N	O	S	0	3	0
			983	637	159	182	5			
1	C	115	Total	C	N	O	S	0	3	0
			984	639	160	180	5			
1	D	115	Total	C	N	O	S	0	2	0
			981	637	160	179	5			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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

-
- The chemical structure of JHL is a complex polycyclic molecule. It features a central benzene ring substituted with a naphthalene-like system on the left and a piperidine ring on the right. The naphthalene system includes a pyrazole ring with an NAC group and an oxygen atom. The piperidine ring is substituted with a CBA group and an OBM group. The molecule is further substituted with various other groups including OAX, CAY, CAU, CAT, CAS, CAV, CAW, CAQ, CAL, CAM, CAH, CAA, CAG, CBF, CBE, CBI, CBJ, CBH, FBK, FBL, CBG, and CBA. The structure is highly symmetrical and complex, with many chiral centers and functional groups.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 39	C 30	F 2	N 4	O 3	0	0
3	B	1	Total 39	C 30	F 2	N 4	O 3	0	0
3	B	1	Total 39	C 30	F 2	N 4	O 3	0	0
3	C	1	Total 39	C 30	F 2	N 4	O 3	0	0
3	C	1	Total 39	C 30	F 2	N 4	O 3	0	0
3	D	1	Total 39	C 30	F 2	N 4	O 3	0	0

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

- Molecule 5 is water.

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

3 Residue-property plots [i](#)

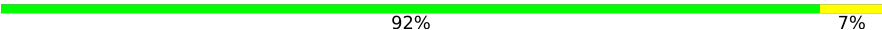
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A:  91% 9%

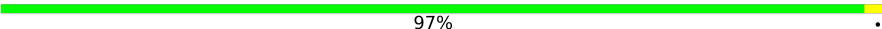


- Molecule 1: CREB-binding protein

Chain B:  92% 7% .

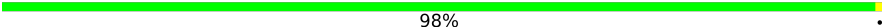


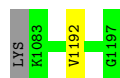
- Molecule 1: CREB-binding protein

Chain C:  97% ..



- Molecule 1: CREB-binding protein

Chain D:  98% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	79.45Å 79.45Å 97.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.44 – 1.87 41.44 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.44-1.87) 91.1 (41.44-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.190 , 0.226 0.186 , 0.223	Depositor 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)	0.36 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	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.*

¹ Intensities estimated from amplitudes.

² 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: EDO, JHL, PO4

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	0.34	0/1025	0.53	0/1390
1	B	0.33	0/1016	0.52	0/1381
1	C	0.35	0/1020	0.50	0/1385
1	D	0.35	0/1011	0.54	0/1372
All	All	0.34	0/4072	0.52	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	10	0
1	B	983	0	963	4	0
1	C	984	0	977	3	0
1	D	981	0	973	1	0
2	A	15	0	0	1	0
2	B	10	0	0	1	0
3	A	39	0	0	0	0
3	B	78	0	0	0	0
3	C	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	B	4	0	6	0	0
4	D	4	0	6	1	0
5	A	110	0	0	4	0
5	B	120	0	0	1	0
5	C	129	0	0	1	0
5	D	104	0	0	1	0
All	All	4673	0	3912	20	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 (20) 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: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:C:1133:MET:HE2	1:C:1133:MET:HB2	1.87	0.44
1:A:1088:GLU:CD	1:A:1092:GLN:HE21	2.26	0.43
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:1133:MET:HB2	1:A:1133:MET:HE2	1.68	0.41
1:B:1116:ASP:CG	1:B:1119:LEU:HG	2.46	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

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	A	117/116 (101%)	116 (99%)	1 (1%)	0	100	100
1	B	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

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%)	111 (100%)	0	100	100
1	B	110/109 (101%)	110 (100%)	0	100	100
1	C	111/109 (102%)	111 (100%)	0	100	100
1	D	110/109 (101%)	110 (100%)	0	100	100
All	All	442/436 (101%)	442 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1146	GLN
1	D	1146	GLN
1	D	1194	GLN

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 ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	EDO	D	1202	-	3,3,3	0.46	0	2,2,2	0.32	0
2	PO4	B	1202	-	4,4,4	0.87	0	6,6,6	0.65	0
4	EDO	B	1203	-	3,3,3	0.45	0	2,2,2	0.29	0
2	PO4	B	1201	-	4,4,4	1.03	0	6,6,6	0.68	0
3	JHL	C	1201	-	42,44,44	2.44	12 (28%)	58,65,65	2.06	14 (24%)
2	PO4	A	1204	-	4,4,4	1.06	0	6,6,6	0.42	0
3	JHL	B	1205	-	42,44,44	2.45	12 (28%)	58,65,65	1.85	15 (25%)
3	JHL	A	1202	-	42,44,44	2.41	13 (30%)	58,65,65	1.82	12 (20%)
3	JHL	D	1201	-	42,44,44	2.44	14 (33%)	58,65,65	1.88	13 (22%)
3	JHL	C	1202	-	42,44,44	2.40	14 (33%)	58,65,65	1.84	14 (24%)
2	PO4	A	1201	-	4,4,4	1.04	0	6,6,6	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	1203	-	4,4,4	0.87	0	6,6,6	0.29	0
3	JHL	B	1204	-	42,44,44	2.48	12 (28%)	58,65,65	1.95	14 (24%)

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	EDO	D	1202	-	-	0/1/1/1	-
4	EDO	B	1203	-	-	1/1/1/1	-
3	JHL	B	1204	-	-	2/18/42/42	0/6/6/6
3	JHL	C	1201	-	-	2/18/42/42	0/6/6/6
3	JHL	B	1205	-	-	0/18/42/42	0/6/6/6
3	JHL	A	1202	-	-	3/18/42/42	0/6/6/6
3	JHL	D	1201	-	-	3/18/42/42	0/6/6/6
3	JHL	C	1202	-	-	0/18/42/42	0/6/6/6

