



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:56 PM UTC

PDB ID : 4N4T / pdb_00004n4t
Title : Co-crystal structure of tankyrase 1 with compound 3 [(4S)-3-{4-[6-amino-5-(pyrimidin-2-yl)pyridin-3-yl]phenyl}-5,5-dimethyl-4-phenyl-1,3-oxazolidin-2-one]
Authors : Huang, X.
Deposited on : 2013-10-08
Resolution : 2.31 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

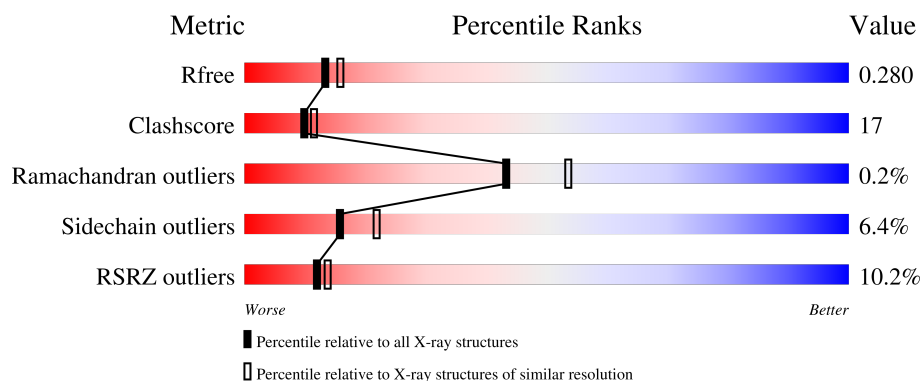
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	217	11% 67% 28% ..
1	B	217	9% 58% 28% 6% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2GV	A	1402	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3501 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 Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1694	1066	309	308	11			
1	B	199	Total	C	N	O	S	0	0	0
			1598	1006	292	290	10			

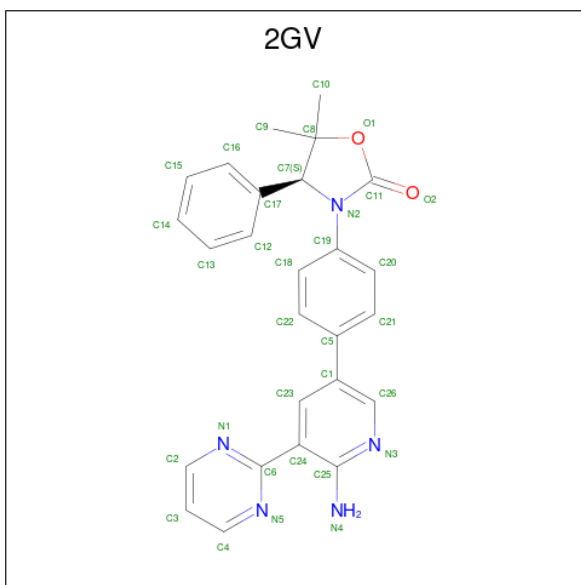
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1315	HIS	-	expression tag	UNP Q6PFX9
A	1316	HIS	-	expression tag	UNP Q6PFX9
A	1317	HIS	-	expression tag	UNP Q6PFX9
A	1318	HIS	-	expression tag	UNP Q6PFX9
A	1319	HIS	-	expression tag	UNP Q6PFX9
A	1320	HIS	-	expression tag	UNP Q6PFX9
B	1315	HIS	-	expression tag	UNP Q6PFX9
B	1316	HIS	-	expression tag	UNP Q6PFX9
B	1317	HIS	-	expression tag	UNP Q6PFX9
B	1318	HIS	-	expression tag	UNP Q6PFX9
B	1319	HIS	-	expression tag	UNP Q6PFX9
B	1320	HIS	-	expression tag	UNP Q6PFX9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (4S)-3-{4-[6-amino-5-(pyrimidin-2-yl)pyridin-3-yl]phenyl}-5,5-dimethyl-4-phenyl-1,3-oxazolidin-2-one (CCD ID: 2GV) (formula: C₂₆H₂₃N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	26	5	2		
3	B	1	Total	C	N	O	0	0
			33	26	5	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	67	Total	O	0	0
			67	67		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.94Å 77.88Å 147.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 50.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.31) 99.2 (50.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.275 0.260 , 0.280	Depositor DCC
R_{free} test set	1111 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3501	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 20.03 % 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 9.5043e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, 2GV

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	0.53	0/1738	1.04	8/2340 (0.3%)
1	B	0.54	1/1637 (0.1%)	0.99	5/2200 (0.2%)
All	All	0.54	1/3375 (0.0%)	1.02	13/4540 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1148	ILE	CB-CG2	5.21	1.69	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	GLY	N-CA-C	-10.30	101.66	115.36
1	B	1252	CYS	N-CA-C	6.59	120.26	109.85
1	A	1281	ARG	N-CA-C	6.37	118.74	110.40
1	A	1288	ALA	N-CA-C	-6.30	105.91	113.97
1	B	1310	ILE	N-CA-C	-6.22	99.30	109.12
1	B	1268	MET	N-CA-C	5.92	118.55	110.55
1	A	1236	THR	N-CA-C	5.78	117.38	111.14
1	B	1203	TYR	N-CA-C	5.62	118.38	109.50
1	A	1252	CYS	N-CA-C	5.37	118.46	110.14
1	A	1208	PHE	N-CA-C	5.15	118.46	110.17
1	A	1293	VAL	N-CA-C	5.13	115.86	108.48
1	B	1143	ASN	N-CA-C	-5.11	107.72	114.31
1	A	1310	ILE	N-CA-C	-5.03	101.22	108.87

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	1694	0	1608	51	0
1	B	1598	0	1504	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	23	3	0
3	B	33	0	23	2	0
4	A	74	0	0	3	0
4	B	67	0	0	6	0
All	All	3501	0	3158	114	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 17.

