



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 2G2F / pdb_00002g2f
Title : A Src-like Inactive Conformation in the Abl Tyrosine Kinase Domain
Authors : Levinson, N.M.; Kuchment, O.
Deposited on : 2006-02-15
Resolution : 2.70 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

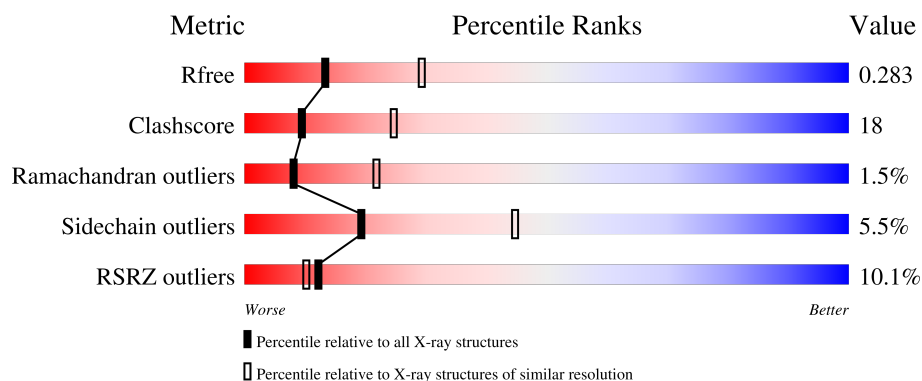
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	287	
1	B	287	
2	C	11	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4586 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 Abl Kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2228	1435	361	415	17			
1	B	264	Total	C	N	O	S	0	0	0
			2150	1388	349	396	17			

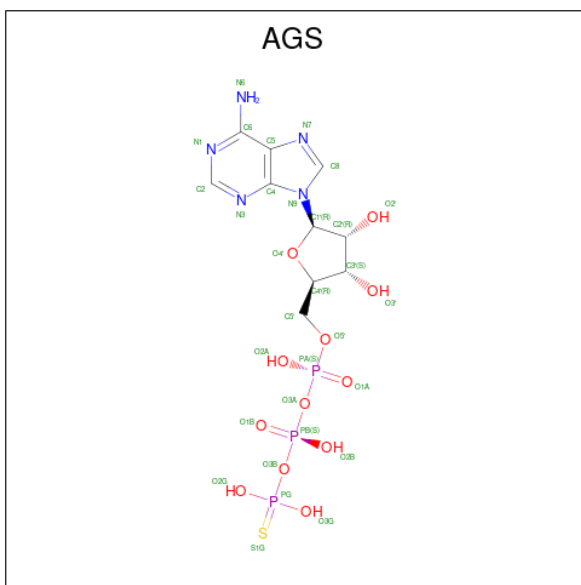
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLY	-	cloning artifact	UNP P00519
A	227	HIS	-	cloning artifact	UNP P00519
A	228	MET	-	cloning artifact	UNP P00519
A	396	PRO	HIS	engineered mutation	UNP P00519
B	226	GLY	-	cloning artifact	UNP P00519
B	227	HIS	-	cloning artifact	UNP P00519
B	228	MET	-	cloning artifact	UNP P00519
B	396	PRO	HIS	engineered mutation	UNP P00519

- Molecule 2 is a protein called ATP-Peptide Conjugate.

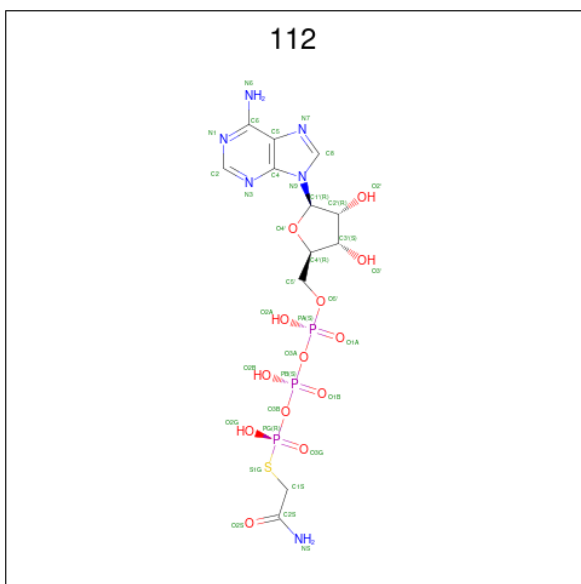
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			57	41	8	8			

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is THIOPHOSPHORIC ACID O-((ADENOSYL-PHOSPHO)PHOSPHO)-S-AC ETAMIDYL-DIESTER (CCD ID: 112) (formula: $C_{12}H_{19}N_6O_{13}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		

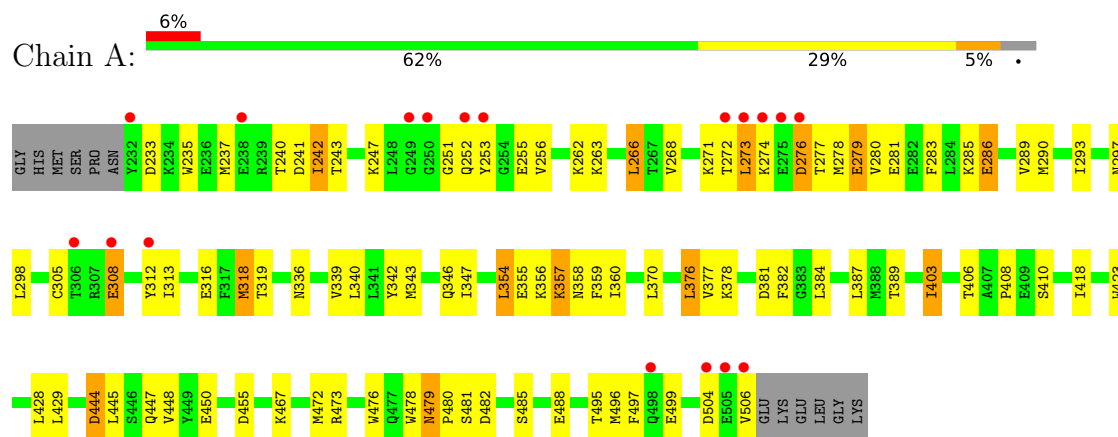
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	30	Total 30	O 30	0	0
5	C	2	Total 2	O 2	0	0

