



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:15 PM UTC

PDB ID : 4DVI / pdb_00004dvi
Title : Crystal structure of Tankyrase 1 with IWR2
Authors : Huang, X.
Deposited on : 2012-02-23
Resolution : 1.90 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

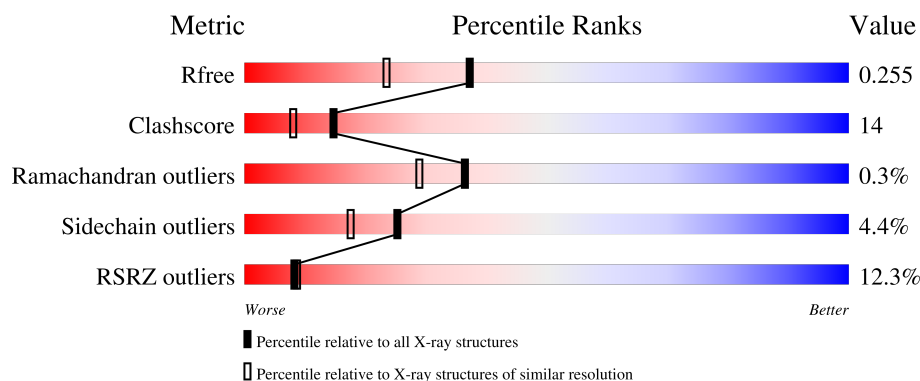
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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% 69% 21% • • 5%
1	B	217	12% 65% 23% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3644 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	206	Total	C	N	O	S	0	0	0
			1664	1047	304	302	11			
1	B	200	Total	C	N	O	S	0	0	0
			1602	1002	297	293	10			

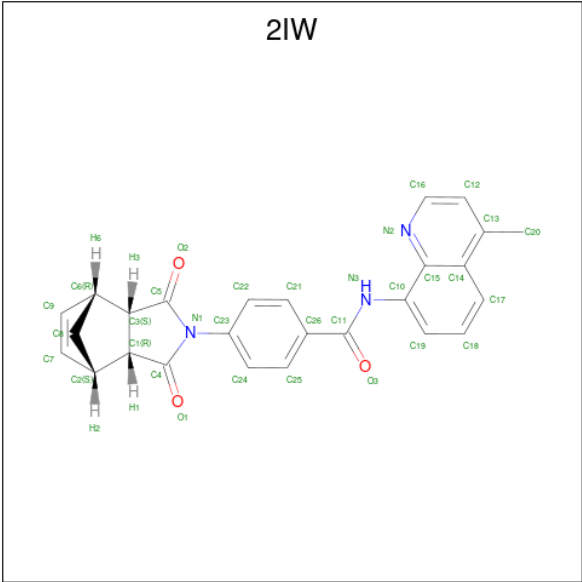
There are 12 discrepancies between the modelled and reference sequences:

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 4-[(3aR,4S,7R,7aS)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2H-4,7-methanoisindol-2-yl]-N-(4-methylquinolin-8-yl)benzamide (CCD ID: 2IW) (formula: C₂₆H₂₁N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	26	3	3		
3	B	1	Total	C	N	O	0	0
			32	26	3	3		

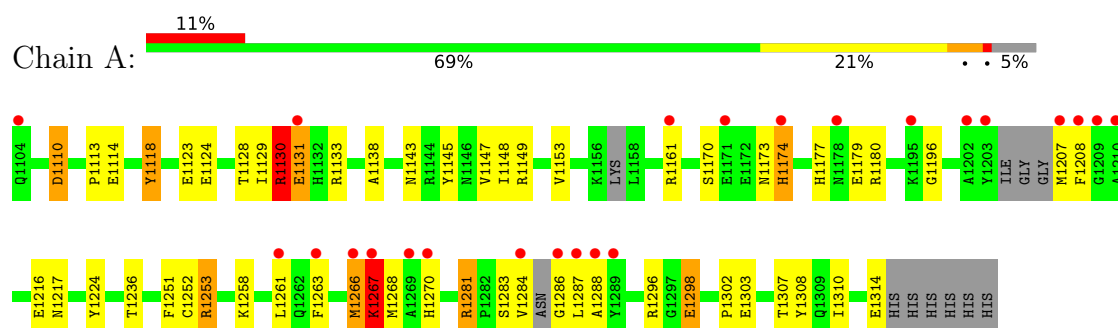
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total	O	0	0
			180	180		
4	B	132	Total	O	0	0
			132	132		

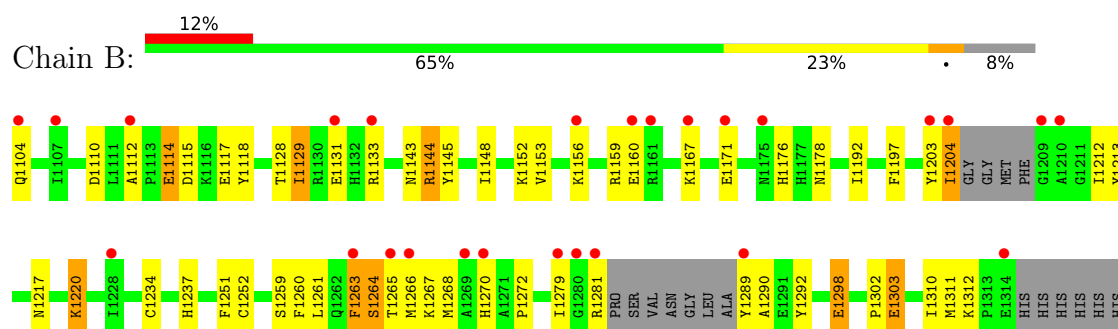
3 Residue-property plots

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: Tankyrase-1



• Molecule 1: Tankyrase-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.47Å 77.94Å 146.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 99.3 (50.00-1.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.91Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.258 0.243 , 0.255	Depositor DCC
R_{free} test set	1889 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtrriage
Anisotropy	0.714	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3644	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.83 % 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 9.9374e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2IW, ZN