All (114) 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:1122:GLU:HG3	1:B:1147:VAL:HG21	1.53	0.89
1:A:1204:ILE:HD13	1:A:1209:GLY:HA2	1.56	0.87
1:B:1104:GLN:O	1:B:1104:GLN:HG3	1.79	0.82
1:B:1144:ARG:HD2	1:B:1311:MET:SD	2.23	0.78
1:A:1281:ARG:NH1	1:B:1259:SER:O	2.17	0.77
1:B:1152:LYS:HD3	4:B:1550:HOH:O	1.87	0.73
1:B:1156:LYS:O	1:B:1160:GLU:HG3	1.89	0.72
1:B:1199:GLU:HG2	1:B:1295:TYR:O	1.90	0.72
1:A:1262:GLN:NE2	1:A:1264:SER:O	2.23	0.71
1:A:1204:ILE:HD11	1:A:1268:MET:O	1.88	0.71
1:B:1131:GLU:H	1:B:1131:GLU:CD	1.97	0.70
1:B:1220:LYS:HB2	1:B:1220:LYS:NZ	2.08	0.69
1:A:1199:GLU:HG2	1:A:1295:TYR:O	1.92	0.69
1:A:1260:PHE:HE2	1:A:1262:GLN:HG2	1.58	0.69
1:A:1146:ASN:ND2	1:A:1148:ILE:HD11	2.07	0.69
1:B:1204:ILE:HD11	1:B:1268:MET:O	1.93	0.69
1:B:1190:ASN:O	1:B:1194:HIS:HD2	1.77	0.67
1:A:1132:HIS:C	1:A:1134:ASP:H	2.01	0.67
1:B:1114:GLU:OE1	1:B:1114:GLU:N	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:GLU:HG3	4:A:1552:HOH:O	1.97	0.65
1:B:1148:ILE:HD11	1:B:1307:THR:HG22	1.78	0.65
1:B:1314:GLU:O	1:B:1315:HIS:HB2	1.96	0.65
1:B:1204:ILE:HD13	1:B:1209:GLY:HA2	1.81	0.62
1:B:1217:ASN:OD1	1:B:1289:TYR:CB	2.47	0.62
1:B:1176:HIS:HB3	4:B:1520:HOH:O	1.98	0.62
1:B:1178:ASN:ND2	1:B:1256:LEU:HB2	2.15	0.62
1:A:1117:GLU:OE2	1:A:1152:LYS:HE2	2.00	0.61
1:B:1199:GLU:CD	1:B:1199:GLU:H	2.06	0.61
1:B:1232:THR:HG22	4:B:1508:HOH:O	2.00	0.60
1:A:1260:PHE:CE2	1:A:1262:GLN:HG2	2.36	0.59
1:B:1117:GLU:CD	1:B:1152:LYS:HZ2	2.11	0.58
1:B:1234:CYS:SG	1:B:1237:HIS:HB2	2.43	0.58
1:B:1235:PRO:O	1:B:1238:LYS:NZ	2.35	0.58
1:B:1167:LYS:O	1:B:1171:GLU:HG3	2.03	0.57
1:A:1199:GLU:HG3	1:A:1297:GLY:H	1.70	0.57
1:B:1216:GLU:HG3	1:B:1292:TYR:HE2	1.70	0.56
1:B:1263:PHE:N	1:B:1263:PHE:CD2	2.74	0.56
1:A:1204:ILE:HD13	1:A:1209:GLY:CA	2.30	0.56
1:A:1184:HIS:HE1	3:A:1402:2GV:H14	1.71	0.55
1:A:1252:CYS:HB3	1:A:1301:TYR:O	2.06	0.55
3:A:1402:2GV:H14	3:A:1402:2GV:O2	2.07	0.54
1:B:1314:GLU:O	1:B:1315:HIS:CB	2.55	0.54
1:A:1128:THR:HB	1:A:1217:ASN:HA	1.90	0.54
1:A:1266:MET:O	1:A:1267:LYS:CB	2.56	0.53
1:A:1178:ASN:HD22	1:A:1178:ASN:C	2.16	0.53
1:A:1189:ILE:HD12	1:A:1250:LEU:HG	1.92	0.52
1:B:1220:LYS:HB2	1:B:1220:LYS:HZ3	1.73	0.52
1:A:1268:MET:HE2	1:A:1278:VAL:HG21	1.92	0.51
1:B:1148:ILE:HD11	1:B:1307:THR:CG2	2.40	0.51
1:B:1279:ILE:HG12	1:B:1292:TYR:CD1	2.45	0.51
1:B:1248:GLN:HA	1:B:1306:ILE:O	2.11	0.51
1:B:1258:LYS:HD3	1:B:1274:GLY:O	2.10	0.51
1:B:1220:LYS:HB2	1:B:1220:LYS:HZ2	1.76	0.51
1:B:1117:GLU:CD	1:B:1152:LYS:NZ	2.69	0.50
1:A:1281:ARG:HD3	4:A:1524:HOH:O	2.12	0.49
1:A:1178:ASN:HA	1:B:1176:HIS:CE1	2.47	0.49
1:B:1267:LYS:N	4:B:1518:HOH:O	2.45	0.49
1:A:1184:HIS:CE1	3:A:1402:2GV:H14	2.48	0.49
1:B:1220:LYS:NZ	1:B:1220:LYS:CB	2.74	0.48
