



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:44 PM UTC

PDB ID : 4KNB / pdb_00004knb
Title : C-Met in complex with OSI ligand
Authors : Wang, J.; Steinig, A.G.; Li, A.H.; Chen, X.; Dong, H.; Ferraro, C.; Jin, M.; Kadalbajoo, M.; Kleinberg, A.; Stolz, K.M.; Tavares-Greco, P.A.; Wang, T.; Albertella, M.R.; Peng, Y.; Crew, L.; Kahler, J.
Deposited on : 2013-05-09
Resolution : 2.40 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

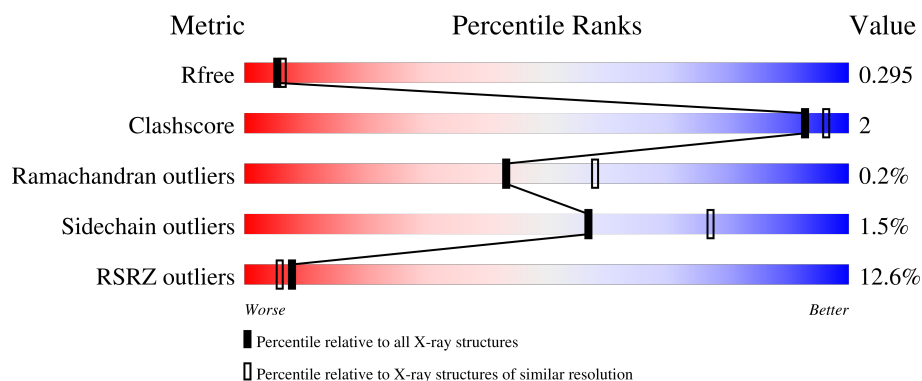
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	5% 91% 5%
1	B	287	15% 85% 5% 11%
1	C	287	8% 87% 6% 6%
1	D	287	18% 82% 14%

2 Entry composition [i](#)

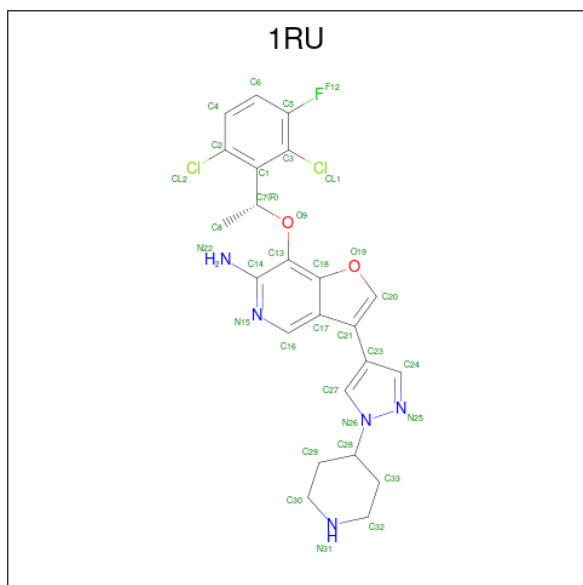
There are 4 unique types of molecules in this entry. The entry contains 8611 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	30	0	0
			2180	1412	370	383	15			
1	B	256	Total	C	N	O	S	19	3	0
			2074	1348	350	360	16			
1	C	271	Total	C	N	O	S	15	0	0
			2168	1408	369	376	15			
1	D	247	Total	C	N	O	S	20	1	0
			1961	1269	339	338	15			

- Molecule 2 is 7-[(1R)-1-(2,6-dichloro-3-fluorophenyl)ethoxy]-3-[1-(piperidin-4-yl)-1H-pyrazol-4-yl]furo[3,2-c]pyridin-6-amine (CCD ID: 1RU) (formula: C₂₃H₂₂Cl₂FN₅O₂).



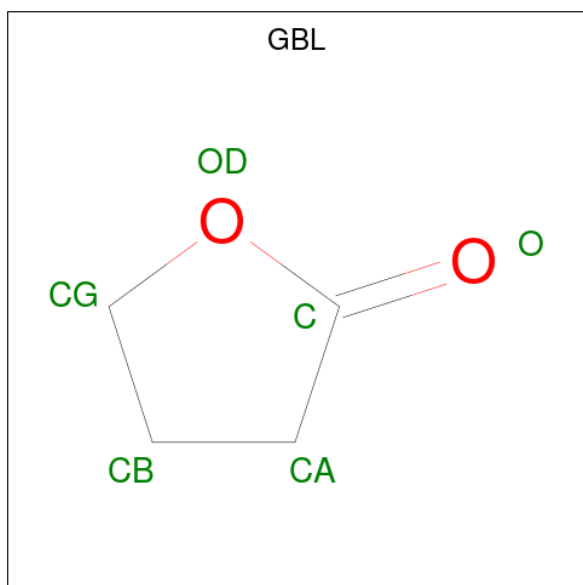
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0
			33	23	2	1	5	2	
2	B	1	Total	C	Cl	F	N	O	0
			33	23	2	1	5	2	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	Cl	F	N	O	0	0
			33	23	2	1	5	2		
2	D	1	Total	C	Cl	F	N	O	0	0
			33	23	2	1	5	2		

- Molecule 3 is GAMMA-BUTYROLACTONE (CCD ID: GBL) (formula: $C_4H_6O_2$).



