



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:58 AM EDT

PDB ID : 1YW2 / pdb_00001yw2
Title : Mutated Mus Musculus P38 Kinase (mP38)
Authors : Laughlin, S.K.; Clark, M.P.; Djung, J.F.; Golebiowski, A.; Brugel, T.A.; Sabat, M.; Bookland, R.G.; Laufersweiler, M.J.; Vanrens, J.C.; Townes, J.A.; De, B.; Hsieh, L.C.; Xu, S.C.; Walter, R.L.; Mekel, M.J.; Janusz, M.J.
Deposited on : 2005-02-16
Resolution : 2.01 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

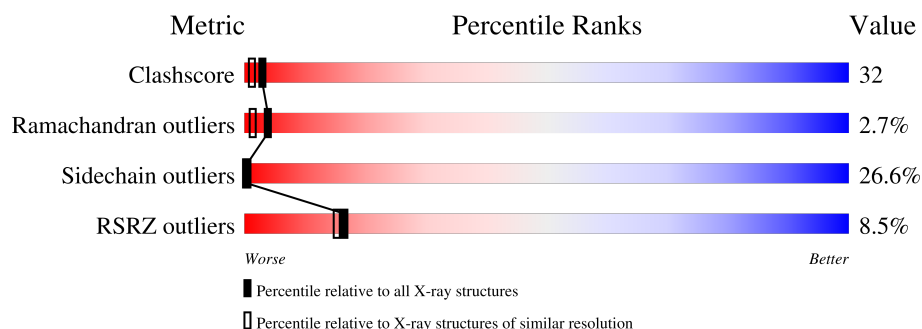
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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))
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	360	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2980 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.

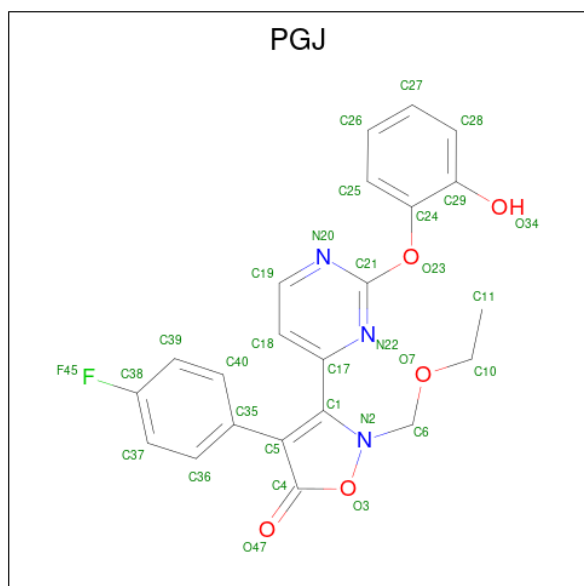
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2754	1765	475	502	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1180	ALA	THR	engineered mutation	UNP P47811
A	1182	PHE	TYR	engineered mutation	UNP P47811

- Molecule 2 is 2-(ETHOXYMETHYL)-4-(4-FLUOROPHENYL)-3-[2-(2-HYDROXYPHENOXY)PYRIMIDIN-4-YL]ISOXAZOL-5(2H)-ONE (CCD ID: PGJ) (formula: C₂₂H₁₈FN₃O₅).

