



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:29 PM EDT

PDB ID : 4RXE / pdb_00004rx
Title : T. Brucei Farnesyl Diphosphate Synthase Complexed with Bisphosphonate BPH-14
Authors : Cao, R.; Liu, Y.-L.; Oldfield, E.
Deposited on : 2014-12-10
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

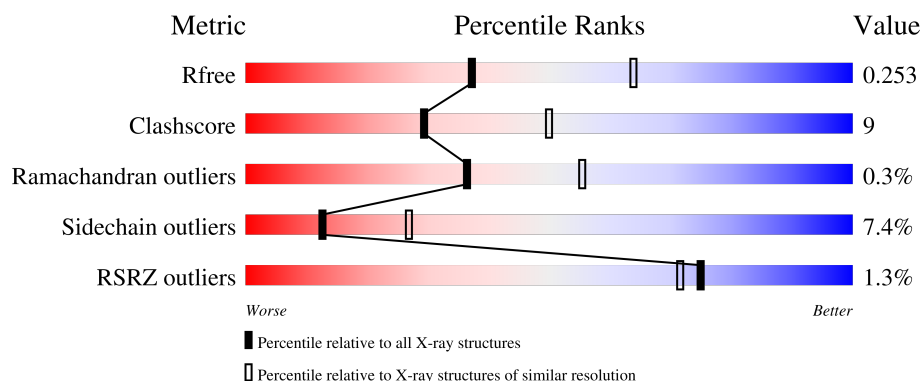
1 Overall quality at a glance

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	390	
1	B	390	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5934 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 Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2864	1826	472	538	28			
1	B	359	Total	C	N	O	S	0	0	0
			2872	1830	474	540	28			

There are 46 discrepancies between the modelled and reference sequences:

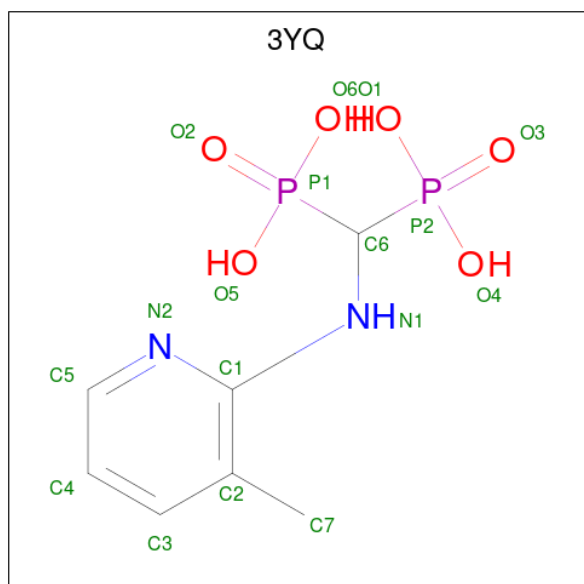
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q86C09
A	-21	GLY	-	expression tag	UNP Q86C09
A	-20	SER	-	expression tag	UNP Q86C09
A	-19	SER	-	expression tag	UNP Q86C09
A	-18	HIS	-	expression tag	UNP Q86C09
A	-17	HIS	-	expression tag	UNP Q86C09
A	-16	HIS	-	expression tag	UNP Q86C09
A	-15	HIS	-	expression tag	UNP Q86C09
A	-14	HIS	-	expression tag	UNP Q86C09
A	-13	HIS	-	expression tag	UNP Q86C09
A	-12	SER	-	expression tag	UNP Q86C09
A	-11	SER	-	expression tag	UNP Q86C09
A	-10	GLY	-	expression tag	UNP Q86C09
A	-9	LEU	-	expression tag	UNP Q86C09
A	-8	VAL	-	expression tag	UNP Q86C09
A	-7	PRO	-	expression tag	UNP Q86C09
A	-6	ARG	-	expression tag	UNP Q86C09
A	-5	GLY	-	expression tag	UNP Q86C09
A	-4	SER	-	expression tag	UNP Q86C09
A	-3	HIS	-	expression tag	UNP Q86C09
A	-2	MET	-	expression tag	UNP Q86C09
A	-1	ALA	-	expression tag	UNP Q86C09
A	0	SER	-	expression tag	UNP Q86C09
B	-22	MET	-	expression tag	UNP Q86C09
B	-21	GLY	-	expression tag	UNP Q86C09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP Q86C09
B	-19	SER	-	expression tag	UNP Q86C09
B	-18	HIS	-	expression tag	UNP Q86C09
B	-17	HIS	-	expression tag	UNP Q86C09
B	-16	HIS	-	expression tag	UNP Q86C09
B	-15	HIS	-	expression tag	UNP Q86C09
B	-14	HIS	-	expression tag	UNP Q86C09
B	-13	HIS	-	expression tag	UNP Q86C09
B	-12	SER	-	expression tag	UNP Q86C09
B	-11	SER	-	expression tag	UNP Q86C09
B	-10	GLY	-	expression tag	UNP Q86C09
B	-9	LEU	-	expression tag	UNP Q86C09
B	-8	VAL	-	expression tag	UNP Q86C09
B	-7	PRO	-	expression tag	UNP Q86C09
B	-6	ARG	-	expression tag	UNP Q86C09
B	-5	GLY	-	expression tag	UNP Q86C09
B	-4	SER	-	expression tag	UNP Q86C09
B	-3	HIS	-	expression tag	UNP Q86C09
B	-2	MET	-	expression tag	UNP Q86C09
B	-1	ALA	-	expression tag	UNP Q86C09
B	0	SER	-	expression tag	UNP Q86C09