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

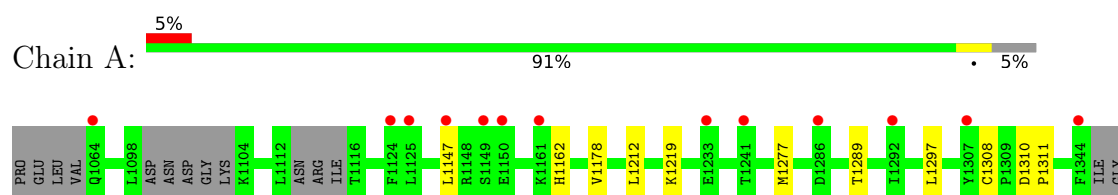
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	20	Total	O	0	0
			20	20		
4	C	11	Total	O	0	0
			11	11		
4	D	15	Total	O	0	0
			15	15		

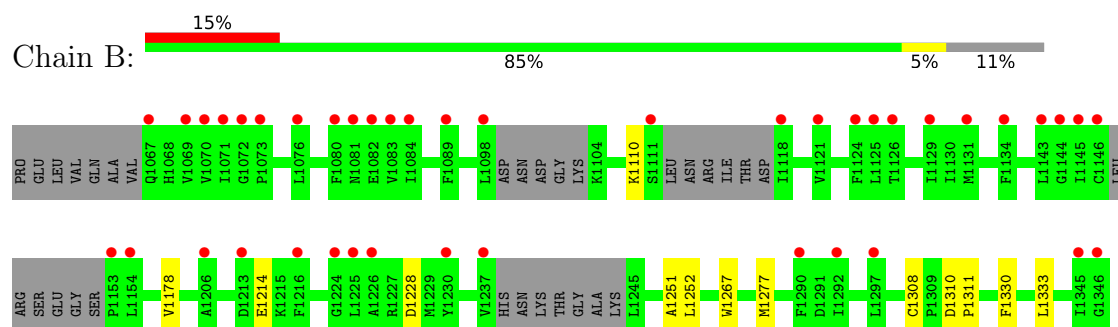
3 Residue-property plots [i](#)

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.

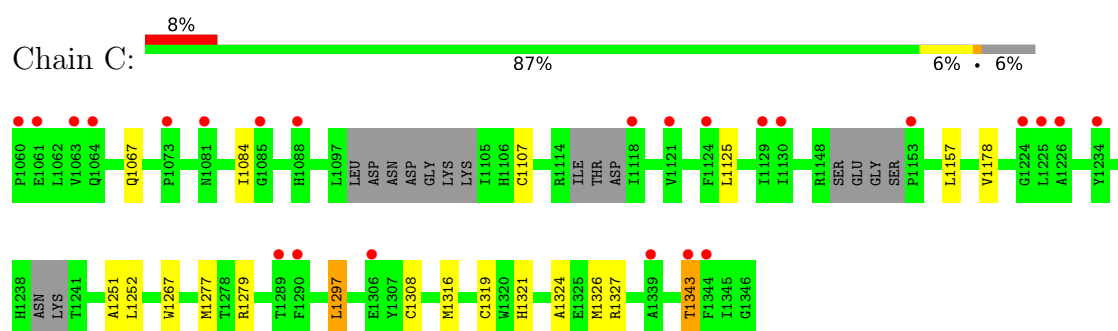
- Molecule 1: Hepatocyte growth factor receptor



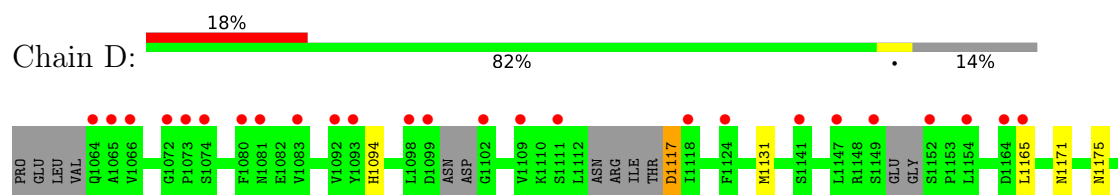
- Molecule 1: Hepatocyte growth factor receptor

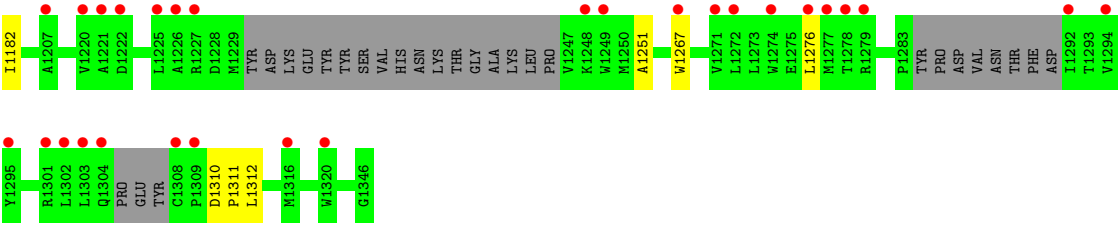


- Molecule 1: Hepatocyte growth factor receptor



- Molecule 1: Hepatocyte growth factor receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.71Å 85.92Å 156.47Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	24.95 – 2.40 24.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.95-2.40) 99.3 (24.95-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.240 , 0.288 0.248 , 0.295	Depositor DCC
R_{free} test set	1062 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8611	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GBL, 1RU

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	0.49	0/2235	0.73	0/3023
1	B	0.46	0/2126	0.72	0/2870
1	C	0.46	0/2222	0.72	0/3003
1	D	0.44	0/2002	0.67	0/2695
All	All	0.46	0/8585	0.71	0/11591

There are no bond length outliers.

There are no bond angle outliers.

