



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:46 AM UTC

PDB ID : 2HZ0 / pdb_00002hz0
Title : Abl kinase domain in complex with NVP-AEG082
Authors : Cowan-Jacob, S.W.; Fendrich, G.; Liebetanz, J.; Fabbro, D.; Manley, P.
Deposited on : 2006-08-08
Resolution : 2.10 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

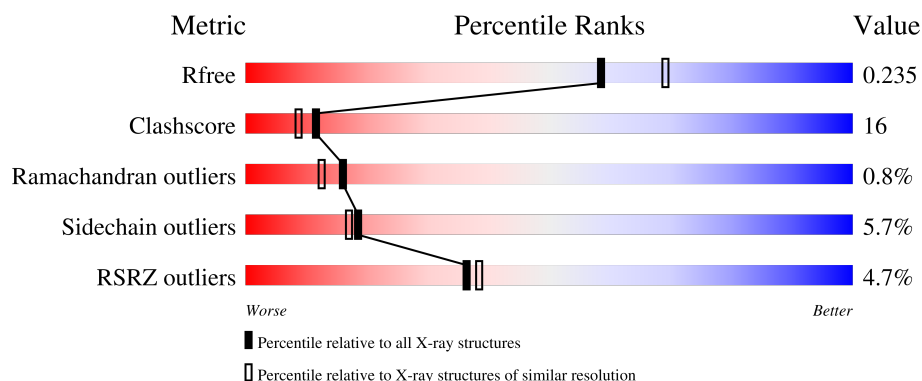
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

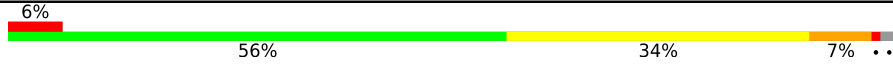
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	270	
1	B	270	

2 Entry composition [i](#)

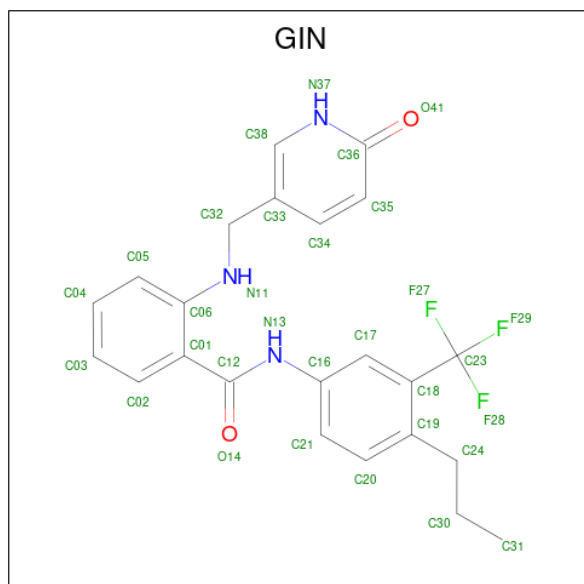
There are 3 unique types of molecules in this entry. The entry contains 4544 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proto-oncogene tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2121	1381	339	384	17			
1	B	243	Total	C	N	O	S	0	1	0
			1974	1291	315	351	17			

- Molecule 2 is 2-[[[(6-OXO-1,6-DIHYDROPYRIDIN-3-YL)METHYL]AMINO}-N-[4-PROPYL-3-(TRIFLUOROMETHYL)PHENYL]BENZAMIDE (CCD ID: GIN) (formula: $C_{23}H_{22}F_3N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	23	3	3	2		
2	B	1	Total	C	F	N	O	0	0
			31	23	3	3	2		

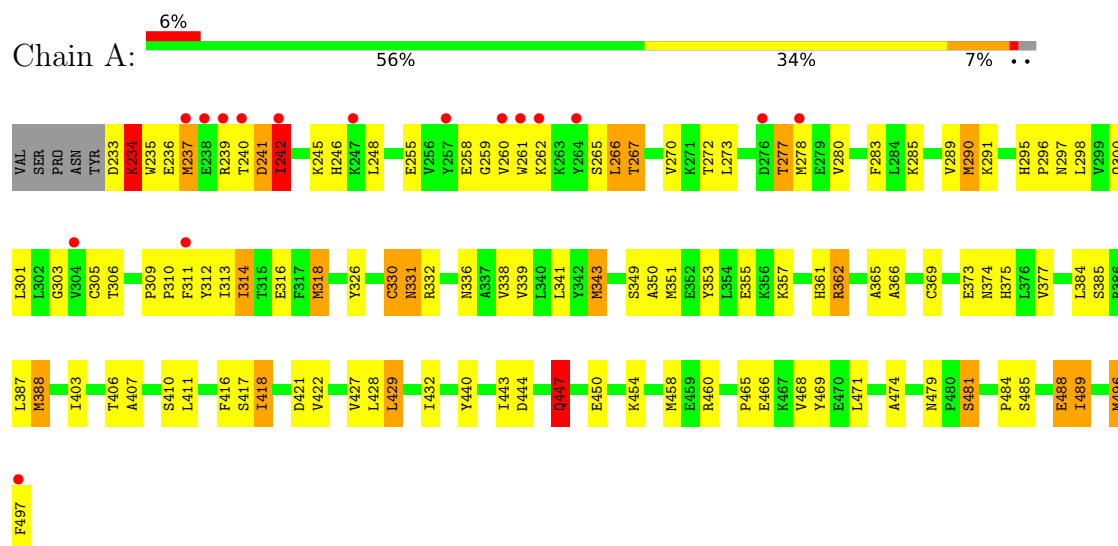
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	192	Total 192	O 192	0	0
3	B	195	Total 195	O 195	0	0