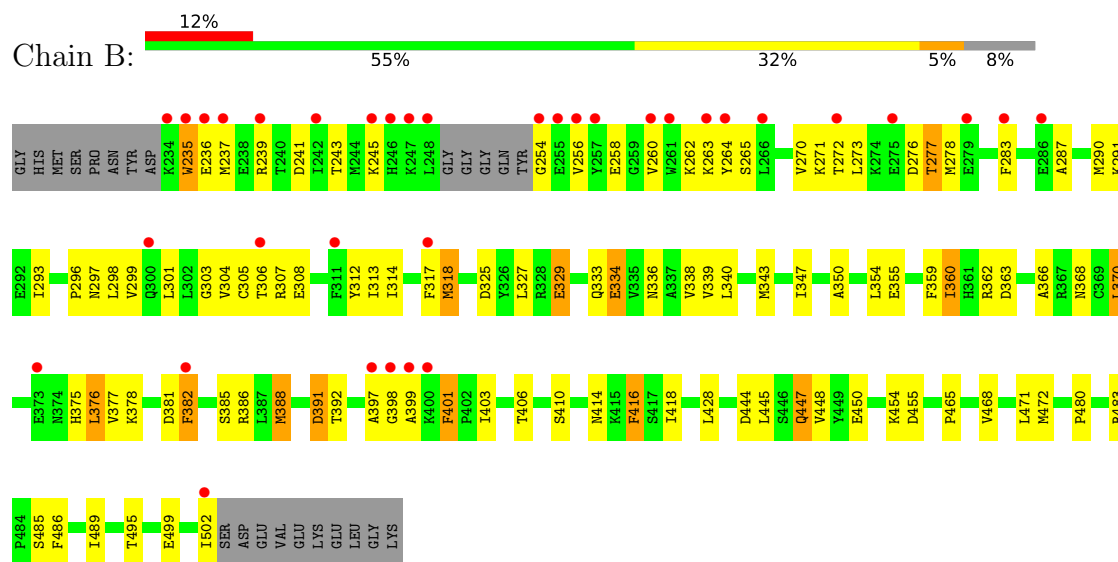
3 Residue-property plots [i](#)

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.

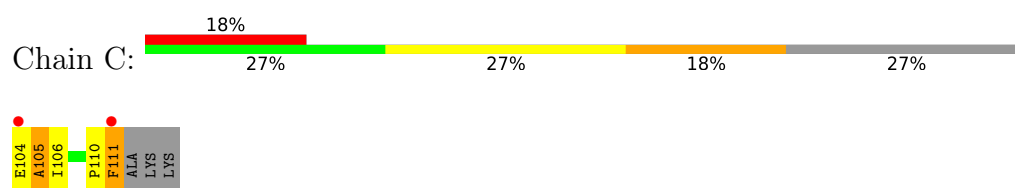
• Molecule 1: Abl Kinase



• Molecule 1: Abl Kinase



• Molecule 2: ATP-Peptide Conjugate



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.67Å 133.32Å 56.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 99.6 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.286 0.229 , 0.283	Depositor DCC
R_{free} test set	1376 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4586	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: 112, AGS

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	0.51	1/2285 (0.0%)	0.96	6/3094 (0.2%)
1	B	0.46	0/2204	0.92	7/2983 (0.2%)
2	C	0.59	0/59	1.12	1/80 (1.2%)
All	All	0.49	1/4548 (0.0%)	0.95	14/6157 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	MET	SD-CE	-5.25	1.66	1.79

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	THR	N-CA-C	6.41	119.08	111.71
1	B	333	GLN	N-CA-C	-6.30	105.72	113.41
2	C	106	ILE	N-CA-C	6.27	116.95	111.56
1	B	391	ASP	N-CA-C	-6.14	105.07	114.16
1	B	306	THR	N-CA-C	5.92	118.01	110.61
1	B	448	VAL	N-CA-C	5.72	116.37	110.36
1	A	479	ASN	CA-C-N	5.66	126.92	119.84
1	A	479	ASN	C-N-CA	5.66	126.92	119.84
1	A	403	ILE	N-CA-C	5.46	120.70	109.34
1	B	334	GLU	N-CA-C	-5.32	102.79	111.04
1	B	235	TRP	N-CA-C	5.29	116.73	111.07
1	A	448	VAL	N-CA-C	5.28	115.48	110.42
1	A	286	GLU	N-CA-C	-5.09	105.62	111.07
1	B	472	MET	N-CA-C	-5.03	105.98	111.82

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	2228	0	2174	73	0
1	B	2150	0	2119	81	0
2	C	57	0	52	3	0
3	B	31	0	12	1	0
4	C	35	0	14	5	0
5	A	53	0	0	1	0
5	B	30	0	0	0	0
5	C	2	0	0	0	0
All	All	4586	0	4371	159	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 18.