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	2180	0	2200	5	0
1	B	2074	0	2094	6	0
1	C	2168	0	2193	9	0
1	D	1961	0	2005	6	0
2	A	33	0	22	0	0
2	B	33	0	22	0	0
2	C	33	0	22	1	0
2	D	33	0	22	0	0
3	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	6	0	0
4	A	32	0	0	1	0
4	B	20	0	0	0	0
4	C	11	0	0	0	0
4	D	15	0	0	0	0
All	All	8611	0	8598	26	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 2.

All (26) 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:1178:VAL:HG13	1:A:1277:MET:HE1	1.80	0.63
1:C:1277:MET:HE2	1:C:1308:CYS:HA	1.83	0.61
1:B:1178:VAL:HG13	1:B:1277:MET:HE1	1.87	0.56
1:B:1110:LYS:NZ	1:B:1228:ASP:OD1	2.38	0.55
1:D:1117:ASP:N	1:D:1117:ASP:OD1	2.41	0.54
1:C:1178:VAL:HG13	1:C:1277:MET:HE1	1.90	0.53
1:C:1251:ALA:HA	1:C:1267:TRP:CD2	2.46	0.51
1:B:1277:MET:HE2	1:B:1308:CYS:HA	1.92	0.51
1:A:1219:LYS:NZ	4:A:1513:HOH:O	2.47	0.48
1:D:1310:ASP:N	1:D:1311:PRO:HD2	2.29	0.48
1:C:1084:ILE:O	2:C:1401:1RU:H7	2.14	0.48
1:A:1277:MET:HE2	1:A:1308:CYS:HA	1.97	0.47
1:C:1252:LEU:HD11	1:C:1297:LEU:HD13	1.96	0.47
1:D:1251:ALA:HA	1:D:1267:TRP:CD2	2.52	0.44
1:C:1321:HIS:CD2	1:C:1326:MET:HB2	2.52	0.43
1:B:1310:ASP:HB2	1:B:1311:PRO:HD3	2.00	0.43
1:B:1251:ALA:HA	1:B:1267:TRP:CD2	2.54	0.43
1:A:1162:HIS:HB2	1:A:1212:LEU:HB3	2.00	0.43
1:D:1251:ALA:HA	1:D:1267:TRP:CG	2.53	0.43
1:C:1107:CYS:HB2	1:C:1157:LEU:O	2.20	0.42
1:D:1182:ILE:HG12	1:D:1312:LEU:HD22	2.01	0.42
1:A:1310:ASP:HB2	1:A:1311:PRO:HD3	2.02	0.41
1:C:1324:ALA:HA	1:C:1327:ARG:CZ	2.50	0.41
1:D:1165:LEU:HD21	1:D:1276:LEU:HD21	2.03	0.41
1:C:1316:MET:O	1:C:1319:CYS:HB2	2.21	0.40
1:B:1330:PHE:HA	1:B:1333:LEU:HD12	2.03	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	267/287 (93%)	260 (97%)	7 (3%)	0	100	100
1	B	248/287 (86%)	240 (97%)	8 (3%)	0	100	100
1	C	261/287 (91%)	252 (97%)	7 (3%)	2 (1%)	16	25
1	D	234/287 (82%)	228 (97%)	6 (3%)	0	100	100
All	All	1010/1148 (88%)	980 (97%)	28 (3%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1343	THR
1	C	1067	GLN

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	242/254 (95%)	239 (99%)	3 (1%)	63	81
1	B	231/254 (91%)	229 (99%)	2 (1%)	70	85
1	C	240/254 (94%)	236 (98%)	4 (2%)	53	74
1	D	218/254 (86%)	213 (98%)	5 (2%)	44	66
All	All	931/1016 (92%)	917 (98%)	14 (2%)	57	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1147	LEU
1	A	1289	THR
1	A	1297	LEU
1	B	1214	GLU
1	B	1252	LEU
1	C	1125	LEU
1	C	1279	ARG
1	C	1297	LEU
1	C	1343	THR
1	D	1094	HIS
1	D	1117	ASP
1	D	1131	MET
1	D	1171	ASN
1	D	1175	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1079	HIS
1	A	1123	GLN
1	A	1167	ASN
1	A	1238	HIS
1	A	1304	GLN
1	B	1068	HIS
1	B	1167	ASN
1	B	1174	HIS
1	B	1304	GLN
1	C	1064	GLN
1	C	1079	HIS
1	C	1081	ASN
1	C	1175	ASN
1	C	1304	GLN
1	C	1321	HIS
1	D	1079	HIS
1	D	1106	HIS
1	D	1167	ASN
1	D	1171	ASN

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 ⓘ

7 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$
3	GBL	A	1402	-	6,6,6	0.59	0	7,7,7	0.82	0
2	1RU	C	1401	-	37,37,37	2.32	8 (21%)	40,54,54	2.42	12 (30%)
2	1RU	D	1401	-	37,37,37	2.31	7 (18%)	40,54,54	2.41	13 (32%)
2	1RU	B	1401	-	37,37,37	2.31	8 (21%)	40,54,54	2.48	13 (32%)
3	GBL	A	1403	-	6,6,6	0.60	0	7,7,7	0.79	0
2	1RU	A	1401	-	37,37,37	2.30	7 (18%)	40,54,54	2.35	13 (32%)
3	GBL	B	1402	-	6,6,6	0.54	0	7,7,7	0.97	1 (14%)