- Molecule 2 is {[(3-methylpyridin-2-yl)amino]methanediyl}bis(phosphonic acid) (CCD ID: 3YQ) (formula: C₇H₁₂N₂O₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			17	7	2	6	2		
2	B	1	Total	C	N	O	P	0	0
			17	7	2	6	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		

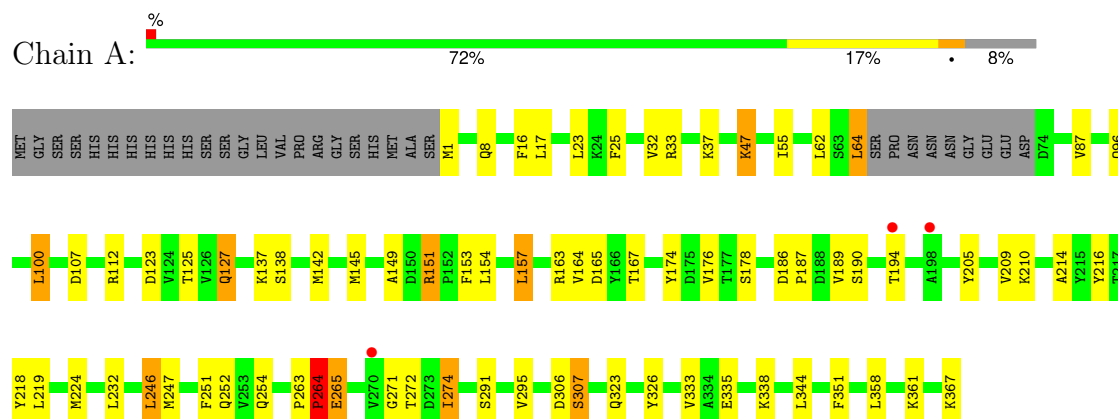
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	92	Total	O	0	0
			92	92		

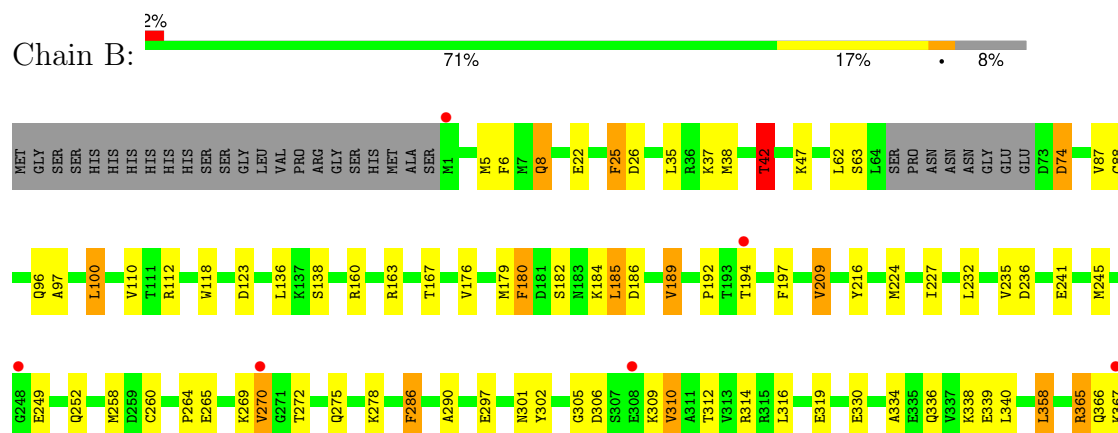
3 Residue-property plots [i](#)