All (159) 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:274:LYS:C	1:A:276:ASP:H	1.86	0.84
1:B:239:ARG:HH12	1:B:308:GLU:HB2	1.42	0.84
1:A:293:ILE:HD13	1:A:384:LEU:HD11	1.58	0.83
1:A:358:ASN:OD1	1:A:389:THR:HG22	1.78	0.82
1:A:247:LYS:HE3	1:A:255:GLU:HB3	1.63	0.81
1:A:403:ILE:HB	1:A:445:LEU:HD22	1.69	0.73
1:A:253:TYR:HA	1:A:277:THR:OG1	1.90	0.72
1:B:298:LEU:HD11	1:B:354:LEU:HD11	1.72	0.70
1:A:293:ILE:HD13	1:A:384:LEU:CD1	2.22	0.70
1:A:279:GLU:OE2	1:A:281:GLU:HB2	1.92	0.70
1:B:276:ASP:O	1:B:277:THR:HG23	1.92	0.69
1:A:271:LYS:HB3	1:A:313:ILE:HB	1.75	0.69
1:B:258:GLU:HG3	1:B:317:PHE:CE1	2.29	0.67
1:A:251:GLY:C	1:A:253:TYR:H	2.02	0.67
1:A:237:MET:HE1	1:A:242:ILE:HD13	1.77	0.66
1:B:391:ASP:OD1	1:B:392:THR:HG23	1.95	0.66
1:A:340:LEU:HA	1:A:343:MET:HE2	1.78	0.66
1:A:318:MET:HG3	1:A:370:LEU:CB	2.26	0.64
1:B:360:ILE:CD1	1:B:385:SER:HB2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:THR:HG22	1:A:273:LEU:N	2.13	0.64
1:A:485:SER:OG	1:A:488:GLU:HG3	1.97	0.63
1:B:495:THR:O	1:B:499:GLU:HG2	1.98	0.63
1:A:479:ASN:HB3	1:A:482:ASP:OD2	2.00	0.61
1:A:243:THR:OG1	1:A:262:LYS:HE2	1.99	0.61
1:A:298:LEU:HD11	1:A:354:LEU:HD13	1.82	0.61
1:B:296:PRO:O	1:B:378:LYS:HE2	2.01	0.61
1:A:336:ASN:OD1	1:A:339:VAL:HG23	2.01	0.60
1:B:293:ILE:HD12	1:B:293:ILE:O	2.00	0.60
1:B:350:ALA:O	1:B:354:LEU:HD13	2.02	0.60
1:A:406:THR:CG2	1:A:410:SER:HB2	2.31	0.60
1:B:360:ILE:HD13	1:B:385:SER:HB2	1.84	0.59
1:B:450:GLU:OE2	1:B:454:LYS:HE3	2.02	0.59
1:A:251:GLY:HA2	4:C:201:112:O2G	2.02	0.59
1:B:485:SER:O	1:B:489:ILE:HG13	2.01	0.59
1:A:305:CYS:HB2	1:A:312:TYR:HB2	1.84	0.59
1:B:318:MET:HA	1:B:318:MET:HE2	1.83	0.59
2:C:111:PHE:CD1	2:C:111:PHE:N	2.71	0.58
1:B:325:ASP:O	1:B:329:GLU:HG3	2.03	0.58
1:B:270:VAL:HG22	1:B:314:ILE:CD1	2.33	0.58
1:B:237:MET:HE1	1:B:314:ILE:HG13	1.85	0.58
1:B:270:VAL:HG22	1:B:314:ILE:HD12	1.86	0.57
1:A:256:VAL:CG1	4:C:201:112:H5'1	2.34	0.57
3:B:601:AGS:O2B	3:B:601:AGS:H3'	2.05	0.56
4:C:201:112:O2B	4:C:201:112:H5'2	2.05	0.56
1:B:471:LEU:O	1:B:471:LEU:HD23	2.06	0.56
1:B:398:GLY:O	1:B:399:ALA:C	2.50	0.55
1:A:318:MET:HG3	1:A:370:LEU:HB3	1.87	0.54
1:B:278:MET:HA	1:B:278:MET:HE2	1.89	0.54
1:A:429:LEU:HB3	1:A:472:MET:HE2	1.89	0.54
1:B:237:MET:CE	1:B:314:ILE:HG13	2.38	0.54
1:B:376:LEU:HD11	1:B:378:LYS:HE3	1.90	0.54
1:A:273:LEU:CD1	1:A:278:MET:HB2	2.37	0.54
1:B:239:ARG:NH1	1:B:308:GLU:HB2	2.18	0.54
1:B:447:GLN:HE21	1:B:447:GLN:CA	2.21	0.53
1:A:376:LEU:HD11	1:A:378:LYS:HE3	1.91	0.53
1:B:343:MET:O	1:B:347:ILE:HG12	2.08	0.53
1:B:303:GLY:H	1:B:314:ILE:HB	1.74	0.53
1:B:290:MET:HE2	1:B:301:LEU:HD13	1.91	0.53
1:B:336:ASN:ND2	1:B:338:VAL:HG12	2.23	0.52
1:B:416:PHE:N	1:B:416:PHE:CD1	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ASN:HD21	1:B:502:ILE:HG23	1.73	0.52
1:A:243:THR:OG1	1:A:262:LYS:CE	2.58	0.52
2:C:104:GLU:O	2:C:105:ALA:CB	2.56	0.52
1:A:273:LEU:HD23	1:A:273:LEU:O	2.10	0.51
1:A:355:GLU:HG3	1:A:418:ILE:HG12	1.92	0.51
1:A:356:LYS:C	1:A:358:ASN:H	2.19	0.51
1:B:336:ASN:HD21	1:B:338:VAL:HG12	1.76	0.51
1:B:287:ALA:O	1:B:291:LYS:HG3	2.11	0.51
1:A:251:GLY:C	1:A:253:TYR:N	2.68	0.50
1:A:286:GLU:HG2	1:A:382:PHE:CD1	2.47	0.50
1:A:297:ASN:ND2	1:A:346:GLN:HB3	2.26	0.50
1:A:423:TRP:CE3	1:A:476:TRP:HA	2.46	0.50
1:A:272:THR:HG22	1:A:273:LEU:H	1.75	0.50
1:A:286:GLU:HG2	1:A:382:PHE:CE1	2.46	0.50
1:A:370:LEU:N	1:A:370:LEU:HD22	2.27	0.50
1:B:340:LEU:HA	1:B:343:MET:HE2	1.93	0.50
1:B:480:PRO:HA	1:B:483:ARG:NE	2.27	0.50
1:A:273:LEU:HD12	1:A:278:MET:HB2	1.93	0.49
1:B:297:ASN:HA	1:B:378:LYS:HG2	1.94	0.49
1:B:366:ALA:N	1:B:428:LEU:HD13	2.27	0.49
1:A:237:MET:O	1:A:305:CYS:SG	2.63	0.49
1:A:274:LYS:C	1:A:276:ASP:N	2.57	0.49
1:B:340:LEU:HD23	1:B:343:MET:HE2	1.92	0.49