1:A:1213:TYR:OH	1:A:1265:THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:ARG:HB2	1:A:1303:GLU:OE1	2.13	0.48
1:A:1134:ASP:C	1:A:1136:GLY:H	2.21	0.47
1:A:1146:ASN:HD21	1:A:1148:ILE:HD11	1.76	0.47
1:B:1289:TYR:O	1:B:1290:ALA:HB3	2.14	0.47
1:B:1128:THR:HB	1:B:1217:ASN:HA	1.95	0.47
1:B:1186:SER:O	1:B:1189:ILE:HG12	2.14	0.47
1:B:1216:GLU:OE1	1:B:1290:ALA:HB3	2.14	0.47
1:A:1132:HIS:C	1:A:1134:ASP:N	2.72	0.47
1:A:1129:ILE:HD11	1:A:1145:TYR:CE2	2.50	0.46
1:A:1207:MET:CB	4:A:1566:HOH:O	2.62	0.46
1:B:1117:GLU:OE2	1:B:1152:LYS:NZ	2.49	0.46
1:A:1199:GLU:HG2	1:A:1296:ARG:HA	1.97	0.46
1:A:1134:ASP:HB3	1:A:1136:GLY:H	1.81	0.45
1:B:1298:GLU:H	1:B:1298:GLU:CD	2.24	0.45
1:B:1228:ILE:C	1:B:1230:GLY:H	2.25	0.45
1:A:1113:PRO:HA	1:A:1118:TYR:CD2	2.52	0.45
1:A:1134:ASP:C	1:A:1136:GLY:N	2.73	0.45
1:A:1153:VAL:HB	1:A:1302:PRO:O	2.16	0.45
1:B:1222:ASN:HA	1:B:1225:VAL:HG23	1.99	0.45
1:B:1253:ARG:HH11	1:B:1253:ARG:HG2	1.81	0.45
1:A:1124:GLU:O	1:A:1128:THR:HG23	2.17	0.44
1:A:1167:LYS:HG2	1:A:1171:GLU:OE2	2.17	0.44
1:A:1198:ASP:OD1	1:A:1200:ARG:HB2	2.17	0.44
1:A:1260:PHE:CE2	1:A:1262:GLN:CG	3.01	0.44
1:B:1209:GLY:HA3	4:B:1564:HOH:O	2.17	0.44
3:B:1402:2GV:O2	3:B:1402:2GV:H14	2.17	0.44
1:B:1178:ASN:CG	1:B:1178:ASN:O	2.60	0.44
1:B:1144:ARG:HD3	1:B:1145:TYR:O	2.17	0.44
1:A:1165:ARG:HB2	1:A:1298:GLU:HG3	2.00	0.43
1:A:1178:ASN:C	1:A:1178:ASN:ND2	2.73	0.43
1:B:1173:ASN:ND2	1:B:1176:HIS:O	2.31	0.43
1:A:1207:MET:C	1:A:1266:MET:HB3	2.43	0.43
1:A:1158:LEU:HD21	1:A:1196:GLY:HA3	2.00	0.43
1:B:1159:ARG:HH22	1:B:1303:GLU:CD	2.26	0.43
1:B:1140:GLY:HA2	1:B:1241:SER:HB2	2.01	0.43
1:A:1188:PHE:O	1:A:1192:ILE:HG13	2.19	0.43
1:A:1262:GLN:OE1	1:A:1268:MET:SD	2.77	0.43
1:B:1131:GLU:CD	1:B:1131:GLU:N	2.71	0.42
1:B:1149:ARG:HB3	1:B:1307:THR:HB	2.02	0.42
1:B:1197:PHE:HB3	1:B:1212:ILE:HD13	2.01	0.42
1:B:1253:ARG:HG2	1:B:1253:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:HIS:O	1:A:1238:LYS:C	2.62	0.42
1:B:1258:LYS:HE2	4:B:1559:HOH:O	2.18	0.42
1:B:1117:GLU:OE1	1:B:1152:LYS:NZ	2.53	0.42
1:B:1158:LEU:HD21	1:B:1196:GLY:CA	2.50	0.42
1:A:1129:ILE:HD11	1:A:1145:TYR:CD2	2.55	0.42
1:A:1268:MET:HE3	1:A:1268:MET:HB3	1.96	0.42
1:A:1204:ILE:HD11	1:A:1268:MET:C	2.45	0.42
1:B:1228:ILE:C	1:B:1230:GLY:N	2.78	0.41
1:A:1173:ASN:HB3	1:A:1176:HIS:O	2.21	0.41
1:A:1148:ILE:O	1:A:1148:ILE:HG23	2.19	0.41
3:B:1402:2GV:N5	3:B:1402:2GV:N4	2.63	0.41
1:B:1204:ILE:HD13	1:B:1209:GLY:CA	2.51	0.41
1:B:1312:LYS:HB2	1:B:1312:LYS:HE2	1.56	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	210/217 (97%)	204 (97%)	6 (3%)	0	100	100
1	B	191/217 (88%)	185 (97%)	5 (3%)	1 (0%)	24	30
All	All	401/434 (92%)	389 (97%)	11 (3%)	1 (0%)	43	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1290	ALA