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	JHL	CAR-NAZ	9.32	1.59	1.47
3	C	1201	JHL	CAR-NAZ	9.02	1.58	1.47
3	D	1201	JHL	CAR-NAZ	8.97	1.58	1.47
3	A	1202	JHL	CAR-NAZ	8.83	1.58	1.47
3	B	1205	JHL	CAR-NAZ	8.49	1.58	1.47
3	C	1202	JHL	CAR-NAZ	8.17	1.57	1.47
3	C	1201	JHL	CBA-NAZ	8.11	1.52	1.36
3	B	1205	JHL	CBA-NAZ	8.08	1.52	1.36
3	B	1204	JHL	CBA-NAZ	8.08	1.52	1.36
3	D	1201	JHL	CBA-NAZ	7.93	1.51	1.36
3	C	1202	JHL	CBA-NAZ	7.92	1.51	1.36
3	A	1202	JHL	CBA-NAZ	7.70	1.51	1.36
3	D	1201	JHL	CAH-CAA	3.65	1.56	1.49
3	C	1202	JHL	CAH-CAA	3.61	1.56	1.49
3	A	1202	JHL	CAH-CAA	3.43	1.56	1.49
3	C	1202	JHL	CBB-CBA	3.36	1.58	1.51
3	B	1205	JHL	CAH-CAA	3.35	1.56	1.49
3	C	1201	JHL	CAL-CAK	3.32	1.44	1.39
3	B	1205	JHL	CBB-CBA	3.24	1.57	1.51
3	B	1204	JHL	CBB-CBA	3.21	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1204	JHL	CAH-CAA	3.16	1.55	1.49
3	A	1202	JHL	CBB-CBA	3.08	1.57	1.51
3	D	1201	JHL	CBB-CBA	3.04	1.57	1.51
3	B	1205	JHL	CBC-CBD	-3.01	1.45	1.53
3	C	1202	JHL	OAD-NAC	-2.95	1.37	1.42
3	D	1201	JHL	CAA-CAE	2.95	1.39	1.36
3	A	1202	JHL	CAO-NAN	2.94	1.35	1.32
3	C	1202	JHL	CBC-CBD	-2.92	1.45	1.53
3	C	1201	JHL	CAH-CAA	2.91	1.55	1.49
3	C	1202	JHL	CBD-CAR	-2.91	1.46	1.53
3	D	1201	JHL	CBC-CBD	-2.88	1.46	1.53
3	C	1201	JHL	CBB-CBA	2.88	1.57	1.51
3	A	1202	JHL	OAD-NAC	-2.87	1.37	1.42
3	A	1202	JHL	CBC-CBD	-2.85	1.46	1.53
3	C	1201	JHL	CBC-CBD	-2.85	1.46	1.53
3	B	1204	JHL	CBC-CBD	-2.84	1.46	1.53
3	B	1205	JHL	OAD-NAC	-2.83	1.37	1.42
3	B	1204	JHL	CBD-CAR	-2.80	1.46	1.53
3	B	1205	JHL	CBE-NAZ	2.80	1.47	1.43
3	C	1201	JHL	CBD-CAR	-2.79	1.46	1.53
3	D	1201	JHL	CBD-CAR	-2.75	1.46	1.53
3	A	1202	JHL	CBD-CAR	-2.74	1.46	1.53
3	B	1205	JHL	CAA-CAE	2.73	1.39	1.36
3	B	1205	JHL	CBD-CAR	-2.71	1.46	1.53
3	B	1204	JHL	CAO-NAN	2.70	1.35	1.32
3	B	1204	JHL	CAL-CAK	2.64	1.43	1.39
3	B	1204	JHL	OAD-NAC	-2.58	1.37	1.42
3	C	1201	JHL	CAO-NAN	2.55	1.35	1.32
3	B	1205	JHL	CAL-CAK	2.54	1.43	1.39
3	A	1202	JHL	CAI-CAJ	2.54	1.43	1.40
3	C	1201	JHL	CAA-CAE	2.47	1.39	1.36
3	C	1202	JHL	CAA-CAE	2.47	1.39	1.36
3	C	1201	JHL	CAI-CAJ	2.46	1.43	1.40
3	C	1202	JHL	CBE-NAZ	2.46	1.47	1.43
3	B	1204	JHL	CAI-CAJ	2.44	1.43	1.40
3	B	1204	JHL	CBE-NAZ	2.42	1.47	1.43
3	D	1201	JHL	OAD-NAC	-2.42	1.38	1.42
3	D	1201	JHL	CBE-NAZ	2.39	1.47	1.43
3	B	1204	JHL	CAA-CAE	2.38	1.39	1.36
3	C	1202	JHL	OBM-CBA	-2.32	1.18	1.23
3	D	1201	JHL	CAO-NAN	2.31	1.35	1.32
3	C	1202	JHL	CAI-CAJ	2.28	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	JHL	CBE-NAZ	2.27	1.46	1.43
3	B	1205	JHL	OBM-CBA	-2.24	1.18	1.23
3	D	1201	JHL	CAL-CAK	2.23	1.43	1.39
3	A	1202	JHL	CAA-CAE	2.22	1.38	1.36
3	C	1202	JHL	CAO-NAN	2.22	1.34	1.32
3	D	1201	JHL	CAI-CAJ	2.20	1.43	1.40
3	C	1201	JHL	CBE-NAZ	2.18	1.46	1.43
3	A	1202	JHL	CAL-CAK	2.17	1.43	1.39
3	A	1202	JHL	OBM-CBA	-2.14	1.18	1.23
3	B	1205	JHL	CAB-NAC	2.12	1.35	1.30
3	C	1202	JHL	CAB-NAC	2.09	1.35	1.30
3	C	1202	JHL	CAL-CAK	2.08	1.42	1.39
3	D	1201	JHL	OBM-CBA	-2.07	1.18	1.23
3	C	1201	JHL	OAD-NAC	-2.03	1.38	1.42
3	D	1201	JHL	CAB-NAC	2.01	1.35	1.30

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1204	JHL	CBE-NAZ-CAR	6.37	126.90	117.50
3	C	1201	JHL	NAP-CAO-NAN	-6.29	108.25	113.13
3	D	1201	JHL	CBE-NAZ-CAR	6.04	126.42	117.50
3	B	1205	JHL	NAP-CAO-NAN	-5.88	108.57	113.13
3	C	1201	JHL	CAE-CAA-CAB	5.58	107.63	104.38
3	C	1201	JHL	CBE-NAZ-CAR	5.56	125.70	117.50
3	A	1202	JHL	CBE-NAZ-CAR	5.38	125.44	117.50
3	C	1202	JHL	NAP-CAO-NAN	-5.32	109.00	113.13
3	B	1204	JHL	NAP-CAO-NAN	-5.14	109.14	113.13
3	D	1201	JHL	NAP-CAO-NAN	-4.98	109.27	113.13
3	B	1204	JHL	CAE-CAA-CAB	4.82	107.19	104.38
3	B	1204	JHL	OAD-CAE-CAG	4.82	124.04	116.59
3	D	1201	JHL	OAD-CAE-CAG	4.79	124.00	116.59
3	A	1202	JHL	OAD-CAE-CAG	4.76	123.95	116.59
3	A	1202	JHL	NAP-CAO-NAN	-4.72	109.47	113.13
3	A	1202	JHL	CAE-CAA-CAB	4.64	107.08	104.38
3	C	1202	JHL	OAD-CAE-CAG	4.57	123.65	116.59
3	B	1205	JHL	CAE-CAA-CAB	4.44	106.96	104.38
3	C	1201	JHL	OAD-CAE-CAG	4.37	123.35	116.59
3	D	1201	JHL	CAE-CAA-CAB	4.27	106.87	104.38
3	B	1205	JHL	OAD-CAE-CAG	4.22	123.11	116.59
3	C	1202	JHL	CAG-CAE-CAA	-4.11	128.27	133.91
3	B	1205	JHL	CAJ-NAN-CAO	3.94	108.96	104.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1204	JHL	CAG-CAE-CAA	-3.88	128.58	133.91
3	D	1201	JHL	CAG-CAE-CAA	-3.87	128.60	133.91
3	C	1202	JHL	CAJ-NAN-CAO	3.81	108.82	104.75
3	C	1202	JHL	CBE-NAZ-CAR	3.70	122.96	117.50
3	C	1202	JHL	CAE-CAA-CAB	3.68	106.53	104.38
3	C	1201	JHL	CAK-NAP-CAO	3.65	109.17	106.75
3	A	1202	JHL	CAG-CAE-CAA	-3.54	129.05	133.91
3	B	1205	JHL	CBE-NAZ-CAR	3.53	122.71	117.50
3	B	1205	JHL	CAG-CAE-CAA	-3.36	129.29	133.91
3	C	1202	JHL	CAJ-CAK-NAP	3.34	107.91	105.12
3	B	1204	JHL	CBD-CAR-CAO	-3.32	103.95	112.74
3	C	1201	JHL	CAJ-NAN-CAO	3.31	108.28	104.75
3	C	1201	JHL	CAF-CAB-NAC	3.27	125.55	119.86
3	C	1201	JHL	CAG-CAE-CAA	-3.25	129.45	133.91
3	A	1202	JHL	CAJ-CAK-NAP	3.22	107.81	105.12
3	C	1201	JHL	CBD-CAR-CAO	-3.09	104.56	112.74
3	B	1205	JHL	CAF-CAB-NAC	3.09	125.23	119.86
3	D	1201	JHL	CAJ-NAN-CAO	3.03	107.99	104.75
3	B	1205	JHL	CAJ-CAK-NAP	2.97	107.60	105.12
3	A	1202	JHL	CBD-CAR-CAO	-2.87	105.14	112.74
3	C	1202	JHL	CAF-CAB-NAC	2.87	124.84	119.86
3	B	1204	JHL	CAF-CAB-NAC	2.82	124.76	119.86
3	A	1202	JHL	CAJ-NAN-CAO	2.81	107.76	104.75
3	B	1204	JHL	CAJ-NAN-CAO	2.81	107.75	104.75
3	D	1201	JHL	CBD-CAR-CAO	-2.77	105.41	112.74
3	C	1202	JHL	CBD-CAR-CAO	-2.70	105.61	112.74
3	C	1201	JHL	CAS-CAQ-NAP	-2.64	105.72	112.27
3	B	1204	JHL	CAJ-CAK-NAP	2.63	107.32	105.12
3	D	1201	JHL	CAJ-CAK-NAP	2.63	107.31	105.12
3	C	1202	JHL	CAK-CAJ-NAN	-2.59	106.90	110.19
3	B	1204	JHL	CBE-NAZ-CBA	-2.58	115.38	119.18
3	B	1205	JHL	CBJ-CBE-NAZ	2.58	122.96	120.14
3	B	1205	JHL	CBD-CAR-CAO	-2.49	106.15	112.74
3	A	1202	JHL	CAF-CAB-NAC	2.47	124.16	119.86
3	C	1201	JHL	CBE-NAZ-CBA	-2.46	115.55	119.18
3	C	1202	JHL	CAL-CAK-CAJ	-2.45	119.40	122.23
3	C	1202	JHL	CAW-CAQ-NAP	-2.45	106.18	112.27
3	C	1201	JHL	OBM-CBA-NAZ	-2.41	119.38	122.52
3	D	1201	JHL	CBJ-CBE-NAZ	2.40	122.77	120.14
3	B	1205	JHL	CBF-CBE-NAZ	-2.40	116.97	119.36
3	D	1201	JHL	CAF-CAB-NAC	2.35	123.94	119.86
3	B	1205	JHL	CAK-CAJ-NAN	-2.33	107.23	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	JHL	CAK-CAJ-NAN	-2.28	107.29	110.19
3	B	1205	JHL	CBD-CBC-CBB	2.24	116.83	111.12
3	B	1204	JHL	CAL-CAK-CAJ	-2.22	119.67	122.23
3	B	1205	JHL	CAW-CAQ-NAP	-2.22	106.76	112.27
3	C	1202	JHL	OBM-CBA-NAZ	-2.18	119.68	122.52
3	B	1204	JHL	CAK-NAP-CAO	2.17	108.19	106.75
3	C	1202	JHL	CBF-CBE-NAZ	-2.17	117.19	119.36
3	D	1201	JHL	CAK-CAJ-NAN	-2.17	107.44	110.19
3	A	1202	JHL	CBJ-CBE-NAZ	2.15	122.49	120.14
3	D	1201	JHL	CBF-CBE-NAZ	-2.13	117.24	119.36
3	B	1204	JHL	CAS-CAQ-NAP	-2.13	106.98	112.27
3	D	1201	JHL	CBE-NAZ-CBA	-2.11	116.07	119.18
3	A	1202	JHL	CBF-CBE-NAZ	-2.07	117.30	119.36
3	C	1201	JHL	CAL-CAK-CAJ	-2.06	119.86	122.23
3	B	1204	JHL	CAK-CAJ-NAN	-2.05	107.58	110.19
3	B	1205	JHL	CAL-CAK-CAJ	-2.04	119.87	122.23
3	C	1201	JHL	OAD-NAC-CAB	2.02	108.30	106.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

