



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 PM UTC

PDB ID : 8SSN / pdb_00008ssn
Title : Abl kinase in complex with SKI and asciminib
Authors : Ludewig, H.; Kim, C.; Kern, D.
Deposited on : 2023-05-08
Resolution : 2.86 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

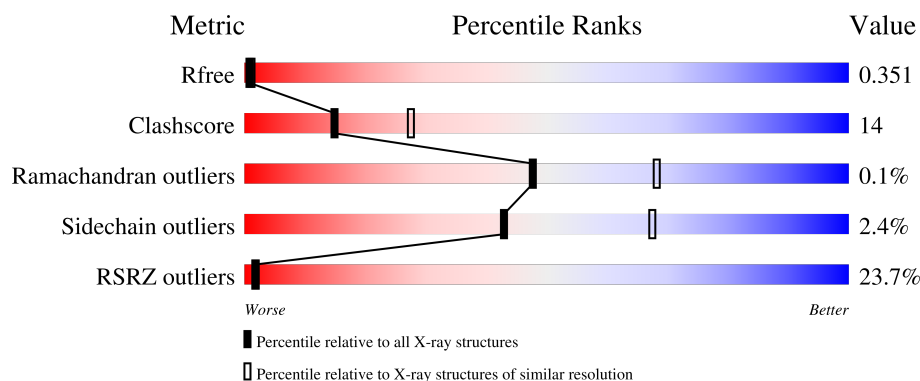
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	448	22% 60% 31% 6%
1	B	448	21% 65% 20% 14%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6667 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.

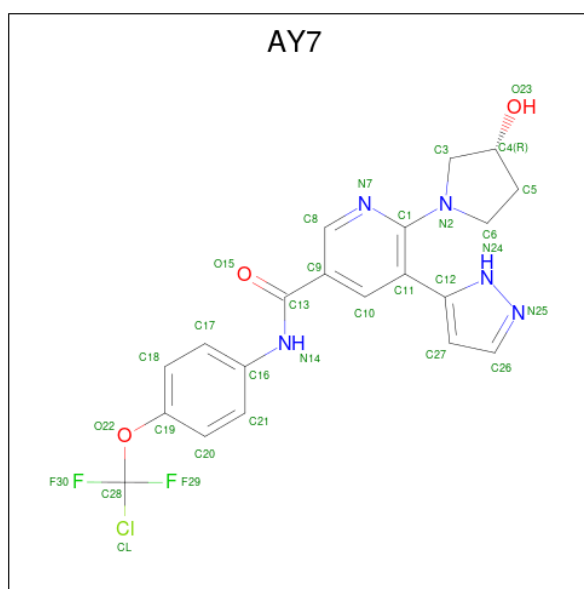
- Molecule 1 is a protein called Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3367	2147	568	635	17			
1	B	386	Total	C	N	O	S	0	0	0
			3099	1977	526	582	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLY	-	expression tag	UNP P00519
B	82	GLY	-	expression tag	UNP P00519

- Molecule 2 is asciminib (CCD ID: AY7) (formula: C₂₀H₁₈ClF₂N₅O₃) (labeled as "Ligand of Interest" by depositor).



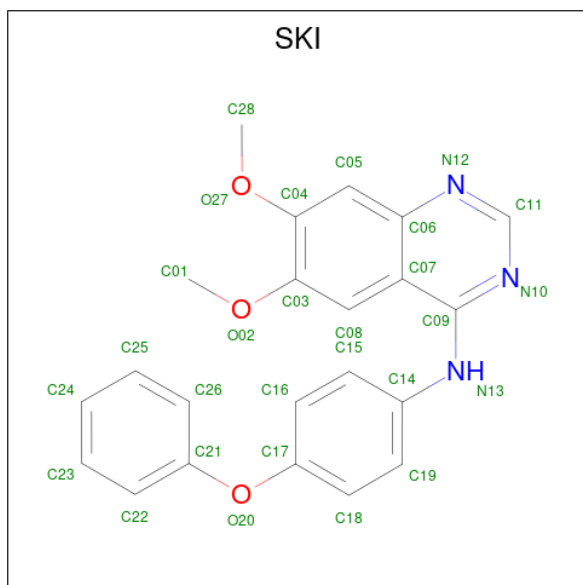
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			31	20	1	2	5	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Cl	F	N	O	0	0
			31	20	1	2	5	3		

- Molecule 3 is 6,7-dimethoxy-N-(4-phenoxyphenyl)quinazolin-4-amine (CCD ID: SKI) (formula: C₂₂H₁₉N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	3	3		
3	B	1	Total	C	N	O	0	0
			28	22	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

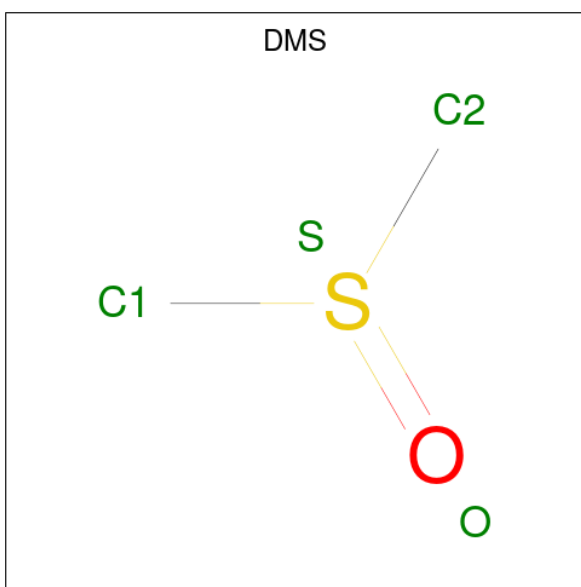
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

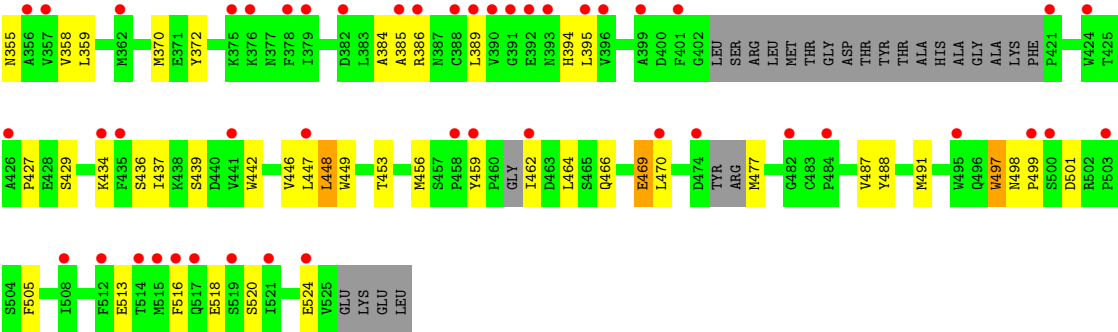
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total 23	O 23	0	0
7	B	28	Total 28	O 28	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.48Å 103.21Å 107.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 2.86 47.83 – 2.86	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.83-2.86) 81.0 (47.83-2.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.21 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.298 , 0.348 0.299 , 0.351	Depositor DCC
R_{free} test set	1189 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 95.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6667	wwPDB-VP
Average B, all atoms (Å ²)	93.0	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 56.63 % 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 2.6637e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, AY7, DMS, SKI, CL