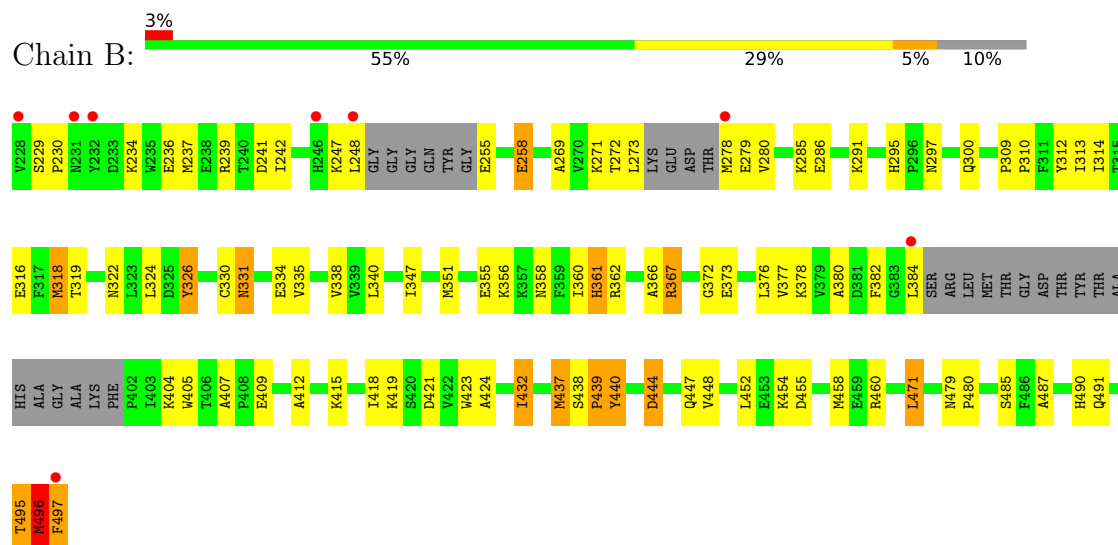
3 Residue-property plots [i](#)

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: Proto-oncogene tyrosine-protein kinase ABL1



- Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.02Å 123.96Å 139.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.10) 99.7 (25.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.195 , 0.256 0.178 , 0.235	Depositor DCC
R_{free} test set	1778 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.7	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	4544	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GIN

