



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 AM UTC

PDB ID : 4N4V / pdb_00004n4v
Title : Co-crystal structure of tankyrase 1 with compound 4 [(4S)-3-{trans-4-[6-amin
o-5-(pyrimidin-2-yl)pyridin-3-yl]cyclohexyl}-5,5-dimethyl-4-phenyl-1,3-oxazol
idin-2-one]
Authors : Huang, X.
Deposited on : 2013-10-08
Resolution : 2.00 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

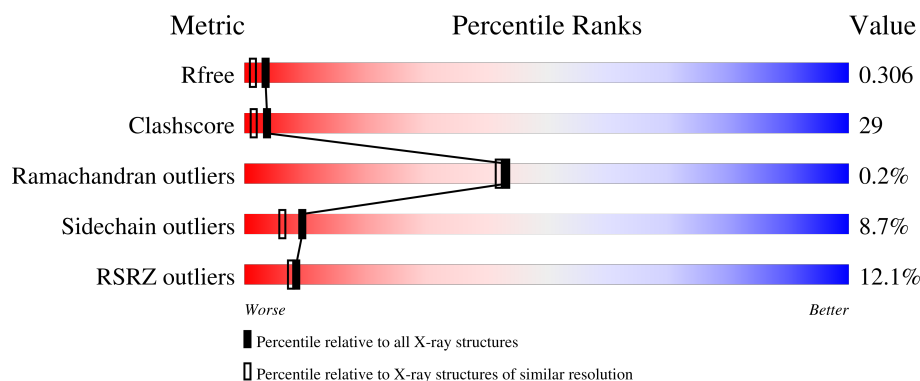
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	9% 63% 29% 5%
1	B	217	14% 50% 34% 6% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3734 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	211	Total	C	N	O	S	0	0	0
			1697	1068	310	307	12			
1	B	202	Total	C	N	O	S	0	0	0
			1615	1016	294	294	11			

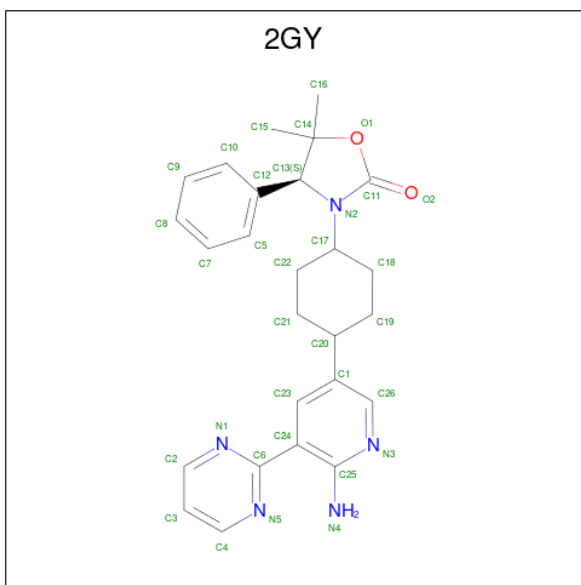
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1315	HIS	-	expression tag	UNP O95271
A	1316	HIS	-	expression tag	UNP O95271
A	1317	HIS	-	expression tag	UNP O95271
A	1318	HIS	-	expression tag	UNP O95271
A	1319	HIS	-	expression tag	UNP O95271
A	1320	HIS	-	expression tag	UNP O95271
B	1315	HIS	-	expression tag	UNP O95271
B	1316	HIS	-	expression tag	UNP O95271
B	1317	HIS	-	expression tag	UNP O95271
B	1318	HIS	-	expression tag	UNP O95271
B	1319	HIS	-	expression tag	UNP O95271
B	1320	HIS	-	expression tag	UNP O95271

- 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-{trans-4-[6-amino-5-(pyrimidin-2-yl)pyridin-3-yl]cyclohexyl}-5,5-dimethyl-4-phenyl-1,3-oxazolidin-2-one (CCD ID: 2GY) (formula: C₂₆H₂₉N₅O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	201	Total O 201 201	0	0
4	B	153	Total O 153 153	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	41.99Å 77.72Å 147.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 94.4 (50.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.97Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.290 0.280 , 0.306	Depositor DCC
R_{free} test set	1666 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.5	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	3734	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.90% 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: ZN, 2GY

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	0.64	0/1740	1.13	16/2339 (0.7%)
1	B	0.82	2/1655 (0.1%)	1.35	24/2225 (1.1%)
All	All	0.73	2/3395 (0.1%)	1.25	40/4564 (0.9%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1266	MET	C-N	14.76	1.53	1.33
1	B	1266	MET	C-O	-6.62	1.15	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1133	ARG	NE-CZ-NH1	-14.63	106.87	121.50
1	B	1133	ARG	NE-CZ-NH2	11.71	129.74	119.20
1	A	1172	GLU	CA-CB-CG	9.94	133.97	114.10
1	B	1133	ARG	CD-NE-CZ	-9.76	110.74	124.40
1	B	1159	ARG	NE-CZ-NH1	-8.80	112.69	121.50
1	B	1267	LYS	CA-C-N	-8.69	106.93	122.74
1	B	1267	LYS	C-N-CA	-8.69	106.93	122.74
1	B	1267	LYS	O-C-N	8.15	132.84	123.31
1	B	1195	LYS	CA-CB-CG	7.39	128.88	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1133	ARG	CA-CB-CG	7.38	128.86	114.10
1	B	1159	ARG	NE-CZ-NH2	7.23	125.71	119.20
1	A	1266	MET	N-CA-C	7.04	121.69	113.18
1	B	1264	SER	N-CA-C	6.87	119.83	110.35
1	B	1178	ASN	CA-CB-CG	6.71	119.31	112.60
1	B	1171	GLU	CA-CB-CG	6.68	127.46	114.10
1	A	1310	ILE	N-CA-C	-6.62	100.42	109.55
1	B	1116	LYS	CA-CB-CG	6.58	127.26	114.10
1	B	1178	ASN	CB-CA-C	6.57	122.20	112.09
1	B	1313	PRO	N-CA-C	-6.35	101.29	111.38
1	A	1258	LYS	CA-CB-CG	6.35	126.79	114.10
1	B	1252	CYS	N-CA-C	6.11	119.50	109.85
1	B	1304	TYR	N-CA-C	6.10	118.84	108.90
1	A	1236	THR	N-CA-C	6.02	117.64	111.14
1	A	1251	PHE	N-CA-C	-5.96	97.43	107.99
1	B	1133	ARG	CG-CD-NE	5.87	124.92	112.00
1	A	1252	CYS	N-CA-C	5.86	119.22	110.14
1	A	1130	ARG	CA-CB-CG	5.76	125.62	114.10
1	A	1134	ASP	N-CA-C	5.74	119.36	112.93
1	B	1236	THR	N-CA-C	5.44	117.20	111.28
1	B	1269	ALA	N-CA-C	-5.37	106.86	113.41
1	A	1253	ARG	N-CA-C	-5.32	100.50	108.96
1	B	1137	ASN	N-CA-C	5.29	118.52	111.75
1	B	1207	MET	N-CA-C	5.25	119.39	113.15
1	B	1292	TYR	N-CA-C	5.25	117.95	109.40
1	A	1293	VAL	N-CA-C	5.22	116.00	108.48
1	A	1298	GLU	CA-CB-CG	5.04	124.19	114.10
1	A	1130	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	A	1129	ILE	CA-C-N	-5.01	114.10	122.21
1	A	1129	ILE	C-N-CA	-5.01	114.10	122.21
1	A	1208	PHE	N-CA-C	5.01	116.99	109.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1159	ARG	Sidechain
1	B	1266	MET	Mainchain