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	0.23	0/3448	0.50	5/4669 (0.1%)
1	B	0.22	0/3171	0.39	1/4289 (0.0%)
All	All	0.23	0/6619	0.45	6/8958 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ARG	CB-CA-C	-6.52	100.19	110.04
1	A	382	ASP	N-CA-C	-6.08	103.23	110.41
1	A	382	ASP	N-CA-CB	5.71	118.64	111.79
1	A	387	ASN	CB-CA-C	5.38	120.05	109.72
1	A	142	GLU	N-CA-C	-5.14	106.51	112.89
1	B	141	LEU	N-CA-C	-5.02	107.54	113.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3367	0	3282	114	0
1	B	3099	0	3010	65	0
2	A	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	0	1	0
3	A	28	0	0	0	0
3	B	28	0	0	1	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	12	0	18	0	0
6	B	4	0	6	0	0
7	A	23	0	0	1	0
7	B	28	0	0	0	0
All	All	6667	0	6316	178	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 14.

All (178) 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:264:LYS:HD2	1:A:279:VAL:HG23	1.44	0.96
1:A:379:ILE:HD11	1:A:381:ARG:HH21	1.39	0.88
1:A:453:THR:HB	1:A:456:MET:HG3	1.68	0.76
1:B:159:LEU:HD21	1:B:239:ARG:HB3	1.68	0.75
1:A:96:ASP:OD1	1:A:97:ASN:N	2.20	0.75
1:B:459:TYR:H	1:B:477:MET:HE2	1.51	0.74
1:A:297:MET:SD	1:A:297:MET:N	2.61	0.73
1:A:324:CYS:HB3	1:A:331:TYR:HB2	1.67	0.73
1:B:313:LYS:N	1:B:372:TYR:HH	1.85	0.73
1:A:261:ILE:HG22	1:A:262:THR:H	1.52	0.72
1:B:427:PRO:HB2	1:B:497:TRP:CH2	2.28	0.69
1:A:140:SER:HB2	1:A:142:GLU:OE1	1.93	0.69
1:B:453:THR:HB	1:B:456:MET:HG3	1.76	0.68
1:A:223:THR:HG22	1:A:224:VAL:HG13	1.77	0.66
1:A:172:GLU:HG3	1:A:180:ARG:HE	1.60	0.66
1:B:122:GLN:HB2	1:B:127:GLN:HG2	1.79	0.65
1:A:141:LEU:HD11	1:A:214:LEU:HB3	1.79	0.64
1:A:428:GLU:HG3	1:A:434:LYS:HD2	1.80	0.64
1:A:360:LEU:HD12	1:A:521:ILE:HD12	1.79	0.63
1:B:277:GLU:HG3	1:B:336:PHE:HE2	1.64	0.63
1:B:180:ARG:HB3	1:B:195:ILE:HD12	1.80	0.63
1:B:354:VAL:HG13	1:B:358:VAL:HG11	1.83	0.61
1:A:264:LYS:HB2	1:A:277:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD11	1:A:373:LEU:HG	1.82	0.61
1:B:239:ARG:HD3	1:B:239:ARG:H	1.65	0.61
1:A:487:VAL:O	1:A:491:MET:HG2	2.01	0.60
1:B:117:GLU:OE2	1:B:245:TYR:HD2	1.82	0.60
1:A:358:VAL:O	1:A:362:MET:HG3	2.01	0.60
1:B:305:GLU:O	1:B:309:MET:HG2	2.00	0.60
1:A:263:MET:HE1	1:A:289:VAL:HG11	1.85	0.59
1:A:492:ARG:NH1	1:A:493:ALA:HB2	2.18	0.58
1:A:391:GLY:N	1:A:395:LEU:O	2.35	0.58
1:A:362:MET:HB3	1:A:396:VAL:HG21	1.85	0.58
1:A:487:VAL:HG22	1:A:515:MET:HE1	1.86	0.57
1:B:436:SER:O	1:B:439:SER:OG	2.23	0.57
1:A:423:LYS:HB3	1:A:459:TYR:HD2	1.70	0.57
1:A:403:LEU:HD11	1:A:406:LEU:HD23	1.86	0.56
1:B:488:TYR:HA	1:B:491:MET:HE3	1.88	0.56
1:A:159:LEU:HD21	1:A:239:ARG:HB3	1.87	0.56
1:A:289:VAL:HG22	1:A:333:ILE:HD12	1.88	0.55
1:A:424:TRP:NE1	1:A:450:GLU:OE2	2.40	0.55
1:B:349:CYS:HB2	1:B:354:VAL:HG21	1.88	0.55
1:B:459:TYR:N	1:B:477:MET:HE2	2.19	0.55
1:A:362:MET:HA	1:A:365:GLN:HE21	1.71	0.55
1:A:380:HIS:O	1:A:381:ARG:HB2	2.06	0.55
1:B:336:PHE:HD1	1:B:337:MET:N	2.05	0.55
1:A:154:ASN:CG	1:A:360:LEU:HD22	2.31	0.55
1:A:387:ASN:HB3	1:A:400:ASP:HB2	1.88	0.54
1:B:498:ASN:HB2	1:B:501:ASP:OD2	2.08	0.54
1:B:141:LEU:HD23	1:B:147:TYR:CE2	2.43	0.54
1:A:407:MET:HE3	1:A:409:GLY:H	1.73	0.53
1:B:277:GLU:HG3	1:B:336:PHE:CE2	2.42	0.53
1:B:459:TYR:O	1:B:462:ILE:N	2.41	0.53
1:A:172:GLU:HG3	1:A:180:ARG:NE	2.23	0.53
1:A:280:TRP:O	1:A:284:SER:N	2.41	0.53
1:A:462:ILE:HG23	1:A:470:LEU:HD13	1.89	0.53
1:A:280:TRP:HB3	1:A:285:LEU:HD23	1.91	0.53
1:A:292:LEU:HD11	1:A:330:PHE:HB2	1.90	0.53
1:B:261:ILE:HG21	1:B:289:VAL:HG21	1.91	0.53
1:A:266:LYS:HA	1:A:276:TYR:HA	1.90	0.52
1:A:203:LEU:HD12	1:A:203:LEU:H	1.75	0.52
1:A:380:HIS:CD2	1:A:401:PHE:HB3	2.46	0.51
1:A:248:SER:HB2	1:A:283:TYR:CE2	2.45	0.51
1:B:497:TRP:O	1:B:499:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LYS:HB3	1:A:459:TYR:CD2	2.45	0.51
1:B:343:LEU:HD23	1:B:386:ARG:HE	1.75	0.51
1:B:442:TRP:O	1:B:446:VAL:HG23	2.11	0.51
1:A:131:PRO:HB3	1:A:244:VAL:HG11	1.92	0.50
1:B:498:ASN:O	1:B:499:PRO:C	2.55	0.50
1:A:280:TRP:O	1:A:284:SER:HA	2.12	0.50
1:B:358:VAL:HG13	1:B:394:HIS:CD2	2.47	0.50
1:B:497:TRP:O	1:B:497:TRP:HE3	1.94	0.50
1:A:490:LEU:HD21	1:A:508:ILE:HG23	1.94	0.49
1:B:101:ILE:HG21	1:B:107:LEU:HD21	1.93	0.49
1:B:310:LYS:HD3	1:B:310:LYS:C	2.37	0.49
1:A:362:MET:HE3	1:A:394:HIS:HB3	1.94	0.49
1:B:280:TRP:O	1:B:284:SER:N	2.45	0.49
1:A:292:LEU:HD13	1:A:297:MET:HG2	1.94	0.49
1:A:370:MET:HB3	1:A:505:PHE:CG	2.47	0.49
1:A:373:LEU:HD22	1:A:378:PHE:HB3	1.93	0.49
1:B:427:PRO:HB2	1:B:497:TRP:CZ3	2.47	0.48