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: Farnesyl pyrophosphate synthase



• Molecule 1: Farnesyl pyrophosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.15Å 119.15Å 62.82Å 90.00° 112.24° 90.00°	Depositor
Resolution (Å)	29.07 – 2.50 29.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.07-2.50) 95.8 (29.07-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.34 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.197 , 0.255 0.204 , 0.253	Depositor DCC
R_{free} test set	1537 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5934	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.27% 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: 3YQ, MG

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	1.03	1/2923 (0.0%)	1.16	11/3952 (0.3%)
1	B	1.03	2/2931 (0.1%)	1.19	5/3963 (0.1%)
All	All	1.03	3/5854 (0.1%)	1.17	16/7915 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	PHE	C-O	-5.39	1.17	1.24
1	B	270	VAL	CA-CB	5.17	1.59	1.53
1	B	25	PHE	CA-C	-5.07	1.46	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	LEU	CA-C-N	-7.10	112.86	119.82
1	A	232	LEU	C-N-CA	-7.10	112.86	119.82
1	A	87	VAL	N-CA-C	-6.69	104.00	110.42
1	A	55	ILE	CB-CA-C	-6.34	103.76	111.88
1	A	1	MET	CA-C-N	-5.90	112.63	119.47
1	A	1	MET	C-N-CA	-5.90	112.63	119.47
1	B	42	THR	N-CA-CB	-5.80	101.56	110.20
1	B	270	VAL	CB-CA-C	5.70	117.38	111.23
1	A	307	SER	N-CA-C	5.58	119.19	112.38
1	A	32	VAL	CB-CA-C	-5.44	104.80	112.14
1	A	265	GLU	N-CA-C	5.38	119.01	112.23
1	A	154	LEU	N-CA-C	5.38	117.84	111.33
1	B	87	VAL	N-CA-C	-5.25	105.27	110.62
1	A	107	ASP	N-CA-C	-5.17	106.75	113.16
1	B	366	GLN	N-CA-C	-5.08	105.82	111.36
1	B	286	PHE	CB-CA-C	-5.00	103.03	110.88

There are no chirality outliers.

There are no planarity outliers.

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	2864	0	2824	46	0
1	B	2872	0	2830	62	0
2	A	17	0	10	0	0
2	B	17	0	9	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	66	0	0	6	0
4	B	92	0	0	14	0
All	All	5934	0	5673	98	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 9.