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	1.79	33/2177 (1.5%)	1.32	20/2950 (0.7%)
1	B	1.92	47/2028 (2.3%)	1.22	7/2742 (0.3%)
All	All	1.85	80/4205 (1.9%)	1.28	27/5692 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	MET	SD-CE	-17.20	1.36	1.79
1	A	318	MET	SD-CE	-16.10	1.39	1.79
1	A	388	MET	SD-CE	-13.43	1.46	1.79
1	B	437	MET	SD-CE	11.24	2.07	1.79
1	A	285	LYS	CA-C	9.45	1.65	1.52
1	B	440	TYR	CA-CB	8.64	1.60	1.52
1	A	440	TYR	CA-CB	8.35	1.58	1.52
1	B	335	VAL	CA-C	-8.24	1.45	1.52
1	B	407	ALA	CA-C	8.14	1.62	1.53
1	A	343	MET	SD-CE	-8.05	1.59	1.79
1	B	378	LYS	CA-C	7.96	1.62	1.52
1	A	361	HIS	CA-CB	7.95	1.66	1.53
1	A	427	VAL	CA-CB	7.66	1.64	1.54
1	B	423	TRP	C-O	-7.62	1.15	1.24
1	A	411	LEU	C-O	-7.32	1.15	1.24
1	B	376	LEU	CA-C	7.24	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	351	MET	SD-CE	7.16	1.97	1.79
1	A	479	ASN	CA-C	-7.11	1.45	1.52
1	B	432	ILE	CB-CG2	7.03	1.75	1.52
1	A	447	GLN	C-O	-7.00	1.14	1.24
1	B	366	ALA	N-CA	6.98	1.54	1.46
1	B	347	ILE	C-O	-6.91	1.16	1.24
1	B	421	ASP	N-CA	6.89	1.54	1.46
1	A	458	MET	SD-CE	6.82	1.96	1.79
1	B	372	GLY	CA-C	6.79	1.59	1.52
1	B	458	MET	SD-CE	6.78	1.96	1.79
1	A	351	MET	C-O	6.78	1.32	1.24
1	B	448	VAL	CA-CB	6.54	1.62	1.54
1	A	339	VAL	CA-C	6.49	1.61	1.52
1	B	360	ILE	CA-C	-6.37	1.45	1.52
1	A	338	VAL	CA-CB	6.25	1.62	1.54
1	A	428	LEU	CA-C	6.24	1.60	1.52
1	B	367	ARG	CG-CD	6.22	1.71	1.52
1	B	360	ILE	CA-CB	6.21	1.61	1.54
1	B	440	TYR	N-CA	6.18	1.51	1.46
1	A	366	ALA	CA-CB	6.12	1.63	1.53
1	B	452	LEU	N-CA	6.09	1.53	1.46
1	B	355	GLU	CA-C	6.08	1.60	1.52
1	B	407	ALA	C-O	-6.07	1.16	1.23
1	B	405	TRP	N-CA	5.99	1.54	1.46
1	B	291	LYS	C-O	-5.97	1.16	1.24
1	A	432	ILE	C-O	-5.96	1.17	1.24
1	A	349	SER	CA-C	5.89	1.60	1.52
1	A	443	ILE	C-O	-5.84	1.18	1.24
1	B	377	VAL	CA-CB	5.82	1.63	1.54
1	B	361	HIS	N-CA	5.79	1.53	1.46
1	B	423	TRP	CA-CB	5.77	1.62	1.53
1	B	460	ARG	C-O	-5.71	1.17	1.24
1	A	298	LEU	C-O	-5.66	1.17	1.24
1	B	380	ALA	CA-CB	5.65	1.61	1.53
1	A	474	ALA	CA-CB	5.63	1.62	1.53
1	B	471	LEU	C-O	-5.60	1.17	1.24
1	B	300	GLN	C-O	-5.60	1.17	1.24
1	B	439	PRO	CA-C	5.54	1.59	1.52
1	A	296	PRO	C-O	-5.46	1.17	1.24
1	B	340	LEU	C-O	-5.45	1.17	1.24
1	B	373	GLU	N-CA	5.42	1.52	1.46
1	A	290	MET	SD-CE	-5.38	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	ASN	CA-C	-5.35	1.45	1.52
1	B	324	LEU	C-O	-5.35	1.18	1.24
1	B	334	GLU	CA-C	5.34	1.59	1.52
1	A	366	ALA	CA-C	-5.30	1.45	1.52
1	A	458	MET	N-CA	-5.30	1.39	1.46
1	A	418	ILE	C-O	-5.27	1.18	1.24
1	A	440	TYR	C-O	-5.27	1.21	1.23
1	B	479	ASN	C-O	-5.26	1.17	1.24
1	B	269	ALA	CA-CB	-5.25	1.45	1.53
1	A	421	ASP	CA-C	5.21	1.59	1.52
1	B	326	TYR	CA-C	-5.21	1.46	1.52
1	A	369	CYS	CA-C	-5.20	1.46	1.52
1	A	407	ALA	CA-CB	5.14	1.60	1.53
1	A	365	ALA	CA-CB	5.14	1.62	1.53
1	B	380	ALA	CA-C	5.11	1.59	1.53
1	B	490	HIS	CA-CB	-5.05	1.45	1.53
1	B	487	ALA	CA-CB	5.05	1.61	1.53
1	A	489	ILE	CG1-CD1	5.03	1.71	1.51
1	A	278	MET	SD-CE	5.02	1.92	1.79
1	B	485	SER	C-O	-5.02	1.17	1.23
1	B	424	ALA	CA-C	5.01	1.59	1.52
1	B	380	ALA	C-O	-5.01	1.18	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ASP	N-CA-C	-15.70	91.63	114.39
1	A	384	LEU	N-CA-C	-9.50	95.70	109.96
1	A	248	LEU	N-CA-C	-8.22	103.84	114.04
1	A	242	ILE	N-CA-C	7.70	119.17	107.77
1	B	319	THR	N-CA-C	7.69	120.34	111.11
1	A	235	TRP	N-CA-C	7.66	120.70	111.82
1	A	266	LEU	N-CA-C	7.06	120.99	109.76
1	A	246	HIS	N-CA-C	7.01	119.04	110.41
1	B	258	GLU	N-CA-C	-6.71	98.76	109.76
1	B	338	VAL	N-CA-C	-6.47	103.94	111.00
1	A	332	ARG	N-CA-C	6.46	120.26	112.38
1	A	234	LYS	N-CA-C	-6.41	97.15	110.80
1	A	300	GLN	N-CA-C	6.39	119.12	108.96
1	A	280	VAL	N-CA-C	6.22	116.70	110.23
1	A	429	LEU	N-CA-C	-6.20	104.52	111.28
1	A	362	ARG	N-CA-C	6.04	122.77	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	SER	N-CA-C	6.01	119.18	110.28
1	B	241	ASP	N-CA-C	-5.96	105.49	112.89
1	B	412	ALA	N-CA-C	5.96	117.58	111.14
1	B	313	ILE	N-CA-C	-5.90	99.04	107.77
1	B	376	LEU	N-CA-C	-5.72	101.93	110.23
1	A	418	ILE	N-CA-C	-5.68	104.82	110.62
1	A	330	CYS	N-CA-C	5.64	117.97	110.53
1	A	267	THR	N-CA-C	-5.63	101.95	110.28
1	A	298	LEU	N-CA-C	-5.55	99.24	108.34
1	A	403	ILE	N-CA-C	5.45	116.83	110.62
1	A	258	GLU	N-CA-C	-5.13	102.88	110.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	409	GLU	Sidechain