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	176/185 (95%)	165 (94%)	11 (6%)	16	22
1	B	166/185 (90%)	155 (93%)	11 (7%)	15	21
All	All	342/370 (92%)	320 (94%)	22 (6%)	16	22

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1104	GLN
1	A	1123	GLU
1	A	1148	ILE
1	A	1161	ARG
1	A	1199	GLU
1	A	1216	GLU
1	A	1252	CYS
1	A	1266	MET
1	A	1283	SER
1	A	1303	GLU
1	A	1315	HIS
1	B	1104	GLN
1	B	1131	GLU
1	B	1144	ARG
1	B	1152	LYS
1	B	1158	LEU
1	B	1199	GLU
1	B	1208	PHE
1	B	1220	LYS
1	B	1249	MET
1	B	1263	PHE
1	B	1312	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1166	GLN
1	A	1173	ASN
1	A	1178	ASN
1	A	1237	HIS
1	A	1262	GLN
1	A	1299	GLN
1	B	1104	GLN
1	B	1143	ASN
1	B	1176	HIS
1	B	1178	ASN
1	B	1190	ASN
1	B	1194	HIS
1	B	1262	GLN
1	B	1270	HIS
1	B	1299	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	2GV	A	1402	-	37,37,37	3.53	22 (59%)	52,54,54	3.49	29 (55%)
3	2GV	B	1402	-	37,37,37	3.53	23 (62%)	52,54,54	3.55	25 (48%)