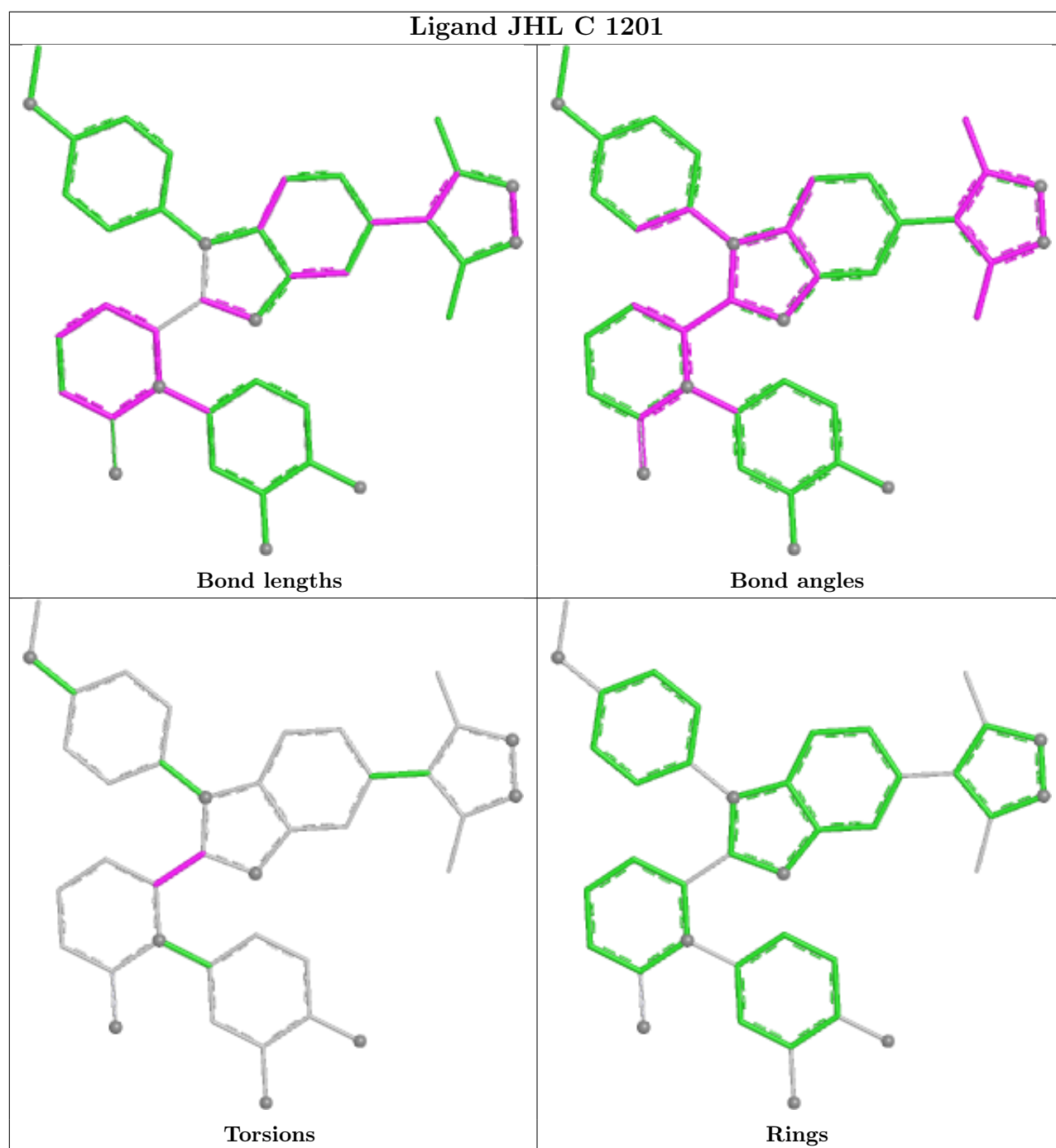
Mol	Chain	Res	Type	Atoms
3	A	1202	JHL	NAP-CAO-CAR-NAZ
3	A	1202	JHL	NAN-CAO-CAR-NAZ
3	B	1204	JHL	NAP-CAO-CAR-NAZ
3	B	1204	JHL	NAN-CAO-CAR-NAZ
3	C	1201	JHL	NAP-CAO-CAR-NAZ
3	C	1201	JHL	NAN-CAO-CAR-NAZ
3	D	1201	JHL	NAP-CAO-CAR-NAZ
3	D	1201	JHL	NAN-CAO-CAR-NAZ
3	A	1202	JHL	CAT-CAU-OAX-CAY
3	D	1201	JHL	CAT-CAU-OAX-CAY
4	B	1203	EDO	O1-C1-C2-O2