1:B:384:ALA:HA	1:B:447:LEU:HD11	1.96	0.48
1:B:516:PHE:CE1	1:B:524:GLU:HG3	2.49	0.48
1:A:318:VAL:HG11	1:A:399:ALA:HB2	1.96	0.48
1:A:379:ILE:CD1	1:A:381:ARG:HE	2.27	0.47
1:A:449:TRP:HD1	1:A:491:MET:HE1	1.78	0.47
1:B:466:GLN:O	1:B:470:LEU:HG	2.14	0.47
1:A:262:THR:OG1	1:A:281:LYS:HE3	2.13	0.47
1:A:479:ARG:HD3	1:A:488:TYR:CD2	2.49	0.47
1:A:280:TRP:O	1:A:284:SER:CA	2.62	0.47
1:A:380:HIS:N	1:A:440:ASP:OD2	2.45	0.47
1:B:337:MET:HG3	1:B:389:LEU:HB2	1.97	0.47
1:A:469:GLU:C	1:A:471:LEU:N	2.71	0.47
1:A:88:LEU:HD11	1:A:136:THR:HB	1.97	0.47
1:A:239:ARG:HG2	1:A:240:ASN:N	2.30	0.47
1:A:196:ASN:ND2	7:A:701:HOH:O	2.33	0.47
1:A:477:MET:O	1:A:488:TYR:OH	2.23	0.47
1:A:224:VAL:HG23	1:A:226:ASP:HB2	1.95	0.46
1:B:83:ASN:OD1	1:B:83:ASN:N	2.43	0.46
1:A:380:HIS:O	1:A:381:ARG:CB	2.63	0.46
1:B:429:SER:OG	1:B:434:LYS:O	2.24	0.46
1:A:442:TRP:CE3	1:A:495:TRP:HA	2.52	0.45
1:A:462:ILE:N	1:B:456:MET:HE1	2.31	0.45
1:A:292:LEU:HB3	1:A:406:LEU:CD2	2.47	0.45
1:B:342:LEU:HB3	1:B:385:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HG2	1:A:311:GLU:OE2	2.16	0.45
1:A:467:VAL:HA	1:A:470:LEU:HD12	1.99	0.45
1:B:88:LEU:HD21	1:B:136:THR:HG22	1.98	0.45
1:B:184:LEU:HD13	1:B:232:LEU:HD23	1.99	0.45
1:A:379:ILE:HD11	1:A:381:ARG:NH2	2.20	0.45
1:B:99:LEU:HB2	1:B:128:GLY:HA3	1.99	0.45
1:A:444:PHE:CE1	1:A:508:ILE:HG21	2.52	0.45
1:B:218:VAL:O	1:B:222:SER:N	2.50	0.45
1:A:468:TYR:HE1	1:A:497:TRP:HH2	1.65	0.45
1:A:384:ALA:C	1:A:447:LEU:HD13	2.41	0.44
1:A:476:ARG:NH2	1:A:495:TRP:O	2.49	0.44
1:A:306:ALA:HA	1:A:309:MET:HB2	1.99	0.44
1:B:334:THR:HG21	3:B:602:SKI:C26	2.46	0.44
1:A:463:ASP:HB3	1:A:466:GLN:HG2	2.00	0.44
1:B:449:TRP:CH2	1:B:456:MET:HB2	2.53	0.44
1:A:496:GLN:O	1:A:502:ARG:NH2	2.44	0.44
1:A:428:GLU:CG	1:A:434:LYS:HD2	2.48	0.44
1:A:429:SER:HA	1:A:434:LYS:H	1.83	0.44
1:B:141:LEU:HD21	1:B:214:LEU:HD23	2.00	0.44
1:B:355:ASN:O	1:B:359:LEU:HG	2.18	0.44
1:A:184:LEU:HD21	1:A:230:THR:HG22	2.00	0.43
1:A:341:ASN:HD21	1:A:343:LEU:HB3	1.81	0.43
1:A:486:LYS:HE2	1:A:486:LYS:HB2	1.75	0.43
1:A:434:LYS:HG3	1:A:435:PHE:N	2.34	0.43
1:B:198:ALA:HB2	1:B:204:TYR:HE1	1.83	0.43
1:A:189:ARG:HA	1:A:189:ARG:HD3	1.90	0.43
1:B:159:LEU:HD11	1:B:239:ARG:HD2	2.00	0.43
1:B:370:MET:HB3	1:B:505:PHE:CG	2.54	0.43
1:A:476:ARG:HE	1:A:495:TRP:HB2	1.84	0.43
1:A:449:TRP:CD1	1:A:491:MET:HE1	2.53	0.43
1:A:463:ASP:OD2	2:B:601:AY7:O23	2.35	0.43
1:A:341:ASN:OD1	1:A:386:ARG:HA	2.19	0.42
1:A:146:TRP:CZ3	1:A:218:VAL:HG21	2.53	0.42
1:A:434:LYS:HZ3	1:A:499:PRO:HG3	1.83	0.42
1:A:437:ILE:O	1:A:441:VAL:HG23	2.19	0.42
1:B:341:ASN:HB3	1:B:344:ASP:HB2	2.01	0.42
1:A:474:ASP:C	1:A:476:ARG:HG2	2.44	0.42
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.79	0.42
1:A:375:LYS:HE3	1:A:375:LYS:HB3	1.90	0.42
1:B:358:VAL:CG1	1:B:394:HIS:CD2	3.02	0.42
1:B:189:ARG:NH1	1:B:520:SER:OG	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:LEU:HD21	1:B:487:VAL:CG2	2.50	0.41
1:B:448:LEU:HD22	1:B:491:MET:HE2	2.01	0.41
1:A:87:ALA:HA	1:A:135:ILE:HG22	2.02	0.41
1:A:468:TYR:CD1	1:A:468:TYR:C	2.98	0.41
1:B:153:ARG:HB3	1:B:513:GLU:OE2	2.20	0.41
1:A:220:HIS:NE2	1:A:226:ASP:OD2	2.36	0.41
1:A:405:ARG:HD3	1:A:405:ARG:HA	1.87	0.41
1:A:468:TYR:HB3	1:A:469:GLU:OE1	2.21	0.41
1:A:195:ILE:HG22	1:A:203:LEU:HB3	2.02	0.41
1:A:316:ASN:HB2	1:A:369:ALA:HB2	2.03	0.41
1:A:491:MET:HE3	1:A:495:TRP:CH2	2.56	0.41
1:A:321:LEU:N	1:A:333:ILE:O	2.53	0.41
1:A:434:LYS:CG	1:A:435:PHE:N	2.84	0.41
1:A:479:ARG:HD3	1:A:488:TYR:HD2	1.85	0.41
1:B:196:ASN:ND2	1:B:204:TYR:CZ	2.89	0.41
1:A:186:TYR:HB3	1:A:191:TYR:HE1	1.86	0.41
1:A:289:VAL:HG22	1:A:333:ILE:CD1	2.50	0.41
1:B:93:ALA:HB2	1:B:99:LEU:C	2.46	0.41
1:A:138:VAL:O	1:A:143:LYS:HD3	2.21	0.40
1:B:453:THR:CB	1:B:456:MET:HG3	2.47	0.40
1:A:328:PRO:HB2	1:A:329:PRO:HD3	2.03	0.40
1:A:354:VAL:O	1:A:454:TYR:OH	2.37	0.40
1:A:137:PRO:O	1:A:140:SER:OG	2.36	0.40
1:A:403:LEU:C	1:A:404:SER:HG	2.28	0.40
1:A:468:TYR:CE1	1:A:497:TRP:HH2	2.39	0.40
1:A:341:ASN:OD1	1:A:342:LEU:N	2.54	0.40
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.93	0.40
1:B:437:ILE:HD13	1:B:437:ILE:HA	1.89	0.40
1:A:434:LYS:NZ	1:A:499:PRO:HG3	2.36	0.40
1:B:204:TYR:HB3	1:B:210:ARG:HA	2.04	0.40
1:B:353:GLU:HG3	1:B:354:VAL:HG23	2.02	0.40
1:B:469:GLU:OE1	1:B:469:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/448 (91%)	385 (94%)	22 (5%)	1 (0%)	43	62
1	B	366/448 (82%)	356 (97%)	10 (3%)	0	100	100
All	All	774/896 (86%)	741 (96%)	32 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	SER