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	GBL	A	1402	-	-	-	0/1/1/1
2	1RU	C	1401	-	-	2/15/24/24	0/5/5/5
2	1RU	D	1401	-	-	4/15/24/24	0/5/5/5
2	1RU	B	1401	-	-	4/15/24/24	0/5/5/5
3	GBL	A	1403	-	-	-	0/1/1/1
2	1RU	A	1401	-	-	3/15/24/24	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GBL	B	1402	-	-	-	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1401	1RU	O19-C18	-8.93	1.22	1.37
2	C	1401	1RU	O19-C18	-8.90	1.23	1.37
2	B	1401	1RU	O19-C18	-8.84	1.23	1.37
2	A	1401	1RU	O19-C18	-8.71	1.23	1.37
2	B	1401	1RU	N26-N25	-5.30	1.26	1.36
2	D	1401	1RU	N26-N25	-5.29	1.26	1.36
2	C	1401	1RU	N26-N25	-5.24	1.26	1.36
2	D	1401	1RU	O19-C20	-5.21	1.23	1.38
2	B	1401	1RU	O19-C20	-5.13	1.23	1.38
2	C	1401	1RU	O19-C20	-5.10	1.23	1.38
2	A	1401	1RU	O19-C20	-5.06	1.23	1.38
2	A	1401	1RU	N26-N25	-5.05	1.27	1.36
2	A	1401	1RU	C17-C21	-4.96	1.36	1.45
2	D	1401	1RU	C17-C21	-4.90	1.37	1.45
2	B	1401	1RU	C17-C21	-4.81	1.37	1.45
2	C	1401	1RU	C17-C21	-4.79	1.37	1.45
2	A	1401	1RU	C20-C21	3.01	1.38	1.35
2	B	1401	1RU	C14-N22	2.88	1.41	1.34
2	C	1401	1RU	C14-N22	2.82	1.41	1.34
2	A	1401	1RU	C14-N22	2.80	1.41	1.34
2	D	1401	1RU	C14-N22	2.75	1.41	1.34
2	B	1401	1RU	C20-C21	2.68	1.38	1.35
2	C	1401	1RU	C20-C21	2.66	1.38	1.35
2	D	1401	1RU	C16-N15	2.44	1.39	1.34
2	B	1401	1RU	C16-N15	2.43	1.39	1.34
2	C	1401	1RU	C21-C23	2.38	1.50	1.47
2	D	1401	1RU	C20-C21	2.36	1.38	1.35
2	C	1401	1RU	C16-N15	2.34	1.39	1.34
2	A	1401	1RU	C16-N15	2.29	1.39	1.34
2	B	1401	1RU	C21-C23	2.08	1.50	1.47

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1401	1RU	C24-N25-N26	9.40	108.97	104.14
2	B	1401	1RU	C24-N25-N26	9.26	108.90	104.14
2	D	1401	1RU	C24-N25-N26	9.04	108.78	104.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	1RU	C24-N25-N26	8.93	108.73	104.14
2	D	1401	1RU	C17-C16-N15	-4.90	117.42	124.32
2	A	1401	1RU	C17-C16-N15	-4.75	117.63	124.32
2	C	1401	1RU	C17-C16-N15	-4.74	117.65	124.32
2	B	1401	1RU	C17-C16-N15	-4.74	117.65	124.32
2	D	1401	1RU	C23-C24-N25	-4.38	108.61	112.09
2	B	1401	1RU	O19-C20-C21	-4.13	110.37	112.68
2	A	1401	1RU	C23-C24-N25	-4.08	108.85	112.09
2	C	1401	1RU	C23-C24-N25	-4.01	108.91	112.09
2	B	1401	1RU	C23-C24-N25	-3.95	108.95	112.09
2	C	1401	1RU	C2-C1-C3	3.82	119.23	114.93
2	D	1401	1RU	C8-C7-C1	-3.75	107.76	113.20
2	B	1401	1RU	C8-C7-C1	-3.67	107.87	113.20
2	B	1401	1RU	O19-C18-C13	3.65	129.00	124.89
2	A	1401	1RU	C8-C7-C1	-3.49	108.13	113.20
2	A	1401	1RU	O19-C18-C13	3.49	128.82	124.89
2	C	1401	1RU	O19-C18-C13	3.47	128.80	124.89
2	D	1401	1RU	O19-C18-C13	3.45	128.78	124.89
2	A	1401	1RU	C2-C1-C3	3.36	118.70	114.93
2	B	1401	1RU	C2-C1-C3	3.31	118.65	114.93
2	C	1401	1RU	C8-C7-C1	-3.30	108.41	113.20
2	D	1401	1RU	C2-C1-C3	3.17	118.49	114.93
2	D	1401	1RU	C16-N15-C14	3.14	121.68	118.64
2	A	1401	1RU	O9-C7-C8	3.03	110.77	105.51
2	D	1401	1RU	O9-C7-C8	2.88	110.50	105.51
2	C	1401	1RU	C16-N15-C14	2.85	121.40	118.64
2	C	1401	1RU	C27-C23-C21	2.83	131.54	126.95
2	B	1401	1RU	C16-N15-C14	2.79	121.34	118.64
2	C	1401	1RU	C27-N26-N25	-2.79	110.58	112.45
2	B	1401	1RU	C27-N26-N25	-2.77	110.58	112.45
2	B	1401	1RU	C27-C23-C21	2.75	131.42	126.95
2	C	1401	1RU	O9-C7-C8	2.73	110.23	105.51
2	D	1401	1RU	C18-O19-C20	2.72	111.41	104.75
2	A	1401	1RU	C27-N26-N25	-2.71	110.63	112.45
2	A	1401	1RU	C16-N15-C14	2.63	121.19	118.64
2	B	1401	1RU	O9-C7-C8	2.61	110.04	105.51
2	A	1401	1RU	C18-O19-C20	2.55	110.98	104.75
2	A	1401	1RU	C28-N26-N25	2.53	123.86	120.41
2	D	1401	1RU	O19-C20-C21	-2.48	111.29	112.68
2	D	1401	1RU	C27-N26-N25	-2.43	110.82	112.45
2	B	1401	1RU	C17-C21-C23	2.34	132.03	128.74
2	C	1401	1RU	C17-C21-C23	2.32	132.00	128.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	1RU	O19-C20-C21	-2.31	111.39	112.68
2	D	1401	1RU	C27-C23-C21	2.31	130.70	126.95
2	C	1401	1RU	C18-O19-C20	2.27	110.31	104.75
2	B	1401	1RU	C18-O19-C20	2.11	109.92	104.75
3	B	1402	GBL	OD-C-O	2.09	125.89	120.43
2	D	1401	1RU	C28-N26-N25	2.06	123.22	120.41
2	A	1401	1RU	C27-C23-C21	2.05	130.29	126.95