All (98) 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:186:ASP:O	1:B:123:ASP:CB	2.01	1.07
1:A:123:ASP:CB	1:B:189:VAL:O	2.22	0.86
1:B:96:GLN:OE1	1:B:100:LEU:HD11	1.73	0.86
1:B:249:GLU:HB3	4:B:4169:HOH:O	1.79	0.82
1:A:137:LYS:HE2	1:A:165:ASP:OD2	1.86	0.75
1:B:22:GLU:HG3	4:B:4172:HOH:O	1.87	0.74
1:A:151:ARG:HG2	1:A:153:PHE:CZ	2.24	0.73
1:A:361:LYS:HE2	4:A:3161:HOH:O	1.93	0.69
1:B:100:LEU:CB	4:B:4179:HOH:O	2.42	0.67
1:B:96:GLN:NE2	1:B:216:TYR:OH	2.26	0.67
1:A:96:GLN:NE2	1:A:100:LEU:HD21	2.10	0.67
1:A:64:LEU:HD21	4:A:3158:HOH:O	1.96	0.66
1:A:167:THR:HG22	1:B:25:PHE:CE1	2.30	0.65
1:A:209:VAL:HG22	1:A:252:GLN:HG2	1.77	0.65
1:B:180:PHE:HB3	4:B:4158:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:MET:HA	1:B:8:GLN:HG3	1.81	0.62
1:B:301:ASN:ND2	1:B:312:THR:HG21	2.15	0.61
1:B:194:THR:HG23	1:B:197:PHE:HA	1.82	0.60
1:B:100:LEU:HD23	4:B:4179:HOH:O	2.00	0.60
1:A:246:LEU:HD11	1:A:333:VAL:HG13	1.83	0.60
1:A:25:PHE:CE1	1:B:167:THR:HG22	2.38	0.59
1:A:254:GLN:HG2	1:A:326:TYR:OH	2.03	0.59
1:B:160:ARG:NH2	1:B:232:LEU:HD21	2.18	0.59
1:B:100:LEU:HB3	4:B:4179:HOH:O	2.02	0.58
1:A:123:ASP:CB	1:B:186:ASP:O	2.53	0.57
1:A:274:ILE:HG13	4:A:3129:HOH:O	2.05	0.56
4:A:3163:HOH:O	1:B:26:ASP:HB2	2.04	0.56
1:B:96:GLN:OE1	1:B:100:LEU:CD1	2.50	0.56
1:A:247:MET:HE1	1:A:358:LEU:HG	1.88	0.56
1:B:38:MET:O	1:B:42:THR:HB	2.06	0.56
1:B:272:THR:O	1:B:275:GLN:HB2	2.06	0.56
1:B:42:THR:HG23	1:B:97:ALA:HB1	1.89	0.55
1:A:25:PHE:HE1	1:B:167:THR:HG22	1.72	0.54
1:B:96:GLN:HE21	1:B:96:GLN:HA	1.72	0.54
1:B:179:MET:CB	4:B:4170:HOH:O	2.54	0.54
1:B:209:VAL:HG22	1:B:252:GLN:HG2	1.89	0.54
1:A:163:ARG:O	1:A:167:THR:HG23	2.07	0.53
1:A:33:ARG:O	1:A:37:LYS:HD2	2.08	0.53
1:B:112:ARG:NH2	2:B:4001:3YQ:O6	2.40	0.53
1:A:100:LEU:HD22	1:A:112:ARG:NH1	2.24	0.52
1:B:110:VAL:HG22	4:B:4143:HOH:O	2.08	0.52
1:B:182:SER:O	1:B:185:LEU:HB2	2.10	0.52
1:A:187:PRO:HG2	1:B:37:LYS:HG2	1.92	0.51
1:B:88:CYS:SG	1:B:224:MET:HE2	2.51	0.51
1:B:336:GLN:NE2	4:B:4171:HOH:O	2.44	0.51
1:B:278:LYS:O	1:B:302:TYR:OH	2.13	0.50
1:B:365:ARG:HA	4:B:4174:HOH:O	2.09	0.50
1:A:47:LYS:NZ	4:A:3121:HOH:O	2.32	0.50
1:B:306:ASP:O	1:B:310:VAL:HG13	2.11	0.50
1:A:210:LYS:O	1:A:214:ALA:HB3	2.12	0.49
1:A:263:PRO:O	1:A:264:PRO:C	2.56	0.49
1:B:96:GLN:O	1:B:100:LEU:HD13	2.12	0.49
1:B:100:LEU:HB2	4:B:4179:HOH:O	2.09	0.49
1:B:258:MET:HE1	1:B:367:LYS:HB3	1.95	0.49