1:B:355:GLU:HG3	1:B:418:ILE:HG12	1.94	0.49
1:B:376:LEU:HD22	1:B:377:VAL:H	1.77	0.49
1:A:273:LEU:HD13	1:A:283:PHE:CD1	2.48	0.49
1:B:245:LYS:NZ	1:B:260:VAL:HG21	2.28	0.49
1:B:304:VAL:HG12	1:B:313:ILE:HD13	1.95	0.49
1:B:293:ILE:HD11	1:B:381:ASP:OD1	2.13	0.49
1:B:376:LEU:HD22	1:B:377:VAL:N	2.27	0.49
1:A:256:VAL:HG12	4:C:201:112:H5'1	1.95	0.49
1:B:235:TRP:O	1:B:236:GLU:C	2.56	0.48
1:A:347:ILE:HD11	1:A:377:VAL:CG1	2.43	0.48
1:B:334:GLU:OE2	1:B:375:HIS:HE1	1.97	0.47
1:A:495:THR:O	1:A:499:GLU:HG2	2.14	0.47
1:B:241:ASP:OD1	1:B:263:LYS:HE3	2.14	0.47
1:A:256:VAL:HG11	4:C:201:112:H5'1	1.96	0.47
1:B:454:LYS:O	1:B:455:ASP:HB2	2.14	0.47
1:A:276:ASP:CG	1:A:277:THR:H	2.22	0.47
1:A:406:THR:HG22	1:A:410:SER:HB2	1.96	0.47
1:B:336:ASN:OD1	1:B:339:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:NH1	1:B:385:SER:OG	2.44	0.47
1:B:381:ASP:O	1:B:382:PHE:C	2.57	0.47
1:A:241:ASP:HB3	1:A:263:LYS:HE3	1.96	0.47
1:B:502:ILE:HG22	1:B:502:ILE:O	2.15	0.47
1:B:264:TYR:O	1:B:265:SER:C	2.59	0.46
1:B:447:GLN:CA	1:B:447:GLN:NE2	2.79	0.46
1:A:318:MET:HG3	1:A:370:LEU:HB2	1.97	0.46
1:B:293:ILE:HD12	1:B:293:ILE:C	2.41	0.46
1:B:318:MET:SD	1:B:378:LYS:HD2	2.56	0.46
1:A:347:ILE:HD11	1:A:377:VAL:HG11	1.97	0.45
2:C:104:GLU:O	2:C:105:ALA:HB3	2.16	0.45
1:B:236:GLU:OE2	1:B:307:ARG:HD2	2.16	0.45
1:A:255:GLU:H	1:A:255:GLU:HG3	1.61	0.45
1:B:340:LEU:HD23	1:B:343:MET:CE	2.46	0.45
1:B:465:PRO:HG2	1:B:468:VAL:CG2	2.47	0.45
1:A:408:PRO:HB3	1:A:478:TRP:CZ3	2.52	0.45
1:A:357:LYS:HB3	1:A:359:PHE:CE1	2.53	0.44
1:A:272:THR:CG2	1:A:273:LEU:N	2.79	0.44
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.99	0.44
1:A:290:MET:HE3	1:A:381:ASP:CG	2.42	0.44
1:B:256:VAL:HG22	1:B:271:LYS:HG3	2.00	0.44
1:B:401:PHE:CD1	1:B:401:PHE:N	2.84	0.44
1:B:243:THR:OG1	1:B:262:LYS:HE3	2.17	0.44
1:B:263:LYS:C	1:B:265:SER:H	2.25	0.44
1:A:285:LYS:O	1:A:289:VAL:HG23	2.18	0.43
1:B:283:PHE:CZ	1:B:313:ILE:HG12	2.53	0.43
1:B:376:LEU:CD1	1:B:378:LYS:HE3	2.48	0.43
1:B:406:THR:HG22	1:B:410:SER:HB2	2.00	0.43
1:B:273:LEU:HD22	1:B:283:PHE:HB2	2.00	0.43
1:B:486:PHE:CD1	1:B:489:ILE:HD12	2.54	0.42
1:A:316:GLU:CD	1:A:318:MET:HE1	2.44	0.42
1:A:316:GLU:OE2	1:A:318:MET:HE1	2.19	0.42
1:A:342:TYR:HB2	1:A:497:PHE:CE1	2.54	0.42
1:A:467:LYS:HD3	1:A:496:MET:SD	2.59	0.42
1:A:473:ARG:HD2	5:A:601:HOH:O	2.18	0.42
1:A:308:GLU:N	1:A:308:GLU:OE2	2.52	0.42
1:B:403:ILE:HB	1:B:445:LEU:HD22	2.01	0.42
1:B:450:GLU:O	1:B:454:LYS:HG2	2.19	0.42
1:B:359:PHE:CZ	1:B:386:ARG:HD2	2.55	0.42
1:B:327:LEU:HD21	1:B:343:MET:HE1	2.02	0.42
1:B:416:PHE:N	1:B:416:PHE:HD1	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:HD12	1:A:428:LEU:O	2.20	0.41
1:B:299:VAL:HG21	1:B:370:LEU:HD23	2.02	0.41
1:A:504:ASP:C	1:A:506:VAL:H	2.29	0.41
1:A:293:ILE:HD11	1:A:381:ASP:HB2	2.01	0.41
1:A:360:ILE:HG21	1:A:387:LEU:HD23	2.01	0.41
1:A:266:LEU:HD13	1:A:268:VAL:CG1	2.51	0.41
1:B:363:ASP:OD2	1:B:368:ASN:ND2	2.54	0.41
1:B:388:MET:HE2	1:B:388:MET:HA	2.01	0.41
1:B:254:GLY:HA3	1:B:272:THR:O	2.21	0.41
1:B:263:LYS:O	1:B:264:TYR:HB2	2.21	0.41
1:A:233:ASP:OD1	1:A:235:TRP:HD1	2.05	0.40
1:A:444:ASP:OD2	1:A:447:GLN:HG3	2.20	0.40
1:A:357:LYS:HB3	1:A:359:PHE:HE1	1.87	0.40
1:A:251:GLY:O	1:A:253:TYR:N	2.55	0.40
1:A:272:THR:CG2	1:A:273:LEU:H	2.34	0.40
1:B:336:ASN:CG	1:B:338:VAL:HG12	2.46	0.40
1:B:406:THR:CG2	1:B:410:SER:HB2	2.52	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	273/287 (95%)	247 (90%)	22 (8%)	4 (2%)	8	22
1	B	260/287 (91%)	232 (89%)	26 (10%)	2 (1%)	16	37
2	C	6/11 (54%)	4 (67%)	0	2 (33%)	0	0
All	All	539/585 (92%)	483 (90%)	48 (9%)	8 (2%)	8	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	ASP
1	B	382	PHE
1	B	397	ALA
2	C	105	ALA
1	A	280	VAL
1	A	252	GLN
1	A	357	LYS
2	C	110	PRO

