



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:31 PM UTC

PDB ID : 3CTJ / pdb_00003ctj
Title : Crystal structure of the tyrosine kinase domain of the hepatocyte growth factor receptor c-met in complex with a aminopyridine based inhibitor
Authors : Sack, J.
Deposited on : 2008-04-14
Resolution : 2.50 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

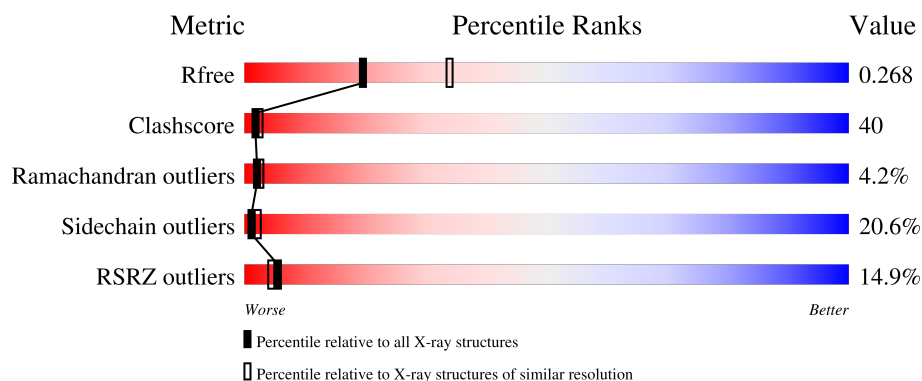
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	314	

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
2	320	A	2001	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2419 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.

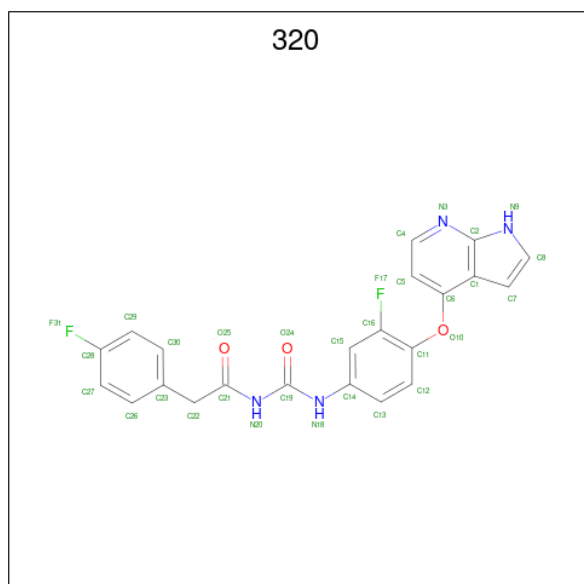
- Molecule 1 is a protein called Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2308	1495	393	406	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	GLY	-	expression tag	UNP P08581
A	1048	ALA	-	expression tag	UNP P08581
A	1194	PHE	TYR	engineered mutation	UNP P08581
A	1234	PHE	TYR	engineered mutation	UNP P08581
A	1235	ASP	TYR	engineered mutation	UNP P08581

- Molecule 2 is 2-(4-fluorophenyl)-N-{[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-yloxy)phenyl]carbamoyl}acetamide (CCD ID: 320) (formula: C₂₂H₁₆F₂N₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	22	2	4	3		

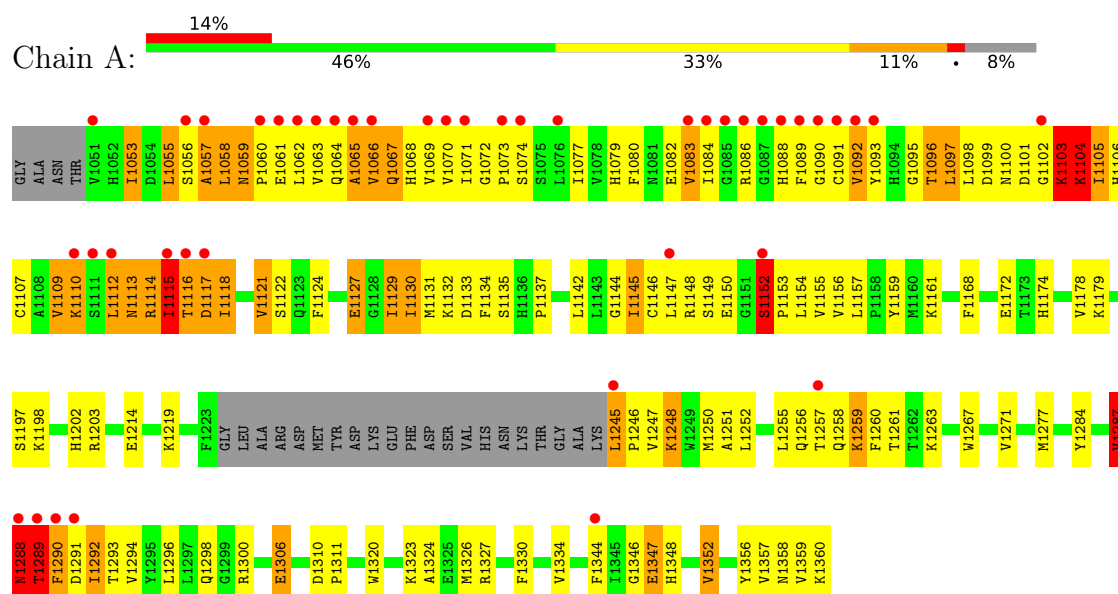
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	0
			80	80		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.81Å 47.11Å 153.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.0 (50.00-2.50) 90.3 (50.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.94 (at 2.51Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.206 , 0.261 0.203 , 0.268	Depositor DCC
R_{free} test set	620 reflections (6.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.3	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	0.93	EDS
Total number of atoms	2419	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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: 320