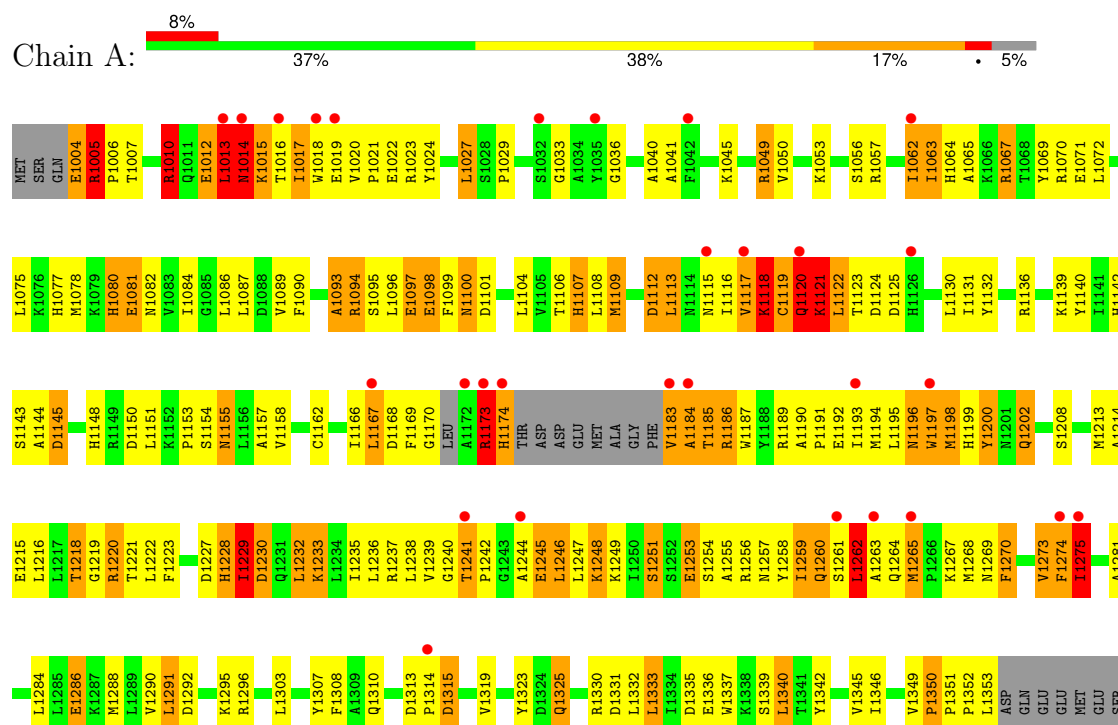


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total 195	O 195	0	0

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: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.04Å 76.95Å 73.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.01 50.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.01) 97.7 (50.00-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.01Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.207 , 0.290 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 112.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.041 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2980	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: PGJ

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	0.68	1/2818 (0.0%)	1.64	57/3823 (1.5%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1170	GLY	N-CA	-25.72	1.04	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1350	PRO	O-C-N	11.93	126.76	121.15
1	A	1169	PHE	CA-C-N	-10.11	103.50	121.70
1	A	1169	PHE	C-N-CA	-10.11	103.50	121.70
1	A	1275	ILE	CA-C-N	8.35	134.15	122.29
1	A	1275	ILE	C-N-CA	8.35	134.15	122.29
1	A	1249	LYS	CA-C-N	-7.46	113.36	122.90
1	A	1249	LYS	C-N-CA	-7.46	113.36	122.90
1	A	1330	ARG	CA-C-N	7.13	134.20	123.23
1	A	1330	ARG	C-N-CA	7.13	134.20	123.23
1	A	1045	LYS	CA-C-N	7.04	135.16	122.06
1	A	1045	LYS	C-N-CA	7.04	135.16	122.06
1	A	1120	GLN	CA-C-N	6.81	134.55	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1120	GLN	C-N-CA	6.81	134.55	121.54
1	A	1199	HIS	N-CA-C	-6.79	104.89	112.57
1	A	1184	ALA	CA-C-N	6.74	134.41	121.54
1	A	1184	ALA	C-N-CA	6.74	134.41	121.54
1	A	1197	TRP	CA-C-N	6.57	133.53	121.70
1	A	1197	TRP	C-N-CA	6.57	133.53	121.70
1	A	1166	ILE	CA-C-N	-6.53	113.99	123.00
1	A	1166	ILE	C-N-CA	-6.53	113.99	123.00
1	A	1124	ASP	CA-C-N	6.51	129.01	120.28
1	A	1124	ASP	C-N-CA	6.51	129.01	120.28
1	A	1260	GLN	CA-C-N	6.46	131.52	122.41
1	A	1260	GLN	C-N-CA	6.46	131.52	122.41
1	A	1345	VAL	N-CA-C	-6.34	104.57	110.53
1	A	1005	ARG	O-C-N	6.26	125.03	121.27
1	A	1112	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	1229	ILE	CA-C-N	6.09	128.76	120.54
1	A	1229	ILE	C-N-CA	6.09	128.76	120.54
1	A	1010	ARG	CD-NE-CZ	6.01	132.81	124.40
1	A	1096	LEU	CA-C-N	5.94	128.56	120.54
1	A	1096	LEU	C-N-CA	5.94	128.56	120.54
1	A	1118	LYS	CA-C-N	5.91	132.34	121.70
1	A	1118	LYS	C-N-CA	5.91	132.34	121.70
1	A	1077	HIS	CA-C-N	-5.77	114.75	122.42
1	A	1077	HIS	C-N-CA	-5.77	114.75	122.42
1	A	1288	MET	CA-C-N	-5.65	114.45	122.41
1	A	1288	MET	C-N-CA	-5.65	114.45	122.41
1	A	1155	ASN	CA-CB-CG	-5.58	107.02	112.60
1	A	1013	LEU	CA-C-N	5.54	132.12	121.54
1	A	1013	LEU	C-N-CA	5.54	132.12	121.54
1	A	1274	PHE	CA-C-N	5.53	131.65	121.70
1	A	1274	PHE	C-N-CA	5.53	131.65	121.70
1	A	1080	HIS	CA-CB-CG	5.50	119.30	113.80
1	A	1027	LEU	CA-C-N	-5.49	115.21	122.56
1	A	1027	LEU	C-N-CA	-5.49	115.21	122.56
1	A	1145	ASP	CA-C-O	5.45	127.74	120.98
1	A	1101	ASP	O-C-N	5.39	129.85	123.27
1	A	1270	PHE	O-C-N	5.38	128.30	122.11
1	A	1228	HIS	CA-CB-CG	-5.35	108.45	113.80
1	A	1109	MET	N-CA-C	-5.35	107.30	113.88
1	A	1219	GLY	CA-C-N	-5.21	112.63	121.85
1	A	1219	GLY	C-N-CA	-5.21	112.63	121.85
1	A	1331	ASP	CA-CB-CG	5.15	117.75	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1230	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	1262	LEU	CA-C-N	-5.03	113.57	120.71
1	A	1262	LEU	C-N-CA	-5.03	113.57	120.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1173	ARG	Sidechain

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	2754	0	2747	178	0
2	A	31	0	18	0	0
3	A	195	0	0	12	0
All	All	2980	0	2765	178	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 32.