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	238/251 (95%)	225 (94%)	13 (6%)	19	45
1	B	232/251 (92%)	220 (95%)	12 (5%)	21	47
2	C	4/7 (57%)	3 (75%)	1 (25%)	0	2
All	All	474/509 (93%)	448 (94%)	26 (6%)	19	45

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

Mol	Chain	Res	Type
1	A	240	THR
1	A	242	ILE
1	A	266	LEU
1	A	273	LEU
1	A	279	GLU
1	A	308	GLU
1	A	354	LEU
1	A	376	LEU
1	A	444	ASP
1	A	450	GLU
1	A	455	ASP
1	A	480	PRO
1	A	481	SER
1	B	277	THR
1	B	318	MET

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Mol	Chain	Res	Type
1	B	329	GLU
1	B	360	ILE
1	B	370	LEU
1	B	376	LEU
1	B	388	MET
1	B	401	PHE
1	B	414	ASN
1	B	416	PHE
1	B	444	ASP
1	B	447	GLN
2	C	111	PHE

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	322	ASN
1	B	375	HIS
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
4	112	C	201	2	34,37,37	3.62	12 (35%)	46,57,57	1.59	11 (23%)
3	AGS	B	601	-	32,33,33	2.69	13 (40%)	45,52,52	1.69	11 (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	112	C	201	2	-	5/23/44/44	0/3/3/3
3	AGS	B	601	-	-	8/21/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	112	PA-O3A	13.24	1.73	1.59
4	C	201	112	C1S-S1G	-12.27	1.69	1.84
3	B	601	AGS	PA-O3A	8.46	1.68	1.59
4	C	201	112	C6-N6	4.79	1.46	1.34
3	B	601	AGS	C5-C4	4.76	1.47	1.39
3	B	601	AGS	C2-N1	4.32	1.41	1.33
3	B	601	AGS	C4-N3	4.25	1.42	1.34
4	C	201	112	C4-N3	4.24	1.42	1.34
3	B	601	AGS	C2-N3	3.92	1.40	1.33
3	B	601	AGS	C6-N6	3.83	1.44	1.34
4	C	201	112	C5-C4	3.61	1.45	1.39
4	C	201	112	PG-O2G	-3.50	1.47	1.56
3	B	601	AGS	PB-O3A	-3.46	1.55	1.59
3	B	601	AGS	C8-N9	3.38	1.43	1.37
3	B	601	AGS	C1'-N9	3.09	1.54	1.46
4	C	201	112	C2-N1	3.03	1.39	1.33
3	B	601	AGS	PB-O1B	2.93	1.61	1.50
3	B	601	AGS	PA-O5'	2.54	1.69	1.59
4	C	201	112	O4'-C4'	-2.39	1.39	1.45
3	B	601	AGS	O2'-C2'	2.38	1.48	1.43
4	C	201	112	C2'-C1'	2.34	1.60	1.53
4	C	201	112	C8-N9	2.26	1.41	1.37
3	B	601	AGS	O4'-C4'	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	112	C2-N3	2.02	1.37	1.33
4	C	201	112	C6-N1	2.01	1.41	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	AGS	C4-N9-C8	-4.31	101.22	105.74
3	B	601	AGS	N9-C8-N7	4.25	119.97	113.94
3	B	601	AGS	C2'-C1'-N9	-4.17	102.95	113.30
4	C	201	112	O3A-PB-O1B	-4.01	98.65	110.70
4	C	201	112	N9-C8-N7	3.42	118.79	113.94
4	C	201	112	C4-N9-C8	-2.98	102.61	105.74
3	B	601	AGS	PB-O3B-PG	-2.79	122.97	133.17
3	B	601	AGS	O2A-PA-O5'	2.62	119.43	107.57
4	C	201	112	O2S-C2S-NS	-2.51	115.83	122.53
3	B	601	AGS	C1'-N9-C8	2.45	132.53	127.09
4	C	201	112	O2'-C2'-C1'	2.34	118.16	110.10
3	B	601	AGS	C4-C5-N7	2.34	113.26	110.58
4	C	201	112	O2G-PG-O3B	-2.31	101.03	107.27
4	C	201	112	C6-C5-C4	-2.29	114.05	117.18
4	C	201	112	N3-C2-N1	-2.29	125.12	128.58
3	B	601	AGS	O2A-PA-O1A	2.13	122.34	112.44
3	B	601	AGS	C3'-C2'-C1'	2.09	105.41	101.46
4	C	201	112	O4'-C4'-C3'	2.06	109.24	105.15
4	C	201	112	O2A-PA-O5'	2.04	116.83	107.57
3	B	601	AGS	C5-N7-C8	-2.02	100.27	103.45
3	B	601	AGS	O3A-PB-O1B	-2.02	104.62	110.70
4	C	201	112	C4-C5-N7	2.02	112.89	110.58