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	0.46	0/2370	0.94	7/3212 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1152	SER	CA-C-N	9.34	130.84	120.66
1	A	1152	SER	C-N-CA	9.34	130.84	120.66
1	A	1057	ALA	N-CA-C	-8.43	102.70	113.16
1	A	1104	LYS	N-CA-C	6.10	119.20	110.10
1	A	1287	VAL	N-CA-C	5.81	116.56	108.89
1	A	1066	VAL	N-CA-C	-5.79	105.19	113.07
1	A	1214	GLU	N-CA-C	5.39	117.91	111.71

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	2308	0	2327	184	0
2	A	31	0	16	2	0
3	A	80	0	0	7	0
All	All	2419	0	2343	186	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 40.

All (186) 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:1059:ASN:HB2	1:A:1062:LEU:HB2	1.19	1.16
1:A:1100:ASN:HB2	1:A:1103:LYS:HD2	1.42	1.01
1:A:1179:LYS:HB2	1:A:1344[B]:PHE:CD2	1.96	0.99
1:A:1288:ASN:H	1:A:1288:ASN:HD22	1.04	0.96
1:A:1102:GLY:HA3	1:A:1103:LYS:HG3	1.47	0.96
1:A:1179:LYS:HB2	1:A:1344[B]:PHE:HD2	1.24	0.96
1:A:1288:ASN:H	1:A:1288:ASN:ND2	1.58	0.94
1:A:1080:PHE:HA	1:A:1093:TYR:HD2	1.38	0.87
1:A:1100:ASN:HB2	1:A:1103:LYS:CD	2.10	0.82
1:A:1080:PHE:HA	1:A:1093:TYR:CD2	2.14	0.81
1:A:1070:VAL:HG21	1:A:1147:LEU:HD12	1.63	0.80
1:A:1114:ARG:HH11	1:A:1114:ARG:HG3	1.47	0.79
1:A:1344[B]:PHE:HE1	1:A:1348:HIS:CD2	2.00	0.79
1:A:1132:LYS:HG3	1:A:1133:ASP:OD1	1.82	0.79
1:A:1059:ASN:CB	1:A:1062:LEU:HB2	2.09	0.78
1:A:1148:ARG:HG2	3:A:44:HOH:O	1.86	0.76
1:A:1071:ILE:HD11	1:A:1146:CYS:HB2	1.67	0.74
1:A:1070:VAL:CG2	1:A:1147:LEU:HD12	2.16	0.74
1:A:1124:PHE:O	1:A:1127:GLU:HG3	1.88	0.74
1:A:1097:LEU:HD23	1:A:1105:ILE:CG2	2.18	0.74
1:A:1131:MET:HE1	1:A:1157:LEU:CD2	2.18	0.73
1:A:1288:ASN:HD22	1:A:1288:ASN:N	1.85	0.73
1:A:1115:ILE:HB	1:A:1116:THR:HA	1.70	0.73
1:A:1102:GLY:HA3	1:A:1103:LYS:CG	2.20	0.72
1:A:1115:ILE:CB	1:A:1116:THR:HA	2.21	0.71
1:A:1259:LYS:HG3	3:A:40:HOH:O	1.90	0.71
1:A:1102:GLY:H	1:A:1103:LYS:HB2	1.57	0.69
1:A:1118:ILE:O	1:A:1118:ILE:HD12	1.93	0.67
1:A:1178:VAL:HG13	1:A:1277:MET:HE1	1.76	0.67
1:A:1257:THR:O	1:A:1259:LYS:N	2.24	0.67
1:A:1114:ARG:HG3	1:A:1114:ARG:NH1	2.05	0.67
1:A:1068:HIS:CE1	1:A:1132:LYS:HE2	2.29	0.67
1:A:1067:GLN:O	1:A:1070:VAL:HG12	1.94	0.66
1:A:1137:PRO:O	1:A:1219:LYS:HE2	1.94	0.66
1:A:1096:THR:HG21	1:A:1104:LYS:NZ	2.11	0.65
1:A:1116:THR:HG23	1:A:1117:ASP:N	2.10	0.65
1:A:1097:LEU:HD23	1:A:1105:ILE:HG22	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344[B]:PHE:CZ	1:A:1348:HIS:HB2	2.33	0.64