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	1697	0	1630	85	0
1	B	1615	0	1532	115	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	28	2	0
3	B	33	0	29	4	0
4	A	201	0	0	27	2
4	B	153	0	0	39	2
All	All	3734	0	3219	191	2

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 29.

All (191) 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:1190:ASN:HB2	4:B:1613:HOH:O	1.25	1.28
1:B:1175:ASN:HB3	4:B:1543:HOH:O	1.40	1.20
1:B:1263:PHE:HB2	4:B:1577:HOH:O	1.38	1.19
1:B:1176:HIS:HD2	4:B:1633:HOH:O	1.26	1.19
1:B:1314:GLU:HB2	4:B:1599:HOH:O	1.49	1.10
1:A:1133:ARG:HD2	4:A:1694:HOH:O	1.48	1.10
1:B:1176:HIS:CD2	4:B:1633:HOH:O	2.01	1.08
1:A:1248:GLN:OE1	4:A:1570:HOH:O	1.74	1.06
1:B:1107:ILE:HG13	4:B:1621:HOH:O	1.55	1.05
1:A:1298:GLU:CG	4:A:1549:HOH:O	2.06	1.03
1:A:1296:ARG:CZ	4:A:1647:HOH:O	2.09	0.98
1:A:1161:ARG:NH2	1:A:1298:GLU:OE2	1.97	0.97
1:B:1263:PHE:CB	4:B:1577:HOH:O	2.01	0.96
1:B:1262:GLN:NE2	4:B:1612:HOH:O	1.89	0.95
1:B:1153:VAL:O	4:B:1596:HOH:O	1.84	0.95
1:A:1116:LYS:HE3	4:A:1685:HOH:O	1.68	0.93
1:A:1172:GLU:OE1	1:A:1276:HIS:NE2	2.01	0.92
1:B:1207:MET:H	1:B:1207:MET:HE2	1.39	0.88
1:A:1298:GLU:HG3	4:A:1549:HOH:O	1.68	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:MET:HE2	1:B:1207:MET:N	1.90	0.86
1:A:1296:ARG:NH2	4:A:1647:HOH:O	2.08	0.86
1:A:1281:ARG:HG2	1:A:1281:ARG:HH11	1.39	0.86
1:B:1314:GLU:C	4:B:1599:HOH:O	2.17	0.86
1:A:1283:SER:HA	1:B:1263:PHE:CE1	2.11	0.85
1:B:1268:MET:HE1	1:B:1278:VAL:HG21	1.57	0.85
1:A:1220:LYS:NZ	4:A:1512:HOH:O	1.92	0.83
1:B:1228:ILE:HD11	3:B:1402:2GY:H9	1.64	0.80
1:B:1252:CYS:HB3	1:B:1301:TYR:O	1.83	0.79
1:B:1178:ASN:ND2	1:B:1257:GLY:O	2.17	0.78
1:A:1130:ARG:HH11	1:A:1217:ASN:HD21	1.31	0.76
1:B:1270:HIS:HD2	4:B:1524:HOH:O	1.66	0.76
1:B:1239:ASP:OD1	4:B:1640:HOH:O	2.04	0.75
1:A:1144:ARG:HG2	1:A:1145:TYR:N	2.01	0.75
1:A:1298:GLU:H	1:A:1298:GLU:CD	1.93	0.75
1:A:1131:GLU:HB3	4:A:1658:HOH:O	1.86	0.75
1:B:1152:LYS:NZ	4:B:1649:HOH:O	2.20	0.74
1:B:1115:ASP:OD2	1:B:1117:GLU:HB3	1.88	0.74
1:A:1253:ARG:HG3	1:A:1303:GLU:HG2	1.70	0.73
1:B:1114:GLU:H	1:B:1114:GLU:CD	1.95	0.73
1:B:1132:HIS:C	1:B:1134:ASP:H	1.97	0.71
1:B:1314:GLU:CA	4:B:1599:HOH:O	2.39	0.71
1:A:1220:LYS:HE3	4:A:1535:HOH:O	1.90	0.71
1:B:1170:SER:O	1:B:1175:ASN:HA	1.88	0.71
1:B:1264:SER:O	4:B:1612:HOH:O	2.08	0.71
1:B:1268:MET:HE1	1:B:1278:VAL:CG2	2.21	0.71
1:A:1201:HIS:HE1	4:A:1629:HOH:O	1.74	0.71
1:A:1284:VAL:HG23	1:B:1263:PHE:HE2	1.56	0.71
1:B:1314:GLU:CB	4:B:1599:HOH:O	2.18	0.71
1:A:1284:VAL:HG23	1:B:1263:PHE:CE2	2.25	0.70
1:B:1128:THR:HB	1:B:1217:ASN:HA	1.73	0.70
1:B:1144:ARG:HD2	1:B:1311:MET:SD	2.31	0.70
1:B:1176:HIS:HB3	4:B:1604:HOH:O	1.91	0.70
1:A:1130:ARG:NH1	4:A:1679:HOH:O	2.23	0.70
1:A:1133:ARG:CZ	1:A:1288:ALA:HB2	2.22	0.70
1:A:1283:SER:OG	1:A:1286:GLY:HA3	1.92	0.70
1:B:1312:LYS:HD3	4:B:1525:HOH:O	1.92	0.69
1:A:1281:ARG:HG2	1:A:1281:ARG:NH1	2.06	0.68
1:B:1175:ASN:CB	4:B:1543:HOH:O	2.15	0.68
1:A:1117:GLU:OE2	1:A:1152:LYS:HE2	1.93	0.68