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	AGS	PB-O3A-PA-O5'
3	B	601	AGS	C5'-O5'-PA-O1A
3	B	601	AGS	C5'-O5'-PA-O3A
4	C	201	112	PB-O3A-PA-O5'
3	B	601	AGS	O4'-C4'-C5'-O5'
4	C	201	112	PG-O3B-PB-O3A
3	B	601	AGS	C3'-C4'-C5'-O5'
3	B	601	AGS	PA-O3A-PB-O1B
3	B	601	AGS	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	C	201	112	PG-O3B-PB-O2B
4	C	201	112	PB-O3A-PA-O2A
3	B	601	AGS	PB-O3A-PA-O2A
4	C	201	112	PB-O3A-PA-O1A

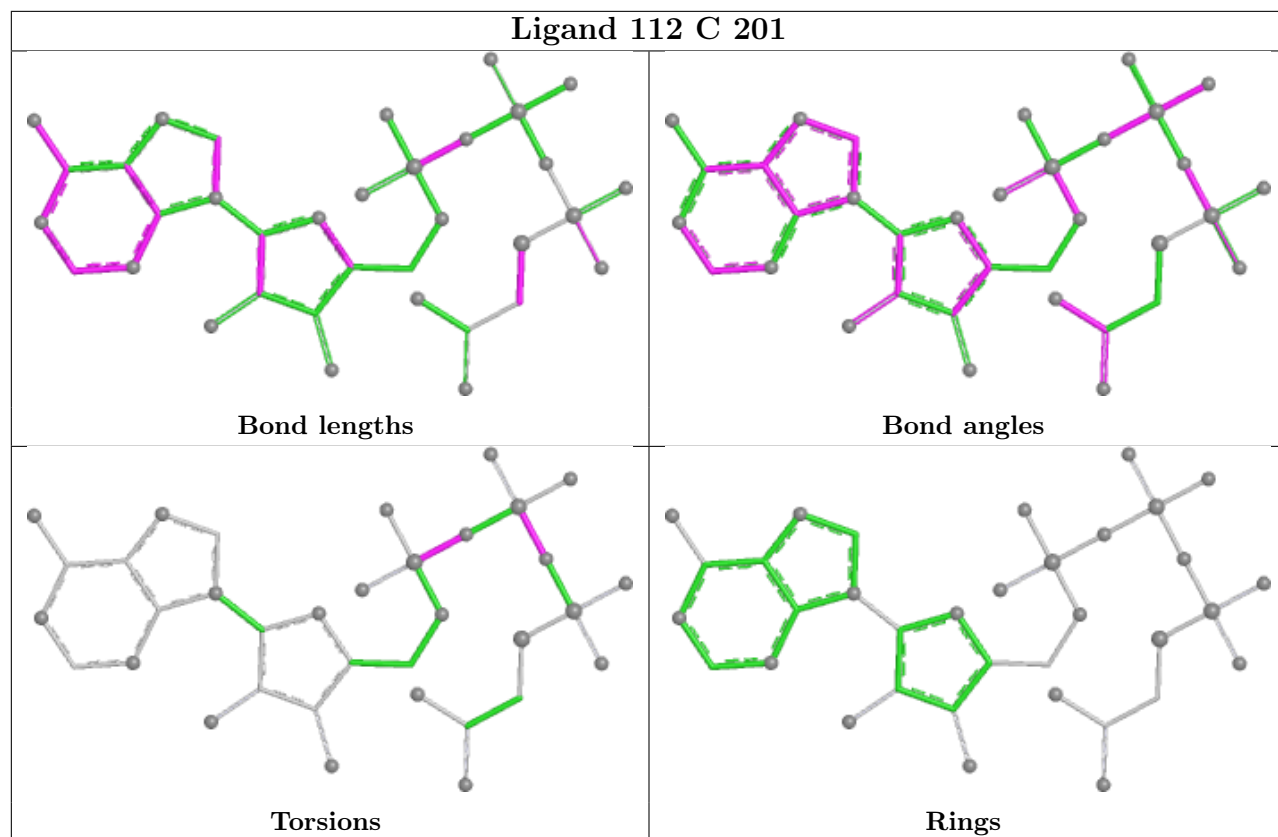
There are no ring outliers.