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	368/390 (94%)	359 (98%)	9 (2%)	43	67
1	B	338/390 (87%)	330 (98%)	8 (2%)	43	67
All	All	706/780 (90%)	689 (98%)	17 (2%)	43	67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	244	VAL
1	A	275	VAL
1	A	320	LEU
1	A	422	ILE
1	A	468	TYR
1	A	469	GLU
1	A	476	ARG
1	A	512	PHE
1	B	139	ASN
1	B	176	SER

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Mol	Chain	Res	Type
1	B	323	VAL
1	B	395	LEU
1	B	448	LEU
1	B	469	GLU
1	B	497	TRP
1	B	518	GLU

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

Mol	Chain	Res	Type
1	A	125	ASN
1	A	496	GLN
1	B	196	ASN
1	B	393	ASN
1	B	394	HIS
1	B	466	GLN
1	B	496	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](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	DMS	A	608	-	3,3,3	0.66	0	3,3,3	0.51	0
3	SKI	A	602	-	31,31,31	2.93	12 (38%)	42,42,42	2.26	17 (40%)
2	AY7	B	601	-	33,34,34	0.68	1 (3%)	41,49,49	0.95	1 (2%)
5	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.08	0
6	DMS	A	606	-	3,3,3	0.67	0	3,3,3	0.54	0
6	DMS	B	604	-	3,3,3	0.67	0	3,3,3	0.53	0
2	AY7	A	601	-	33,34,34	0.68	1 (3%)	41,49,49	0.84	1 (2%)
5	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	B	603	-	4,4,4	0.24	0	6,6,6	0.08	0
6	DMS	A	607	-	3,3,3	0.67	0	3,3,3	0.53	0
3	SKI	B	602	-	31,31,31	2.91	12 (38%)	42,42,42	2.18	15 (35%)