1:A:1104:GLN:HB3	4:A:1560:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:GLU:OE2	4:A:1561:HOH:O	2.10	0.67
1:A:1173:ASN:ND2	1:A:1258:LYS:HE3	2.09	0.67
1:A:1153:VAL:O	4:A:1529:HOH:O	2.12	0.67
1:B:1311:MET:O	4:B:1552:HOH:O	2.12	0.66
1:B:1228:ILE:HD11	3:B:1402:2GY:C15	2.26	0.65
1:A:1149:ARG:HB3	1:A:1307:THR:HB	1.78	0.65
1:A:1161:ARG:CZ	1:A:1298:GLU:OE2	2.45	0.64
1:B:1113:PRO:HD2	1:B:1114:GLU:OE2	1.96	0.64
1:A:1216:GLU:HG3	4:A:1567:HOH:O	1.98	0.63
1:A:1128:THR:HB	1:A:1217:ASN:HA	1.81	0.63
1:A:1298:GLU:HG2	4:A:1549:HOH:O	1.87	0.62
1:A:1263:PHE:CD1	1:A:1283:SER:HB3	2.35	0.61
1:A:1158:LEU:HD21	1:A:1196:GLY:CA	2.31	0.61
1:B:1146:ASN:ND2	1:B:1148:ILE:HD11	2.15	0.61
1:A:1173:ASN:HD22	1:A:1258:LYS:HE3	1.67	0.60
1:B:1114:GLU:CG	4:B:1508:HOH:O	2.49	0.60
1:B:1228:ILE:CD1	3:B:1402:2GY:H9	2.31	0.60
1:A:1279:ILE:HG22	1:A:1281:ARG:HD2	1.83	0.60
1:A:1188:PHE:O	1:A:1192:ILE:HG13	2.01	0.59
1:B:1114:GLU:CD	1:B:1114:GLU:N	2.61	0.59
1:A:1130:ARG:HD2	1:A:1217:ASN:ND2	2.17	0.59
1:B:1163:CYS:SG	4:B:1502:HOH:O	2.04	0.58
1:A:1284:VAL:CG2	1:B:1263:PHE:HE2	2.15	0.58
1:A:1117:GLU:O	1:A:1121:VAL:HG23	2.04	0.58
1:A:1159:ARG:NH2	1:A:1303:GLU:OE2	2.37	0.58
1:B:1199:GLU:HG2	1:B:1295:TYR:O	2.04	0.58
1:A:1284:VAL:O	1:A:1285:ASN:CB	2.51	0.57
1:B:1245:CYS:HB2	4:B:1519:HOH:O	2.03	0.57
1:A:1159:ARG:HH12	1:A:1253:ARG:HE	1.50	0.57
1:A:1159:ARG:HH12	1:A:1253:ARG:NE	2.04	0.56
1:A:1180:ARG:NH1	4:A:1668:HOH:O	2.39	0.56
1:B:1114:GLU:HG3	4:B:1508:HOH:O	2.06	0.56
1:A:1283:SER:HA	1:B:1263:PHE:CZ	2.41	0.55
1:B:1195:LYS:CA	1:B:1195:LYS:HE3	2.35	0.55
1:B:1132:HIS:C	1:B:1134:ASP:N	2.66	0.54
1:B:1190:ASN:CB	4:B:1613:HOH:O	2.06	0.54
1:B:1146:ASN:HD21	1:B:1148:ILE:HD11	1.73	0.53
1:B:1268:MET:CE	1:B:1278:VAL:HG21	2.33	0.53
1:B:1144:ARG:HD3	1:B:1145:TYR:O	2.08	0.53
1:A:1155:ASN:ND2	1:A:1158:LEU:HD13	2.24	0.52
1:A:1137:ASN:ND2	4:A:1604:HOH:O	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:GLU:OE1	4:B:1637:HOH:O	2.19	0.52
1:A:1164:HIS:HE1	4:A:1547:HOH:O	1.92	0.51
1:B:1262:GLN:O	1:B:1262:GLN:HG3	2.08	0.51
1:B:1234:CYS:SG	1:B:1237:HIS:HB2	2.50	0.51
1:A:1253:ARG:HG3	1:A:1303:GLU:CG	2.41	0.50
1:B:1177:HIS:CD2	1:B:1178:ASN:N	2.79	0.50
1:B:1160:GLU:HG2	4:B:1570:HOH:O	2.11	0.50
1:B:1268:MET:CE	1:B:1272:PRO:HD3	2.42	0.50
1:B:1144:ARG:HG3	1:B:1311:MET:HB2	1.95	0.49
1:B:1172:GLU:HB3	4:B:1588:HOH:O	2.12	0.49
1:B:1152:LYS:HE2	4:B:1593:HOH:O	2.11	0.49
1:B:1263:PHE:HB3	4:B:1577:HOH:O	1.89	0.49
1:B:1177:HIS:HD2	1:B:1178:ASN:N	2.11	0.49
1:A:1166:GLN:HG3	1:A:1177:HIS:HB2	1.95	0.48
1:A:1186:SER:O	1:A:1189:ILE:HG12	2.13	0.48
1:B:1298:GLU:H	1:B:1298:GLU:HG3	1.30	0.48
1:A:1130:ARG:NH1	1:A:1217:ASN:HD21	2.07	0.48
1:A:1158:LEU:HD21	1:A:1196:GLY:HA2	1.96	0.48
1:A:1144:ARG:NE	1:A:1311:MET:SD	2.87	0.48
1:A:1180:ARG:CZ	1:B:1174:HIS:CE1	2.97	0.47
1:B:1115:ASP:CG	1:B:1117:GLU:H	2.22	0.47
1:B:1112:ALA:HB1	1:B:1114:GLU:OE2	2.15	0.47
1:B:1228:ILE:CD1	3:B:1402:2GY:C15	2.90	0.47
1:B:1115:ASP:HB2	4:B:1558:HOH:O	2.15	0.46
1:B:1262:GLN:CD	4:B:1612:HOH:O	2.47	0.46
1:B:1207:MET:C	1:B:1267:LYS:HE3	2.39	0.46