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	1RU	C18-C13-O9-C7
2	B	1401	1RU	C18-C13-O9-C7
2	B	1401	1RU	C14-C13-O9-C7
2	C	1401	1RU	C18-C13-O9-C7
2	D	1401	1RU	C18-C13-O9-C7
2	A	1401	1RU	C14-C13-O9-C7
2	C	1401	1RU	C14-C13-O9-C7
2	D	1401	1RU	C14-C13-O9-C7
2	D	1401	1RU	C17-C21-C23-C27
2	D	1401	1RU	C17-C21-C23-C24
2	B	1401	1RU	C17-C21-C23-C27
2	B	1401	1RU	C17-C21-C23-C24
2	A	1401	1RU	C29-C28-N26-C27

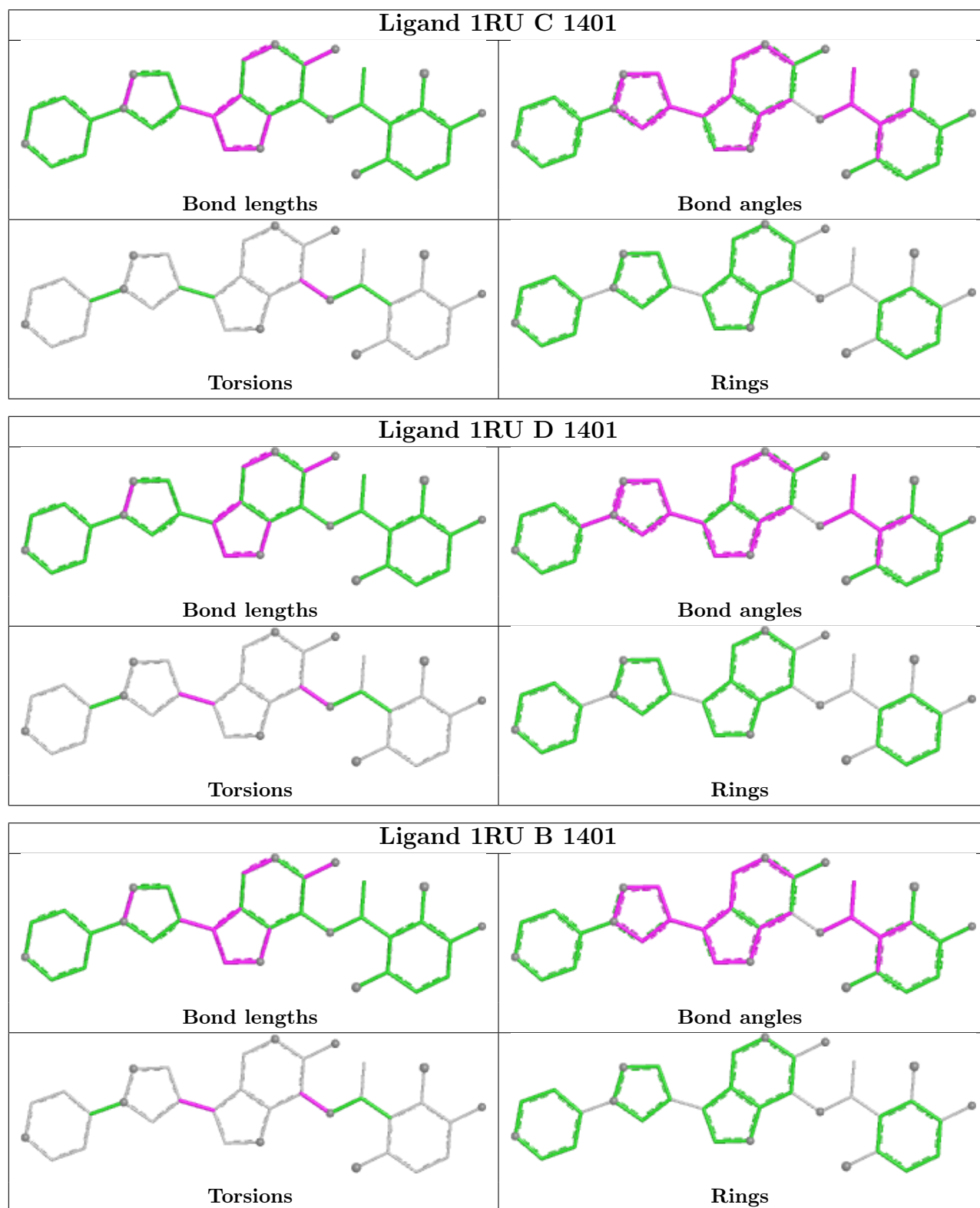
There are no ring outliers.