1:A:174:TYR:O	1:A:178:SER:HB3	2.14	0.48
1:A:291:SER:O	1:A:295:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HE2	1:A:165:ASP:CG	2.39	0.48
1:A:271:GLY:N	4:A:3117:HOH:O	2.42	0.48
1:A:157:LEU:HD21	1:A:224:MET:CE	2.44	0.47
1:A:167:THR:HG22	1:B:25:PHE:HE1	1.75	0.47
1:A:246:LEU:CD1	1:A:333:VAL:HG13	2.44	0.47
1:B:74:ASP:OD2	1:B:74:ASP:N	2.48	0.47
1:B:305:GLY:O	1:B:306:ASP:C	2.58	0.46
1:B:236:ASP:OD1	1:B:236:ASP:C	2.55	0.46
1:B:97:ALA:HA	1:B:100:LEU:HD22	1.98	0.46
1:A:157:LEU:HD21	1:A:224:MET:HE3	1.98	0.46
1:A:125:THR:HB	1:A:127:GLN:HG2	1.99	0.45
1:B:286:PHE:O	1:B:290:ALA:HB2	2.17	0.45
1:B:179:MET:HB2	4:B:4170:HOH:O	2.16	0.45
1:B:297:GLU:HG2	1:B:316:LEU:HD11	1.99	0.45
1:A:344:LEU:HD21	1:A:351:PHE:CD2	2.52	0.44
1:B:301:ASN:HD22	1:B:312:THR:HG21	1.81	0.44
1:A:138:SER:O	1:A:142:MET:HG2	2.17	0.44
1:A:218:TYR:CE2	1:A:247:MET:HE2	2.52	0.44
1:B:96:GLN:CD	1:B:100:LEU:CD1	2.91	0.44
1:A:142:MET:HE1	1:B:163:ARG:NH1	2.32	0.44
1:B:330:GLU:OE1	4:B:4137:HOH:O	2.20	0.44
1:B:42:THR:HG21	1:B:136:LEU:HD11	2.00	0.44
1:B:160:ARG:HD2	1:B:227:ILE:HD11	1.99	0.43
1:B:334:ALA:O	1:B:338:LYS:HG2	2.18	0.43
1:A:263:PRO:O	1:A:265:GLU:N	2.52	0.43
1:B:38:MET:HA	1:B:118:TRP:CH2	2.53	0.43
1:B:194:THR:CG2	1:B:197:PHE:HA	2.49	0.43
1:B:358:LEU:HD22	1:B:358:LEU:O	2.19	0.43
1:A:137:LYS:CE	1:A:165:ASP:OD2	2.63	0.42
1:B:5:MET:O	1:B:6:PHE:C	2.61	0.42
1:B:241:GLU:O	1:B:245:MET:HG2	2.19	0.42
1:A:145:MET:O	1:A:149:ALA:HB2	2.20	0.42
1:A:157:LEU:CD2	1:A:224:MET:HE3	2.49	0.42
1:A:96:GLN:O	1:A:100:LEU:HG	2.20	0.42
1:A:164:VAL:HG11	1:A:216:TYR:HA	2.01	0.41
1:A:189:VAL:O	1:B:123:ASP:CB	2.69	0.41
1:A:16:PHE:CE2	1:A:17:LEU:HD23	2.55	0.41
1:B:260:CYS:O	1:B:314:ARG:NH1	2.53	0.41
1:B:264:PRO:HG3	1:B:270:VAL:HA	2.03	0.41
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.56	0.41
1:A:306:ASP:OD1	1:A:306:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLU:CB	4:B:4111:HOH:O	2.69	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	354/390 (91%)	338 (96%)	15 (4%)	1 (0%)	36	55
1	B	355/390 (91%)	341 (96%)	13 (4%)	1 (0%)	36	55
All	All	709/780 (91%)	679 (96%)	28 (4%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PRO
1	B	192	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	311/340 (92%)	289 (93%)	22 (7%)	13	29
1	B	312/340 (92%)	288 (92%)	24 (8%)	12	25
All	All	623/680 (92%)	577 (93%)	46 (7%)	13	27