1:B:1233:GLY:CA	1:B:1240:ARG:HG2	2.45	0.46
1:B:1115:ASP:CB	4:B:1558:HOH:O	2.64	0.46
1:B:1110:ASP:OD2	1:B:1110:ASP:N	2.48	0.46
1:B:1122:GLU:O	1:B:1122:GLU:HG3	2.12	0.46
1:A:1114:GLU:H	1:A:1114:GLU:HG3	1.30	0.46
1:A:1133:ARG:CD	4:A:1694:HOH:O	2.29	0.46
1:A:1133:ARG:NH1	1:A:1288:ALA:HB2	2.30	0.45
1:B:1258:LYS:HG2	1:B:1275:HIS:CD2	2.51	0.45
1:B:1268:MET:HE1	1:B:1272:PRO:HD3	1.98	0.45
1:A:1144:ARG:HG2	1:A:1145:TYR:H	1.80	0.45
1:B:1188:PHE:O	1:B:1192:ILE:HG13	2.16	0.45
1:B:1207:MET:HE3	1:B:1207:MET:HB2	1.53	0.45
1:B:1134:ASP:HB2	4:B:1530:HOH:O	2.17	0.45
1:A:1220:LYS:CE	4:A:1535:HOH:O	2.57	0.45
1:B:1117:GLU:OE2	1:B:1152:LYS:NZ	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1233:GLY:HA2	1:B:1240:ARG:HG2	1.99	0.44
1:A:1243:TYR:HB3	4:A:1523:HOH:O	2.18	0.44
1:B:1116:LYS:HB3	1:B:1116:LYS:HE3	1.52	0.44
1:B:1177:HIS:HD2	1:B:1179:GLU:H	1.66	0.44
1:B:1155:ASN:HB3	1:B:1158:LEU:HB2	1.99	0.44
1:B:1173:ASN:O	1:B:1174:HIS:C	2.59	0.44
1:A:1220:LYS:HZ2	1:A:1220:LYS:HG2	1.57	0.44
1:A:1106:THR:HG21	1:A:1153:VAL:HG13	1.98	0.43
1:B:1125:MET:HE2	1:B:1145:TYR:CD2	2.53	0.43
1:B:1184:HIS:HB2	1:B:1214:PHE:CD1	2.52	0.43
1:B:1195:LYS:CE	1:B:1195:LYS:HA	2.48	0.43
1:B:1312:LYS:HB2	1:B:1312:LYS:HE2	1.65	0.43
1:B:1106:THR:HG22	1:B:1107:ILE:N	2.32	0.43
1:B:1106:THR:HA	1:B:1154:VAL:O	2.19	0.43
1:B:1262:GLN:NE2	1:B:1264:SER:O	2.52	0.43
1:A:1130:ARG:HG3	4:A:1666:HOH:O	2.18	0.43
1:B:1253:ARG:O	1:B:1300:ALA:HA	2.19	0.43
1:B:1295:TYR:CD2	1:B:1295:TYR:N	2.87	0.43
1:A:1239:ASP:HB3	1:A:1242:CYS:HB2	2.01	0.43
1:B:1205:GLY:O	1:B:1206:GLY:C	2.61	0.43
1:B:1216:GLU:CD	1:B:1290:ALA:HB3	2.43	0.43
1:B:1146:ASN:HB2	1:B:1311:MET:SD	2.58	0.43
1:A:1189:ILE:HD12	1:A:1250:LEU:HG	2.00	0.42
1:A:1284:VAL:HG22	4:A:1677:HOH:O	2.19	0.42
1:B:1279:ILE:HG12	1:B:1292:TYR:CD1	2.54	0.42
1:A:1253:ARG:O	1:A:1300:ALA:HA	2.20	0.42
1:B:1118:TYR:CD2	1:B:1118:TYR:C	2.97	0.42
1:B:1237:HIS:O	1:B:1238:LYS:C	2.63	0.42
1:A:1178:ASN:HD22	1:B:1176:HIS:CE1	2.38	0.42
1:A:1155:ASN:CG	1:A:1158:LEU:HD13	2.45	0.42
1:A:1220:LYS:NZ	4:A:1535:HOH:O	2.53	0.42
1:A:1263:PHE:CZ	1:B:1263:PHE:HB3	2.55	0.42
1:B:1106:THR:HG21	1:B:1153:VAL:HG13	2.02	0.42
1:A:1134:ASP:C	1:A:1134:ASP:OD1	2.61	0.41
1:A:1129:ILE:HD11	1:A:1145:TYR:CE2	2.56	0.41
1:B:1239:ASP:CG	4:B:1640:HOH:O	2.59	0.41
1:A:1184:HIS:HE1	3:A:1402:2GY:H15	1.84	0.41
1:A:1281:ARG:NH1	1:A:1281:ARG:CG	2.78	0.41
1:B:1125:MET:HG2	1:B:1145:TYR:CD2	2.56	0.41
1:A:1184:HIS:CE1	3:A:1402:2GY:H15	2.55	0.41
1:B:1173:ASN:ND2	1:B:1176:HIS:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:CYS:SG	1:A:1244:ILE:HB	2.60	0.41
1:B:1314:GLU:N	4:B:1580:HOH:O	2.44	0.41
1:A:1147:VAL:HG11	1:A:1150:ILE:HD11	2.02	0.41
1:B:1125:MET:HE3	1:B:1249:MET:HE3	2.02	0.41
1:B:1107:ILE:CG1	4:B:1621:HOH:O	2.37	0.41
1:A:1184:HIS:HA	4:A:1508:HOH:O	2.20	0.41
1:A:1263:PHE:CZ	1:B:1261:LEU:HG	2.56	0.40
1:B:1104:GLN:N	4:B:1624:HOH:O	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1516:HOH:O	4:B:1508:HOH:O[4_455]	2.10	0.10
4:A:1579:HOH:O	4:B:1607:HOH:O[4_455]	2.16	0.04