2 monomers are involved in 6 short contacts:

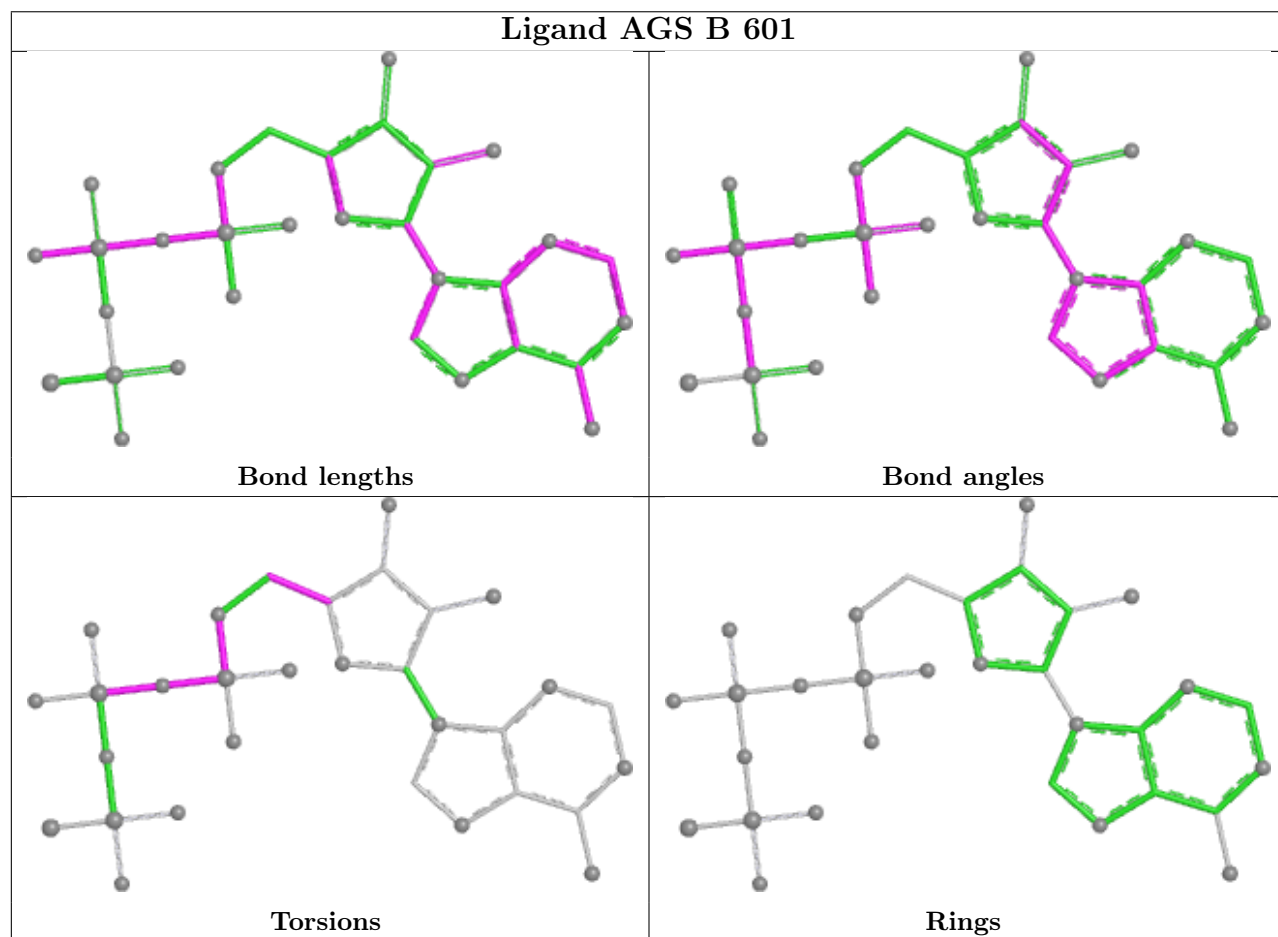
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	112	5	0
3	B	601	AGS	1	0

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.

Ligand 112 C 201



Ligand AGS B 601



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	275/287 (95%)	0.31	18 (6%) 25 22	21, 41, 81, 93	0
1	B	264/287 (91%)	0.71	35 (13%) 7 6	25, 52, 104, 117	0
2	C	8/11 (72%)	0.96	2 (25%) 2 1	49, 55, 63, 66	0
All	All	547/585 (93%)	0.52	55 (10%) 12 10	21, 47, 98, 117	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	VAL	5.2
1	B	382	PHE	4.8
1	A	274	LYS	4.5
1	B	502	ILE	4.4
1	B	254	GLY	4.4
1	A	505	GLU	4.4
1	A	238	GLU	3.9
1	B	248	LEU	3.7
1	B	256	VAL	3.6
1	A	249	GLY	3.5
1	B	234	LYS	3.5
1	B	236	GLU	3.3
1	A	253	TYR	3.2
1	B	397	ALA	3.1
1	B	255	GLU	3.0
1	A	273	LEU	3.0
1	A	250	GLY	3.0
2	C	111	PHE	2.9
1	A	308	GLU	2.8
1	A	272	THR	2.8
1	A	232	TYR	2.8
1	B	279	GLU	2.7
1	B	266	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	276	ASP	2.6
1	B	245	LYS	2.6
1	B	275	GLU	2.6
2	C	104	GLU	2.6
1	B	235	TRP	2.5
1	B	247	LYS	2.5
1	B	373	GLU	2.5
1	B	300	GLN	2.5
1	B	242	ILE	2.5
1	B	246	HIS	2.5
1	B	399	ALA	2.5
1	B	286	GLU	2.4
1	B	260	VAL	2.4
1	B	283	PHE	2.4
1	B	237	MET	2.3
1	A	275	GLU	2.3
1	A	306	THR	2.3
1	B	272	THR	2.2
1	B	317	PHE	2.2
1	B	264	TYR	2.2
1	A	252	GLN	2.2
1	B	398	GLY	2.2
1	B	306	THR	2.1
1	B	400	LYS	2.1
1	B	261	TRP	2.1
1	A	312	TYR	2.1
1	B	263	LYS	2.0
1	A	498	GLN	2.0
1	B	311	PHE	2.0
1	A	504	ASP	2.0
1	B	239	ARG	2.0
1	B	257	TYR	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](#)