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	23	LEU
1	A	47	LYS
1	A	62	LEU
1	A	64	LEU
1	A	100	LEU
1	A	127	GLN
1	A	151	ARG
1	A	157	LEU
1	A	176	VAL
1	A	190	SER
1	A	194	THR
1	A	219	LEU
1	A	246	LEU
1	A	264	PRO
1	A	272	THR
1	A	274	ILE
1	A	307	SER
1	A	323	GLN
1	A	335	GLU
1	A	338	LYS
1	A	367	LYS
1	B	8	GLN
1	B	35	LEU
1	B	42	THR
1	B	47	LYS
1	B	62	LEU
1	B	63	SER
1	B	74	ASP
1	B	100	LEU
1	B	138	SER
1	B	176	VAL
1	B	180	PHE
1	B	184	LYS
1	B	185	LEU
1	B	189	VAL
1	B	209	VAL
1	B	235	VAL
1	B	269	LYS
1	B	309	LYS
1	B	310	VAL
1	B	319	GLU

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Mol	Chain	Res	Type
1	B	339	GLU
1	B	340	LEU
1	B	358	LEU
1	B	365	ARG

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	108	ASN
1	A	162	ASN
1	A	323	GLN
1	A	336	GLN
1	B	96	GLN
1	B	108	ASN
1	B	131	ASN
1	B	155	GLN

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](#)

Of 8 ligands modelled in this entry, 6 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
2	3YQ	A	3001	3	17,17,17	2.74	10 (58%)	22,26,26	3.11	11 (50%)
2	3YQ	B	4001	3	17,17,17	3.45	8 (47%)	22,26,26	2.85	14 (63%)

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	3YQ	A	3001	3	-	0/16/16/16	0/1/1/1
2	3YQ	B	4001	3	-	0/16/16/16	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4001	3YQ	P1-C6	8.98	1.90	1.83
2	B	4001	3YQ	P1-O6	-6.23	1.45	1.54
2	A	3001	3YQ	P2-O1	-5.24	1.46	1.54
2	A	3001	3YQ	P1-C6	5.21	1.87	1.83
2	A	3001	3YQ	C6-N1	-4.99	1.40	1.46
2	B	4001	3YQ	P2-O1	-4.35	1.48	1.54
2	B	4001	3YQ	C7-C2	-4.31	1.42	1.51
2	B	4001	3YQ	P1-O5	-4.07	1.48	1.54
2	B	4001	3YQ	P2-O3	-3.52	1.44	1.49
2	A	3001	3YQ	C7-C2	-3.35	1.44	1.51
2	A	3001	3YQ	P2-C6	3.11	1.85	1.83
2	B	4001	3YQ	C5-N2	2.61	1.40	1.34
2	A	3001	3YQ	P1-O5	-2.40	1.51	1.54
2	A	3001	3YQ	P2-O3	-2.39	1.45	1.49
2	A	3001	3YQ	C5-N2	2.23	1.39	1.34
2	A	3001	3YQ	P1-O6	-2.19	1.51	1.54
2	A	3001	3YQ	P1-O2	-2.18	1.46	1.49
2	B	4001	3YQ	C6-N1	-2.10	1.44	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	3YQ	O2-P1-C6	-8.22	94.78	110.20
2	B	4001	3YQ	O2-P1-C6	-5.86	99.20	110.20
2	A	3001	3YQ	O4-P2-O1	4.85	120.76	107.58
2	B	4001	3YQ	O6-P1-C6	-4.70	93.11	104.77
2	B	4001	3YQ	O3-P2-C6	-4.63	101.51	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	3YQ	O3-P2-C6	-4.62	101.53	110.20
2	A	3001	3YQ	O6-P1-C6	-4.58	93.40	104.77
2	A	3001	3YQ	O6-P1-O5	4.08	118.65	107.58
2	B	4001	3YQ	O6-P1-O2	3.84	123.08	113.45
2	B	4001	3YQ	P2-C6-P1	-3.42	110.34	116.24
2	B	4001	3YQ	O5-P1-C6	-3.39	96.37	104.77
2	A	3001	3YQ	C4-C5-N2	-3.35	118.12	123.42
2	A	3001	3YQ	C2-C1-N2	-3.06	120.34	123.68
2	B	4001	3YQ	C3-C2-C1	3.02	119.13	116.16
2	B	4001	3YQ	C2-C1-N2	-2.93	120.49	123.68
2	B	4001	3YQ	N1-C1-N2	2.87	122.08	118.00
2	A	3001	3YQ	C7-C2-C1	2.84	124.59	122.10
2	A	3001	3YQ	C5-N2-C1	2.79	122.17	116.74
2	A	3001	3YQ	N1-C1-N2	2.79	121.96	118.00
2	B	4001	3YQ	O4-P2-O3	2.75	120.34	113.45
2	B	4001	3YQ	O5-P1-O2	2.61	120.00	113.45
2	A	3001	3YQ	O5-P1-O2	2.53	119.79	113.45
2	B	4001	3YQ	C4-C5-N2	-2.43	119.57	123.42
2	B	4001	3YQ	C5-N2-C1	2.16	120.95	116.74
2	B	4001	3YQ	O6-P1-O5	2.12	113.35	107.58

There are no chirality outliers.