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	2121	0	2051	78	0
1	B	1974	0	1933	54	0
2	A	31	0	22	0	0
2	B	31	0	22	3	0
3	A	192	0	0	2	0
3	B	195	0	0	11	0
All	All	4544	0	4028	131	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 16.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ILE:CG2	1:B:432:ILE:CB	1.75	1.53
1:B:437:MET:CE	1:B:437:MET:SD	2.07	1.42
1:B:295:HIS:HD2	1:B:297:ASN:H	1.15	0.94
1:A:388:MET:HE1	1:A:416:PHE:HB2	1.51	0.92
1:B:404:LYS:HE2	1:B:440:TYR:HB2	1.49	0.92
1:A:295:HIS:HD2	1:A:297:ASN:H	1.18	0.90
1:A:444:ASP:H	1:A:447:GLN:HE21	1.16	0.90
1:A:496:MET:HE3	1:A:497:PHE:CE1	2.12	0.84
1:A:362:ARG:HD3	1:A:388:MET:HE2	1.57	0.84
1:A:306:THR:HA	1:A:311:PHE:HD2	1.42	0.84
1:B:295:HIS:CD2	1:B:297:ASN:H	1.98	0.80
1:A:290:MET:HE1	1:A:313:ILE:CG2	2.13	0.78
1:A:245:LYS:HE3	1:A:260:VAL:HG23	1.65	0.78
1:A:485:SER:OG	1:A:488:GLU:HG2	1.85	0.77
1:A:290:MET:HE1	1:A:313:ILE:HG21	1.68	0.75
1:A:316:GLU:HG3	1:A:318:MET:HE3	1.68	0.74
1:A:388:MET:HE1	1:A:416:PHE:CB	2.17	0.74
1:A:362:ARG:HD3	1:A:388:MET:CE	2.18	0.73
1:A:341:LEU:HD11	1:A:496:MET:HE1	1.70	0.73
1:B:318:MET:HA	1:B:318:MET:HE2	1.71	0.72
1:B:432:ILE:CG2	1:B:432:ILE:CG1	2.68	0.71
1:A:444:ASP:H	1:A:447:GLN:NE2	1.90	0.69
1:B:316:GLU:HG3	1:B:318:MET:HE3	1.75	0.69
1:A:417:SER:HB2	3:A:675:HOH:O	1.93	0.69
1:A:272:THR:HG22	1:A:273:LEU:O	1.93	0.68
1:A:362:ARG:CD	1:A:388:MET:HE2	2.23	0.68
1:B:491:GLN:O	1:B:495:THR:HB	1.95	0.67
1:B:418:ILE:HG23	3:B:726:HOH:O	1.94	0.67
1:A:295:HIS:CD2	1:A:297:ASN:H	2.09	0.66
1:A:306:THR:HA	1:A:311:PHE:CD2	2.29	0.66
1:B:418:ILE:HG12	3:B:726:HOH:O	1.96	0.65
1:A:233:ASP:OD2	1:A:291:LYS:NZ	2.29	0.65
1:B:444:ASP:OD1	1:B:447:GLN:HG3	1.97	0.65
1:A:314:ILE:HD12	1:A:314:ILE:N	2.11	0.64
1:B:255:GLU:N	1:B:384:LEU:HD21	2.12	0.64
1:A:318:MET:HA	1:A:318:MET:HE2	1.81	0.62
1:A:290:MET:CE	1:A:301:LEU:HD13	2.30	0.62
1:B:432:ILE:CG2	1:B:432:ILE:CA	2.75	0.62
1:A:233:ASP:O	1:A:234:LYS:HB3	2.00	0.61
1:A:237:MET:HE1	1:A:303:GLY:HA3	1.81	0.61
1:A:272:THR:HG22	1:A:273:LEU:N	2.16	0.61
1:B:272:THR:HG23	1:B:312:TYR:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LYS:HE3	3:B:748:HOH:O	2.01	0.60
1:A:237:MET:CE	1:A:303:GLY:HA3	2.32	0.59
1:B:362:ARG:NE	3:B:735:HOH:O	2.35	0.59
1:A:313:ILE:C	1:A:314:ILE:HD12	2.28	0.59
1:A:242:ILE:HG13	1:A:261:TRP:HA	1.84	0.58
1:A:465:PRO:HG2	1:A:468:VAL:CG2	2.34	0.58
1:A:460:ARG:HG3	1:A:469:TYR:HB2	1.86	0.58
1:A:316:GLU:CG	1:A:318:MET:HE3	2.34	0.58
1:A:312:TYR:HB3	1:A:314:ILE:HD11	1.87	0.56
1:B:331:ASN:HD22	1:B:331:ASN:C	2.13	0.56
1:A:273:LEU:HD22	1:A:277:THR:HG21	1.87	0.56
1:B:404:LYS:HD2	3:B:778:HOH:O	2.05	0.55
1:B:361:HIS:O	1:B:362:ARG:HB2	2.06	0.55
1:B:229:SER:HB2	1:B:230:PRO:HD2	1.89	0.55
1:B:279:GLU:HB2	3:B:782:HOH:O	2.07	0.55
1:B:229:SER:HB2	1:B:230:PRO:CD	2.38	0.54
1:B:272:THR:HG22	1:B:273:LEU:N	2.23	0.53
1:A:245:LYS:CE	1:A:260:VAL:HG23	2.38	0.53
1:A:331:ASN:HD22	1:A:331:ASN:C	2.15	0.53
1:A:362:ARG:HD2	1:A:416:PHE:CD2	2.44	0.53
1:B:318:MET:HE2	1:B:318:MET:CA	2.37	0.53
1:B:272:THR:HG23	1:B:312:TYR:CE2	2.44	0.53
1:B:247:LYS:HB3	3:B:727:HOH:O	2.07	0.53
1:B:316:GLU:OE2	1:B:318:MET:HE1	2.09	0.52