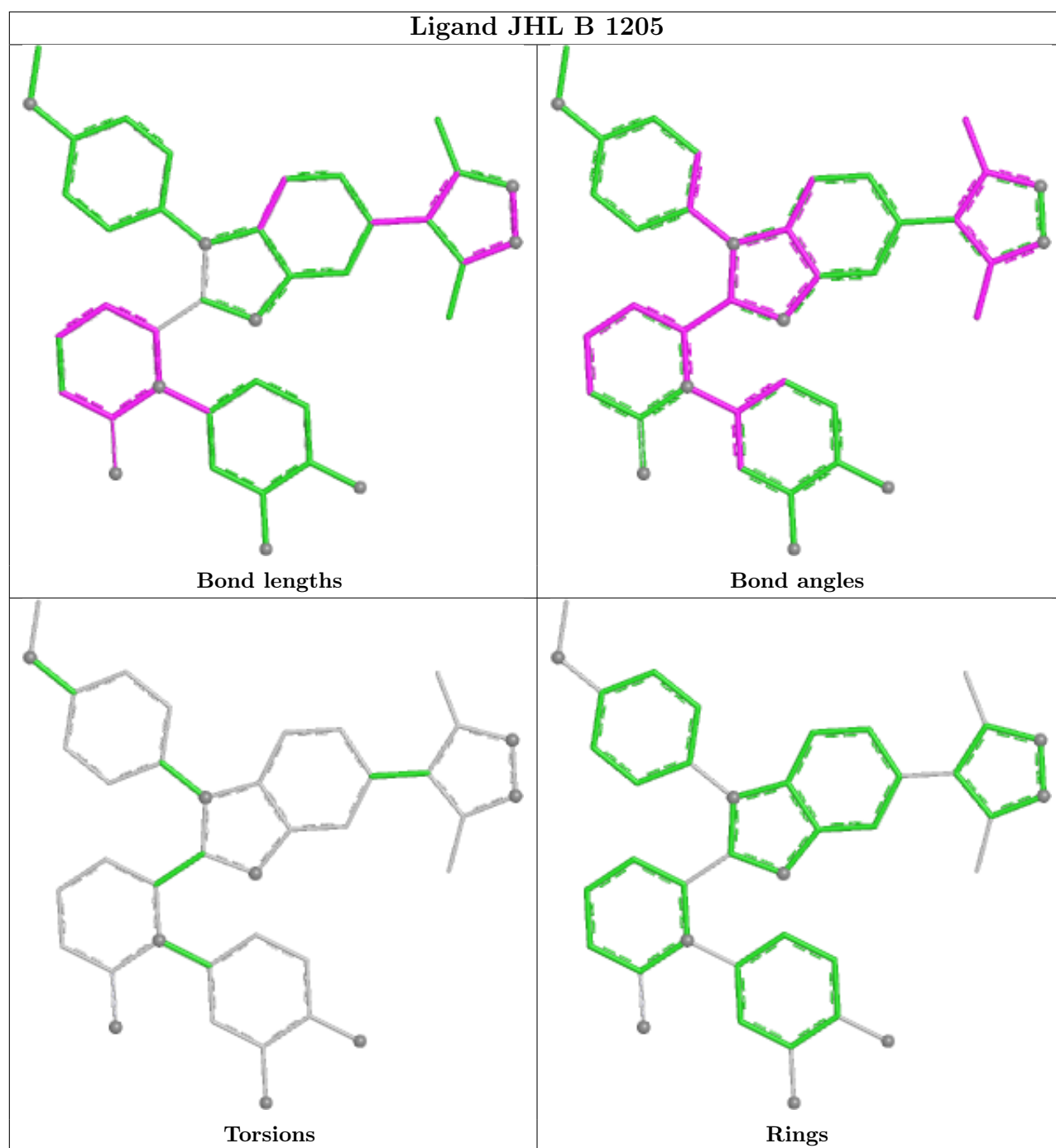
There are no ring outliers.

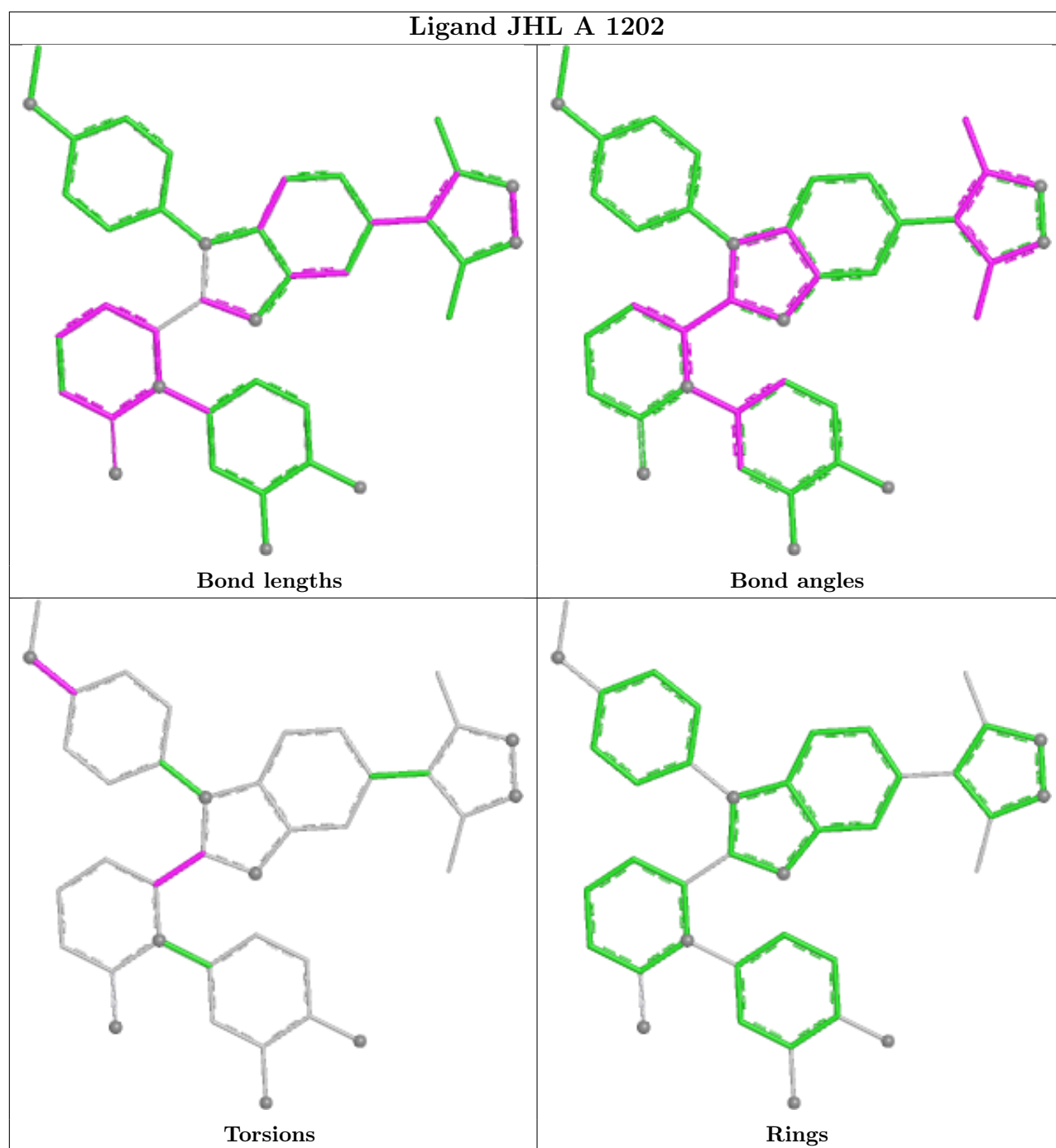
3 monomers are involved in 3 short contacts:

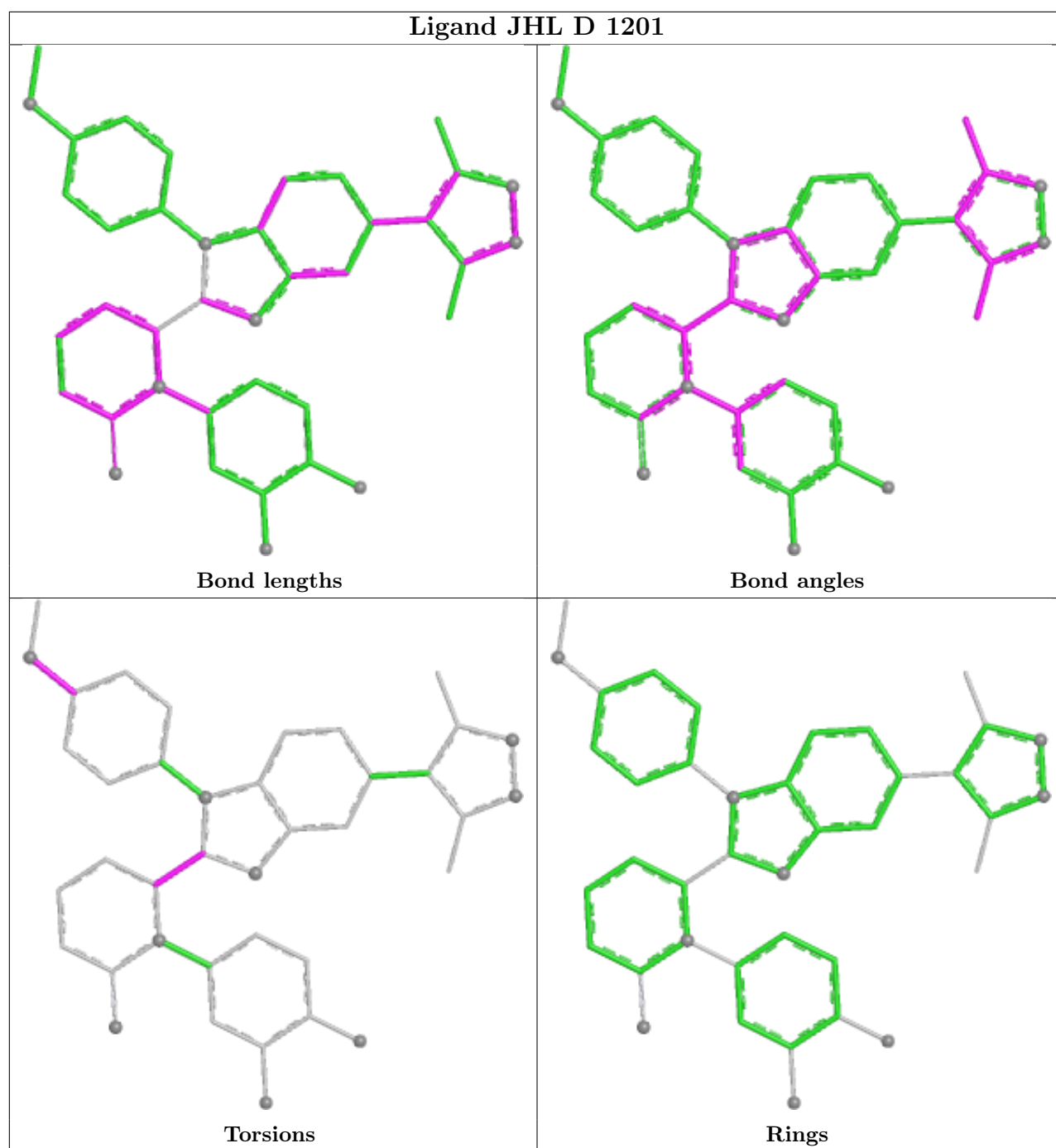
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1202	EDO	1	0
2	B	1202	PO4	1	0
2	A	1203	PO4	1	0

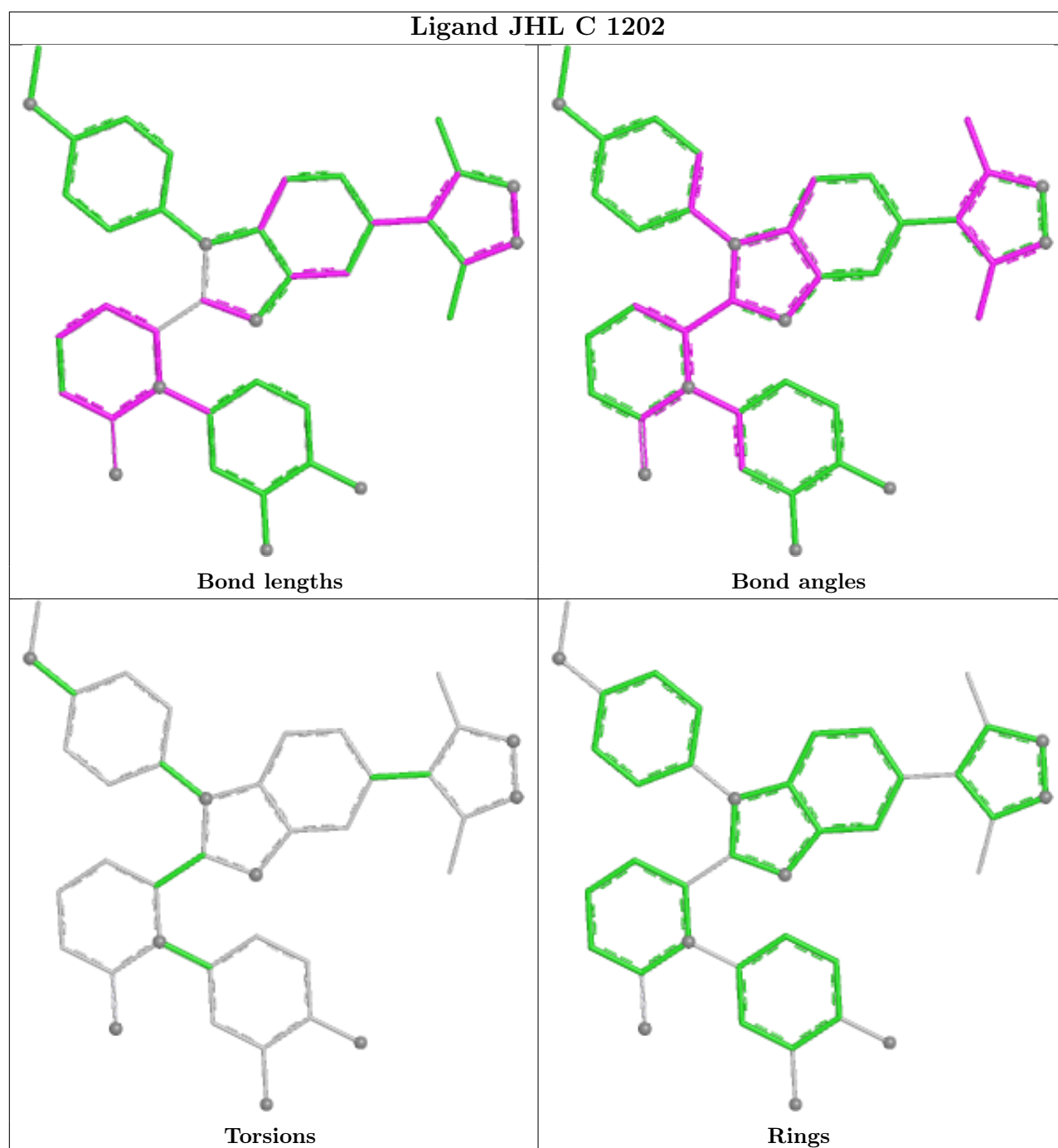
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