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	0.99	10/1704 (0.6%)	1.05	8/2288 (0.3%)
1	B	0.91	9/1639 (0.5%)	1.02	6/2203 (0.3%)
All	All	0.95	19/3343 (0.6%)	1.03	14/4491 (0.3%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1110	ASP	CA-C	-9.59	1.40	1.52
1	A	1131	GLU	CA-C	-9.32	1.40	1.52
1	A	1174	HIS	CA-C	-8.16	1.42	1.53
1	A	1147	VAL	CA-C	-7.55	1.44	1.53
1	B	1131	GLU	CA-C	7.17	1.62	1.52
1	B	1148	ILE	CA-CB	6.72	1.62	1.54
1	B	1129	ILE	CA-C	-6.43	1.44	1.52
1	B	1263	PHE	CA-C	-5.87	1.45	1.52
1	A	1130	ARG	CZ-NH2	-5.84	1.25	1.33
1	B	1290	ALA	CA-C	-5.77	1.45	1.53
1	A	1253	ARG	CA-C	-5.68	1.46	1.52
1	B	1133	ARG	CA-C	-5.54	1.45	1.52
1	A	1161	ARG	CA-C	5.48	1.59	1.52
1	B	1212	ILE	CA-CB	-5.42	1.47	1.54
1	B	1143	ASN	CA-C	-5.42	1.45	1.52
1	B	1267	LYS	CA-C	-5.26	1.46	1.52
1	A	1118	TYR	CA-C	-5.12	1.46	1.52
1	A	1148	ILE	CA-CB	5.09	1.61	1.54
1	A	1143	ASN	CA-C	5.01	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1268	MET	N-CA-C	9.80	123.67	110.35
1	B	1290	ALA	N-CA-C	7.73	120.98	110.55
1	A	1252	CYS	N-CA-C	7.68	122.05	110.14
1	A	1236	THR	N-CA-C	7.14	119.15	111.36
1	B	1252	CYS	N-CA-C	6.68	120.41	109.85
1	B	1133	ARG	N-CA-C	6.40	120.30	112.23
1	A	1310	ILE	N-CA-C	-6.09	100.92	109.21
1	B	1267	LYS	N-CA-C	-5.93	100.95	110.14
1	A	1287	LEU	N-CA-C	5.88	118.30	110.53
1	A	1138	ALA	N-CA-C	5.56	117.15	111.14
1	A	1267	LYS	N-CA-C	5.50	117.35	111.36
1	A	1308	TYR	N-CA-C	5.43	115.72	108.38
1	B	1303	GLU	N-CA-C	5.30	116.74	111.07
1	B	1251	PHE	N-CA-C	-5.26	98.68	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1664	0	1588	45	0
1	B	1602	0	1514	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	21	4	0
3	B	32	0	21	2	0
4	A	180	0	0	7	0
4	B	132	0	0	5	0
All	All	3644	0	3144	90	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 (90) 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:1283:SER:OG	1:A:1286:GLY:HA3	1.69	0.93
1:B:1268:MET:HE1	1:B:1272:PRO:HD3	1.55	0.86
1:B:1144:ARG:HD2	1:B:1311:MET:SD	2.20	0.81
1:A:1263:PHE:CZ	1:B:1261:LEU:HG	2.21	0.74
1:A:1179:GLU:OE2	1:A:1253:ARG:NH1	2.20	0.74
1:A:1207:MET:CB	1:A:1266:MET:HB2	2.17	0.74
1:A:1298:GLU:H	1:A:1298:GLU:CD	1.95	0.71
1:B:1112:ALA:HB1	1:B:1114:GLU:OE2	1.91	0.70
1:B:1128:THR:HB	1:B:1217:ASN:HA	1.75	0.69
1:B:1220:LYS:HZ2	1:B:1220:LYS:HB2	1.59	0.67
1:A:1180:ARG:NH2	1:A:1216:GLU:OE1	2.27	0.67
1:A:1173:ASN:ND2	1:A:1258:LYS:HB2	2.11	0.66
1:B:1217:ASN:OD1	1:B:1289:TYR:CB	2.46	0.63
1:A:1266:MET:HE3	1:A:1267:LYS:HD2	1.78	0.63
1:B:1203:TYR:HD1	1:B:1204:ILE:O	1.83	0.61
1:B:1312:LYS:HD3	4:B:1545:HOH:O	2.01	0.61
1:A:1130:ARG:HD2	1:A:1217:ASN:ND2	2.16	0.60
1:A:1217:ASN:HB2	4:A:1582:HOH:O	2.02	0.60
1:B:1281:ARG:CB	1:B:1281:ARG:HH11	2.14	0.59
1:B:1259:SER:HB3	1:B:1279:ILE:HG13	1.83	0.59
1:B:1178:ASN:ND2	4:B:1547:HOH:O	2.28	0.59
1:B:1234:CYS:SG	1:B:1237:HIS:HB2	2.44	0.58
1:A:1130:ARG:HH11	1:A:1217:ASN:HD21	1.53	0.56
1:A:1173:ASN:HD21	1:A:1258:LYS:HB2	1.69	0.56
1:B:1114:GLU:H	1:B:1114:GLU:CD	2.12	0.56
1:B:1279:ILE:HG12	1:B:1292:TYR:CD1	2.41	0.56
1:B:1289:TYR:N	4:B:1606:HOH:O	2.39	0.55
1:B:1167:LYS:HD2	1:B:1171:GLU:OE1	2.08	0.54
1:B:1281:ARG:HH11	1:B:1281:ARG:HB3	1.72	0.54