1:A:1131:MET:HE1	1:A:1157:LEU:HD22	1.80	0.63
1:A:1072:GLY:O	1:A:1074:SER:N	2.29	0.63
1:A:1098:LEU:HD12	1:A:1098:LEU:N	2.14	0.63
1:A:1344[B]:PHE:HZ	1:A:1348:HIS:H	1.47	0.62
1:A:1248:LYS:HE3	1:A:1289:THR:HB	1.81	0.62
1:A:1292:ILE:O	1:A:1292:ILE:HG13	1.99	0.62
1:A:1092:VAL:HG13	1:A:1109:VAL:O	2.00	0.61
1:A:1145:ILE:HD11	1:A:1147:LEU:CD2	2.31	0.61
1:A:1131:MET:HE1	1:A:1157:LEU:HD21	1.81	0.61
1:A:1168:PHE:O	1:A:1174:HIS:HD2	1.84	0.61
1:A:1059:ASN:OD1	1:A:1059:ASN:N	2.34	0.60
1:A:1066:VAL:HG23	1:A:1129:ILE:HD11	1.84	0.60
1:A:1102:GLY:N	1:A:1103:LYS:HB2	2.16	0.60
1:A:1288:ASN:ND2	1:A:1288:ASN:N	2.38	0.59
1:A:1071:ILE:HD12	1:A:1071:ILE:O	2.03	0.59
1:A:1124:PHE:CE2	1:A:1155:VAL:HG23	2.38	0.59
1:A:1257:THR:OG1	1:A:1259:LYS:HG2	2.01	0.59
1:A:1291:ASP:OD2	1:A:1294:VAL:N	2.27	0.59
1:A:1288:ASN:O	1:A:1290:PHE:N	2.30	0.58
1:A:1097:LEU:HD23	1:A:1105:ILE:HG21	1.83	0.58
1:A:1145:ILE:HD11	1:A:1147:LEU:HD23	1.84	0.58
1:A:1259:LYS:HG3	1:A:1259:LYS:O	2.04	0.58
1:A:1130:ILE:HG22	1:A:1131:MET:HG3	1.86	0.58
1:A:1145:ILE:HG13	1:A:1145:ILE:O	2.05	0.56
1:A:1344[B]:PHE:HZ	1:A:1348:HIS:N	2.03	0.56
2:A:2001:320:O24	2:A:2001:320:H15	2.05	0.56
1:A:1150:GLU:HB2	3:A:43:HOH:O	2.05	0.56
1:A:1055:LEU:HD12	1:A:1118:ILE:CD1	2.36	0.55
1:A:1102:GLY:CA	1:A:1103:LYS:CB	2.84	0.55
1:A:1356:TYR:O	1:A:1359:VAL:HG23	2.06	0.55
1:A:1096:THR:HG21	1:A:1104:LYS:HZ1	1.73	0.54
1:A:1289:THR:O	1:A:1290:PHE:O	2.26	0.54
1:A:1344[B]:PHE:HZ	1:A:1348:HIS:HB2	1.73	0.54
1:A:1107:CYS:HB2	1:A:1157:LEU:O	2.08	0.53
1:A:1068:HIS:HE1	1:A:1132:LYS:HE2	1.71	0.53
1:A:1102:GLY:HA3	1:A:1103:LYS:CB	2.39	0.53
1:A:1069:VAL:HG22	1:A:1144:GLY:HA2	1.91	0.53
1:A:1055:LEU:HD12	1:A:1118:ILE:HD11	1.92	0.52
1:A:1089:PHE:CD1	1:A:1090:GLY:N	2.77	0.52
1:A:1248:LYS:HB2	3:A:23:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1357:VAL:O	1:A:1358:ASN:HB2	2.09	0.51
1:A:1287:VAL:O	1:A:1289:THR:N	2.39	0.51
1:A:1102:GLY:CA	1:A:1103:LYS:HB2	2.41	0.51
1:A:1251:ALA:HA	1:A:1267:TRP:CD2	2.46	0.51
1:A:1064:GLN:O	1:A:1065:ALA:HB3	2.11	0.51
1:A:1060:PRO:HA	3:A:49:HOH:O	2.11	0.51
1:A:1344[B]:PHE:CE1	1:A:1348:HIS:CG	2.98	0.51
1:A:1055:LEU:HD11	1:A:1121:VAL:HG11	1.93	0.50
1:A:1248:LYS:HG2	1:A:1284:TYR:HD2	1.76	0.50
1:A:1287:VAL:C	1:A:1289:THR:H	2.18	0.50
1:A:1344[B]:PHE:HZ	1:A:1348:HIS:CB	2.24	0.50