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	209/217 (96%)	203 (97%)	6 (3%)	0	100	100
1	B	198/217 (91%)	190 (96%)	7 (4%)	1 (0%)	24	21
All	All	407/434 (94%)	393 (97%)	13 (3%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1266	MET

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	178/185 (96%)	166 (93%)	12 (7%)	15	11
1	B	168/185 (91%)	150 (89%)	18 (11%)	6	4
All	All	346/370 (94%)	316 (91%)	30 (9%)	9	6

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1109	LEU
1	A	1114	GLU
1	A	1130	ARG
1	A	1148	ILE
1	A	1170	SER
1	A	1178	ASN
1	A	1180	ARG
1	A	1207	MET
1	A	1216	GLU
1	A	1220	LYS
1	A	1281	ARG
1	A	1298	GLU
1	B	1114	GLU
1	B	1116	LYS
1	B	1118	TYR
1	B	1131	GLU
1	B	1133	ARG
1	B	1144	ARG
1	B	1152	LYS
1	B	1167	LYS
1	B	1178	ASN
1	B	1195	LYS
1	B	1199	GLU
1	B	1204	ILE
1	B	1207	MET
1	B	1249	MET
1	B	1252	CYS

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Mol	Chain	Res	Type
1	B	1262	GLN
1	B	1298	GLU
1	B	1312	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1164	HIS
1	A	1173	ASN
1	A	1176	HIS
1	A	1177	HIS
1	A	1178	ASN
1	A	1190	ASN
1	A	1201	HIS
1	A	1217	ASN
1	A	1248	GLN
1	B	1104	GLN
1	B	1143	ASN
1	B	1146	ASN
1	B	1174	HIS
1	B	1177	HIS
1	B	1178	ASN
1	B	1190	ASN
1	B	1270	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	2GY	A	1402	-	37,37,37	3.40	21 (56%)	47,54,54	3.93	27 (57%)
3	2GY	B	1402	-	37,37,37	4.24	23 (62%)	47,54,54	4.06	26 (55%)

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	2GY	A	1402	-	-	1/16/45/45	0/5/5/5
3	2GY	B	1402	-	-	0/16/45/45	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	2GY	C14-C13	15.90	1.73	1.55
3	B	1402	2GY	C6-N1	7.34	1.46	1.34
3	A	1402	2GY	C6-N1	6.98	1.45	1.34
3	B	1402	2GY	O1-C14	-6.82	1.38	1.48
3	A	1402	2GY	C10-C12	6.47	1.49	1.39
3	B	1402	2GY	C10-C12	6.32	1.49	1.39
3	A	1402	2GY	O1-C11	6.17	1.45	1.35
3	A	1402	2GY	C5-C12	5.83	1.48	1.39
3	A	1402	2GY	C6-N5	5.37	1.43	1.34
3	A	1402	2GY	C11-N2	-5.32	1.28	1.35
3	B	1402	2GY	C5-C12	4.91	1.46	1.39
3	B	1402	2GY	C6-N5	4.85	1.42	1.34
3	B	1402	2GY	C17-N2	-4.77	1.41	1.48
3	B	1402	2GY	C26-C1	4.67	1.45	1.39
3	B	1402	2GY	O1-C11	4.66	1.43	1.35
3	A	1402	2GY	C1-C20	-4.63	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	2GY	C9-C10	4.56	1.46	1.38
3	A	1402	2GY	C17-N2	-4.50	1.41	1.48
3	B	1402	2GY	C7-C5	4.36	1.46	1.38
3	A	1402	2GY	C7-C5	4.19	1.46	1.38
3	A	1402	2GY	C8-C7	4.04	1.47	1.38
3	A	1402	2GY	O1-C14	3.95	1.54	1.48
3	A	1402	2GY	C9-C8	3.89	1.46	1.38
3	B	1402	2GY	C9-C8	3.83	1.46	1.38
3	B	1402	2GY	C11-N2	-3.77	1.30	1.35
3	B	1402	2GY	C8-C7	3.65	1.46	1.38
3	A	1402	2GY	C23-C1	3.58	1.44	1.39
3	B	1402	2GY	C23-C1	3.53	1.44	1.39
3	B	1402	2GY	C9-C10	3.45	1.44	1.38
3	A	1402	2GY	C2-N1	3.26	1.41	1.34
3	A	1402	2GY	C26-C1	3.10	1.43	1.39
3	B	1402	2GY	O2-C11	-3.00	1.16	1.21
3	B	1402	2GY	C4-N5	2.86	1.40	1.34
3	A	1402	2GY	C4-N5	2.84	1.40	1.34
3	B	1402	2GY	C2-N1	2.78	1.40	1.34
3	A	1402	2GY	C3-C4	2.74	1.45	1.37
3	B	1402	2GY	C3-C2	2.70	1.45	1.37
3	A	1402	2GY	C13-N2	-2.66	1.45	1.47
3	B	1402	2GY	C15-C14	2.51	1.56	1.52
3	B	1402	2GY	C3-C4	2.50	1.44	1.37
3	A	1402	2GY	C3-C2	2.34	1.44	1.37
3	B	1402	2GY	C23-C24	2.31	1.43	1.39
3	B	1402	2GY	C1-C20	-2.20	1.47	1.52
3	A	1402	2GY	O2-C11	-2.03	1.18	1.21