1:A:1128:THR:HB	1:A:1217:ASN:HA	1.89	0.54
1:A:1207:MET:N	4:A:1649:HOH:O	2.42	0.53
1:A:1284:VAL:O	1:A:1286:GLY:N	2.42	0.52
1:A:1270:HIS:CD2	1:A:1270:HIS:C	2.88	0.52
1:A:1196:GLY:O	3:A:1402:2IW:H18	2.10	0.50
3:A:1402:2IW:O3	3:A:1402:2IW:H19	2.11	0.50
1:B:1204:ILE:C	4:B:1601:HOH:O	2.54	0.50
1:A:1208:PHE:CD2	3:A:1402:2IW:H8	2.47	0.50
1:A:1253:ARG:HG3	1:A:1303:GLU:OE2	2.12	0.50
1:A:1153:VAL:HB	1:A:1302:PRO:O	2.12	0.49
1:A:1130:ARG:CD	1:A:1217:ASN:ND2	2.75	0.49
1:A:1266:MET:HG2	1:A:1267:LYS:N	2.25	0.48
1:B:1159:ARG:HG3	1:B:1159:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:GLU:CD	1:A:1298:GLU:N	2.69	0.48
1:B:1298:GLU:H	1:B:1298:GLU:CD	2.20	0.48
1:A:1133:ARG:CZ	1:A:1288:ALA:HB2	2.44	0.47
1:B:1281:ARG:CB	1:B:1281:ARG:NH1	2.77	0.47
1:A:1130:ARG:NH1	1:A:1217:ASN:HD21	2.13	0.47
1:A:1177:HIS:CE1	4:A:1658:HOH:O	2.67	0.47
1:A:1296:ARG:HD3	4:A:1549:HOH:O	2.14	0.47
1:B:1192:ILE:HD13	1:B:1197:PHE:CE1	2.50	0.47
1:B:1268:MET:HE3	1:B:1270:HIS:O	2.16	0.46
1:A:1149:ARG:HB3	1:A:1307:THR:HB	1.97	0.46
1:B:1159:ARG:NH2	1:B:1303:GLU:OE2	2.49	0.46
1:B:1144:ARG:HD3	1:B:1145:TYR:O	2.15	0.46
1:B:1281:ARG:NH1	1:B:1281:ARG:HB2	2.30	0.46
1:A:1113:PRO:HA	1:A:1118:TYR:CG	2.50	0.46
1:B:1117:GLU:OE2	1:B:1152:LYS:HE2	2.15	0.45
1:A:1110:ASP:CG	4:A:1633:HOH:O	2.60	0.45
1:A:1124:GLU:HG2	1:A:1251:PHE:CZ	2.52	0.45
1:B:1104:GLN:O	1:B:1104:GLN:HG3	2.17	0.45
1:B:1213:TYR:CD1	3:B:1402:2IW:H1	2.52	0.45
1:B:1167:LYS:HD2	1:B:1167:LYS:C	2.43	0.44
1:B:1129:ILE:HD11	1:B:1145:TYR:CE2	2.53	0.44
1:B:1167:LYS:HB3	1:B:1167:LYS:HE3	1.82	0.43
1:B:1176:HIS:HD2	4:B:1543:HOH:O	2.01	0.43
1:B:1153:VAL:HB	1:B:1302:PRO:O	2.18	0.43
1:B:1167:LYS:CD	1:B:1171:GLU:OE1	2.66	0.43
1:A:1263:PHE:CE2	1:B:1261:LEU:HG	2.53	0.43
1:A:1208:PHE:HZ	1:A:1224:TYR:HH	1.65	0.43
1:B:1112:ALA:O	1:B:1115:ASP:CB	2.66	0.43
1:B:1203:TYR:CD1	1:B:1204:ILE:O	2.69	0.42
1:B:1264:SER:OG	1:B:1265:THR:N	2.52	0.42
1:B:1310:ILE:O	1:B:1310:ILE:HG13	2.19	0.42
3:B:1402:2IW:H19	3:B:1402:2IW:O3	2.17	0.42
1:A:1261:LEU:HD23	1:A:1281:ARG:NH1	2.34	0.42
1:A:1123:GLU:OE1	1:A:1123:GLU:HA	2.18	0.42
1:A:1173:ASN:O	1:A:1174:HIS:HB2	2.19	0.42
1:A:1180:ARG:HG3	1:A:1180:ARG:NH1	2.35	0.42
1:B:1118:TYR:CD2	1:B:1118:TYR:C	2.97	0.42
1:A:1314:GLU:C	4:A:1679:HOH:O	2.63	0.42
1:A:1130:ARG:HD2	1:A:1217:ASN:HD22	1.85	0.42
1:A:1177:HIS:HE1	4:A:1658:HOH:O	2.01	0.42
1:A:1129:ILE:HD11	1:A:1145:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:ARG:HG3	1:B:1159:ARG:HH11	1.86	0.41
1:B:1156:LYS:O	1:B:1160:GLU:HG3	2.20	0.41
1:A:1113:PRO:HA	1:A:1118:TYR:CD2	2.56	0.41
1:A:1208:PHE:CE2	3:A:1402:2IW:H8	2.55	0.41
1:A:1296:ARG:HB3	1:A:1298:GLU:OE2	2.21	0.41
1:A:1263:PHE:CZ	1:B:1263:PHE:CB	3.04	0.40
1:B:1260:PHE:CG	1:B:1272:PRO:HG2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/217 (91%)	194 (98%)	4 (2%)	0	100	100
1	B	194/217 (89%)	188 (97%)	5 (3%)	1 (0%)	24	16
All	All	392/434 (90%)	382 (97%)	9 (2%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1266	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/185 (95%)	167 (95%)	8 (5%)	24	16
1	B	166/185 (90%)	159 (96%)	7 (4%)	26	19
All	All	341/370 (92%)	326 (96%)	15 (4%)	25	17