All (178) 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:1173:ARG:O	1:A:1174:HIS:HB3	1.32	1.05
1:A:1087:LEU:HD23	1:A:1106:THR:HA	1.52	0.90
1:A:1263:ALA:HB3	1:A:1265:MET:HE3	1.55	0.89
1:A:1173:ARG:O	1:A:1174:HIS:CB	2.16	0.87
1:A:1218:THR:HG22	1:A:1220:ARG:H	1.46	0.81
1:A:1131:ILE:HG21	1:A:1213:MET:HE3	1.62	0.80
1:A:1236:LEU:HD12	1:A:1262:LEU:HD12	1.64	0.79
1:A:1155:ASN:HA	1:A:1167:LEU:HD11	1.67	0.77
1:A:1080:HIS:HD2	1:A:1082:ASN:H	1.29	0.76
1:A:1230:ASP:HA	1:A:1233:LYS:HG3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:HIS:ND1	1:A:1174:HIS:C	2.44	0.73
1:A:1227:ASP:OD1	1:A:1229:ILE:HG13	1.89	0.73
1:A:1117:VAL:HG13	1:A:1120:GLN:HG3	1.72	0.72
1:A:1214:ALA:O	1:A:1218:THR:HB	1.90	0.72
1:A:1004:GLU:OE1	1:A:1006:PRO:HD3	1.89	0.72
1:A:1095:SER:OG	1:A:1097:GLU:HB2	1.90	0.71
1:A:1062:ILE:HG22	1:A:1063:ILE:HD13	1.72	0.71
1:A:1123:THR:HG22	1:A:1125:ASP:H	1.56	0.71
1:A:1198:MET:HB3	1:A:1200:TYR:H	1.56	0.71
1:A:1155:ASN:O	1:A:1167:LEU:HG	1.91	0.70
1:A:1198:MET:HB3	1:A:1200:TYR:N	2.07	0.69
1:A:1333:LEU:HB3	3:A:3079:HOH:O	1.90	0.69
1:A:1230:ASP:HA	1:A:1233:LYS:HE2	1.73	0.69
1:A:1232:LEU:O	1:A:1236:LEU:HG	1.93	0.69
1:A:1131:ILE:HG13	1:A:1213:MET:HE3	1.75	0.69
1:A:1191:PRO:HG3	1:A:1235:ILE:HD13	1.73	0.69
1:A:1218:THR:HG22	1:A:1220:ARG:N	2.07	0.68
1:A:1336:GLU:O	1:A:1340:LEU:HD22	1.93	0.68
1:A:1118:LYS:HG3	1:A:1119:CYS:HA	1.77	0.67
1:A:1197:TRP:HB3	1:A:1198:MET:HG3	1.76	0.66
1:A:1120:GLN:NE2	1:A:1216:LEU:HA	2.11	0.66
1:A:1261:SER:O	1:A:1262:LEU:HD23	1.97	0.65
1:A:1121:LYS:HE2	1:A:1122:LEU:O	1.97	0.65
1:A:1253:GLU:HB2	1:A:1256:ARG:HH21	1.62	0.64
1:A:1184:ALA:HB3	1:A:1187:TRP:CD2	2.33	0.64
1:A:1242:PRO:HG3	1:A:1259:ILE:HG21	1.80	0.63
1:A:1078:MET:HA	1:A:1078:MET:HE2	1.81	0.63
1:A:1087:LEU:HD21	1:A:1107:HIS:CE1	2.34	0.63
1:A:1080:HIS:CD2	1:A:1082:ASN:H	2.15	0.62
1:A:1142:HIS:CG	1:A:1202:GLN:HG2	2.34	0.62
1:A:1247:LEU:HD13	1:A:1260:GLN:NE2	2.15	0.62
1:A:1117:VAL:HG22	1:A:1122:LEU:HD21	1.82	0.62
1:A:1235:ILE:O	1:A:1239:VAL:HG22	2.00	0.61
1:A:1155:ASN:HD22	1:A:1167:LEU:HD11	1.66	0.60
1:A:1244:ALA:O	1:A:1248:LYS:HG2	2.01	0.60
1:A:1093:ALA:HB1	1:A:1098:GLU:HG3	1.83	0.60
1:A:1120:GLN:HE22	1:A:1216:LEU:HA	1.67	0.59
1:A:1239:VAL:HG21	1:A:1291:LEU:HD13	1.85	0.59
1:A:1323:TYR:CD2	1:A:1325:GLN:HG2	2.37	0.59
1:A:1062:ILE:HD11	1:A:1332:LEU:O	2.04	0.58
1:A:1255:ALA:O	1:A:1259:ILE:HG13	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:SER:O	1:A:1258:TYR:HD1	1.87	0.57
1:A:1049:ARG:HH21	1:A:1049:ARG:HB2	1.69	0.56
1:A:1229:ILE:HG13	1:A:1230:ASP:H	1.70	0.56
1:A:1087:LEU:HD21	1:A:1107:HIS:NE2	2.20	0.56
1:A:1107:HIS:H	1:A:1107:HIS:CD2	2.23	0.56
1:A:1120:GLN:NE2	1:A:1216:LEU:HD23	2.20	0.56
1:A:1230:ASP:CA	1:A:1233:LYS:HG3	2.35	0.56
1:A:1148:HIS:CE1	1:A:1168:ASP:HA	2.41	0.56
1:A:1349:VAL:HG13	1:A:1350:PRO:HD2	1.88	0.56
1:A:1153:PRO:HB2	1:A:1183:VAL:HG23	1.88	0.55
1:A:1167:LEU:HD12	1:A:1167:LEU:O	2.06	0.55
1:A:1242:PRO:HG2	1:A:1247:LEU:HD21	1.88	0.55
1:A:1117:VAL:CG1	1:A:1120:GLN:HG3	2.36	0.55
1:A:1142:HIS:CD2	1:A:1202:GLN:HG2	2.42	0.55
1:A:1154:SER:OG	1:A:1183:VAL:HG21	2.07	0.54
1:A:1195:LEU:HD13	1:A:1197:TRP:CH2	2.43	0.54
1:A:1151:LEU:HB2	3:A:3003:HOH:O	2.08	0.54
1:A:1087:LEU:HD13	1:A:1351:PRO:HG3	1.90	0.53
1:A:1197:TRP:HB3	1:A:1198:MET:CG	2.38	0.53
1:A:1274:PHE:HA	1:A:1275:ILE:HB	1.89	0.53
1:A:1081:GLU:CG	1:A:1136:ARG:HH12	2.21	0.53
1:A:1244:ALA:O	1:A:1247:LEU:HB2	2.08	0.53
1:A:1184:ALA:HB3	1:A:1187:TRP:CE3	2.44	0.53
1:A:1263:ALA:O	1:A:1265:MET:HG2	2.10	0.52
1:A:1027:LEU:HD23	3:A:3017:HOH:O	2.08	0.52
1:A:1053:LYS:HE2	1:A:1071:GLU:OE2	2.09	0.52
1:A:1148:HIS:HD2	1:A:1150:ASP:H	1.54	0.52
1:A:1081:GLU:HG2	3:A:3010:HOH:O	2.08	0.52
1:A:1080:HIS:HE1	3:A:3041:HOH:O	1.93	0.52
1:A:1087:LEU:HD23	1:A:1106:THR:CA	2.35	0.52
1:A:1281:ALA:HB2	1:A:1307:TYR:CE1	2.46	0.51
1:A:1232:LEU:HD23	1:A:1236:LEU:HG	1.92	0.51
1:A:1244:ALA:HA	1:A:1247:LEU:HD12	1.93	0.50
1:A:1253:GLU:HG3	1:A:1254:SER:N	2.25	0.50
1:A:1247:LEU:HD13	1:A:1260:GLN:HE22	1.76	0.50
1:A:1117:VAL:HG13	1:A:1117:VAL:O	2.12	0.49
1:A:1267:LYS:HD2	3:A:3150:HOH:O	2.12	0.49
1:A:1012:GLU:OE2	1:A:1015:LYS:HA	2.13	0.49
1:A:1081:GLU:HG2	1:A:1136:ARG:HH12	1.76	0.49
1:A:1131:ILE:HG13	1:A:1213:MET:CE	2.42	0.49