1:A:316:GLU:CD	1:A:318:MET:HE3	2.34	0.52
1:A:484:PRO:HB2	1:A:488:GLU:HG3	1.89	0.52
1:A:233:ASP:HB2	1:A:236:GLU:HG2	1.92	0.52
1:B:326:TYR:O	1:B:330:CYS:HB3	2.10	0.51
1:A:239:ARG:HG3	1:A:312:TYR:HE1	1.75	0.51
1:B:358:ASN:HA	1:B:418:ILE:HD11	1.92	0.51
1:B:419:LYS:HG3	1:B:480:PRO:O	2.11	0.50
1:B:248:LEU:HD21	1:B:258:GLU:HB2	1.93	0.50
1:B:367:ARG:NE	3:B:697:HOH:O	2.21	0.50
1:A:355:GLU:HG3	1:A:418:ILE:HG21	1.94	0.49
1:B:454:LYS:O	1:B:455:ASP:HB2	2.10	0.49
1:A:341:LEU:CD1	1:A:496:MET:HE1	2.41	0.49
1:A:242:ILE:HA	1:A:260:VAL:O	2.12	0.48
1:A:233:ASP:CB	1:A:236:GLU:HG2	2.44	0.48
1:B:454:LYS:NZ	3:B:763:HOH:O	2.46	0.48
1:A:273:LEU:HG	1:A:283:PHE:CD1	2.49	0.47
1:A:481:SER:OG	1:B:239:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:N	1:A:314:ILE:CD1	2.78	0.47
1:A:326:TYR:O	1:A:330:CYS:HB3	2.15	0.46
1:A:362:ARG:NE	1:A:388:MET:HE2	2.30	0.46
1:A:290:MET:CE	1:A:313:ILE:HG21	2.42	0.46
1:A:485:SER:H	1:A:488:GLU:CG	2.28	0.46
1:A:266:LEU:HG	1:A:267:THR:O	2.16	0.46
1:A:343:MET:HG2	1:A:377:VAL:HG13	1.98	0.46
1:A:272:THR:CG2	1:A:273:LEU:N	2.80	0.45
1:A:336:ASN:HB2	3:A:770:HOH:O	2.16	0.45
1:A:343:MET:HG2	1:A:377:VAL:CG1	2.47	0.45
1:B:230:PRO:HG2	1:B:236:GLU:HB3	1.98	0.44
1:B:255:GLU:N	1:B:384:LEU:CD2	2.79	0.44
1:A:387:LEU:C	1:A:387:LEU:HD12	2.42	0.44
1:A:242:ILE:O	1:A:242:ILE:HG22	2.18	0.44
1:A:290:MET:HE3	1:A:301:LEU:HD13	1.99	0.44
1:A:305:CYS:O	1:A:311:PHE:HA	2.18	0.44
1:A:239:ARG:HG2	1:A:240:THR:H	1.82	0.44
1:A:465:PRO:HG2	1:A:468:VAL:HB	1.99	0.43
1:A:460:ARG:NH1	1:A:466:GLU:CG	2.82	0.43
1:A:326:TYR:OH	1:A:375:HIS:HD2	2.02	0.43
1:B:278:MET:HE1	3:B:747:HOH:O	2.17	0.43
1:B:438:SER:HA	1:B:439:PRO:HD3	1.89	0.42
1:B:496:MET:C	1:B:497:PHE:CD1	2.97	0.42
1:A:309:PRO:HA	1:A:310:PRO:C	2.44	0.42
1:B:316:GLU:CG	1:B:318:MET:HE3	2.48	0.42
1:B:242:ILE:HD11	1:B:314:ILE:HD13	2.01	0.42
1:B:404:LYS:CE	1:B:440:TYR:HB2	2.34	0.42
1:A:270:VAL:HG22	1:A:314:ILE:HG13	2.00	0.42
1:A:422:VAL:HG13	1:A:489:ILE:HD11	2.01	0.42
1:B:309:PRO:HA	1:B:310:PRO:C	2.45	0.42
1:A:484:PRO:CB	1:A:488:GLU:HG3	2.51	0.41
1:B:495:THR:O	1:B:495:THR:HG23	2.19	0.41
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.80	0.41
1:B:471:LEU:C	1:B:471:LEU:HD23	2.46	0.41
1:B:382:PHE:CE2	2:B:600:GIN:H34	2.56	0.41
1:A:290:MET:HB2	1:A:290:MET:HE2	1.82	0.41
1:B:230:PRO:HG3	1:B:236:GLU:HG2	2.01	0.41
1:B:404:LYS:HG3	3:B:621:HOH:O	2.21	0.41
1:A:373:GLU:O	1:A:374:ASN:HB2	2.21	0.40
1:B:286:GLU:CD	2:B:600:GIN:H21	2.46	0.40
1:A:406:THR:HG22	1:A:410:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LYS:HE3	1:B:234:LYS:HB2	1.77	0.40
1:B:271:LYS:HB2	2:B:600:GIN:C04	2.51	0.40
1:B:285:LYS:O	1:B:285:LYS:HG3	2.18	0.40
1:A:245:LYS:HG3	1:A:259:GLY:HA2	2.02	0.40
1:A:312:TYR:HB3	1:A:314:ILE:CD1	2.52	0.40
1:A:350:ALA:O	1:A:353:TYR:HB3	2.22	0.40
1:A:273:LEU:HD11	1:A:283:PHE:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/270 (97%)	247 (94%)	13 (5%)	3 (1%)	11	8
1	B	236/270 (87%)	225 (95%)	10 (4%)	1 (0%)	30	28
All	All	499/540 (92%)	472 (95%)	23 (5%)	4 (1%)	16	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LYS
1	A	262	LYS
1	A	265	SER
1	B	496	MET