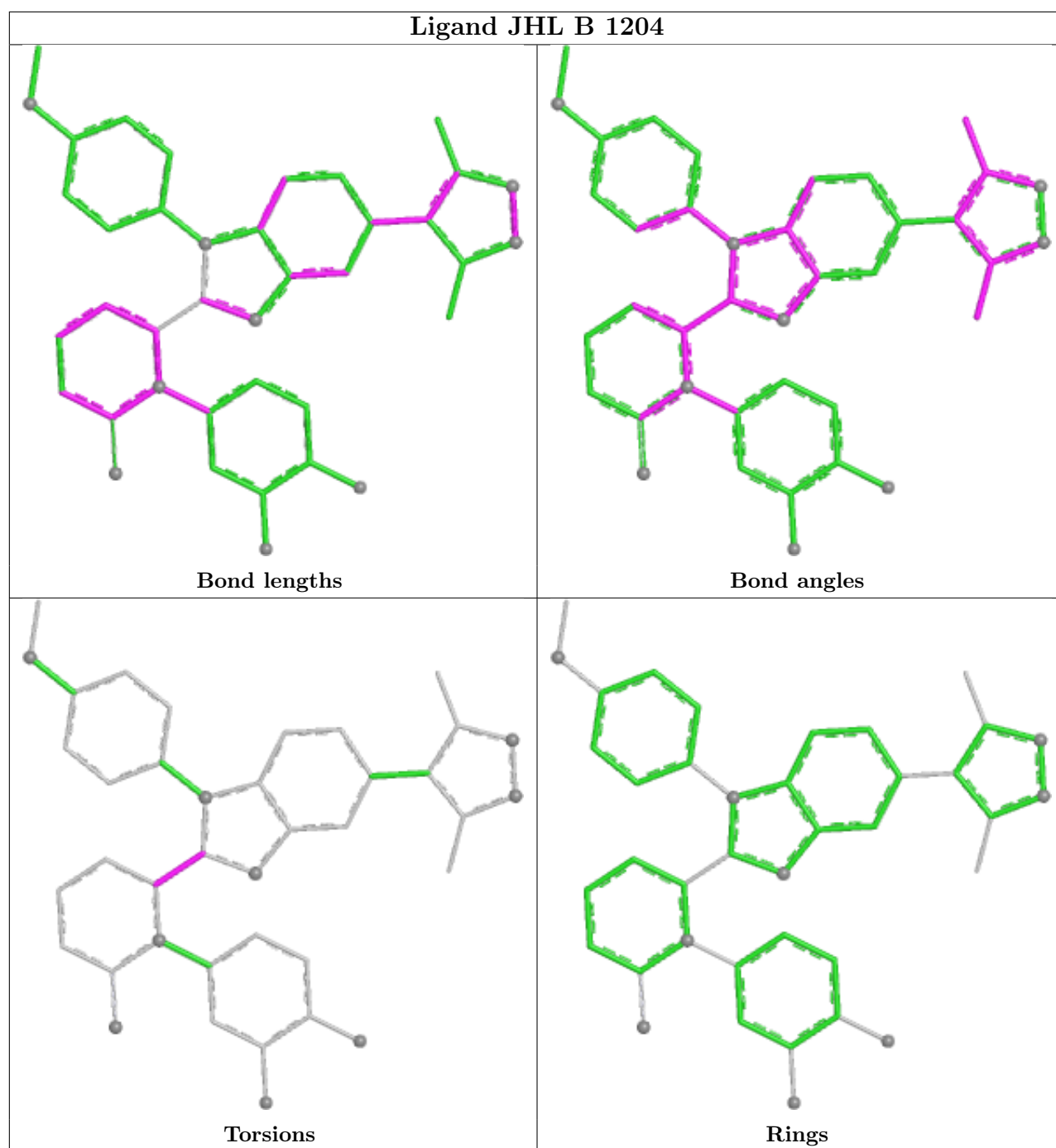












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	116/116 (100%)	-1.44	0 100 100	9, 19, 40, 64	3 (2%)
1	B	115/116 (99%)	-1.52	0 100 100	9, 17, 29, 42	3 (2%)
1	C	115/116 (99%)	-1.52	0 100 100	10, 17, 28, 44	3 (2%)
1	D	115/116 (99%)	-1.42	0 100 100	8, 19, 38, 45	2 (1%)
All	All	461/464 (99%)	-1.47	0 100 100	8, 18, 35, 64	11 (2%)

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
2	PO4	A	1201	5/5	0.99	0.04	30,36,39,45	0
2	PO4	A	1203	5/5	0.99	0.06	30,38,44,52	0
2	PO4	B	1201	5/5	0.99	0.05	30,36,40,50	0
2	PO4	B	1202	5/5	0.99	0.07	31,40,46,47	0

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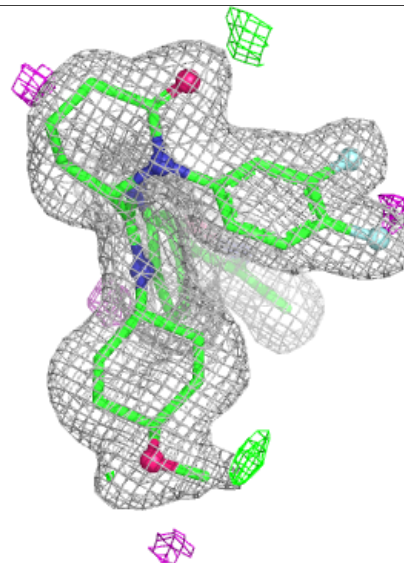
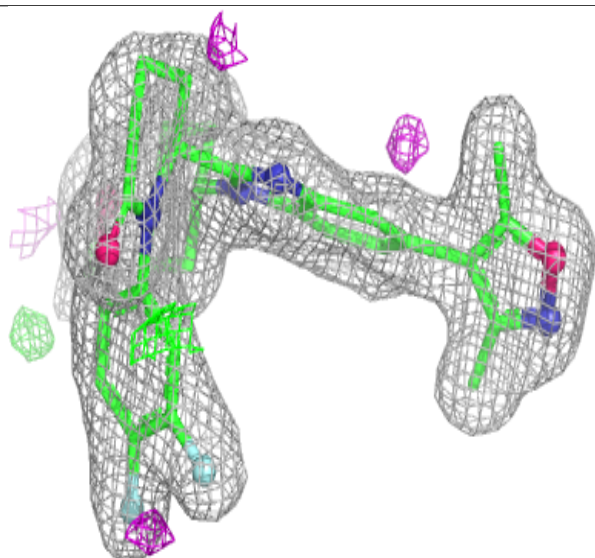
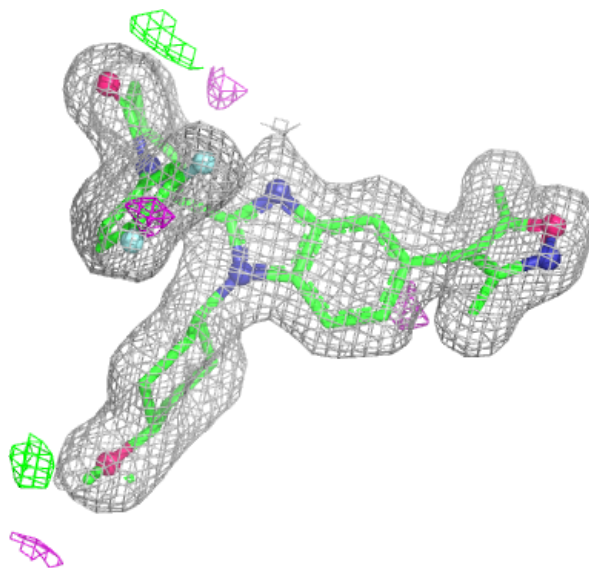
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JHL	A	1202	39/39	0.99	0.03	15,20,26,28	0
3	JHL	B	1204	39/39	0.99	0.03	14,20,26,27	0
3	JHL	B	1205	39/39	0.99	0.03	14,19,25,33	0
3	JHL	C	1201	39/39	0.99	0.03	14,20,27,28	0
3	JHL	C	1202	39/39	0.99	0.03	13,19,25,30	0
3	JHL	D	1201	39/39	0.99	0.03	15,21,28,31	0
4	EDO	B	1203	4/4	0.99	0.04	33,36,40,41	0
4	EDO	D	1202	4/4	0.99	0.04	39,43,43,44	0
2	PO4	A	1204	5/5	1.00	0.03	31,41,53,58	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.