1:A:1109:VAL:HG13	1:A:1156:VAL:HG22	1.93	0.50
2:A:2001:320:O25	2:A:2001:320:N18	2.42	0.50
1:A:1083:VAL:HA	1:A:1093:TYR:HA	1.93	0.50
1:A:1057:ALA:O	1:A:1058:LEU:O	2.29	0.50
1:A:1059:ASN:HB2	1:A:1062:LEU:CB	2.13	0.50
1:A:1115:ILE:HA	1:A:1116:THR:O	2.12	0.50
1:A:1344[B]:PHE:HE1	1:A:1348:HIS:CG	2.28	0.50
1:A:1092:VAL:C	1:A:1093:TYR:HD1	2.21	0.49
1:A:1089:PHE:CE1	1:A:1112:LEU:HD23	2.47	0.49
1:A:1288:ASN:O	1:A:1289:THR:HG23	2.13	0.49
1:A:1059:ASN:HD22	1:A:1062:LEU:HD13	1.78	0.49
1:A:1344[B]:PHE:CE2	1:A:1346:GLY:HA2	2.48	0.49
1:A:1066:VAL:CG2	1:A:1129:ILE:HD11	2.42	0.49
1:A:1292:ILE:O	1:A:1296:LEU:HG	2.13	0.48
1:A:1259:LYS:HE3	1:A:1261:THR:CG2	2.43	0.48
1:A:1114:ARG:C	1:A:1115:ILE:HG23	2.37	0.48
1:A:1069:VAL:HG13	1:A:1069:VAL:O	2.13	0.48
1:A:1145:ILE:HD12	1:A:1146:CYS:O	2.14	0.48
1:A:1252:LEU:CD2	1:A:1293:THR:HG23	2.44	0.48
1:A:1055:LEU:O	1:A:1058:LEU:HB2	2.14	0.47
1:A:1271:VAL:HG23	1:A:1320:TRP:HE1	1.80	0.47
1:A:1093:TYR:CD1	1:A:1093:TYR:N	2.81	0.47
1:A:1069:VAL:HG22	1:A:1069:VAL:O	2.14	0.47
1:A:1145:ILE:HA	1:A:1154:LEU:O	2.14	0.47
1:A:1344[B]:PHE:CZ	1:A:1348:HIS:CB	2.97	0.47
1:A:1068:HIS:CE1	1:A:1132:LYS:CE	2.98	0.47
1:A:1202:HIS:O	1:A:1203:ARG:HB2	2.15	0.47
1:A:1178:VAL:HG13	1:A:1277:MET:CE	2.45	0.47
1:A:1089:PHE:CE1	1:A:1112:LEU:CD2	2.98	0.46
1:A:1116:THR:O	1:A:1117:ASP:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:LEU:C	1:A:1057:ALA:H	2.23	0.46
1:A:1112:LEU:HD12	1:A:1124:PHE:CB	2.46	0.46
1:A:1112:LEU:CD1	1:A:1124:PHE:HB2	2.46	0.46
1:A:1133:ASP:O	1:A:1135:SER:N	2.49	0.46
1:A:1098:LEU:N	1:A:1098:LEU:CD1	2.79	0.45
1:A:1115:ILE:HG13	1:A:1116:THR:N	2.30	0.45
1:A:1058:LEU:HB3	1:A:1059:ASN:H	1.47	0.45
1:A:1106:HIS:CD2	1:A:1159:TYR:CD2	3.05	0.45
1:A:1060:PRO:CA	3:A:49:HOH:O	2.65	0.45
1:A:1096:THR:HG21	1:A:1104:LYS:HZ3	1.79	0.45
1:A:1115:ILE:CG1	1:A:1116:THR:HA	2.47	0.45
1:A:1112:LEU:HD12	1:A:1124:PHE:CG	2.51	0.45
1:A:1132:LYS:HD2	1:A:1132:LYS:C	2.41	0.45
1:A:1306:GLU:HB3	3:A:52:HOH:O	2.17	0.45
1:A:1288:ASN:C	1:A:1290:PHE:H	2.23	0.45
1:A:1114:ARG:NH2	1:A:1150:GLU:O	2.50	0.45
1:A:1330:PHE:O	1:A:1334:VAL:HG23	2.16	0.45
1:A:1263:LYS:HA	1:A:1263:LYS:HD3	1.64	0.44
1:A:1089:PHE:CZ	1:A:1112:LEU:HG	2.53	0.44
1:A:1250:MET:HE3	1:A:1260:PHE:CZ	2.53	0.44
1:A:1310:ASP:N	1:A:1311:PRO:HD2	2.33	0.44
1:A:1132:LYS:HD2	1:A:1132:LYS:O	2.18	0.44