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	215/236 (91%)	199 (93%)	16 (7%)	13	10
1	B	207/236 (88%)	199 (96%)	8 (4%)	28	31
All	All	422/472 (89%)	398 (94%)	24 (6%)	18	17

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	MET
1	A	241	ASP
1	A	242	ILE
1	A	255	GLU
1	A	277	THR
1	A	289	VAL
1	A	314	ILE
1	A	331	ASN
1	A	357	LYS
1	A	447	GLN
1	A	450	GLU
1	A	454	LYS
1	A	471	LEU
1	A	481	SER
1	A	488	GLU
1	A	496	MET
1	B	237	MET
1	B	280	VAL
1	B	331	ASN
1	B	415	LYS
1	B	444	ASP
1	B	495	THR
1	B	496	MET
1	B	497	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	HIS
1	A	331	ASN
1	A	358	ASN

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Mol	Chain	Res	Type
1	A	375	HIS
1	A	396	HIS
1	A	447	GLN
1	B	295	HIS
1	B	297	ASN
1	B	331	ASN
1	B	447	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	GIN	B	600	-	32,33,33	1.67	10 (31%)	40,46,46	0.88	1 (2%)
2	GIN	A	600	-	32,33,33	1.64	8 (25%)	40,46,46	0.98	1 (2%)

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	GIN	B	600	-	-	0/21/22/22	0/3/3/3
2	GIN	A	600	-	-	1/21/22/22	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	GIN	C36-N37	4.17	1.43	1.37
2	A	600	GIN	C17-C18	3.80	1.44	1.39
2	A	600	GIN	C20-C19	3.80	1.45	1.39
2	A	600	GIN	C04-C05	2.79	1.43	1.38
2	B	600	GIN	C01-C12	-2.71	1.44	1.50
2	B	600	GIN	C32-N11	2.67	1.49	1.45
2	B	600	GIN	C38-N37	2.59	1.40	1.36
2	A	600	GIN	C21-C16	2.46	1.43	1.39
2	A	600	GIN	C38-N37	2.39	1.40	1.36
2	A	600	GIN	C36-N37	2.37	1.40	1.37
2	B	600	GIN	C05-C06	-2.32	1.36	1.39
2	A	600	GIN	C21-C20	2.27	1.42	1.38
2	B	600	GIN	C17-C18	2.18	1.42	1.39
2	B	600	GIN	C21-C16	2.17	1.42	1.39
2	B	600	GIN	C35-C34	2.12	1.40	1.35
2	B	600	GIN	C06-N11	2.10	1.43	1.37
2	A	600	GIN	C23-C18	2.03	1.55	1.50
2	B	600	GIN	C02-C01	-2.01	1.36	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	GIN	O41-C36-N37	2.75	122.97	119.33
2	B	600	GIN	O41-C36-N37	2.19	122.22	119.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