1:A:1184:ALA:HB3	1:A:1187:TRP:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:VAL:HG12	1:A:1090:PHE:CZ	2.48	0.48
1:A:1229:ILE:HD12	1:A:1233:LYS:NZ	2.28	0.48
1:A:1223:PHE:HZ	1:A:1238:LEU:HD23	1.77	0.48
1:A:1132:TYR:CE1	1:A:1303:LEU:HD22	2.49	0.48
1:A:1069:TYR:CE2	1:A:1340:LEU:HB3	2.49	0.47
1:A:1154:SER:H	1:A:1183:VAL:HG21	1.79	0.47
1:A:1192:GLU:CD	1:A:1296:ARG:HH12	2.22	0.47
1:A:1245:GLU:HG2	1:A:1246:LEU:H	1.79	0.47
1:A:1020:VAL:HG12	1:A:1090:PHE:CE1	2.49	0.47
1:A:1089:VAL:HG23	1:A:1104:LEU:HD23	1.96	0.47
1:A:1112:ASP:H	1:A:1115:ASN:HB2	1.79	0.47
1:A:1229:ILE:HG13	1:A:1230:ASP:N	2.30	0.47
1:A:1308:PHE:HA	3:A:3019:HOH:O	2.14	0.46
1:A:1140:TYR:O	1:A:1143:SER:OG	2.31	0.46
1:A:1155:ASN:HA	1:A:1155:ASN:HD22	1.40	0.46
1:A:1232:LEU:HD23	1:A:1236:LEU:CG	2.45	0.46
1:A:1113:LEU:O	1:A:1117:VAL:HB	2.16	0.46
1:A:1014:ASN:HA	1:A:1015:LYS:HA	1.37	0.46
1:A:1120:GLN:HE22	1:A:1215:GLU:C	2.24	0.46
1:A:1023:ARG:HG2	1:A:1024:TYR:CE1	2.50	0.46
1:A:1195:LEU:O	1:A:1196:ASN:HB2	2.15	0.45
1:A:1230:ASP:HA	1:A:1233:LYS:CE	2.41	0.45
1:A:1192:GLU:HA	1:A:1197:TRP:CE3	2.51	0.45
1:A:1094:ARG:HB2	3:A:3165:HOH:O	2.16	0.45
1:A:1263:ALA:CB	1:A:1265:MET:HE3	2.38	0.45
1:A:1194:MET:HG2	1:A:1228:HIS:CD2	2.52	0.45
1:A:1251:SER:O	1:A:1256:ARG:NH1	2.50	0.45
1:A:1263:ALA:O	1:A:1265:MET:N	2.50	0.45
1:A:1014:ASN:OD1	1:A:1014:ASN:N	2.50	0.45
1:A:1036:GLY:N	1:A:1056:SER:OG	2.50	0.45
1:A:1241:THR:HG21	3:A:3037:HOH:O	2.16	0.45
1:A:1067:ARG:NH2	1:A:1071:GLU:OE1	2.50	0.45
1:A:1190:ALA:HB1	1:A:1192:GLU:CD	2.42	0.45
1:A:1247:LEU:HB2	1:A:1248:LYS:NZ	2.32	0.45
1:A:1010:ARG:HA	1:A:1018:TRP:O	2.17	0.45
1:A:1013:LEU:HG	1:A:1029:PRO:HD3	2.00	0.44
1:A:1050:VAL:C	1:A:1108:LEU:HB2	2.41	0.44
1:A:1213:MET:HE1	1:A:1284:LEU:HD23	1.99	0.44
1:A:1139:LYS:HE2	1:A:1319:VAL:HG13	1.98	0.44
1:A:1186:ARG:HA	1:A:1189:ARG:HG3	1.99	0.44
1:A:1012:GLU:HG3	1:A:1017:ILE:HD13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:LEU:HD23	1:A:1151:LEU:HA	1.82	0.44
1:A:1155:ASN:ND2	1:A:1167:LEU:HD11	2.30	0.44
1:A:1192:GLU:OE2	1:A:1296:ARG:NH2	2.50	0.44
1:A:1084:ILE:HG13	1:A:1167:LEU:HB3	1.99	0.44
1:A:1087:LEU:HD21	1:A:1107:HIS:CD2	2.52	0.44
1:A:1273:VAL:HG12	1:A:1274:PHE:CD1	2.52	0.44
1:A:1021:PRO:HD3	1:A:1090:PHE:CE1	2.52	0.44
1:A:1315:ASP:OD1	1:A:1315:ASP:N	2.50	0.44
1:A:1087:LEU:HD13	1:A:1087:LEU:HA	1.85	0.44
1:A:1117:VAL:CG2	1:A:1122:LEU:HD21	2.47	0.44
1:A:1080:HIS:CD2	1:A:1082:ASN:HB2	2.53	0.43
1:A:1117:VAL:HG21	1:A:1216:LEU:HD22	2.00	0.43
1:A:1075:LEU:HB3	1:A:1086:LEU:HG	2.01	0.43
1:A:1313:ASP:HA	1:A:1314:PRO:HD3	1.84	0.43
1:A:1112:ASP:OD1	1:A:1154:SER:HA	2.19	0.43
1:A:1198:MET:HB2	1:A:1200:TYR:HB3	2.01	0.43
1:A:1120:GLN:NE2	1:A:1215:GLU:O	2.52	0.43
1:A:1270:PHE:O	1:A:1274:PHE:N	2.49	0.42
1:A:1144:ALA:O	1:A:1145:ASP:HB2	2.19	0.42
1:A:1065:ALA:HB1	1:A:1337:TRP:HB2	2.00	0.42
1:A:1013:LEU:HB3	1:A:1029:PRO:HG3	2.02	0.42
1:A:1040:ALA:O	1:A:1041:ALA:HB2	2.20	0.42
1:A:1275:ILE:HD12	1:A:1275:ILE:HG21	1.75	0.42
1:A:1236:LEU:O	1:A:1240:GLY:N	2.50	0.42
1:A:1098:GLU:H	1:A:1098:GLU:HG2	1.68	0.42
1:A:1196:ASN:HD22	1:A:1196:ASN:HA	1.48	0.42
1:A:1197:TRP:HB3	1:A:1198:MET:CB	2.49	0.41
1:A:1241:THR:HG23	1:A:1265:MET:H	1.85	0.41
1:A:1131:ILE:CG2	1:A:1213:MET:HE3	2.43	0.41
1:A:1291:LEU:HA	1:A:1291:LEU:HD12	1.62	0.41
1:A:1109:MET:HE2	1:A:1157:ALA:O	2.21	0.41
1:A:1122:LEU:HD23	1:A:1122:LEU:N	2.35	0.41
1:A:1235:ILE:HD13	1:A:1235:ILE:HG21	1.81	0.41
1:A:1290:VAL:HG12	1:A:1292:ASP:H	1.85	0.41
1:A:1120:GLN:CG	1:A:1121:LYS:H	2.34	0.41
1:A:1242:PRO:HD2	3:A:3089:HOH:O	2.20	0.41
1:A:1005:ARG:HD3	1:A:1094:ARG:HD3	2.03	0.41
1:A:1198:MET:C	1:A:1200:TYR:H	2.28	0.41
1:A:1099:PHE:CD2	1:A:1342:TYR:HB2	2.56	0.40
1:A:1005:ARG:HA	1:A:1006:PRO:HD2	1.78	0.40
1:A:1270:PHE:CE1	1:A:1286:GLU:HA	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:ALA:CB	1:A:1222:LEU:HD22	2.51	0.40
1:A:1033:GLY:HA3	3:A:3080:HOH:O	2.21	0.40
1:A:1070:ARG:NH1	3:A:3168:HOH:O	2.54	0.40
1:A:1191:PRO:HG3	1:A:1235:ILE:HG21	2.03	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	335/360 (93%)	310 (92%)	16 (5%)	9 (3%)	4 1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	ASN
1	A	1121	LYS
1	A	1185	THR
1	A	1275	ILE
1	A	1173	ARG
1	A	1200	TYR
1	A	1093	ALA
1	A	1100	ASN
1	A	1352	PRO