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1114	GLU
1	A	1130	ARG
1	A	1131	GLU
1	A	1170	SER
1	A	1266	MET
1	A	1267	LYS
1	A	1281	ARG
1	A	1298	GLU
1	B	1110	ASP
1	B	1114	GLU
1	B	1144	ARG
1	B	1204	ILE
1	B	1220	LYS
1	B	1264	SER
1	B	1298	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1104	GLN
1	A	1119	GLN
1	A	1166	GLN
1	A	1173	ASN
1	A	1190	ASN
1	A	1217	ASN
1	A	1270	HIS
1	B	1143	ASN
1	B	1178	ASN
1	B	1201	HIS
1	B	1223	GLN
1	B	1270	HIS
1	B	1299	GLN

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	2IW	A	1402	-	37,37,37	2.96	18 (48%)	56,56,56	3.15	22 (39%)
3	2IW	B	1402	-	37,37,37	2.84	18 (48%)	56,56,56	3.27	27 (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	2IW	A	1402	-	-	4/12/49/49	0/7/6/6
3	2IW	B	1402	-	-	4/12/49/49	0/7/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	2IW	C15-N2	6.42	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	2IW	C23-N1	-5.97	1.35	1.44
3	B	1402	2IW	C23-N1	-5.64	1.35	1.44
3	B	1402	2IW	C15-N2	5.15	1.43	1.37
3	A	1402	2IW	C18-C17	4.57	1.46	1.36
3	A	1402	2IW	C25-C26	4.52	1.46	1.39
3	A	1402	2IW	C14-C15	4.44	1.53	1.42
3	B	1402	2IW	C16-N2	4.40	1.41	1.32
3	A	1402	2IW	C19-C10	4.36	1.47	1.38
3	B	1402	2IW	C14-C15	4.32	1.53	1.42
3	A	1402	2IW	C16-N2	4.29	1.40	1.32
3	B	1402	2IW	C18-C19	4.22	1.46	1.38
3	B	1402	2IW	C21-C26	4.21	1.45	1.39
3	B	1402	2IW	C25-C26	4.11	1.45	1.39
3	B	1402	2IW	C12-C16	4.10	1.46	1.38
3	A	1402	2IW	C12-C13	4.09	1.45	1.37
3	B	1402	2IW	C12-C13	4.03	1.45	1.37
3	B	1402	2IW	C19-C10	3.99	1.46	1.38
3	A	1402	2IW	C12-C16	3.98	1.46	1.38
3	B	1402	2IW	C22-C23	3.83	1.46	1.39
3	B	1402	2IW	C18-C17	3.67	1.44	1.36
3	A	1402	2IW	C25-C24	3.64	1.44	1.38
3	B	1402	2IW	C25-C24	3.62	1.44	1.38
3	A	1402	2IW	C21-C26	3.47	1.44	1.39
3	B	1402	2IW	C22-C21	3.36	1.44	1.38
3	A	1402	2IW	C22-C23	3.35	1.45	1.39
3	A	1402	2IW	C22-C21	3.30	1.44	1.38
3	B	1402	2IW	C24-C23	3.28	1.45	1.39
3	A	1402	2IW	C18-C19	3.16	1.44	1.38
3	A	1402	2IW	C24-C23	3.01	1.45	1.39
3	A	1402	2IW	C6-C3	2.91	1.62	1.56
3	A	1402	2IW	C13-C14	2.50	1.47	1.42
3	B	1402	2IW	C6-C3	2.38	1.61	1.56
3	A	1402	2IW	C10-C15	2.34	1.48	1.42
3	B	1402	2IW	C6-C9	2.25	1.57	1.51
3	B	1402	2IW	C13-C14	2.09	1.46	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1402	2IW	C10-C15-N2	9.97	125.50	117.50
3	A	1402	2IW	C10-C15-N2	9.77	125.34	117.50
3	A	1402	2IW	C2-C1-C3	-8.38	94.55	102.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1402	2IW	C16-N2-C15	8.04	126.79	117.31
3	B	1402	2IW	C2-C1-C3	-7.88	95.05	102.85
3	B	1402	2IW	C6-C3-C1	7.63	110.42	102.85
3	A	1402	2IW	C16-N2-C15	7.56	126.22	117.31
3	A	1402	2IW	C6-C3-C1	7.27	110.06	102.85
3	A	1402	2IW	C8-C2-C1	5.78	107.55	99.90
3	A	1402	2IW	O1-C4-N1	5.48	130.28	124.30
3	B	1402	2IW	O1-C4-N1	5.35	130.14	124.30
3	B	1402	2IW	O2-C5-N1	5.00	129.75	124.30
3	B	1402	2IW	C8-C2-C1	4.89	106.37	99.90
3	A	1402	2IW	C25-C26-C21	4.82	124.70	118.57
3	B	1402	2IW	C25-C26-C21	4.77	124.64	118.57
3	B	1402	2IW	O1-C4-C1	-4.55	121.70	127.51
3	B	1402	2IW	O2-C5-C3	-4.49	121.78	127.51
3	A	1402	2IW	O2-C5-N1	4.30	129.00	124.30
3	A	1402	2IW	O1-C4-C1	-4.27	122.06	127.51
3	A	1402	2IW	O2-C5-C3	-4.16	122.20	127.51
3	B	1402	2IW	C12-C16-N2	-4.07	118.55	124.60
3	B	1402	2IW	C14-C15-N2	-4.04	115.37	122.58
3	A	1402	2IW	C12-C16-N2	-4.00	118.65	124.60
3	A	1402	2IW	C22-C21-C26	-3.95	116.58	120.80
3	A	1402	2IW	C14-C15-N2	-3.82	115.76	122.58
3	B	1402	2IW	C2-C7-C9	-3.73	98.77	107.97
3	B	1402	2IW	C22-C21-C26	-3.48	117.08	120.80
3	A	1402	2IW	C2-C7-C9	-3.22	100.03	107.97
3	B	1402	2IW	C12-C13-C14	3.20	122.51	118.06
3	B	1402	2IW	C8-C6-C3	-3.17	95.70	99.90
3	A	1402	2IW	C12-C13-C14	3.01	122.23	118.06
3	B	1402	2IW	C24-C23-C22	2.79	124.50	119.18
3	B	1402	2IW	C8-C6-C9	-2.79	92.31	99.72
3	B	1402	2IW	C6-C9-C7	2.70	114.62	107.97
3	B	1402	2IW	C18-C17-C14	2.62	124.46	120.91
3	A	1402	2IW	C24-C23-C22	2.62	124.18	119.18
3	A	1402	2IW	C8-C6-C9	-2.61	92.78	99.72
3	A	1402	2IW	C25-C24-C23	-2.60	117.00	120.30
3	B	1402	2IW	C25-C24-C23	-2.57	117.04	120.30
3	B	1402	2IW	C6-C3-C5	-2.49	110.72	114.57
3	A	1402	2IW	C22-C23-N1	-2.48	116.69	119.65
3	B	1402	2IW	C22-C23-N1	-2.47	116.69	119.65
3	A	1402	2IW	C6-C3-C5	-2.40	110.86	114.57
3	B	1402	2IW	C15-C10-N3	2.32	120.13	115.25
3	A	1402	2IW	C24-C25-C26	-2.31	118.33	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1402	2IW	C17-C18-C19	-2.25	117.54	121.00
3	B	1402	2IW	C24-C25-C26	-2.23	118.42	120.80
3	A	1402	2IW	C18-C17-C14	2.11	123.77	120.91
3	B	1402	2IW	C8-C2-C7	2.02	105.10	99.72