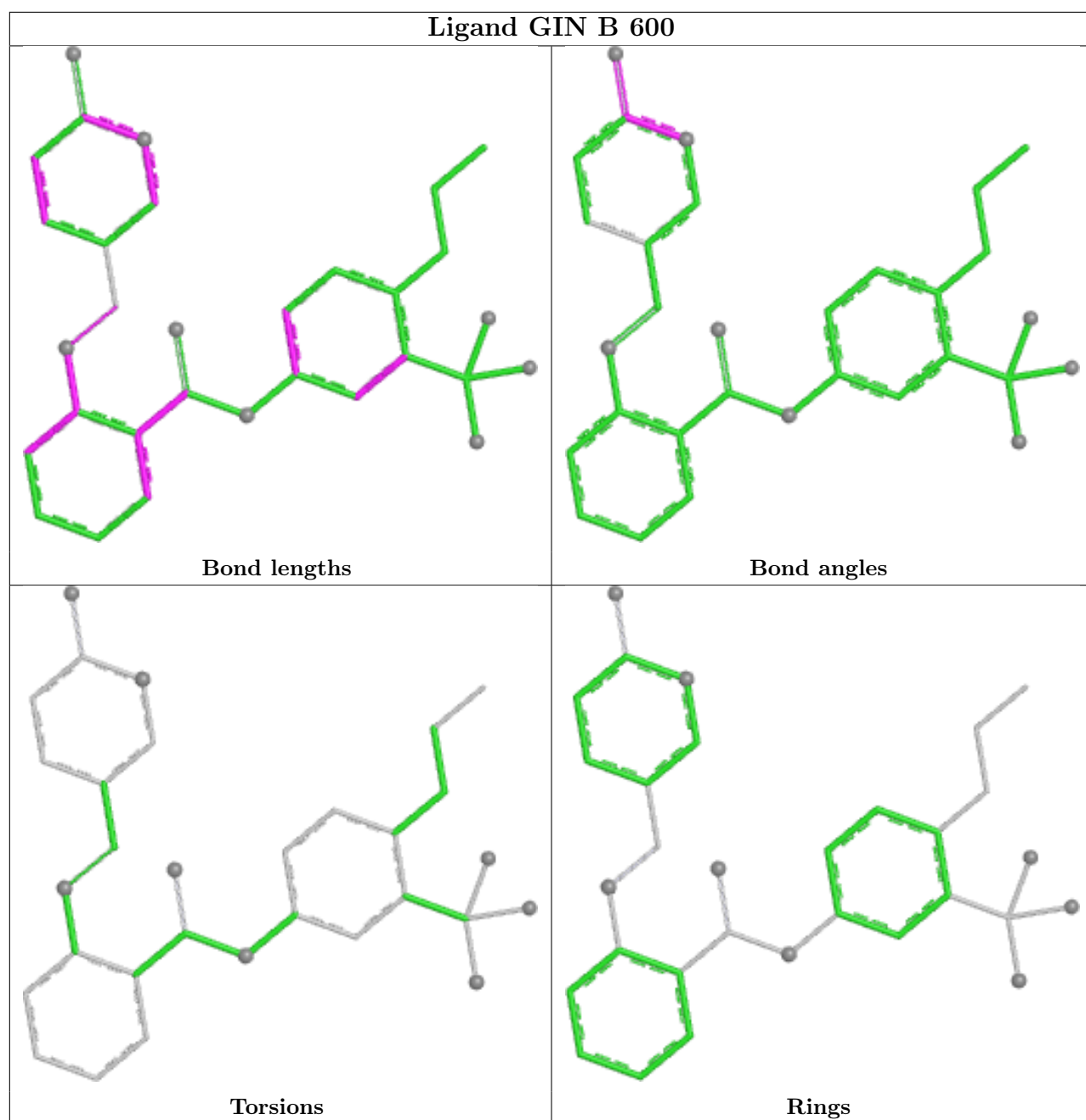
Mol	Chain	Res	Type	Atoms
2	A	600	GIN	C01-C06-N11-C32

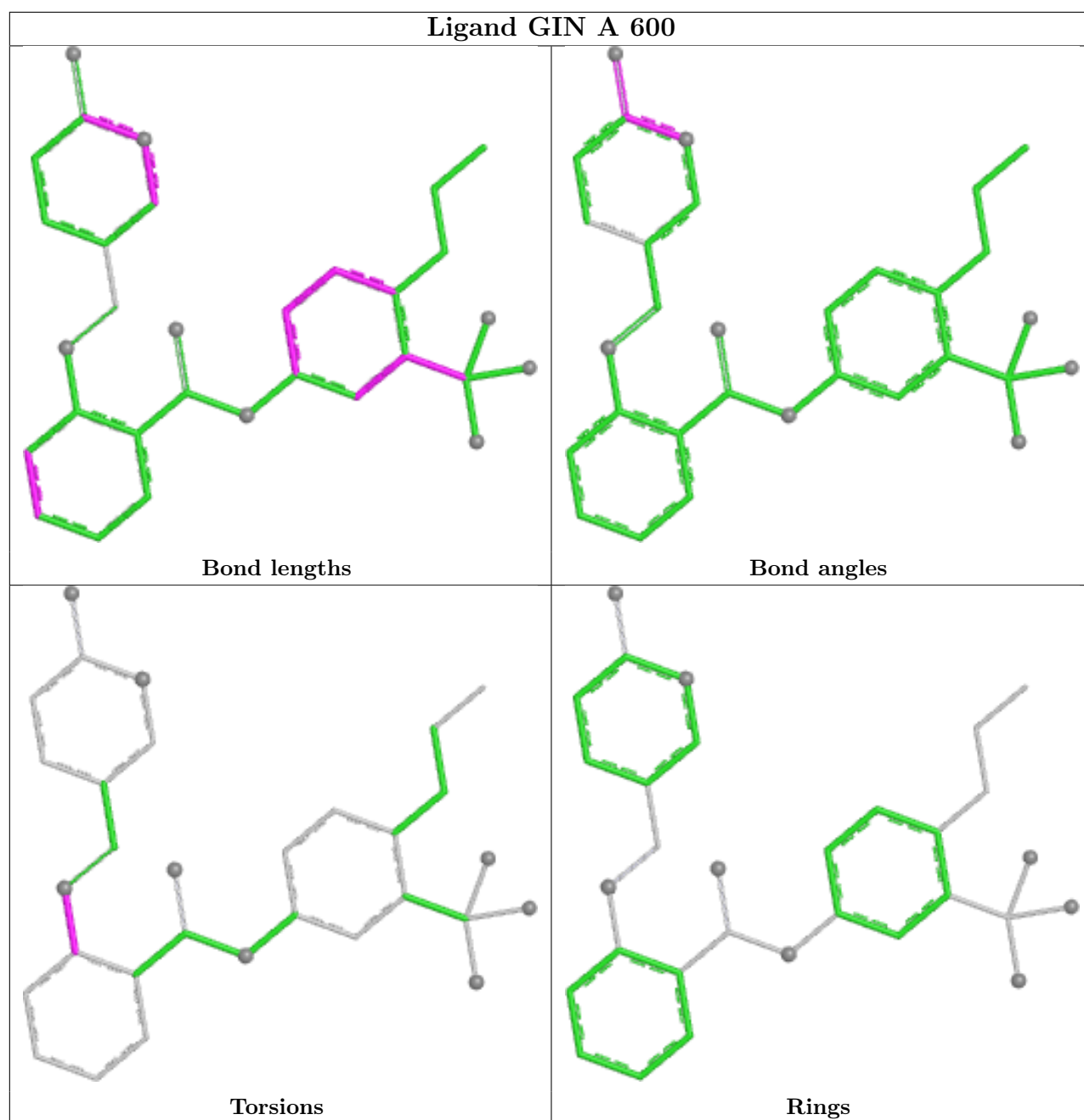
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	GIN	3	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