1:A:1252:LEU:HA	1:A:1252:LEU:HD23	1.75	0.43
1:A:1068:HIS:CE1	1:A:1132:LYS:NZ	2.87	0.43
1:A:1112:LEU:HD11	1:A:1124:PHE:HB2	2.01	0.43
1:A:1245:LEU:HD22	1:A:1246:PRO:HD2	1.99	0.43
1:A:1284:TYR:HB3	1:A:1287:VAL:HG13	2.00	0.43
1:A:1130:ILE:CG2	1:A:1131:MET:HG3	2.47	0.43
1:A:1263:LYS:NZ	1:A:1327:ARG:O	2.51	0.43
1:A:1326:MET:HA	1:A:1326:MET:HE3	2.00	0.43
1:A:1129:ILE:HG22	1:A:1129:ILE:O	2.18	0.42
1:A:1055:LEU:CD1	1:A:1118:ILE:CD1	2.97	0.42
1:A:1055:LEU:CD1	1:A:1118:ILE:HD13	2.50	0.42
1:A:1352:VAL:HG21	1:A:1357:VAL:HG22	2.00	0.42
1:A:1352:VAL:HG21	1:A:1357:VAL:CG2	2.49	0.42
1:A:1110:LYS:HB3	1:A:1155:VAL:HB	2.02	0.42
1:A:1344[B]:PHE:HE2	1:A:1346:GLY:HA2	1.85	0.42
1:A:1089:PHE:CG	1:A:1090:GLY:N	2.88	0.41
1:A:1116:THR:HG23	1:A:1117:ASP:H	1.82	0.41
1:A:1298:GLN:OE1	1:A:1300:ARG:NE	2.45	0.41
1:A:1347:GLU:HG2	1:A:1348:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:VAL:CG2	1:A:1357:VAL:CG2	2.99	0.41
1:A:1112:LEU:HD23	1:A:1113:ASN:H	1.84	0.41
1:A:1324:ALA:HA	1:A:1327:ARG:CZ	2.51	0.41
1:A:1344[B]:PHE:CE1	1:A:1348:HIS:CD2	2.92	0.41
1:A:1065:ALA:HB1	1:A:1068:HIS:HB3	2.02	0.41
1:A:1115:ILE:CB	1:A:1116:THR:CA	2.97	0.41
1:A:1079:HIS:CD2	1:A:1095:GLY:HA2	2.56	0.41
1:A:1179:LYS:CB	1:A:1344[B]:PHE:CD2	2.86	0.41
1:A:1058:LEU:HD22	1:A:1059:ASN:OD1	2.20	0.41
1:A:1114:ARG:HH11	1:A:1114:ARG:CG	2.21	0.41
1:A:1197:SER:OG	1:A:1198:LYS:HD3	2.21	0.41
1:A:1259:LYS:CE	1:A:1261:THR:CG2	2.99	0.41
1:A:1287:VAL:HG21	1:A:1292:ILE:HD12	2.02	0.41
1:A:1288:ASN:C	1:A:1290:PHE:N	2.79	0.41
1:A:1112:LEU:C	1:A:1152:SER:HG	2.21	0.41
1:A:1067:GLN:HE21	1:A:1067:GLN:HB2	1.73	0.40
1:A:1104:LYS:HB3	1:A:1104:LYS:HE2	1.83	0.40
1:A:1247:VAL:HB	1:A:1255:LEU:HD21	2.03	0.40
1:A:1310:ASP:HB2	1:A:1311:PRO:CD	2.52	0.40
1:A:1053:ILE:CD1	1:A:1055:LEU:HD13	2.50	0.40
1:A:1152:SER:HA	1:A:1153:PRO:HD3	1.67	0.40
1:A:1124:PHE:CD2	1:A:1124:PHE:C	2.99	0.40
1:A:1257:THR:C	1:A:1259:LYS:N	2.79	0.40
1:A:1053:ILE:HD13	1:A:1055:LEU:HD13	2.03	0.40
1:A:1114:ARG:O	1:A:1115:ILE:HG12	2.22	0.40
1:A:1257:THR:C	1:A:1259:LYS:H	2.23	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	286/314 (91%)	252 (88%)	22 (8%)	12 (4%)	2 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1058	LEU
1	A	1103	LYS
1	A	1115	ILE
1	A	1117	ASP
1	A	1258	GLN
1	A	1288	ASN
1	A	1290	PHE
1	A	1065	ALA
1	A	1134	PHE
1	A	1289	THR
1	A	1073	PRO
1	A	1116	THR