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	2GY	C1-C26-N3	-9.29	113.17	124.47
3	B	1402	2GY	C1-C26-N3	-9.13	113.37	124.47
3	B	1402	2GY	C2-N1-C6	8.81	124.78	116.07
3	B	1402	2GY	C4-N5-C6	8.14	124.11	116.07
3	A	1402	2GY	O1-C14-C13	-7.89	95.78	102.61
3	B	1402	2GY	C15-C14-C13	7.86	132.27	113.43
3	B	1402	2GY	C24-C6-N1	7.80	126.37	117.22
3	A	1402	2GY	C4-N5-C6	7.49	123.47	116.07
3	A	1402	2GY	C24-C6-N1	7.45	125.96	117.22
3	B	1402	2GY	O1-C14-C15	-7.25	98.88	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	2GY	C21-C20-C19	6.96	124.81	109.68
3	A	1402	2GY	C2-N1-C6	6.94	122.93	116.07
3	B	1402	2GY	C23-C24-C25	-6.52	111.73	117.36
3	A	1402	2GY	O1-C14-C16	-6.30	99.91	106.77
3	A	1402	2GY	C22-C17-N2	-6.16	102.17	112.75
3	A	1402	2GY	C26-N3-C25	6.11	124.54	118.64
3	B	1402	2GY	O1-C14-C13	-6.03	97.39	102.61
3	A	1402	2GY	C23-C24-C25	-5.89	112.27	117.36
3	B	1402	2GY	N5-C6-N1	-5.84	112.87	125.54
3	B	1402	2GY	C21-C20-C19	5.57	121.78	109.68
3	A	1402	2GY	N5-C6-N1	-5.30	114.05	125.54
3	B	1402	2GY	C22-C17-N2	-5.26	103.72	112.75
3	B	1402	2GY	C26-N3-C25	5.23	123.70	118.64
3	A	1402	2GY	C22-C17-C18	4.94	122.33	111.17
3	B	1402	2GY	C14-O1-C11	4.84	114.96	110.04
3	A	1402	2GY	C16-C14-C13	4.84	125.03	113.43
3	A	1402	2GY	O1-C11-O2	4.73	128.23	122.54
3	B	1402	2GY	C23-C1-C20	-4.19	110.51	120.88
3	B	1402	2GY	O1-C14-C16	-3.69	102.75	106.77
3	B	1402	2GY	C14-C13-C12	-3.68	111.59	115.70
3	A	1402	2GY	O2-C11-N2	-3.50	123.71	128.17
3	B	1402	2GY	C10-C12-C5	3.46	122.59	118.30
3	B	1402	2GY	C9-C8-C7	3.38	124.50	119.87
3	A	1402	2GY	C15-C14-C13	3.28	121.29	113.43
3	B	1402	2GY	C12-C13-N2	-3.20	110.56	113.76
3	B	1402	2GY	C22-C17-C18	3.08	118.14	111.17
3	B	1402	2GY	C16-C14-C15	-2.86	104.06	110.76
3	A	1402	2GY	C5-C12-C13	-2.81	114.93	120.74
3	A	1402	2GY	C23-C1-C20	-2.80	113.94	120.88
3	B	1402	2GY	C24-C6-N5	2.80	120.50	117.22
3	B	1402	2GY	C23-C24-C6	2.68	122.93	117.47
3	A	1402	2GY	C18-C19-C20	2.64	115.46	110.61
3	A	1402	2GY	C16-C14-C15	-2.61	104.65	110.76
3	A	1402	2GY	C10-C12-C5	2.57	121.50	118.30
3	A	1402	2GY	C9-C8-C7	2.54	123.34	119.87
3	B	1402	2GY	C8-C7-C5	-2.52	117.13	120.24
3	A	1402	2GY	C19-C20-C1	-2.38	107.04	112.67
3	A	1402	2GY	C18-C17-N2	-2.31	108.78	112.75
3	A	1402	2GY	O1-C11-N2	-2.31	107.98	110.04
3	A	1402	2GY	N4-C25-N3	-2.22	113.44	118.38
3	A	1402	2GY	C24-C6-N5	2.21	119.81	117.22
3	B	1402	2GY	C9-C10-C12	-2.20	118.01	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1402	2GY	C18-C19-C20	2.08	114.42	110.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

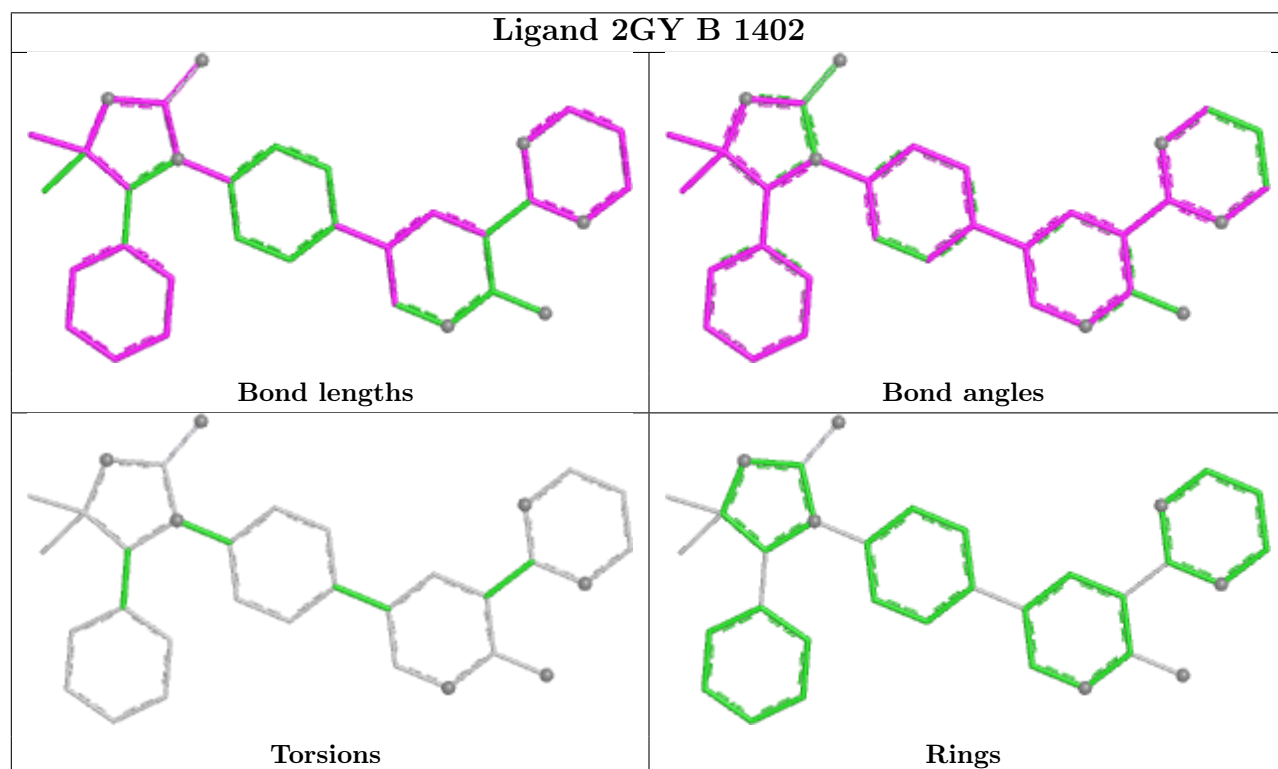
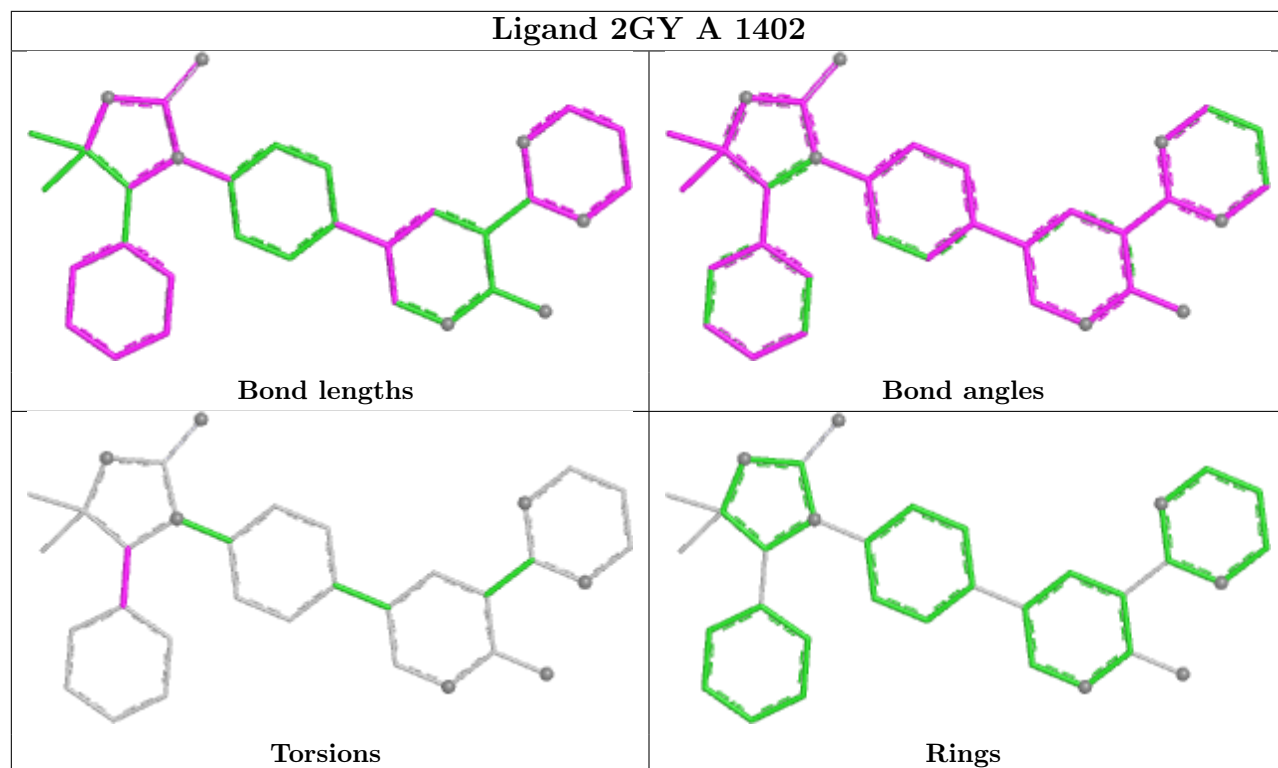
Mol	Chain	Res	Type	Atoms
3	A	1402	2GY	C5-C12-C13-N2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	2GY	2	0
3	B	1402	2GY	4	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 ⓘ