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	SKI	A	602	-	-	3/12/12/12	0/4/4/4
2	AY7	B	601	-	-	7/20/30/30	0/4/4/4
2	AY7	A	601	-	-	6/20/30/30	0/4/4/4
3	SKI	B	602	-	-	2/12/12/12	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	SKI	O27-C04	8.00	1.50	1.37
3	A	602	SKI	O27-C04	7.99	1.50	1.37
3	A	602	SKI	C09-N13	6.55	1.46	1.36
3	B	602	SKI	C09-N13	6.47	1.46	1.36
3	A	602	SKI	C11-N12	5.08	1.40	1.32
3	B	602	SKI	C11-N12	4.95	1.39	1.32
3	A	602	SKI	C15-C14	4.95	1.47	1.39
3	B	602	SKI	C15-C14	4.88	1.47	1.39
3	A	602	SKI	C25-C26	4.34	1.46	1.38
3	B	602	SKI	C25-C26	4.30	1.46	1.38
3	B	602	SKI	C18-C17	4.20	1.46	1.38
3	A	602	SKI	C18-C17	4.15	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	SKI	C04-C03	3.57	1.48	1.40
3	A	602	SKI	C04-C03	3.48	1.48	1.40
3	A	602	SKI	C09-N10	2.88	1.37	1.34
3	B	602	SKI	C09-N10	2.86	1.37	1.34
3	A	602	SKI	O20-C17	-2.75	1.33	1.39
3	B	602	SKI	O20-C17	-2.57	1.34	1.39
3	A	602	SKI	C22-C21	2.41	1.43	1.38
3	B	602	SKI	C22-C21	2.39	1.43	1.38
3	B	602	SKI	C19-C18	2.36	1.42	1.38
3	A	602	SKI	C19-C18	2.28	1.42	1.38
3	B	602	SKI	C16-C15	2.15	1.42	1.38
3	A	602	SKI	C16-C15	2.12	1.42	1.38
2	B	601	AY7	N24-N25	-2.07	1.33	1.36
2	A	601	AY7	N24-N25	-2.00	1.33	1.36

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	SKI	C11-N10-C09	4.87	120.38	116.60
3	A	602	SKI	C11-N10-C09	4.71	120.25	116.60
3	A	602	SKI	C09-C07-C06	4.51	118.53	115.86
3	B	602	SKI	N12-C11-N10	-4.48	122.59	128.67
3	A	602	SKI	N12-C11-N10	-4.37	122.74	128.67
3	B	602	SKI	O02-C03-C08	-4.36	119.64	125.16
3	A	602	SKI	O02-C03-C08	-4.30	119.71	125.16
3	B	602	SKI	C11-N12-C06	4.22	120.23	115.43
3	A	602	SKI	C11-N12-C06	4.17	120.17	115.43
3	A	602	SKI	C08-C07-C09	-4.17	121.45	124.84
3	B	602	SKI	O27-C04-C05	-4.03	120.05	125.16
3	B	602	SKI	C09-C07-C06	3.93	118.18	115.86
3	A	602	SKI	O27-C04-C05	-3.83	120.30	125.16
3	B	602	SKI	O27-C04-C03	3.68	120.39	115.40
3	B	602	SKI	C08-C07-C09	-3.55	121.95	124.84
3	A	602	SKI	C07-C06-N12	-3.49	119.12	122.82
3	B	602	SKI	O02-C03-C04	3.48	120.12	115.40
3	A	602	SKI	O27-C04-C03	3.44	120.08	115.40
2	B	601	AY7	C1-C11-C12	3.39	124.35	120.92
3	A	602	SKI	O02-C03-C04	3.35	119.94	115.40
3	B	602	SKI	C07-C06-N12	-3.30	119.32	122.82
3	A	602	SKI	C21-O20-C17	-3.18	111.51	118.78
3	A	602	SKI	C07-C09-N10	-2.92	119.19	121.35
3	B	602	SKI	C07-C09-N10	-2.79	119.28	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AY7	C1-C11-C12	2.59	123.55	120.92
3	A	602	SKI	C05-C06-N12	2.56	120.95	118.01
3	B	602	SKI	C05-C06-N12	2.36	120.73	118.01
3	B	602	SKI	C14-N13-C09	-2.35	122.20	128.22
3	A	602	SKI	N13-C09-N10	2.29	121.29	118.71
3	A	602	SKI	C01-O02-C03	-2.25	114.21	117.51
3	A	602	SKI	C14-N13-C09	-2.24	122.49	128.22
3	A	602	SKI	C28-O27-C04	-2.16	114.35	117.51
3	B	602	SKI	C01-O02-C03	-2.13	114.38	117.51
3	B	602	SKI	C21-O20-C17	-2.03	114.15	118.78

There are no chirality outliers.

All (18) torsion outliers are listed below:

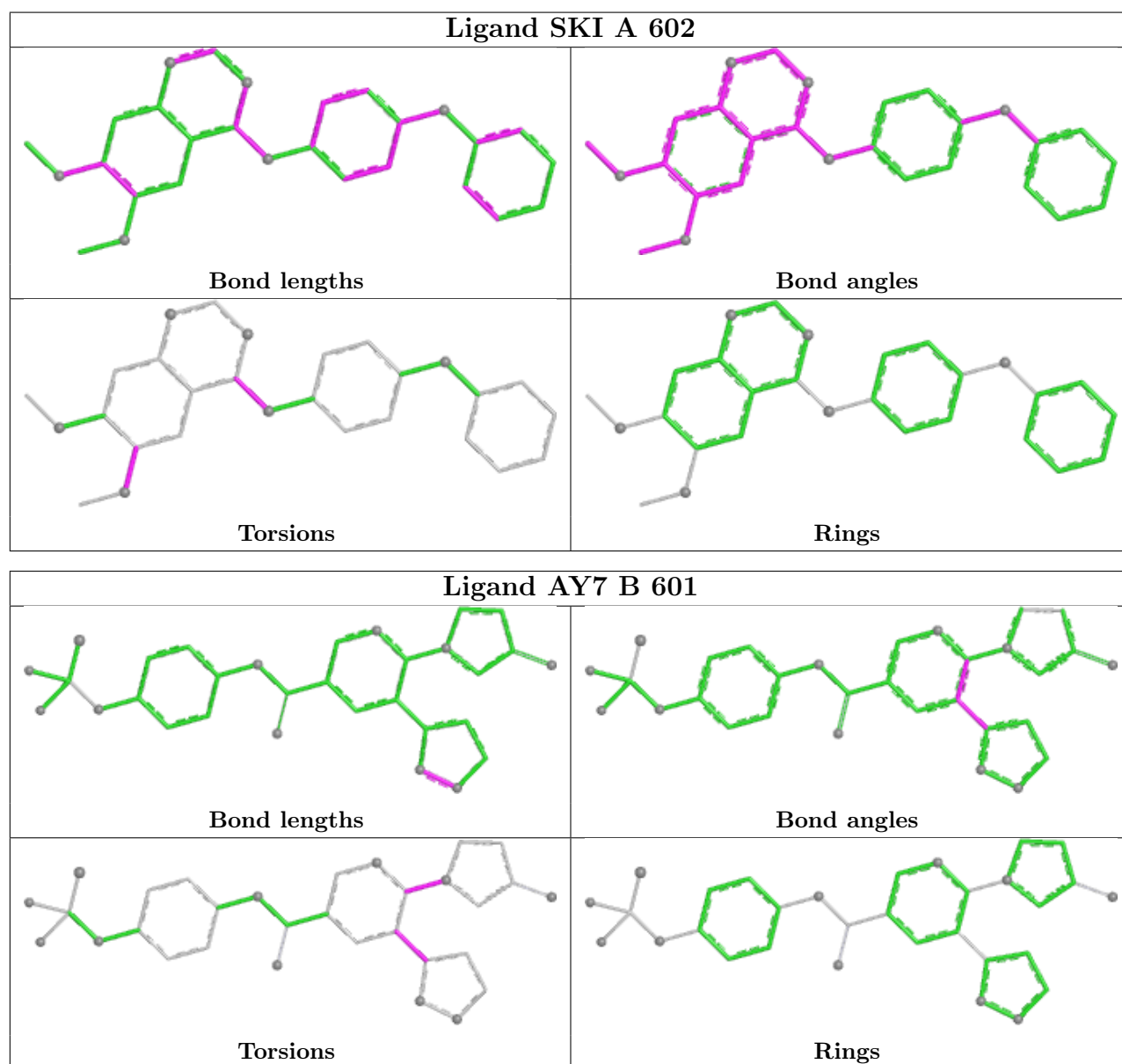
Mol	Chain	Res	Type	Atoms
2	A	601	AY7	C11-C1-N2-C3
2	A	601	AY7	C11-C1-N2-C6
2	A	601	AY7	N7-C1-N2-C3
2	A	601	AY7	N7-C1-N2-C6
2	A	601	AY7	C1-C11-C12-N24
2	A	601	AY7	C10-C11-C12-N24
2	B	601	AY7	C11-C1-N2-C3
2	B	601	AY7	C11-C1-N2-C6
2	B	601	AY7	N7-C1-N2-C3
2	B	601	AY7	N7-C1-N2-C6
2	B	601	AY7	C1-C11-C12-N24
2	B	601	AY7	C10-C11-C12-N24
3	B	602	SKI	C08-C03-O02-C01
3	B	602	SKI	C04-C03-O02-C01
3	A	602	SKI	N10-C09-N13-C14
3	A	602	SKI	C07-C09-N13-C14
3	A	602	SKI	C04-C03-O02-C01
2	B	601	AY7	C10-C11-C12-C27