There are no chirality outliers.

All (8) torsion outliers are listed below:

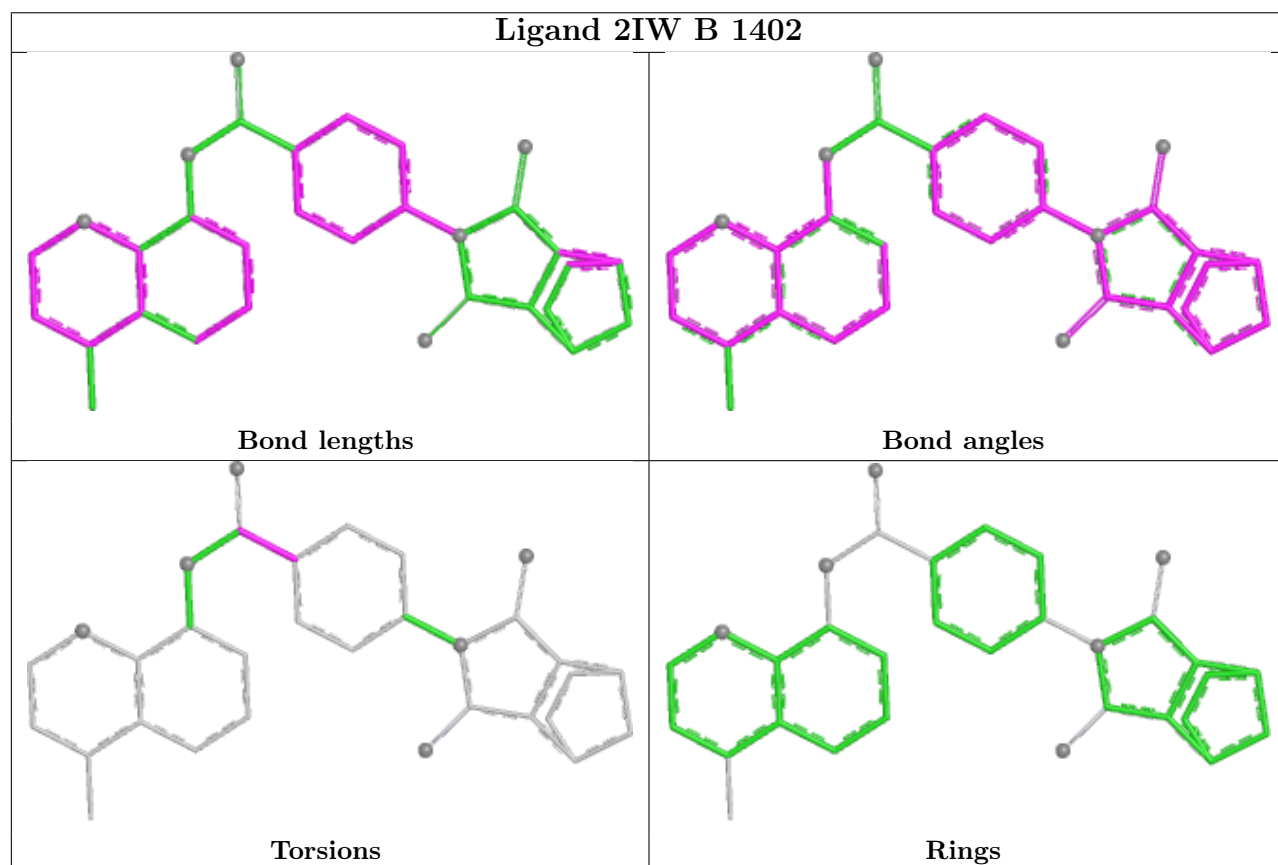
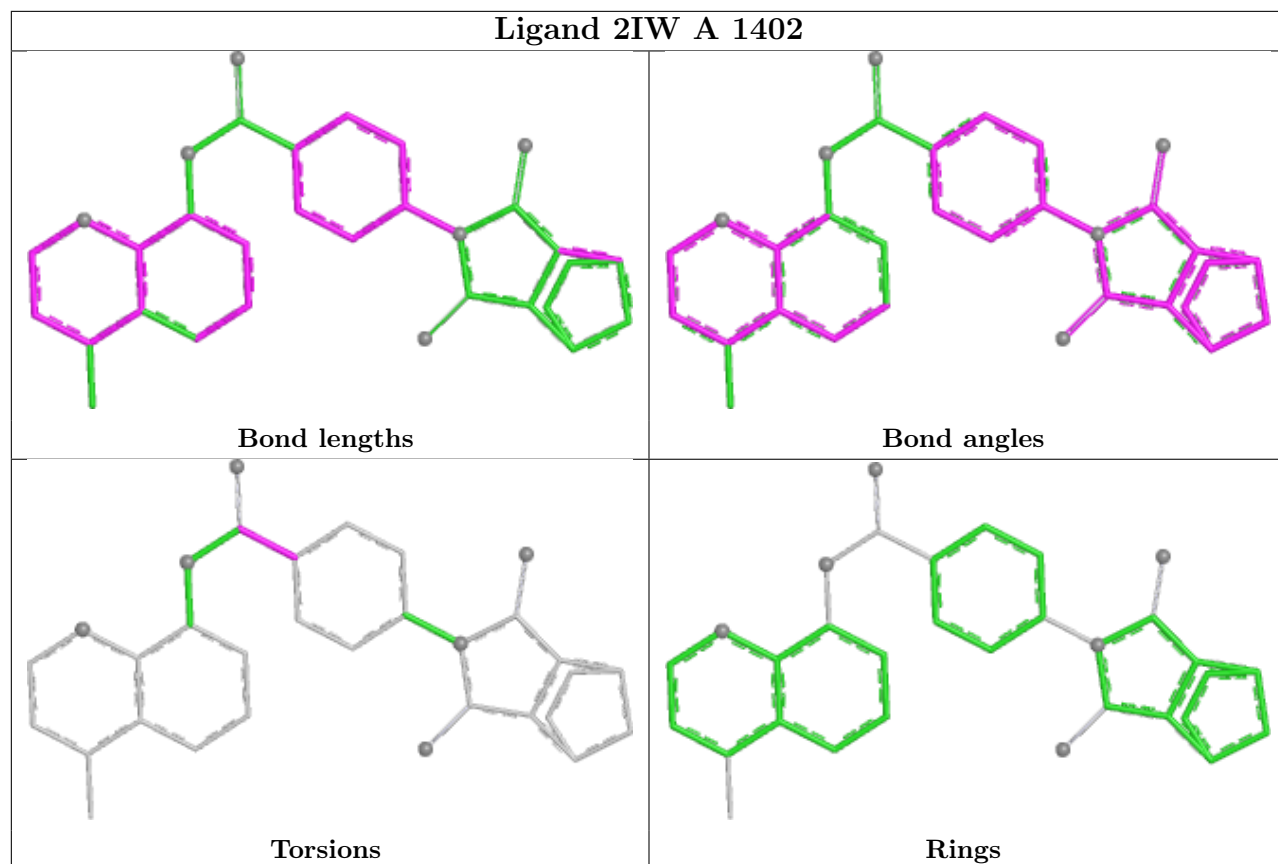
Mol	Chain	Res	Type	Atoms
3	B	1402	2IW	N3-C11-C26-C21
3	B	1402	2IW	O3-C11-C26-C21
3	A	1402	2IW	N3-C11-C26-C25
3	A	1402	2IW	O3-C11-C26-C25
3	B	1402	2IW	N3-C11-C26-C25
3	B	1402	2IW	O3-C11-C26-C25
3	A	1402	2IW	N3-C11-C26-C21
3	A	1402	2IW	O3-C11-C26-C21