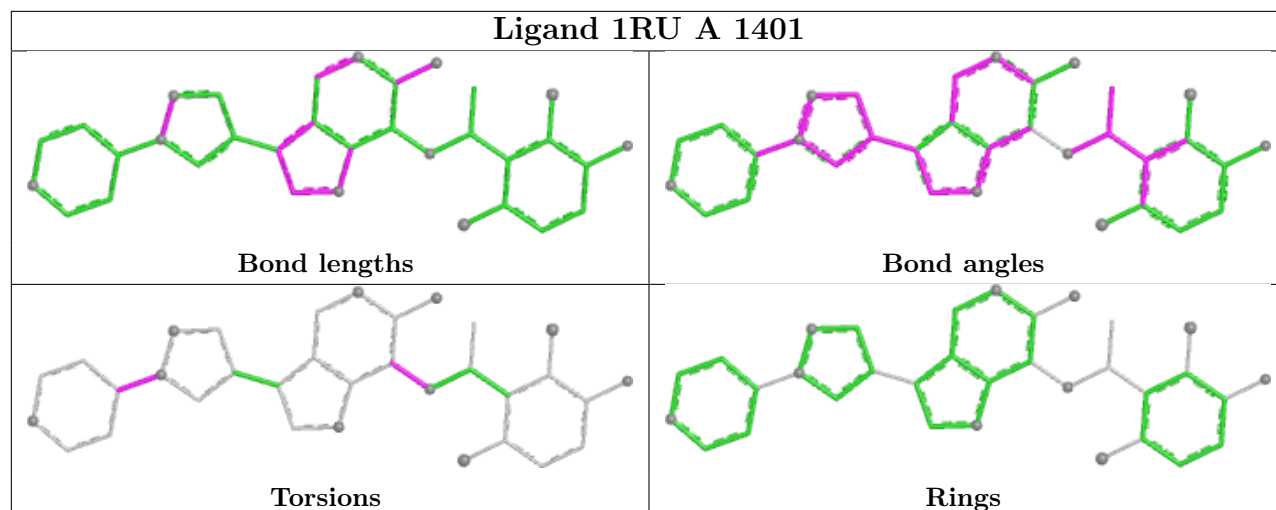
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1401	1RU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/287 (95%)	0.52	13 (4%) 35 32	35, 64, 116, 151	10 (3%)
1	B	256/287 (89%)	1.00	42 (16%) 4 4	35, 75, 163, 272	10 (3%)
1	C	271/287 (94%)	0.75	24 (8%) 15 12	44, 76, 141, 240	6 (2%)
1	D	247/287 (86%)	1.17	53 (21%) 2 2	52, 85, 135, 194	8 (3%)
All	All	1047/1148 (91%)	0.85	132 (12%) 8 6	35, 75, 140, 272	34 (3%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1144	GLY	5.2
1	D	1303	LEU	5.1
1	B	1225	LEU	5.1
1	D	1164	ASP	4.9
1	C	1226	ALA	4.6
1	B	1118	ILE	4.4
1	B	1290	PHE	4.4
1	B	1070	VAL	4.1
1	B	1237	VAL	4.1
1	D	1249	TRP	4.0
1	D	1267	TRP	4.0
1	B	1067	GLN	3.9
1	D	1073	PRO	3.9
1	B	1230	TYR	3.8
1	B	1111	SER	3.8
1	D	1152	SER	3.8
1	B	1069	VAL	3.6
1	C	1060	PRO	3.5
1	C	1118	ILE	3.5
1	B	1346	GLY	3.5
1	D	1222	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1224	GLY	3.4
1	C	1306	GLU	3.4
1	D	1118	ILE	3.3
1	D	1304	GLN	3.3
1	D	1308	CYS	3.3
1	D	1309	PRO	3.3
1	B	1153	PRO	3.2
1	D	1277	MET	3.2
1	D	1316	MET	3.2
1	D	1294	VAL	3.2
1	B	1073	PRO	3.2
1	D	1302	LEU	3.2
1	B	1083	VAL	3.2
1	B	1121	VAL	3.2
1	A	1286	ASP	3.1
1	B	1345	ILE	3.1
1	D	1099	ASP	3.1
1	D	1165	LEU	3.1
1	A	1124	PHE	3.0
1	A	1064	GLN	3.0
1	B	1082	GLU	3.0
1	D	1292	ILE	3.0
1	D	1278	THR	3.0
1	B	1146[A]	CYS	3.0
1	D	1102	GLY	3.0
1	C	1344	PHE	2.9
1	C	1290	PHE	2.9
1	B	1145	ILE	2.9
1	C	1130	ILE	2.9
1	B	1125	LEU	2.9
1	B	1124	PHE	2.9
1	B	1098	LEU	2.9
1	A	1161	LYS	2.8
1	C	1063	VAL	2.8
1	D	1066	VAL	2.8
1	B	1071	ILE	2.8
1	C	1289	THR	2.8
1	D	1064	GLN	2.8
1	D	1274	TRP	2.8
1	B	1206	ALA	2.8
1	D	1147	LEU	2.8
1	D	1248	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1216	PHE	2.8
1	D	1320	TRP	2.7
1	D	1276	LEU	2.7
1	D	1225	LEU	2.7
1	C	1081	ASN	2.6
1	D	1226	ALA	2.6
1	B	1129	ILE	2.6
1	C	1225	LEU	2.6
1	D	1092	VAL	2.6
1	D	1207	ALA	2.6
1	D	1295	TYR	2.6
1	B	1131	MET	2.5
1	A	1150	GLU	2.5
1	C	1124	PHE	2.5
1	B	1226	ALA	2.5
1	D	1272	LEU	2.5
1	B	1292	ILE	2.5
1	D	1154	LEU	2.5
1	B	1126	THR	2.5
1	D	1080	PHE	2.4
1	A	1241	THR	2.4
1	D	1149	SER	2.3
1	B	1297	LEU	2.3
1	C	1064	GLN	2.3
1	A	1147	LEU	2.3
1	D	1271	VAL	2.3
1	C	1061	GLU	2.3
1	C	1073	PRO	2.3
1	D	1072	GLY	2.3
1	D	1124	PHE	2.3
1	B	1154	LEU	2.2
1	D	1279	ARG	2.2
1	D	1301	ARG	2.2
1	D	1081	ASN	2.2
1	C	1234	TYR	2.2
1	B	1213	ASP	2.2
1	D	1109	VAL	2.2
1	D	1065	ALA	2.2
1	B	1076	LEU	2.2
1	D	1141	SER	2.2
1	D	1221	ALA	2.2
1	B	1143	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1093	TYR	2.2
1	A	1292	ILE	2.2
1	C	1129	ILE	2.2
1	D	1227	ARG	2.1
1	C	1153	PRO	2.1
1	B	1081	ASN	2.1
1	A	1125	LEU	2.1
1	D	1098	LEU	2.1
1	A	1233	GLU	2.1
1	A	1149	SER	2.1
1	B	1134	PHE	2.1
1	B	1072	GLY	2.1
1	C	1085	GLY	2.1
1	C	1224	GLY	2.1
1	B	1080	PHE	2.1
1	D	1220	VAL	2.1
1	A	1307	TYR	2.1
1	B	1089	PHE	2.0
1	C	1121	VAL	2.0
1	B	1084	ILE	2.0
1	C	1343	THR	2.0
1	D	1111	SER	2.0
1	A	1344	PHE	2.0
1	D	1083	VAL	2.0
1	C	1339	ALA	2.0
1	C	1088	HIS	2.0
1	D	1074[A]	SER	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.