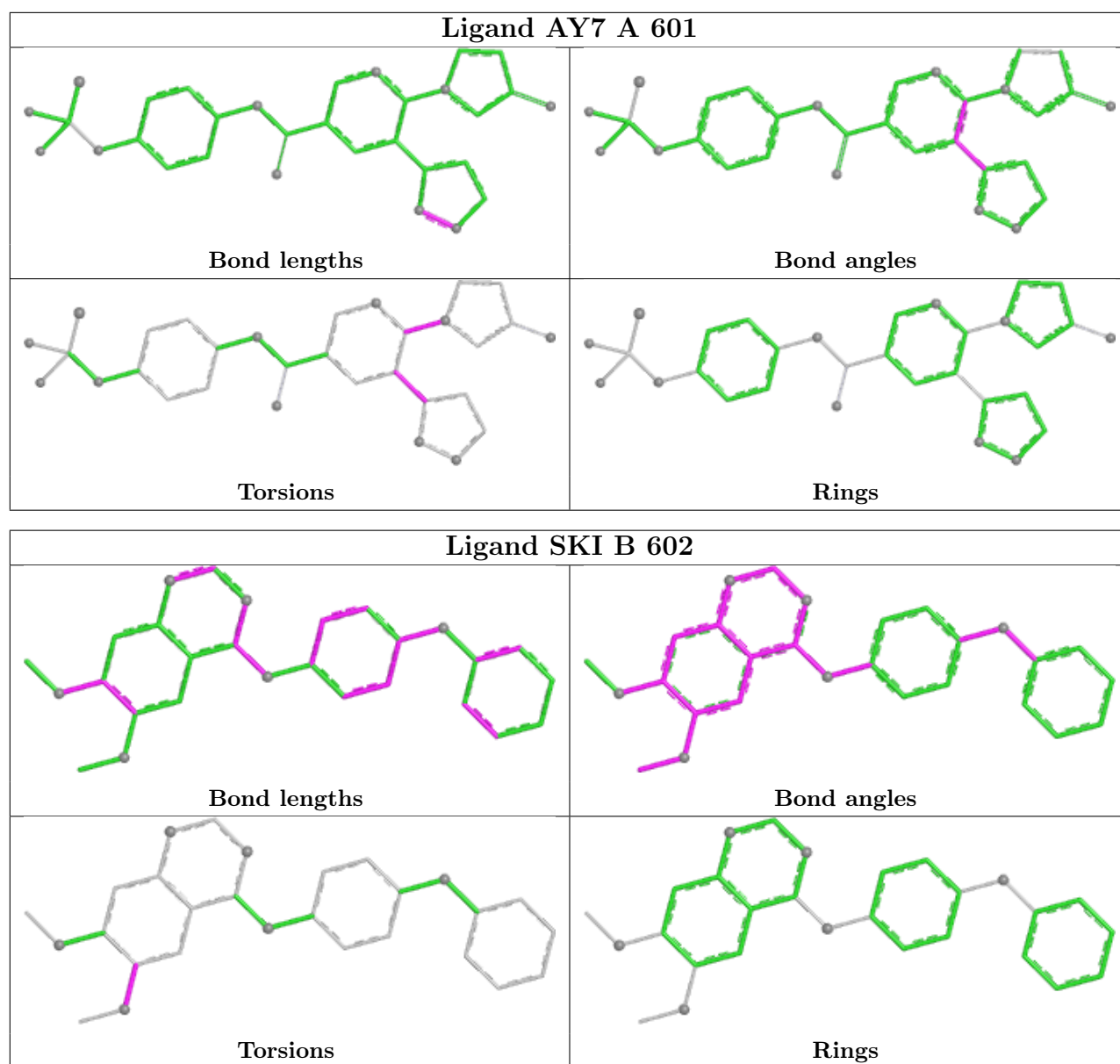
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	AY7	1	0
3	B	602	SKI	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