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	301/318 (95%)	221 (73%)	80 (27%)	0 0

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	GLU
1	A	1005	ARG
1	A	1007	THR
1	A	1010	ARG
1	A	1012	GLU
1	A	1013	LEU
1	A	1014	ASN
1	A	1015	LYS
1	A	1016	THR
1	A	1017	ILE
1	A	1019	GLU
1	A	1022	GLU
1	A	1049	ARG
1	A	1057	ARG
1	A	1062	ILE
1	A	1063	ILE
1	A	1064	HIS
1	A	1067	ARG
1	A	1072	LEU
1	A	1081	GLU
1	A	1094	ARG
1	A	1097	GLU
1	A	1098	GLU
1	A	1100	ASN
1	A	1107	HIS
1	A	1113	LEU
1	A	1116	ILE
1	A	1117	VAL
1	A	1118	LYS
1	A	1119	CYS
1	A	1120	GLN
1	A	1121	LYS
1	A	1122	LEU
1	A	1130	LEU
1	A	1158	VAL
1	A	1162	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1167	LEU
1	A	1174	HIS
1	A	1183	VAL
1	A	1185	THR
1	A	1186	ARG
1	A	1193	ILE
1	A	1196	ASN
1	A	1198	MET
1	A	1202	GLN
1	A	1208	SER
1	A	1218	THR
1	A	1220	ARG
1	A	1221	THR
1	A	1229	ILE
1	A	1232	LEU
1	A	1233	LYS
1	A	1237	ARG
1	A	1241	THR
1	A	1245	GLU
1	A	1246	LEU
1	A	1248	LYS
1	A	1251	SER
1	A	1253	GLU
1	A	1257	ASN
1	A	1259	ILE
1	A	1262	LEU
1	A	1264	GLN
1	A	1265	MET
1	A	1268	MET
1	A	1269	ASN
1	A	1273	VAL
1	A	1275	ILE
1	A	1286	GLU
1	A	1291	LEU
1	A	1295	LYS
1	A	1310	GLN
1	A	1315	ASP
1	A	1325	GLN
1	A	1333	LEU
1	A	1335	ASP
1	A	1339	SER
1	A	1340	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1346	ILE
1	A	1353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1060	GLN
1	A	1064	HIS
1	A	1080	HIS
1	A	1107	HIS
1	A	1115	ASN
1	A	1148	HIS
1	A	1155	ASN
1	A	1196	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	PGJ	A	2001	-	32,34,34	1.38	4 (12%)	37,47,47	3.70	11 (29%)