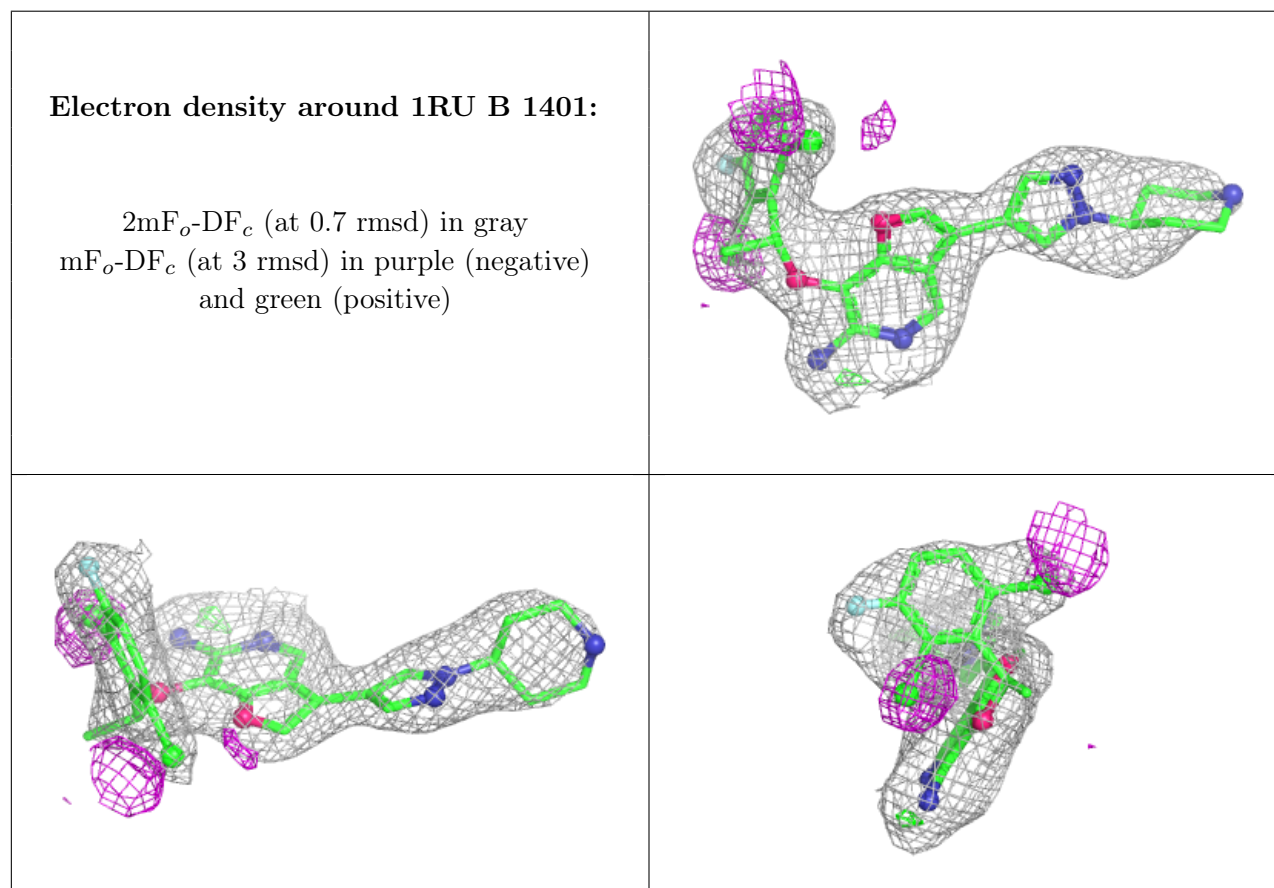
6.4 Ligands [i](#)

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.