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	258/277 (93%)	205 (80%)	53 (20%)	1 2

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1053	ILE
1	A	1055	LEU
1	A	1056	SER
1	A	1059	ASN
1	A	1061	GLU
1	A	1063	VAL
1	A	1067	GLN
1	A	1077	ILE
1	A	1082	GLU

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Mol	Chain	Res	Type
1	A	1083	VAL
1	A	1084	ILE
1	A	1086	ARG
1	A	1088	HIS
1	A	1091	CYS
1	A	1092	VAL
1	A	1096	THR
1	A	1097	LEU
1	A	1099	ASP
1	A	1101	ASP
1	A	1103	LYS
1	A	1104	LYS
1	A	1105	ILE
1	A	1109	VAL
1	A	1110	LYS
1	A	1112	LEU
1	A	1113	ASN
1	A	1114	ARG
1	A	1115	ILE
1	A	1118	ILE
1	A	1121	VAL
1	A	1122	SER
1	A	1127	GLU
1	A	1129	ILE
1	A	1130	ILE
1	A	1142	LEU
1	A	1145	ILE
1	A	1149	SER
1	A	1152	SER
1	A	1161	LYS
1	A	1172	GLU
1	A	1245	LEU
1	A	1248	LYS
1	A	1256	GLN
1	A	1259	LYS
1	A	1287	VAL
1	A	1288	ASN
1	A	1289	THR
1	A	1292	ILE
1	A	1306	GLU
1	A	1323	LYS
1	A	1347	GLU

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Mol	Chain	Res	Type
1	A	1352	VAL
1	A	1360	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1067	GLN
1	A	1068	HIS
1	A	1079	HIS
1	A	1094	HIS
1	A	1100	ASN
1	A	1106	HIS
1	A	1167	ASN
1	A	1174	HIS
1	A	1288	ASN

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](#)

1 ligand is 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
2	320	A	2001	-	34,34,34	3.19	19 (55%)	47,47,47	2.84	22 (46%)

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
2	320	A	2001	-	-	3/16/16/16	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	320	C1-C2	-6.70	1.32	1.41
2	A	2001	320	C30-C23	6.02	1.50	1.38
2	A	2001	320	C11-C16	5.73	1.50	1.38
2	A	2001	320	C2-N9	5.25	1.44	1.36
2	A	2001	320	C29-C28	4.92	1.46	1.37
2	A	2001	320	C8-N9	4.70	1.46	1.38
2	A	2001	320	C26-C23	-4.37	1.30	1.38
2	A	2001	320	O10-C11	4.29	1.48	1.39
2	A	2001	320	C5-C4	4.24	1.46	1.38
2	A	2001	320	C15-C14	3.87	1.45	1.39
2	A	2001	320	C26-C27	3.77	1.44	1.38
2	A	2001	320	O10-C6	3.19	1.46	1.39
2	A	2001	320	C22-C23	2.72	1.56	1.51
2	A	2001	320	C30-C29	-2.42	1.34	1.38
2	A	2001	320	O25-C21	2.38	1.28	1.23
2	A	2001	320	C4-N3	-2.34	1.29	1.34
2	A	2001	320	F17-C16	2.30	1.41	1.35
2	A	2001	320	C19-N20	-2.22	1.34	1.39
2	A	2001	320	C22-C21	2.12	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	320	C1-C2-N3	-9.00	119.36	126.40
2	A	2001	320	C6-C1-C2	6.08	121.53	115.58
2	A	2001	320	O25-C21-N20	-5.07	112.83	122.44
2	A	2001	320	C2-N9-C8	-4.90	105.29	108.11
2	A	2001	320	C5-C4-N3	-4.85	118.03	123.97
2	A	2001	320	C2-C1-C7	4.66	108.70	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	320	C4-N3-C2	4.23	124.96	116.74
2	A	2001	320	C22-C21-N20	4.08	119.37	114.40
2	A	2001	320	C1-C2-N9	4.01	110.60	108.33
2	A	2001	320	O10-C11-C16	-3.51	112.08	119.33
2	A	2001	320	C21-N20-C19	-3.35	124.70	129.02
2	A	2001	320	O24-C19-N20	-3.06	113.45	120.69
2	A	2001	320	C23-C22-C21	-2.82	103.90	112.33
2	A	2001	320	C15-C16-C11	-2.69	119.23	122.86
2	A	2001	320	O10-C11-C12	2.69	127.79	120.74
2	A	2001	320	O25-C21-C22	2.65	127.73	121.99
2	A	2001	320	C13-C14-C15	2.51	122.69	119.66
2	A	2001	320	N18-C19-N20	2.30	119.21	114.22
2	A	2001	320	C30-C29-C28	-2.16	116.16	118.38
2	A	2001	320	O24-C19-N18	2.07	127.32	123.64
2	A	2001	320	N9-C2-N3	2.06	130.02	126.69
2	A	2001	320	C6-C1-C7	-2.04	129.76	134.84