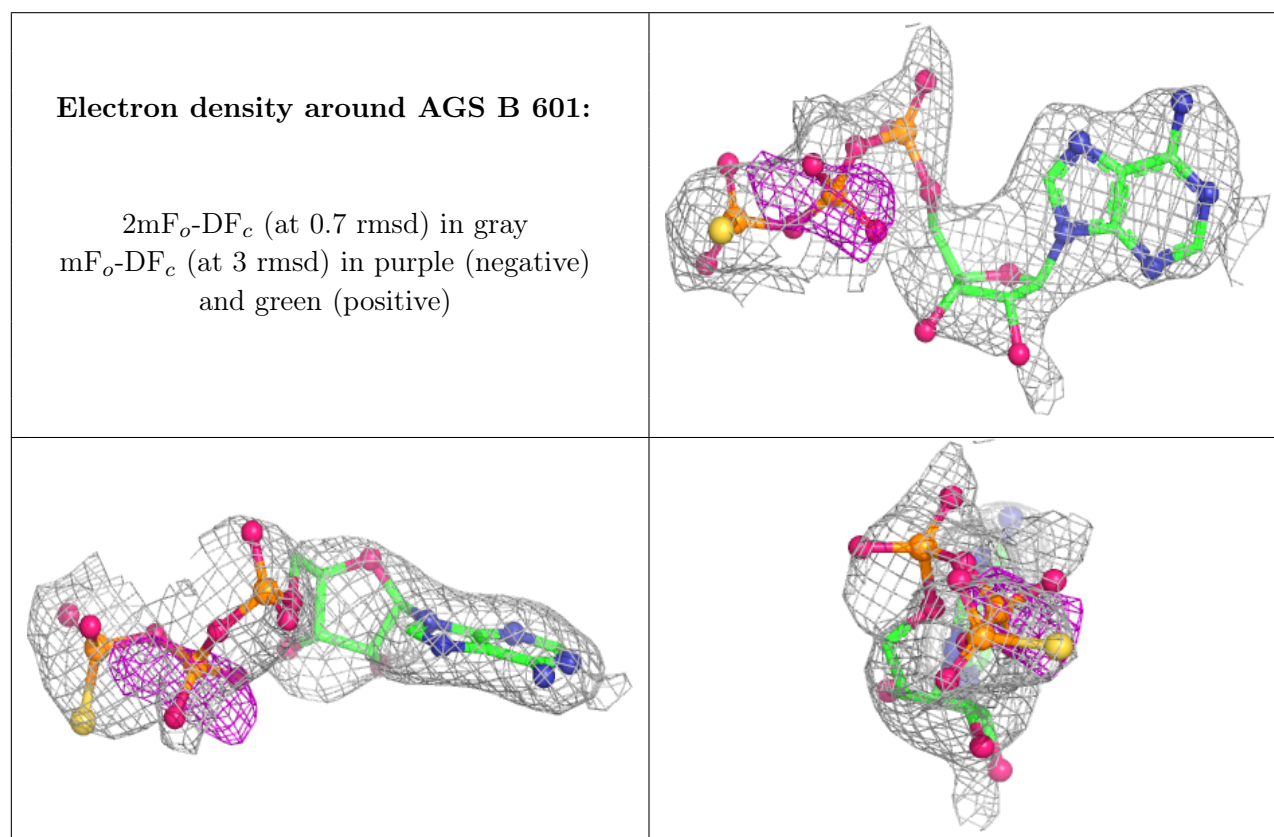
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

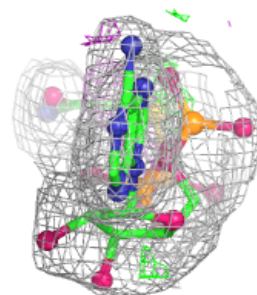
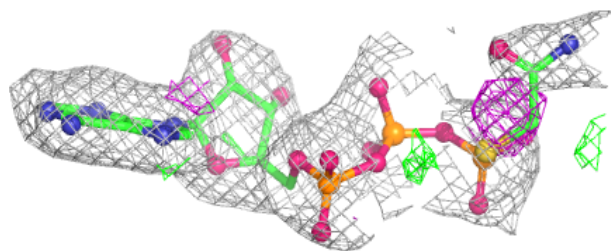
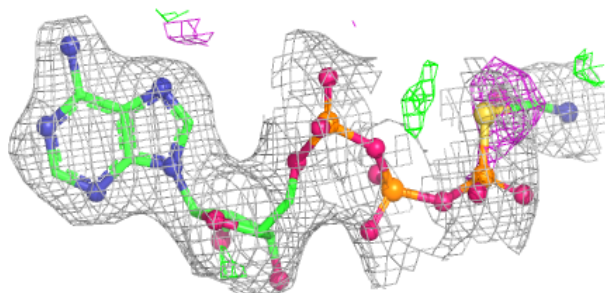
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AGS	B	601	31/31	0.73	0.14	73,87,107,108	0
4	112	C	201	35/35	0.88	0.11	30,51,77,78	0

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 112 C 201:

$2mF_o-DF_c$ (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.