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	211/217 (97%)	0.95	19 (9%) 15 14	18, 25, 34, 42	0
1	B	202/217 (93%)	1.27	31 (15%) 5 4	20, 28, 36, 43	0
All	All	413/434 (95%)	1.10	50 (12%) 8 8	18, 26, 36, 43	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1265	THR	6.8
1	B	1263	PHE	6.5
1	A	1104	GLN	4.6
1	B	1104	GLN	4.5
1	B	1280	GLY	4.4
1	B	1123	GLU	4.4
1	A	1177	HIS	4.2
1	B	1176	HIS	3.8
1	A	1284	VAL	3.7
1	A	1133	ARG	3.6
1	B	1107	ILE	3.4
1	B	1207	MET	3.3
1	B	1148	ILE	3.2
1	A	1263	PHE	3.1
1	A	1174	HIS	3.1
1	B	1115	ASP	3.0
1	B	1262	GLN	3.0
1	B	1171	GLU	3.0
1	B	1161	ARG	3.0
1	A	1109	LEU	2.9
1	A	1158	LEU	2.9
1	B	1267	LYS	2.9
1	B	1264	SER	2.7
1	B	1175	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1190	ASN	2.7
1	A	1298	GLU	2.7
1	A	1156	LYS	2.7
1	B	1261	LEU	2.6
1	B	1290	ALA	2.6
1	B	1109	LEU	2.6
1	B	1233	GLY	2.5
1	B	1159	ARG	2.5
1	B	1178	ASN	2.5
1	B	1238	LYS	2.5
1	A	1161	ARG	2.5
1	B	1266	MET	2.4
1	B	1228	ILE	2.4
1	A	1169	VAL	2.4
1	A	1195	LYS	2.4
1	A	1114	GLU	2.3
1	B	1131	GLU	2.3
1	B	1224	TYR	2.3
1	A	1143	ASN	2.3
1	B	1132	HIS	2.3
1	B	1105	GLY	2.3
1	B	1298	GLU	2.2
1	A	1131	GLU	2.1
1	A	1314	GLU	2.1
1	B	1134	ASP	2.1
1	A	1207	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](#)