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	PGJ	A	2001	-	-	5/15/16/16	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	PGJ	C21-N20	4.99	1.38	1.32
2	A	2001	PGJ	C21-N22	3.17	1.39	1.33
2	A	2001	PGJ	C5-C1	-2.80	1.34	1.39
2	A	2001	PGJ	C17-C1	-2.07	1.46	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	PGJ	N20-C21-N22	-15.94	114.62	128.35
2	A	2001	PGJ	C19-N20-C21	11.07	121.78	114.46
2	A	2001	PGJ	O3-C4-O47	5.38	127.72	118.84
2	A	2001	PGJ	C18-C17-N22	-4.10	118.13	122.92
2	A	2001	PGJ	C1-C17-N22	3.95	120.26	115.57
2	A	2001	PGJ	O23-C24-C29	3.31	122.19	116.59
2	A	2001	PGJ	O47-C4-C5	-3.15	124.27	130.71
2	A	2001	PGJ	O23-C21-N22	2.79	125.68	116.09
2	A	2001	PGJ	C35-C5-C1	2.78	132.41	127.01
2	A	2001	PGJ	C36-C35-C5	-2.51	116.84	120.79
2	A	2001	PGJ	C35-C5-C4	-2.43	117.81	122.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	PGJ	O7-C6-N2-C1
2	A	2001	PGJ	C11-C10-O7-C6
2	A	2001	PGJ	C29-C24-O23-C21
2	A	2001	PGJ	N20-C21-O23-C24