6.1 Protein, DNA and RNA chains

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	265/270 (98%)	0.03	16 (6%) 27 29	13, 28, 67, 84	0
1	B	243/270 (90%)	-0.23	8 (3%) 49 51	11, 25, 50, 80	1 (0%)
All	All	508/540 (94%)	-0.10	24 (4%) 36 38	11, 26, 60, 84	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	THR	4.1
1	B	497	PHE	4.0
1	A	264	TYR	3.9
1	A	311	PHE	3.6
1	A	497	PHE	3.4
1	A	238	GLU	3.3
1	A	242	ILE	3.3
1	B	246	HIS	3.0
1	B	384	LEU	2.9
1	A	278	MET	2.9
1	B	248	LEU	2.8
1	B	228	VAL	2.8
1	A	239	ARG	2.6
1	A	260	VAL	2.4
1	A	247	LYS	2.4
1	A	262	LYS	2.3
1	B	232	TYR	2.3
1	A	257	TYR	2.2
1	A	276	ASP	2.2
1	A	304	VAL	2.2
1	A	261	TRP	2.2
1	B	231	ASN	2.1
1	A	237	MET	2.1
1	B	278	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

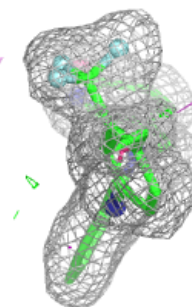
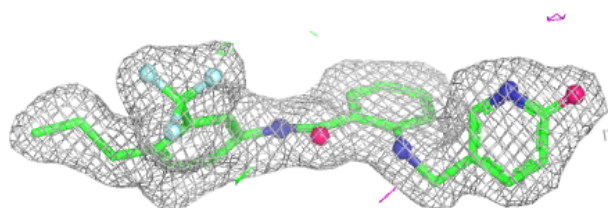
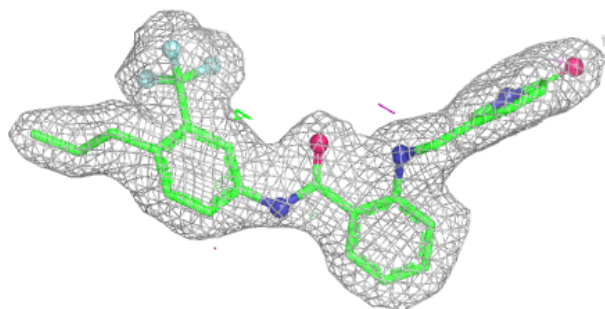
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GIN	A	600	31/31	0.95	0.06	11,20,29,35	0
2	GIN	B	600	31/31	0.97	0.05	6,18,27,32	0

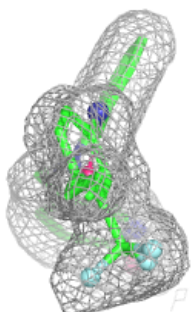
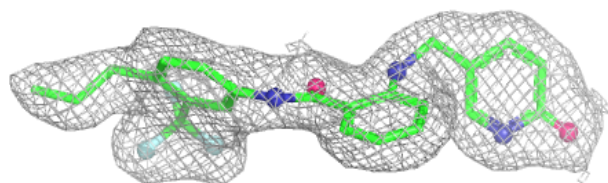
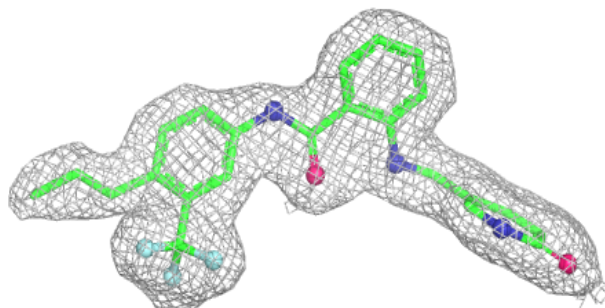
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GIN A 600:

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

**Electron density around GIN B 600:**

$2mF_o-DF_c$ (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.