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	2IW	4	0
3	B	1402	2IW	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	206/217 (94%)	0.81	24 (11%) 9 10	19, 26, 42, 47	0
1	B	200/217 (92%)	0.90	26 (13%) 7 7	20, 30, 45, 51	0
All	All	406/434 (93%)	0.85	50 (12%) 8 9	19, 28, 43, 51	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1203	TYR	6.5
1	A	1208	PHE	6.4
1	A	1207	MET	6.3
1	B	1265	THR	4.4
1	B	1289	TYR	4.2
1	B	1280	GLY	4.2
1	B	1104	GLN	4.0
1	A	1263	PHE	3.9
1	A	1161	ARG	3.8
1	A	1210	ALA	3.8
1	A	1104	GLN	3.5
1	A	1174	HIS	3.5
1	A	1267	LYS	3.5
1	B	1266	MET	3.5
1	B	1171	GLU	3.5
1	B	1203	TYR	3.4
1	A	1270	HIS	3.4
1	B	1204	ILE	3.3
1	A	1266	MET	3.2
1	B	1112	ALA	3.1
1	B	1161	ARG	3.0
1	B	1209	GLY	2.9
1	A	1286	GLY	2.8
1	B	1133	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1269	ALA	2.8
1	B	1160	GLU	2.8
1	A	1202	ALA	2.7
1	B	1263	PHE	2.7
1	B	1228	ILE	2.6
1	A	1209	GLY	2.6
1	A	1289	TYR	2.5
1	A	1287	LEU	2.5
1	A	1178	ASN	2.5
1	A	1171	GLU	2.4
1	B	1270	HIS	2.4
1	A	1131	GLU	2.4
1	B	1131	GLU	2.4
1	A	1284	VAL	2.4
1	B	1107	ILE	2.3
1	B	1269	ALA	2.3
1	B	1167	LYS	2.3
1	B	1314	GLU	2.3
1	A	1261	LEU	2.2
1	B	1210	ALA	2.2
1	A	1195	LYS	2.1
1	B	1175	ASN	2.1
1	B	1279	ILE	2.1
1	A	1288	ALA	2.1
1	B	1156	LYS	2.0
1	B	1281	ARG	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](#)

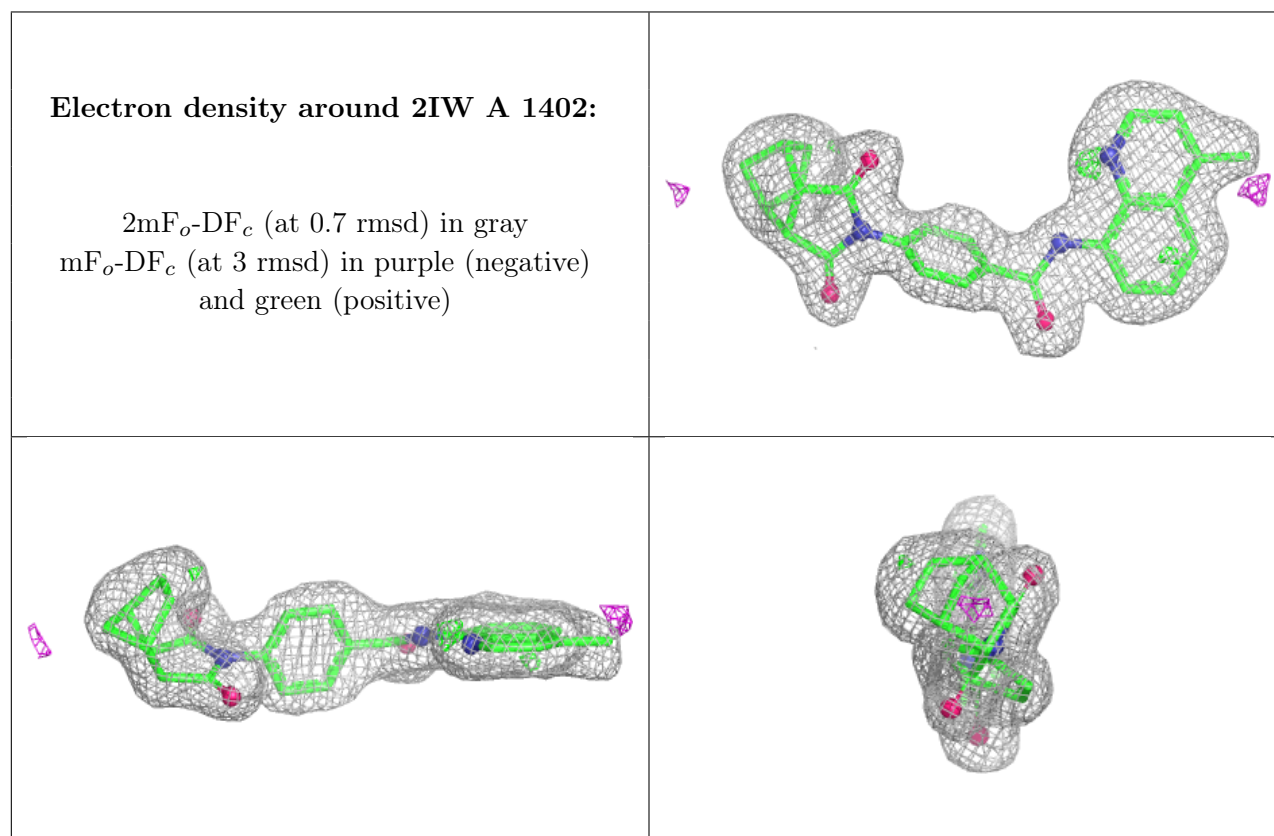
There are no oligosaccharides in this entry.