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	2GV	A	1402	-	-	2/16/35/35	0/5/5/5
3	2GV	B	1402	-	-	0/16/35/35	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	2GV	O1-C8	7.80	1.59	1.48
3	B	1402	2GV	C8-C7	-7.20	1.47	1.55
3	A	1402	2GV	C19-N2	-6.91	1.31	1.43
3	B	1402	2GV	O1-C11	6.62	1.46	1.35
3	A	1402	2GV	C8-C7	-6.40	1.48	1.55
3	A	1402	2GV	C6-N1	6.26	1.44	1.34
3	B	1402	2GV	C19-N2	-6.25	1.32	1.43
3	A	1402	2GV	C16-C17	5.96	1.48	1.39
3	B	1402	2GV	C6-N5	5.61	1.43	1.34
3	B	1402	2GV	C16-C17	5.57	1.47	1.39
3	B	1402	2GV	C6-N1	5.41	1.43	1.34
3	B	1402	2GV	C12-C17	5.14	1.47	1.39
3	A	1402	2GV	C6-N5	4.78	1.42	1.34
3	A	1402	2GV	C26-C1	4.65	1.47	1.39
3	B	1402	2GV	O1-C8	4.47	1.55	1.48
3	B	1402	2GV	C26-C1	4.37	1.47	1.39
3	B	1402	2GV	C22-C5	4.34	1.48	1.39
3	A	1402	2GV	C22-C5	4.26	1.47	1.39
3	A	1402	2GV	C12-C17	4.10	1.45	1.39
3	B	1402	2GV	C23-C1	4.03	1.46	1.39
3	A	1402	2GV	C14-C13	3.99	1.47	1.38
3	A	1402	2GV	C15-C14	3.95	1.46	1.38
3	B	1402	2GV	C20-C19	3.89	1.46	1.39
3	A	1402	2GV	C21-C5	3.80	1.47	1.39
3	B	1402	2GV	C13-C12	3.62	1.45	1.38
3	B	1402	2GV	C21-C5	3.44	1.46	1.39
3	A	1402	2GV	C13-C12	3.38	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	2GV	C18-C19	3.36	1.45	1.39
3	A	1402	2GV	O1-C11	3.35	1.41	1.35
3	A	1402	2GV	C18-C19	3.35	1.45	1.39
3	A	1402	2GV	C20-C19	3.27	1.45	1.39
3	B	1402	2GV	C14-C13	3.24	1.45	1.38
3	B	1402	2GV	C15-C16	3.23	1.44	1.38
3	B	1402	2GV	C15-C14	3.21	1.45	1.38
3	A	1402	2GV	C3-C4	3.05	1.46	1.37
3	A	1402	2GV	C3-C2	2.99	1.46	1.37
3	A	1402	2GV	C15-C16	2.97	1.44	1.38
3	B	1402	2GV	C7-N2	2.89	1.53	1.48
3	B	1402	2GV	C3-C4	2.82	1.45	1.37
3	B	1402	2GV	C3-C2	2.71	1.45	1.37
3	A	1402	2GV	C17-C7	-2.50	1.47	1.51
3	A	1402	2GV	C22-C18	2.37	1.42	1.38
3	B	1402	2GV	C22-C18	2.31	1.42	1.38
3	B	1402	2GV	C17-C7	-2.15	1.48	1.51
3	A	1402	2GV	C4-N5	2.01	1.38	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1402	2GV	O1-C8-C7	-9.78	94.14	102.61
3	B	1402	2GV	C8-C7-N2	9.14	108.48	100.50
3	A	1402	2GV	O2-C11-N2	9.07	139.59	128.52
3	B	1402	2GV	O2-C11-N2	7.43	137.59	128.52
3	B	1402	2GV	C26-N3-C25	7.25	125.64	118.64
3	A	1402	2GV	O1-C8-C7	-7.12	96.45	102.61
3	B	1402	2GV	O1-C11-N2	-7.00	103.17	108.75
3	B	1402	2GV	C4-N5-C6	6.70	122.69	116.07
3	A	1402	2GV	C4-N5-C6	6.56	122.55	116.07
3	A	1402	2GV	C24-C6-N1	6.28	124.59	117.22
3	B	1402	2GV	C2-N1-C6	5.93	121.93	116.07
3	A	1402	2GV	C2-N1-C6	5.88	121.88	116.07
3	B	1402	2GV	C24-C6-N1	5.81	124.03	117.22
3	A	1402	2GV	O1-C11-N2	-5.46	104.40	108.75
3	A	1402	2GV	O1-C11-O2	-5.42	116.01	122.54
3	A	1402	2GV	C26-N3-C25	5.31	123.77	118.64
3	B	1402	2GV	C1-C26-N3	-5.22	115.98	124.28
3	A	1402	2GV	C8-C7-N2	5.13	104.98	100.50
3	A	1402	2GV	C1-C26-N3	-4.88	116.52	124.28
3	A	1402	2GV	C20-C19-N2	-4.65	115.05	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	2GV	C9-C8-C7	4.49	124.20	113.43
3	B	1402	2GV	C8-O1-C11	4.24	114.35	110.04
3	A	1402	2GV	C21-C5-C1	-4.20	114.01	121.25
3	B	1402	2GV	N5-C6-N1	-4.04	116.78	125.54
3	A	1402	2GV	N5-C6-N1	-3.90	117.08	125.54
3	B	1402	2GV	C8-C7-C17	-3.88	111.36	115.70
3	B	1402	2GV	C15-C14-C13	3.87	125.17	119.87
3	A	1402	2GV	C22-C18-C19	-3.86	115.41	120.30
3	A	1402	2GV	C16-C17-C12	3.71	122.90	118.30
3	A	1402	2GV	O1-C8-C10	3.56	110.65	106.77
3	A	1402	2GV	C12-C17-C7	-3.46	113.59	120.74
3	A	1402	2GV	C23-C24-C25	-3.39	114.43	117.36
3	B	1402	2GV	C16-C17-C12	3.30	122.39	118.30
3	A	1402	2GV	C20-C19-C18	3.25	125.37	119.18
3	A	1402	2GV	N4-C25-N3	-3.07	111.54	118.38
3	B	1402	2GV	C22-C18-C19	-2.98	116.53	120.30
3	A	1402	2GV	C15-C14-C13	2.94	123.90	119.87
3	A	1402	2GV	C24-C25-N4	2.92	125.81	121.23
3	A	1402	2GV	C23-C1-C26	2.82	120.12	117.10
3	B	1402	2GV	O1-C11-O2	-2.75	119.23	122.54
3	B	1402	2GV	C12-C17-C7	-2.63	115.30	120.74
3	A	1402	2GV	C22-C5-C21	2.58	122.29	117.68
3	B	1402	2GV	C20-C19-C18	2.43	123.82	119.18
3	A	1402	2GV	C14-C15-C16	-2.42	117.26	120.24
3	A	1402	2GV	C20-C21-C5	-2.37	118.08	121.12
3	B	1402	2GV	C23-C24-C25	-2.37	115.31	117.36
3	B	1402	2GV	C22-C5-C21	2.27	121.74	117.68
3	B	1402	2GV	C14-C13-C12	-2.23	117.49	120.24
3	B	1402	2GV	C9-C8-C7	2.18	118.65	113.43
3	A	1402	2GV	C17-C7-N2	-2.17	110.49	113.16
3	A	1402	2GV	C8-C7-C17	-2.17	113.27	115.70
3	B	1402	2GV	C14-C15-C16	-2.16	117.58	120.24
3	B	1402	2GV	C17-C7-N2	-2.05	110.64	113.16
3	B	1402	2GV	C20-C21-C5	-2.03	118.52	121.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