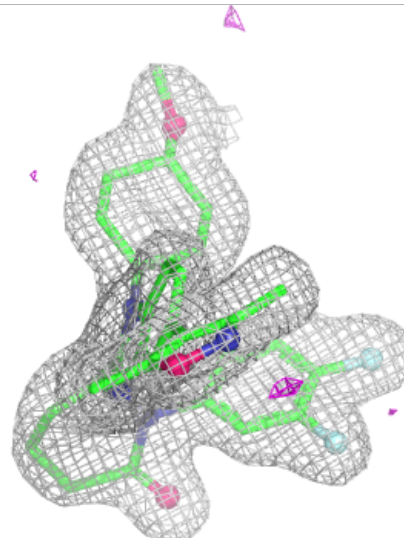
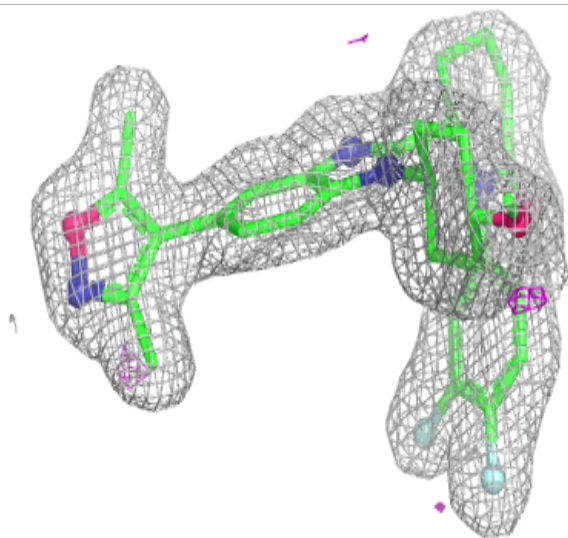
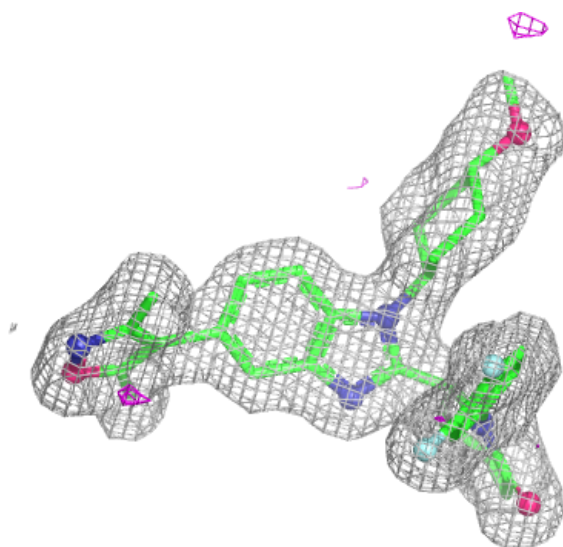
Electron density around JHL A 1202:

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



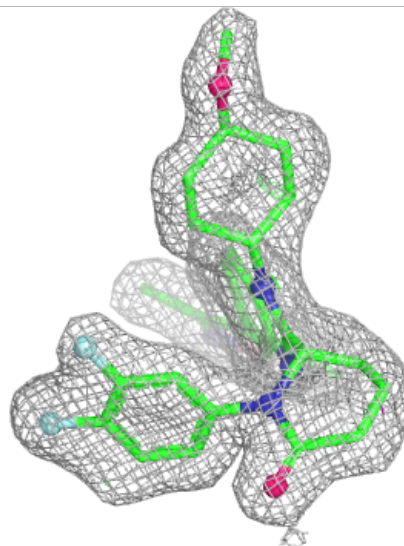
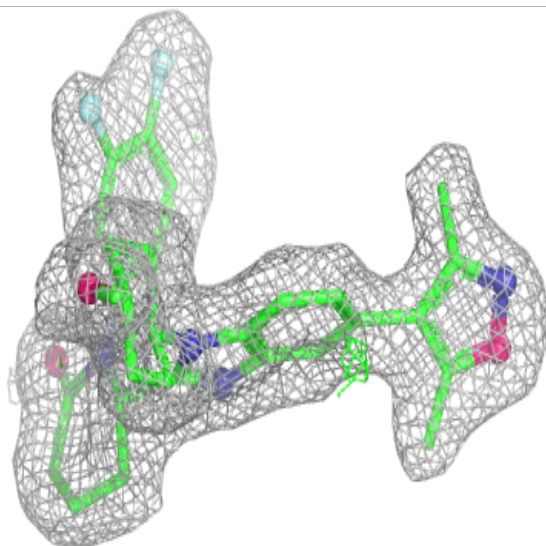
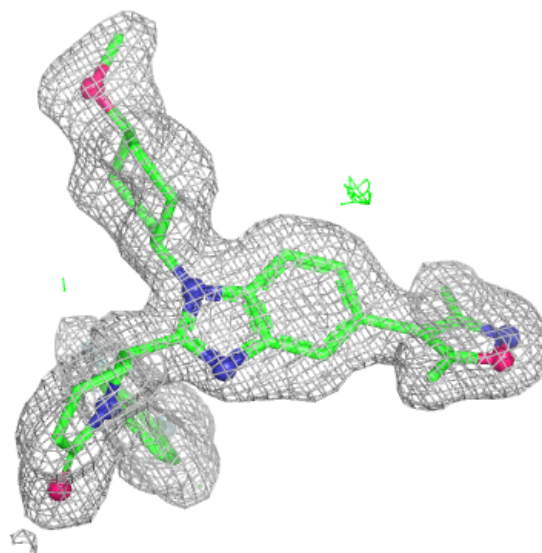
Electron density around JHL B 1204:

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



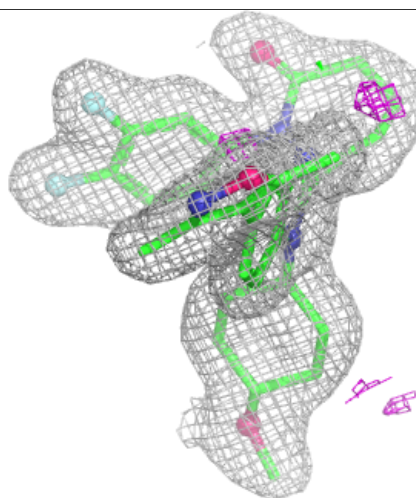
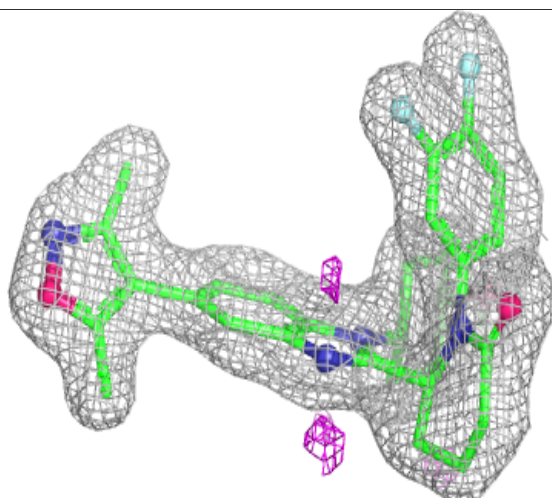
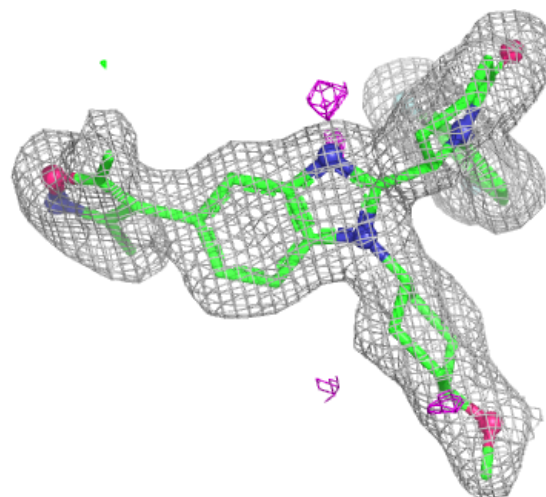
Electron density around JHL B 1205:

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



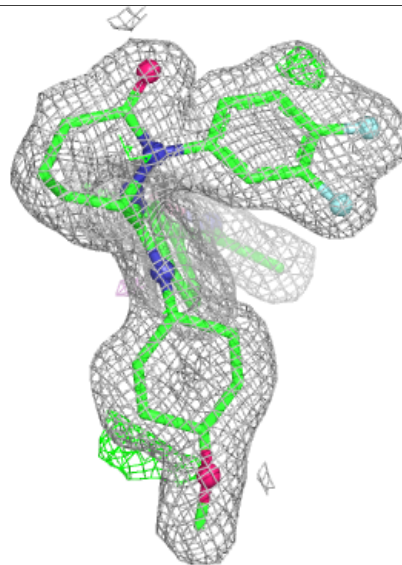
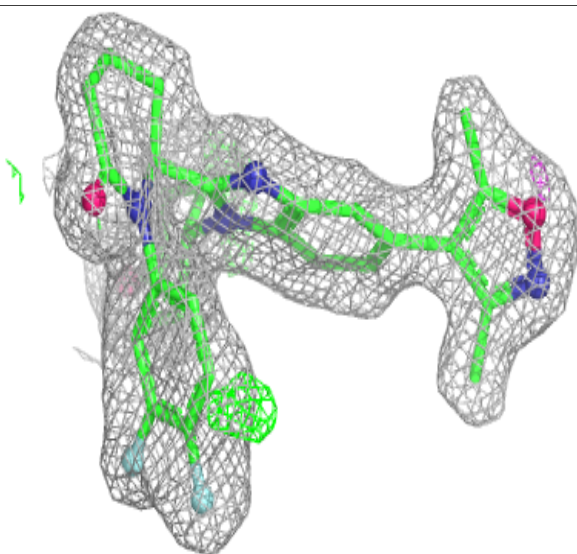
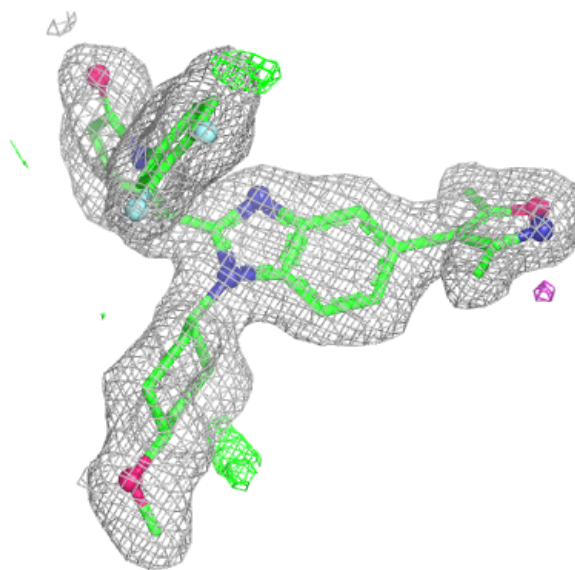
Electron density around JHL C 1201:

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



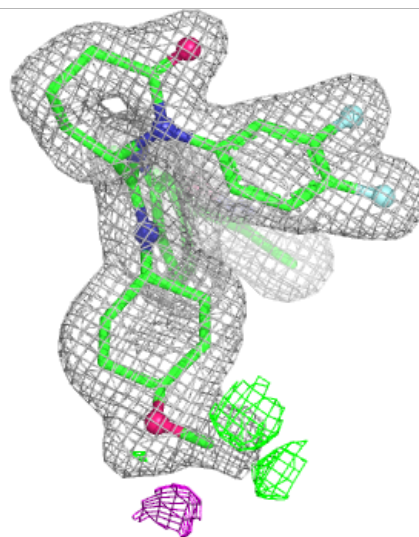
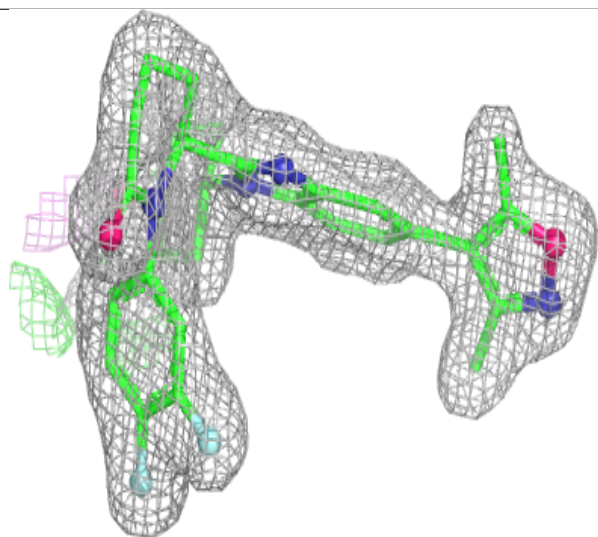
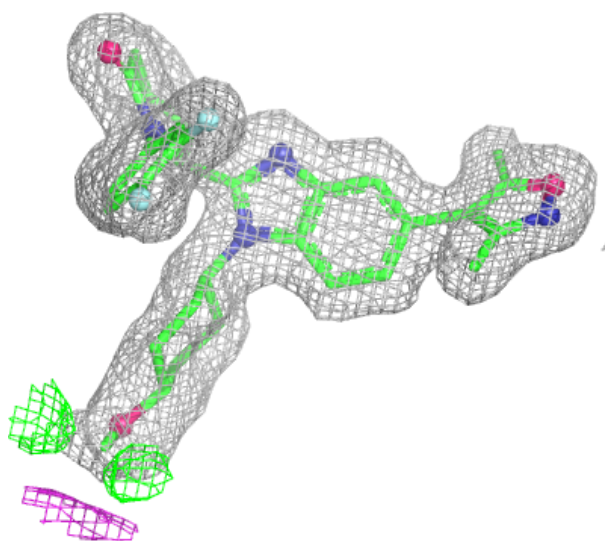
Electron density around JHL C 1202:

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



Electron density around JHL D 1201:

$2mF_o-DF_c$ (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.