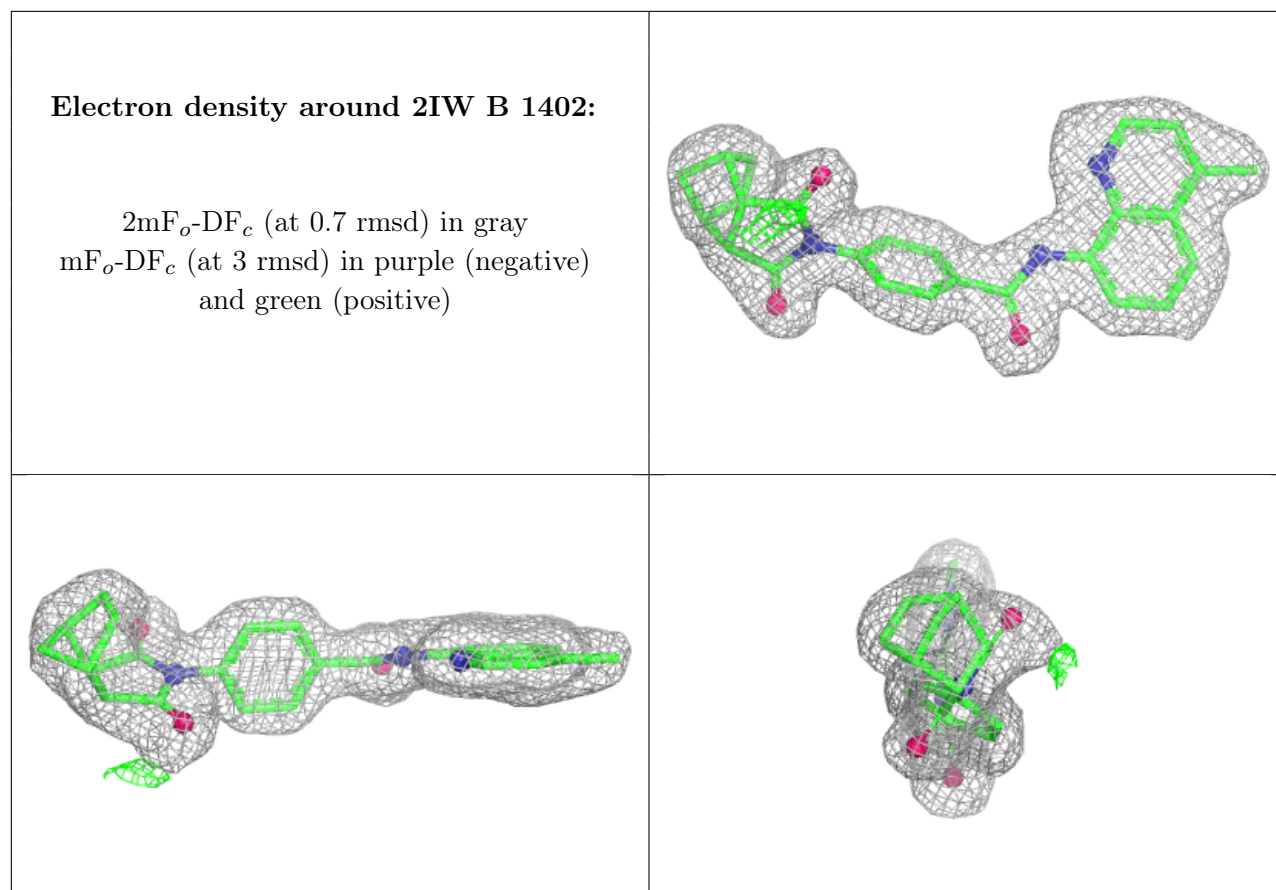
6.4 Ligands [i](#)

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	2IW	A	1402	32/32	0.90	0.10	23,26,28,29	0
3	2IW	B	1402	32/32	0.93	0.08	23,27,31,33	0
2	ZN	B	1401	1/1	0.99	0.02	30,30,30,30	0
2	ZN	A	1401	1/1	1.00	0.03	20,20,20,20	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 ⓘ

There are no such residues in this entry.