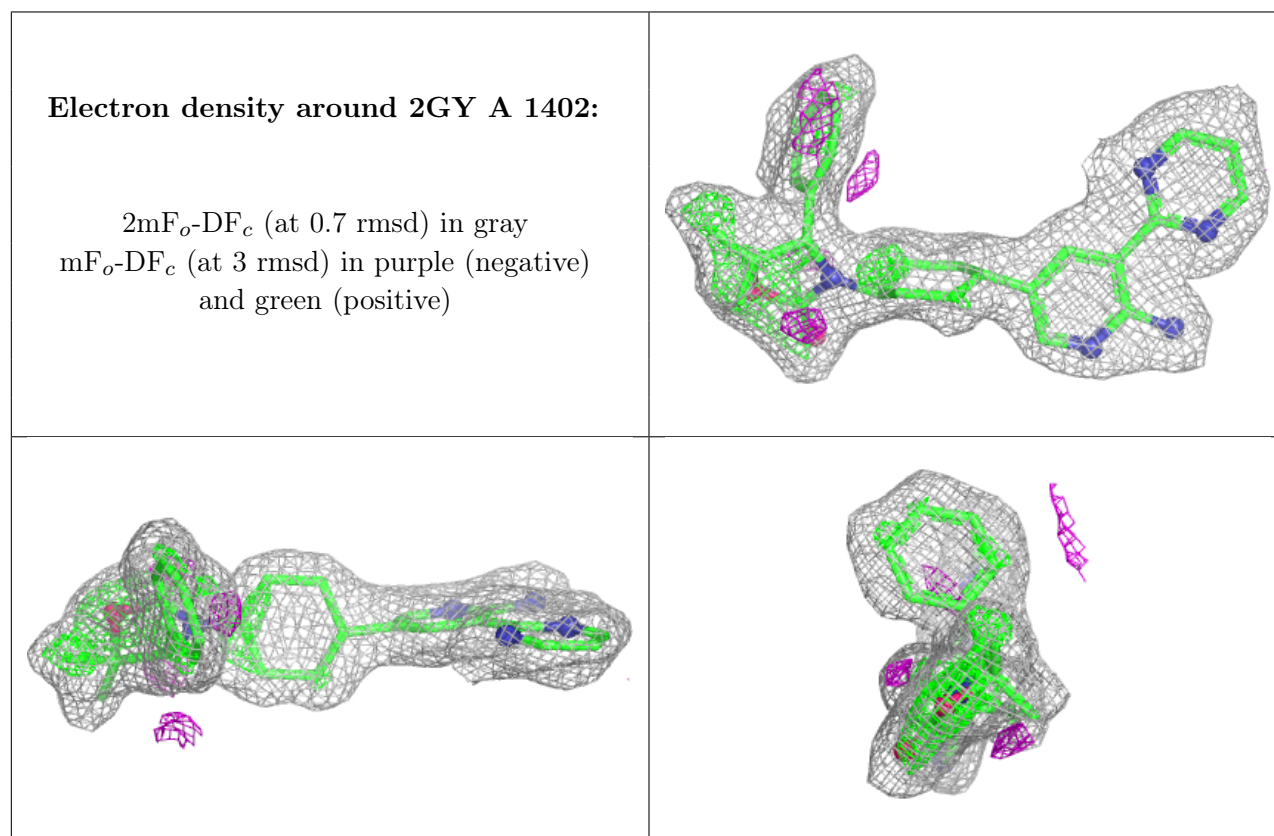
There are no oligosaccharides in this entry.

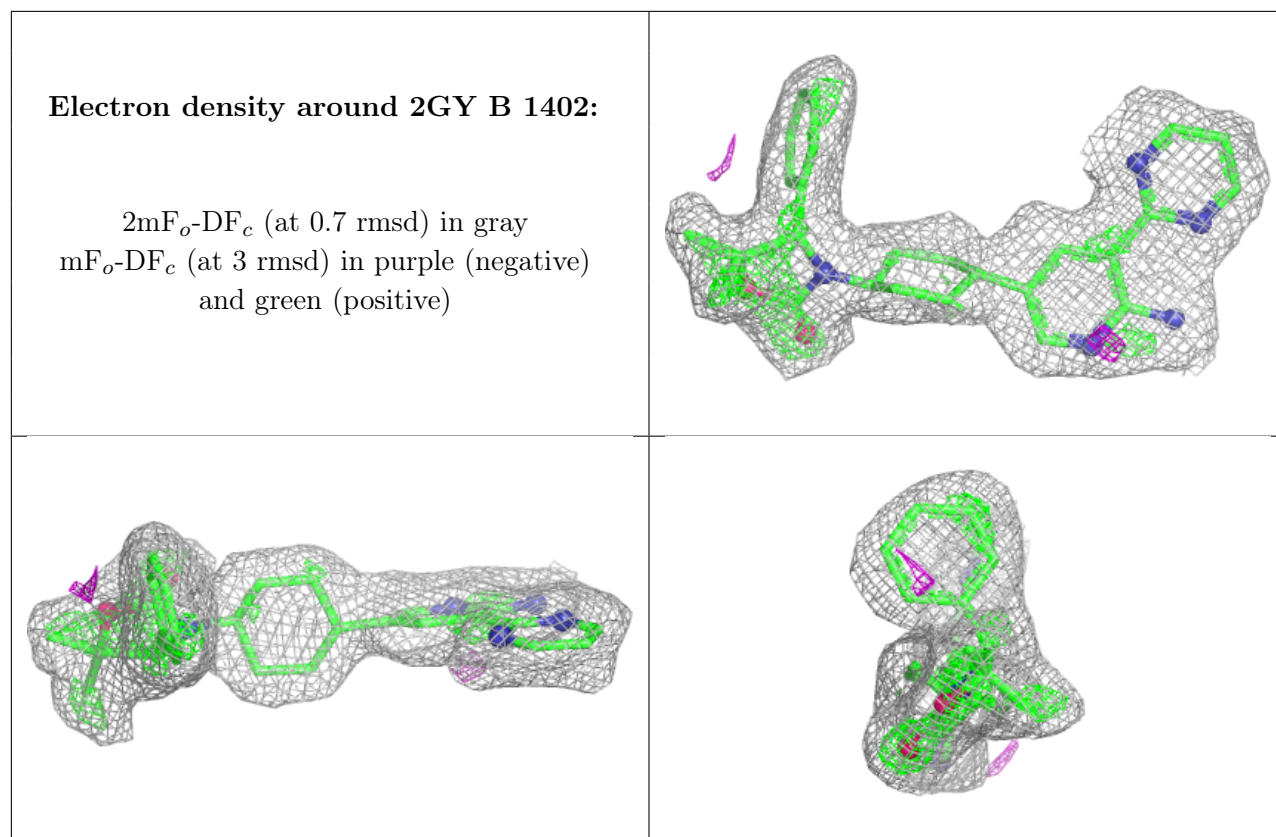
6.4 Ligands [i](#)

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
3	2GY	A	1402	33/33	0.85	0.24	29,42,59,63	0
3	2GY	B	1402	33/33	0.85	0.25	35,47,64,68	0
2	ZN	A	1401	1/1	0.99	0.03	26,26,26,26	0
2	ZN	B	1401	1/1	0.99	0.03	29,29,29,29	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.