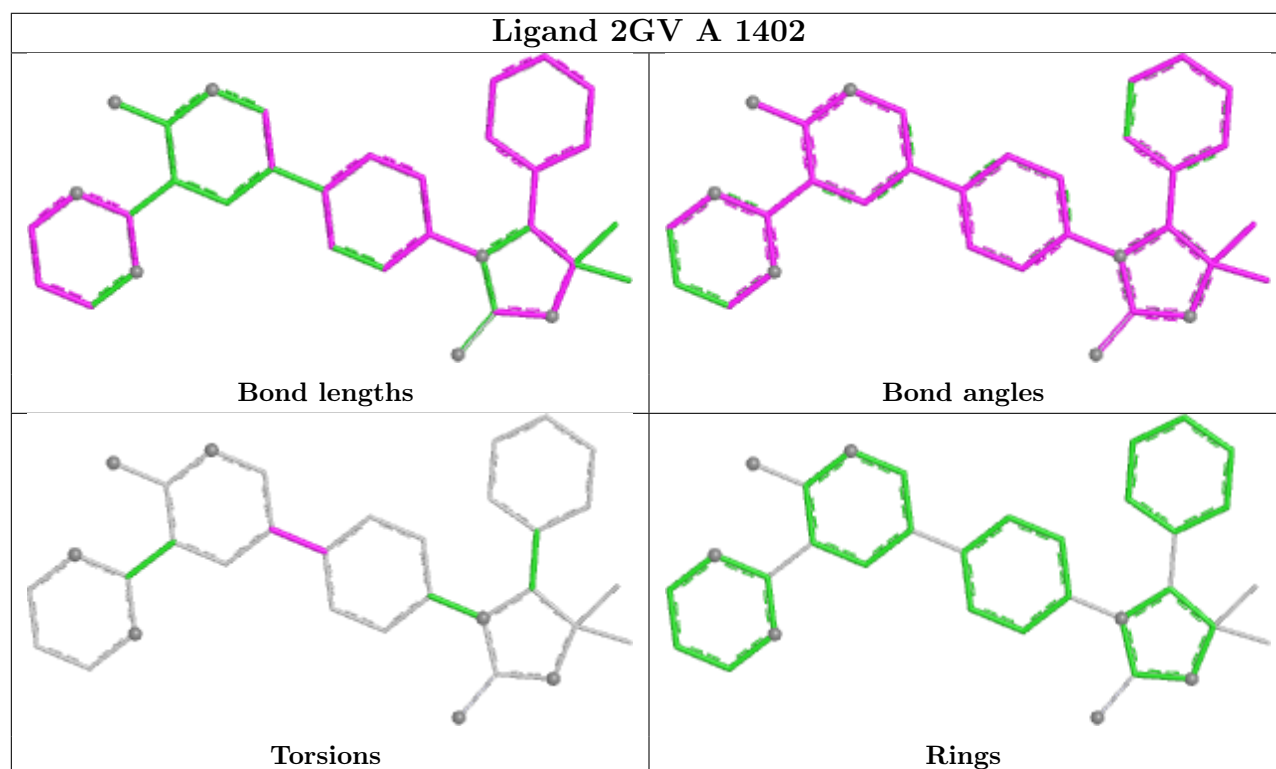
Mol	Chain	Res	Type	Atoms
3	A	1402	2GV	C23-C1-C5-C22
3	A	1402	2GV	C23-C1-C5-C21