Continued on next page...

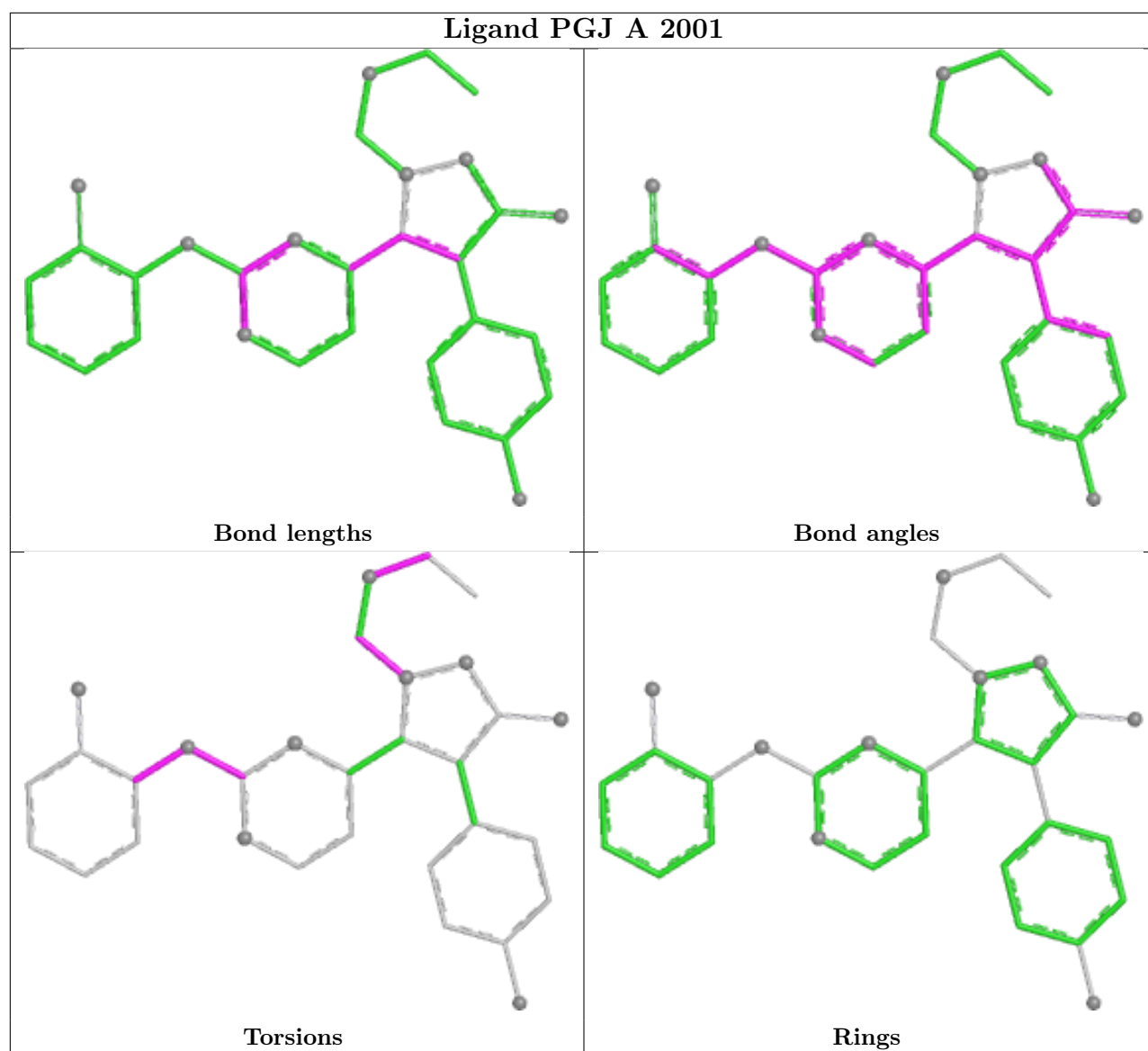
Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2001	PGJ	N22-C21-O23-C24

There are no ring outliers.