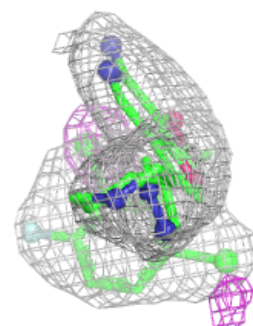
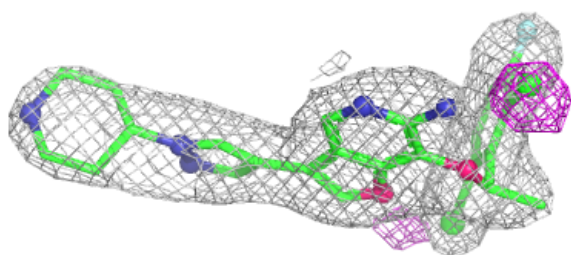
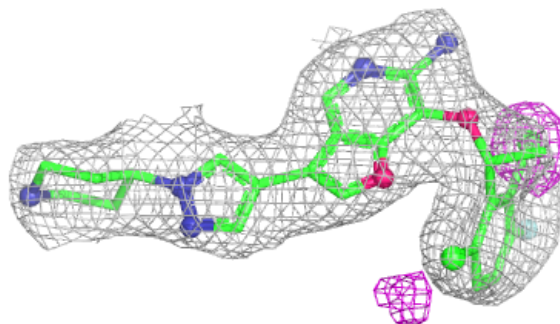
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GBL	A	1402	6/6	0.81	0.14	81,81,81,81	0
2	1RU	B	1401	33/33	0.83	0.15	79,84,87,90	0
2	1RU	D	1401	33/33	0.85	0.14	79,85,94,94	0
2	1RU	C	1401	33/33	0.88	0.13	70,74,82,84	0
3	GBL	B	1402	6/6	0.88	0.14	78,80,80,81	0
2	1RU	A	1401	33/33	0.89	0.11	64,68,75,76	0
3	GBL	A	1403	6/6	0.90	0.11	77,77,78,78	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.

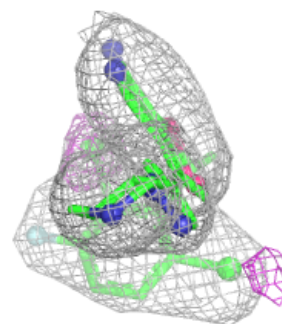
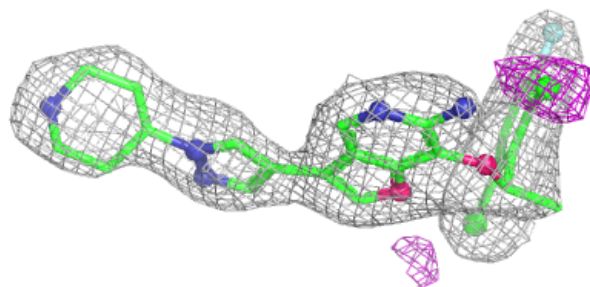
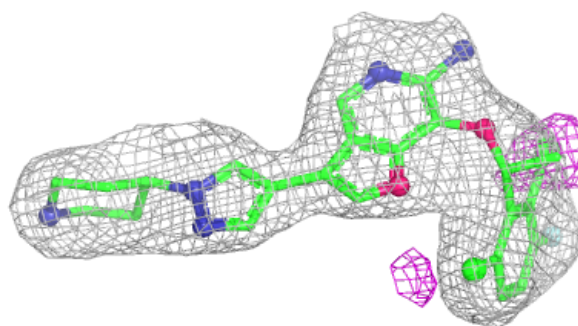


Electron density around 1RU D 1401:

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

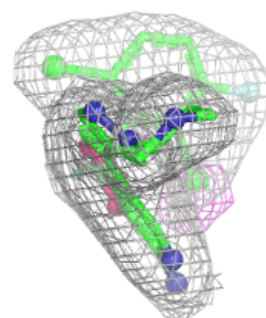
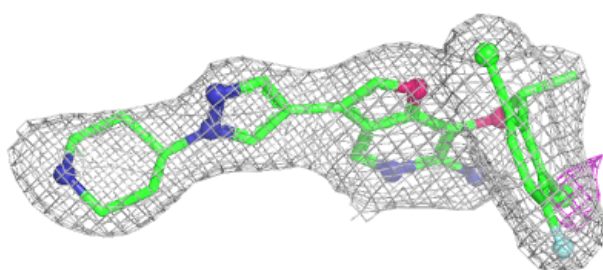
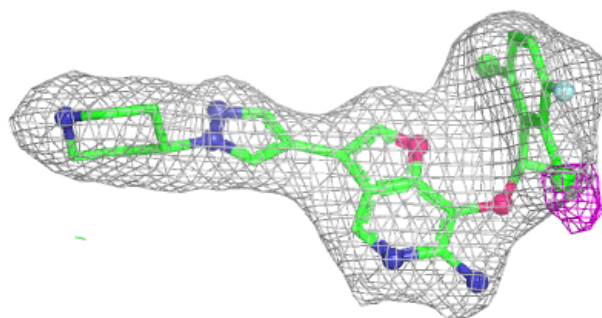
**Electron density around 1RU C 1401:**

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



Electron density around 1RU A 1401:

$2mF_o-DF_c$ (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.