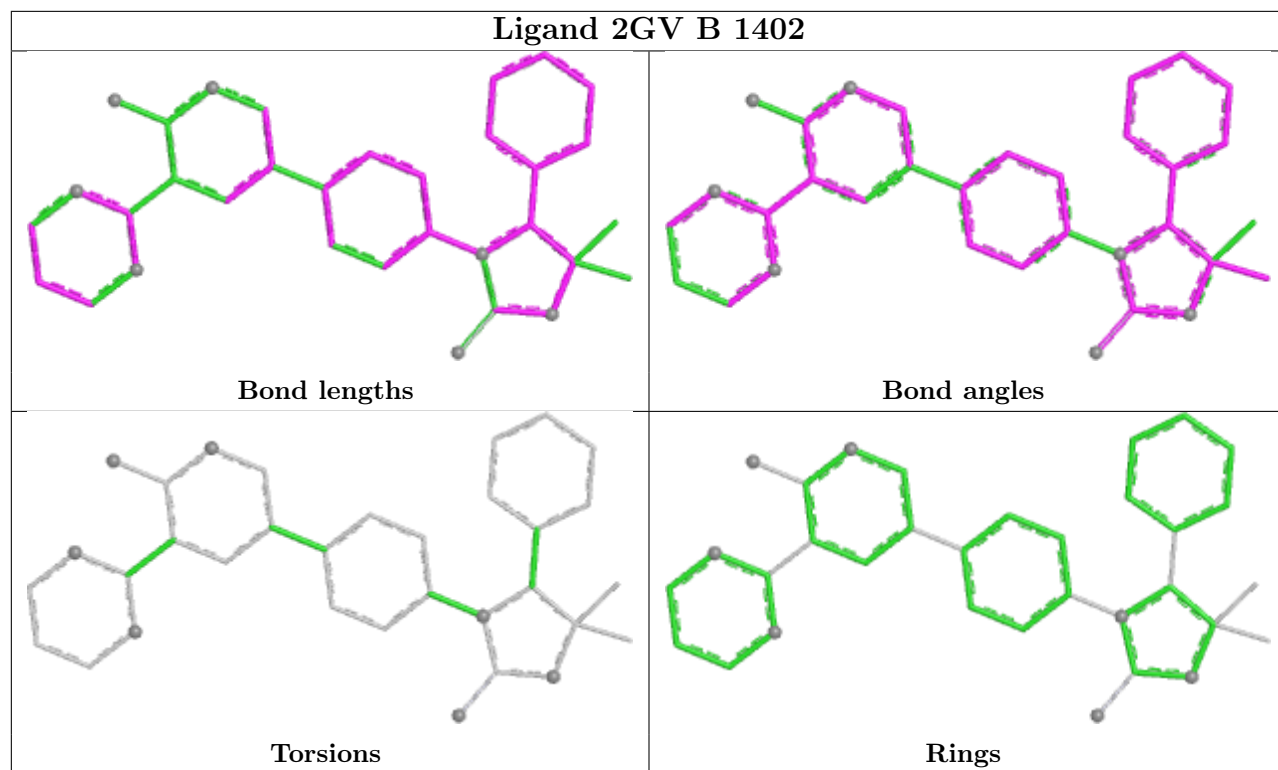
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	2GV	3	0
3	B	1402	2GV	2	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	212/217 (97%)	0.73	23 (10%) 11 12	17, 26, 37, 41	0
1	B	199/217 (91%)	0.82	19 (9%) 14 16	18, 29, 39, 44	0
All	All	411/434 (94%)	0.78	42 (10%) 12 14	17, 27, 38, 44	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1206	GLY	6.2
1	B	1289	TYR	4.0
1	B	1104	GLN	3.8
1	B	1208	PHE	3.5
1	B	1204	ILE	3.5
1	B	1315	HIS	3.4
1	A	1207	MET	3.3
1	A	1315	HIS	3.3
1	B	1123	GLU	3.1
1	B	1264	SER	3.0
1	B	1115	ASP	2.9
1	B	1280	GLY	2.9
1	B	1131	GLU	2.9
1	A	1283	SER	2.9
1	A	1262	GLN	2.8
1	B	1171	GLU	2.8
1	B	1134	ASP	2.7
1	A	1161	ARG	2.7
1	A	1281	ARG	2.6
1	A	1205	GLY	2.6
1	A	1167	LYS	2.6
1	A	1291	GLU	2.6
1	B	1279	ILE	2.6
1	A	1303	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1177	HIS	2.5
1	B	1159	ARG	2.4
1	A	1314	GLU	2.3
1	B	1161	ARG	2.3
1	A	1171	GLU	2.2
1	A	1264	SER	2.2
1	B	1267	LYS	2.2
1	A	1131	GLU	2.2
1	A	1104	GLN	2.2
1	A	1156	LYS	2.2
1	A	1208	PHE	2.1
1	B	1312	LYS	2.1
1	B	1160	GLU	2.1
1	A	1203	TYR	2.1
1	A	1285	ASN	2.1
1	B	1178	ASN	2.1
1	A	1160	GLU	2.1
1	A	1174	HIS	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](#)

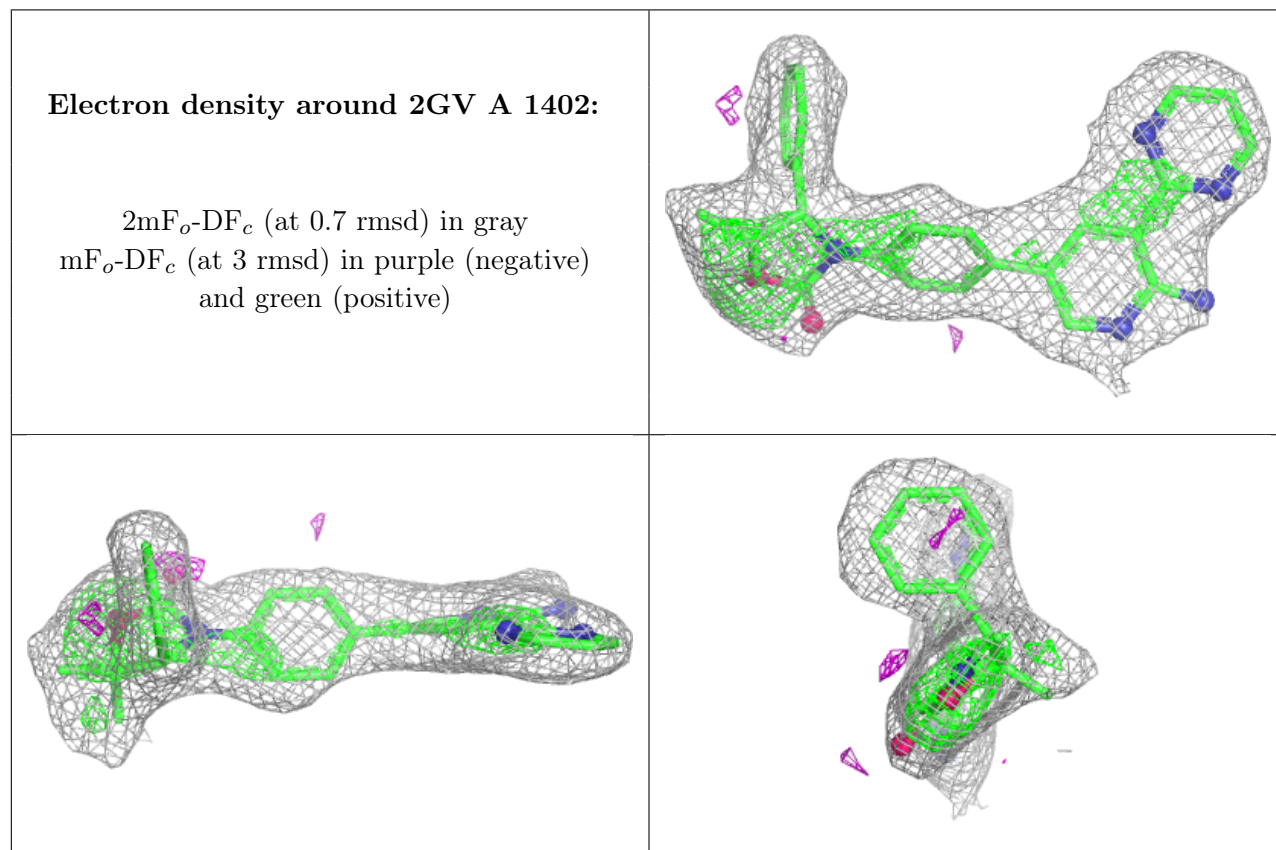
There are no oligosaccharides in this entry.