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	420/448 (93%)	1.46	97 (23%) 2 2	53, 87, 132, 157	0
1	B	386/448 (86%)	1.45	94 (24%) 2 1	55, 90, 137, 155	0
All	All	806/896 (89%)	1.45	191 (23%) 2 2	53, 88, 134, 157	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	ILE	5.2
1	A	401	PHE	4.5
1	A	435	PHE	4.3
1	A	298	GLU	4.3
1	A	494	CYS	4.2
1	A	381	ARG	4.0
1	B	482	GLY	3.8
1	A	299	VAL	3.8
1	B	515	MET	3.8
1	A	332	ILE	3.8
1	A	282	LYS	3.7
1	B	205	VAL	3.6
1	A	447	LEU	3.6
1	B	196	ASN	3.5
1	A	408	THR	3.4
1	A	203	LEU	3.4
1	A	279	VAL	3.4
1	A	483	CYS	3.4
1	A	400	ASP	3.4
1	B	401	PHE	3.3
1	A	338	THR	3.2
1	B	519	SER	3.2
1	A	490	LEU	3.2
1	A	392	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	391	GLY	3.2
1	A	82	GLY	3.1
1	A	385	ALA	3.1
1	B	434	LYS	3.1
1	B	385	ALA	3.1
1	B	524	GLU	3.0
1	A	156	ALA	3.0
1	A	404	SER	3.0
1	B	388	CYS	3.0
1	B	260	ASP	3.0
1	B	514	THR	2.9
1	B	345	TYR	2.9
1	B	216	GLU	2.9
1	B	118	TRP	2.9
1	B	280	TRP	2.9
1	A	519	SER	2.9
1	B	435	PHE	2.9
1	A	395	LEU	2.9
1	A	134	TYR	2.8
1	B	395	LEU	2.8
1	A	424	TRP	2.8
1	B	512	PHE	2.8
1	B	141	LEU	2.8
1	B	382	ASP	2.8
1	B	206	SER	2.8
1	B	517	GLN	2.8
1	A	497	TRP	2.8
1	B	390	VAL	2.8
1	B	245	TYR	2.8
1	A	521	ILE	2.8
1	A	85	PHE	2.7
1	B	342	LEU	2.7
1	B	376	LYS	2.7
1	B	338	THR	2.7
1	A	292	LEU	2.7
1	A	406	LEU	2.7
1	A	283	TYR	2.7
1	A	231	THR	2.7
1	A	296	THR	2.7
1	B	286	THR	2.7
1	B	82	GLY	2.7
1	B	333	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	224	VAL	2.7
1	B	261	ILE	2.6
1	A	498	ASN	2.6
1	A	280	TRP	2.6
1	A	396	VAL	2.6
1	A	309	MET	2.6
1	B	516	PHE	2.6
1	B	175	SER	2.6
1	B	283	TYR	2.6
1	A	464	LEU	2.6
1	A	302	PHE	2.6
1	A	163	GLY	2.6
1	A	399	ALA	2.6
1	A	457	SER	2.5
1	A	421	PRO	2.5
1	A	261	ILE	2.5
1	A	382	ASP	2.5
1	B	199	SER	2.5
1	B	284	SER	2.5
1	A	270	GLY	2.5
1	B	178	GLY	2.5
1	A	370	MET	2.5
1	A	379	ILE	2.5
1	B	441	VAL	2.5
1	B	155	ALA	2.5
1	A	436	SER	2.5
1	A	402	GLY	2.5
1	A	275	VAL	2.5
1	A	516	PHE	2.5
1	B	393	ASN	2.5
1	B	346	LEU	2.5
1	B	421	PRO	2.5
1	B	500	SER	2.5
1	B	459	TYR	2.5
1	B	136	THR	2.5
1	B	332	ILE	2.4
1	B	521	ILE	2.4
1	B	154	ASN	2.4
1	A	135	ILE	2.4
1	A	517	GLN	2.4
1	A	403	LEU	2.4
1	B	309	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	458	PRO	2.4
1	A	96	ASP	2.4
1	B	375	LYS	2.4
1	B	424	TRP	2.4
1	A	456	MET	2.4
1	B	341	ASN	2.4
1	A	525	VAL	2.4
1	B	357	VAL	2.4
1	B	396	VAL	2.4
1	A	197	THR	2.4
1	A	164	ILE	2.4
1	A	312	ILE	2.4
1	A	177	PRO	2.4
1	A	377	ASN	2.3
1	A	487	VAL	2.3
1	A	444	PHE	2.3
1	B	208	GLU	2.3
1	A	146	TRP	2.3
1	B	134	TYR	2.3
1	B	503	PRO	2.3
1	A	391	GLY	2.3
1	B	200	ASP	2.3
1	A	434	LYS	2.3
1	B	474	ASP	2.3
1	B	389	LEU	2.3
1	B	447	LEU	2.3
1	A	218	VAL	2.3
1	A	503	PRO	2.3
1	B	156	ALA	2.3
1	A	383	LEU	2.3
1	A	468	TYR	2.3
1	B	289	VAL	2.3
1	A	240	ASN	2.2
1	A	321	LEU	2.2
1	B	470	LEU	2.2
1	A	344	ASP	2.2
1	B	462	ILE	2.2
1	A	398	VAL	2.2
1	B	378	PHE	2.2
1	A	462	ILE	2.2
1	B	177	PRO	2.2
1	B	339	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	302	PHE	2.2
1	B	399	ALA	2.2
1	A	171	ARG	2.2
1	B	179	GLN	2.2
1	B	508	ILE	2.2
1	B	193	TYR	2.2
1	A	512	PHE	2.2
1	A	448	LEU	2.2
1	B	495	TRP	2.2
1	B	392	GLU	2.2
1	A	133	ASN	2.1
1	B	484	PRO	2.1
1	A	206	SER	2.1
1	A	366	ILE	2.1
1	A	380	HIS	2.1
1	A	130	VAL	2.1
1	A	480	PRO	2.1
1	A	505	PHE	2.1
1	B	217	LEU	2.1
1	B	379	ILE	2.1
1	A	509	HIS	2.1
1	B	362	MET	2.1
1	B	225	ALA	2.1
1	A	300	GLU	2.1
1	A	378	PHE	2.1
1	A	334	THR	2.1
1	B	426	ALA	2.1
1	A	174	GLU	2.1
1	A	245	TYR	2.1
1	B	499	PRO	2.0
1	B	228	LEU	2.0
1	B	356	ALA	2.0
1	B	241	LYS	2.0
1	A	297	MET	2.0
1	A	247	VAL	2.0
1	A	346	LEU	2.0
1	B	115	ASN	2.0
1	B	386	ARG	2.0
1	A	369	ALA	2.0
1	B	226	ASP	2.0
1	B	290	LYS	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](#)