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	320	O25-C21-N20-C19
2	A	2001	320	C22-C21-N20-C19
2	A	2001	320	O24-C19-N18-C14

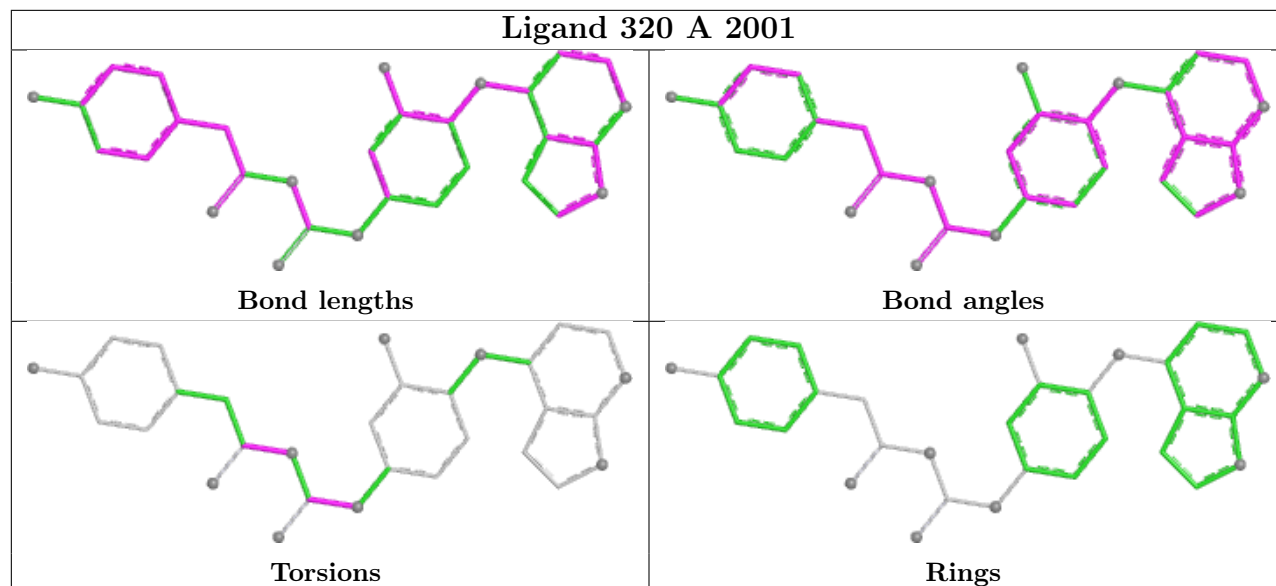
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	320	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	289/314 (92%)	0.54	43 (14%) 5 4	12, 38, 98, 122	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1085	GLY	5.3
1	A	1102	GLY	3.9
1	A	1089	PHE	3.8
1	A	1065	ALA	3.5
1	A	1088	HIS	3.5
1	A	1063	VAL	3.4
1	A	1090	GLY	3.3
1	A	1091	CYS	3.3
1	A	1056	SER	3.2
1	A	1064	GLN	3.1
1	A	1062	LEU	3.1
1	A	1152	SER	3.1
1	A	1093	TYR	3.0
1	A	1288	ASN	2.9
1	A	1112	LEU	2.9
1	A	1060	PRO	2.8
1	A	1061	GLU	2.8
1	A	1069	VAL	2.8
1	A	1084	ILE	2.7
1	A	1116	THR	2.7
1	A	1115	ILE	2.7
1	A	1076	LEU	2.7
1	A	1057	ALA	2.6
1	A	1291	ASP	2.6
1	A	1344[A]	PHE	2.6
1	A	1117	ASP	2.6
1	A	1110	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1290	PHE	2.5
1	A	1147	LEU	2.5
1	A	1071	ILE	2.4
1	A	1289	THR	2.4
1	A	1074	SER	2.4
1	A	1066	VAL	2.3
1	A	1086	ARG	2.3
1	A	1087	GLY	2.3
1	A	1092	VAL	2.3
1	A	1111	SER	2.2
1	A	1051	VAL	2.1
1	A	1245	LEU	2.1
1	A	1083	VAL	2.1
1	A	1257	THR	2.1
1	A	1070	VAL	2.0
1	A	1073	PRO	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](#)