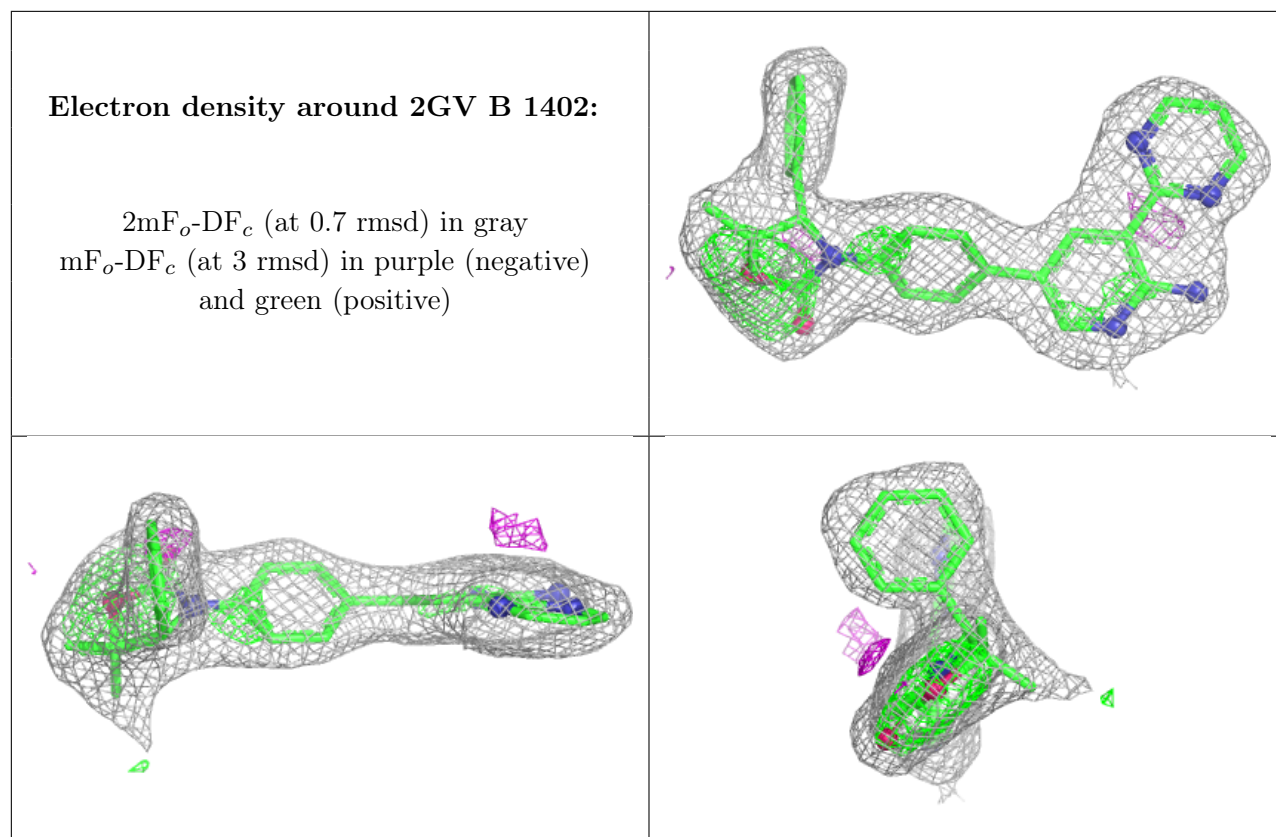
6.4 Ligands [i](#)

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
3	2GV	A	1402	33/33	0.86	0.27	39,49,63,67	0
3	2GV	B	1402	33/33	0.87	0.25	44,53,67,71	0
2	ZN	A	1401	1/1	0.99	0.05	24,24,24,24	0
2	ZN	B	1401	1/1	0.99	0.06	30,30,30,30	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.