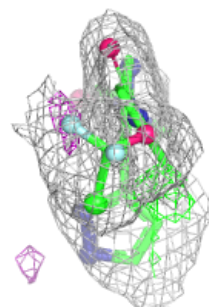
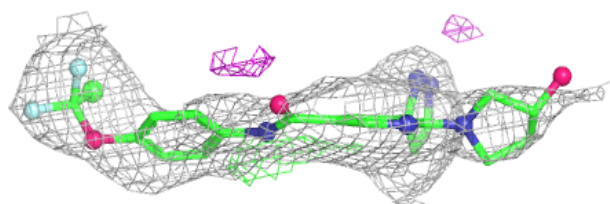
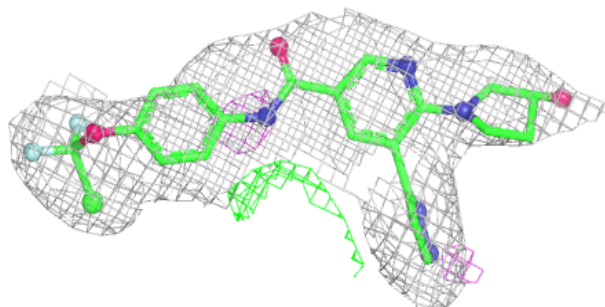
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	DMS	B	604	4/4	0.39	0.28	44,82,97,124	0
6	DMS	A	606	4/4	0.43	0.20	79,84,94,133	0
6	DMS	A	608	4/4	0.58	0.23	55,76,91,142	0
5	SO4	B	603	5/5	0.72	0.20	94,105,119,128	0
5	SO4	A	604	5/5	0.75	0.13	83,88,120,131	0
6	DMS	A	607	4/4	0.76	0.17	63,65,84,97	0
2	AY7	A	601	31/31	0.77	0.18	87,101,118,129	0
3	SKI	B	602	28/28	0.78	0.16	73,108,119,122	0
5	SO4	A	605	5/5	0.79	0.19	85,94,107,123	0
3	SKI	A	602	28/28	0.79	0.20	69,97,107,117	0
4	CL	A	603	1/1	0.88	0.18	90,90,90,90	0
2	AY7	B	601	31/31	0.88	0.14	75,103,130,135	0

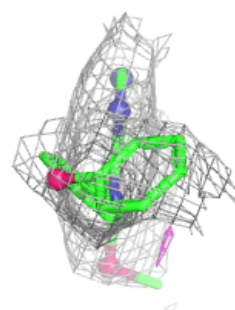
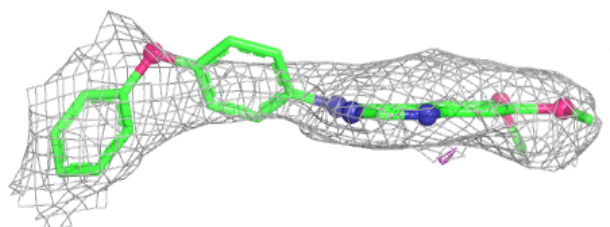
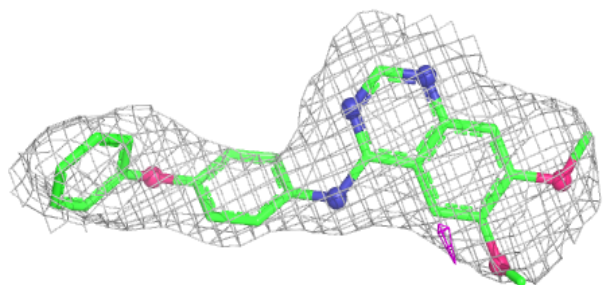
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AY7 A 601:

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

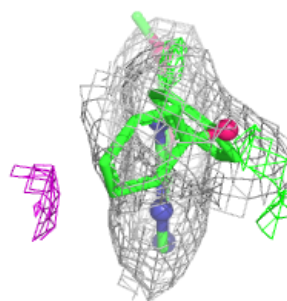
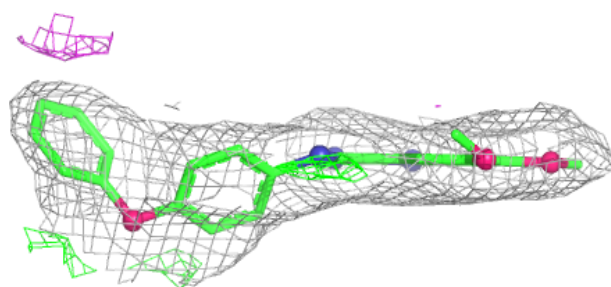
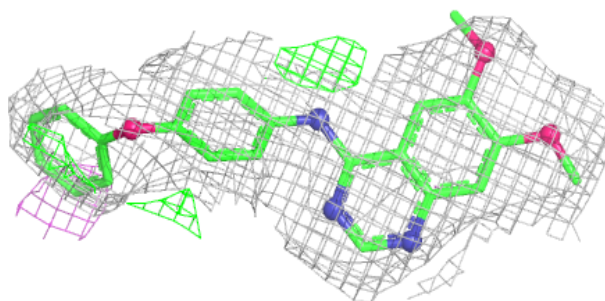
**Electron density around SKI B 602:**

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

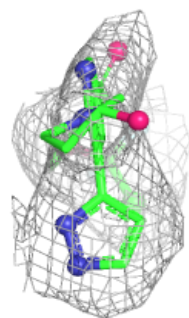
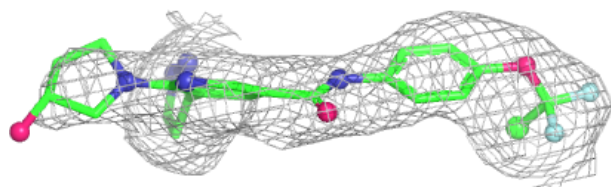
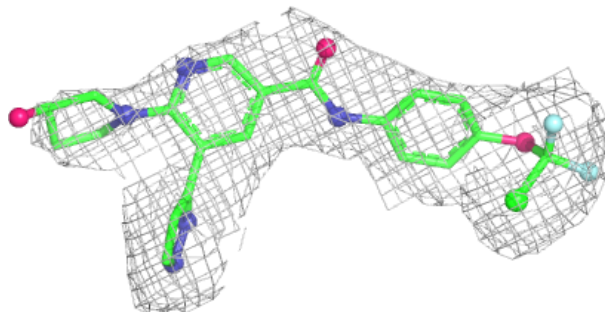


Electron density around SKI A 602:

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

**Electron density around AY7 B 601:**

$2mF_o-DF_c$ (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.