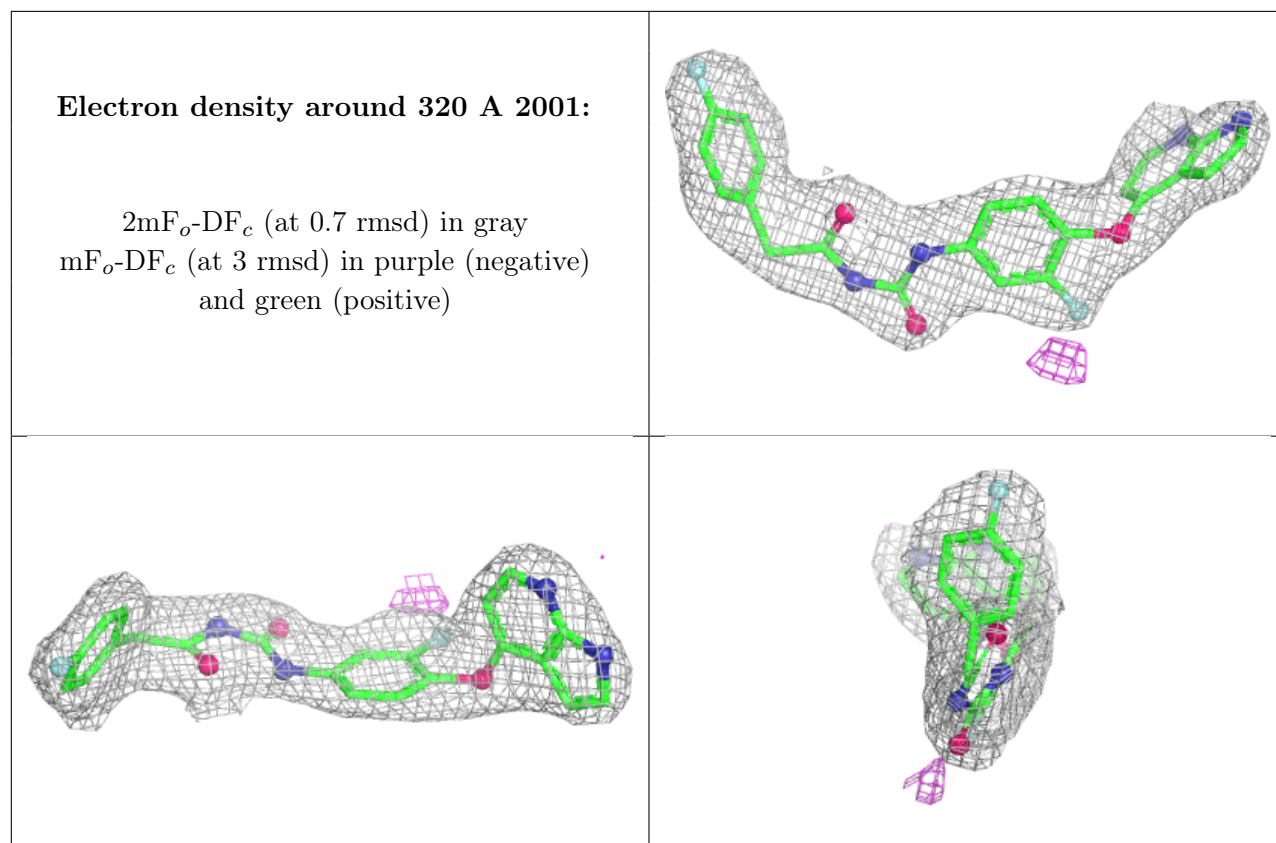
There are no oligosaccharides in this entry.

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
2	320	A	2001	31/31	0.92	0.09	28,36,43,46	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.