No monomer is involved in short contacts.

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	341/360 (94%)	0.78	29 (8%) 16 15	20, 51, 94, 149	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1172	ALA	9.1
1	A	1174	HIS	7.8
1	A	1275	ILE	6.1
1	A	1197	TRP	5.4
1	A	1120	GLN	3.4
1	A	1062	ILE	3.3
1	A	1173	ARG	3.3
1	A	1019	GLU	3.1
1	A	1184	ALA	3.0
1	A	1263	ALA	2.8
1	A	1013	LEU	2.7
1	A	1117	VAL	2.7
1	A	1167	LEU	2.7
1	A	1014	ASN	2.7
1	A	1035	TYR	2.7
1	A	1183	VAL	2.7
1	A	1261	SER	2.6
1	A	1193	ILE	2.5
1	A	1265	MET	2.4
1	A	1115	ASN	2.4
1	A	1032	SER	2.4
1	A	1016	THR	2.3
1	A	1018	TRP	2.2
1	A	1241	THR	2.2
1	A	1042	PHE	2.2
1	A	1274	PHE	2.1
1	A	1244	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1126	HIS	2.1
1	A	1314	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](#)

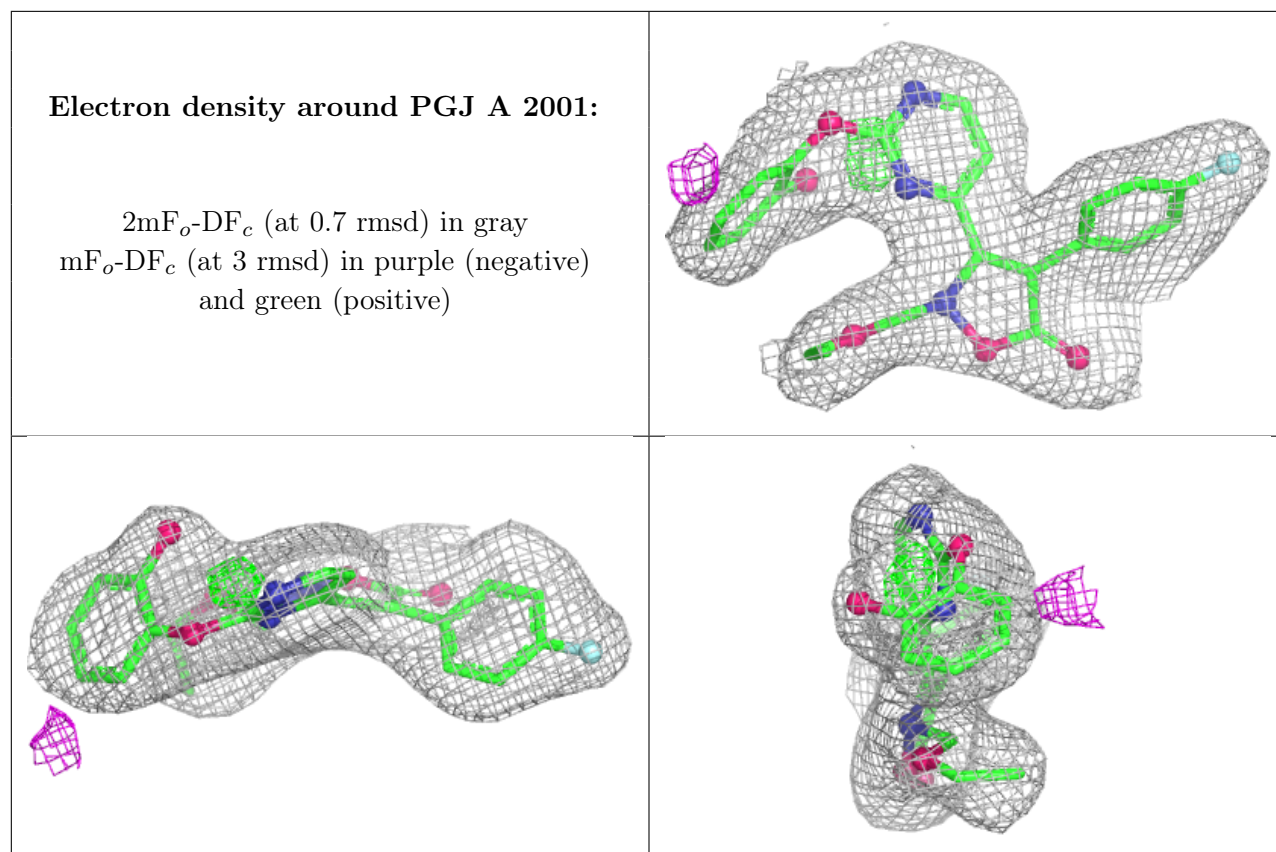
There are no oligosaccharides in this entry.

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	PGJ	A	2001	31/31	0.93	0.08	21,40,61,71	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.