There are no torsion outliers.

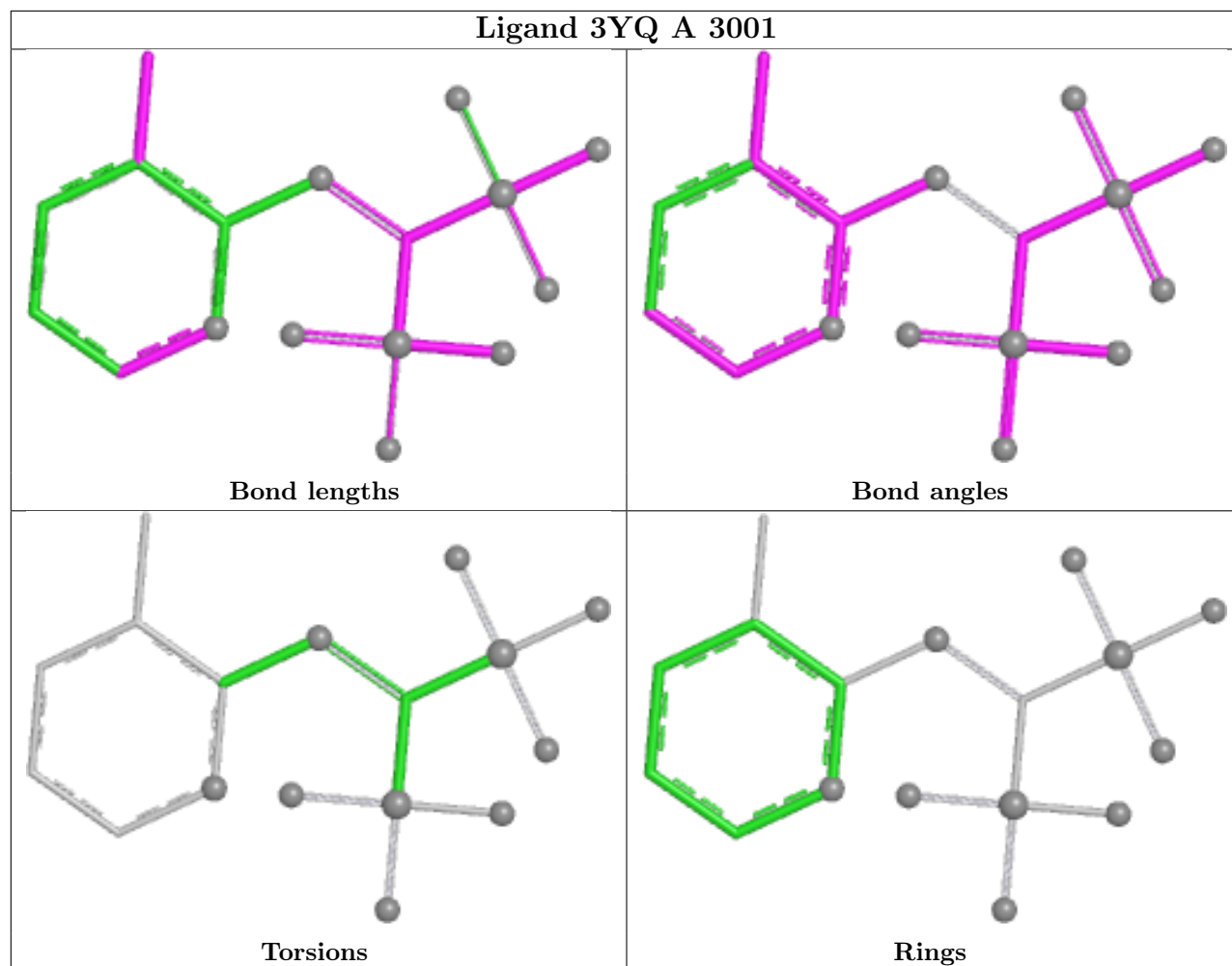
There are no ring outliers.

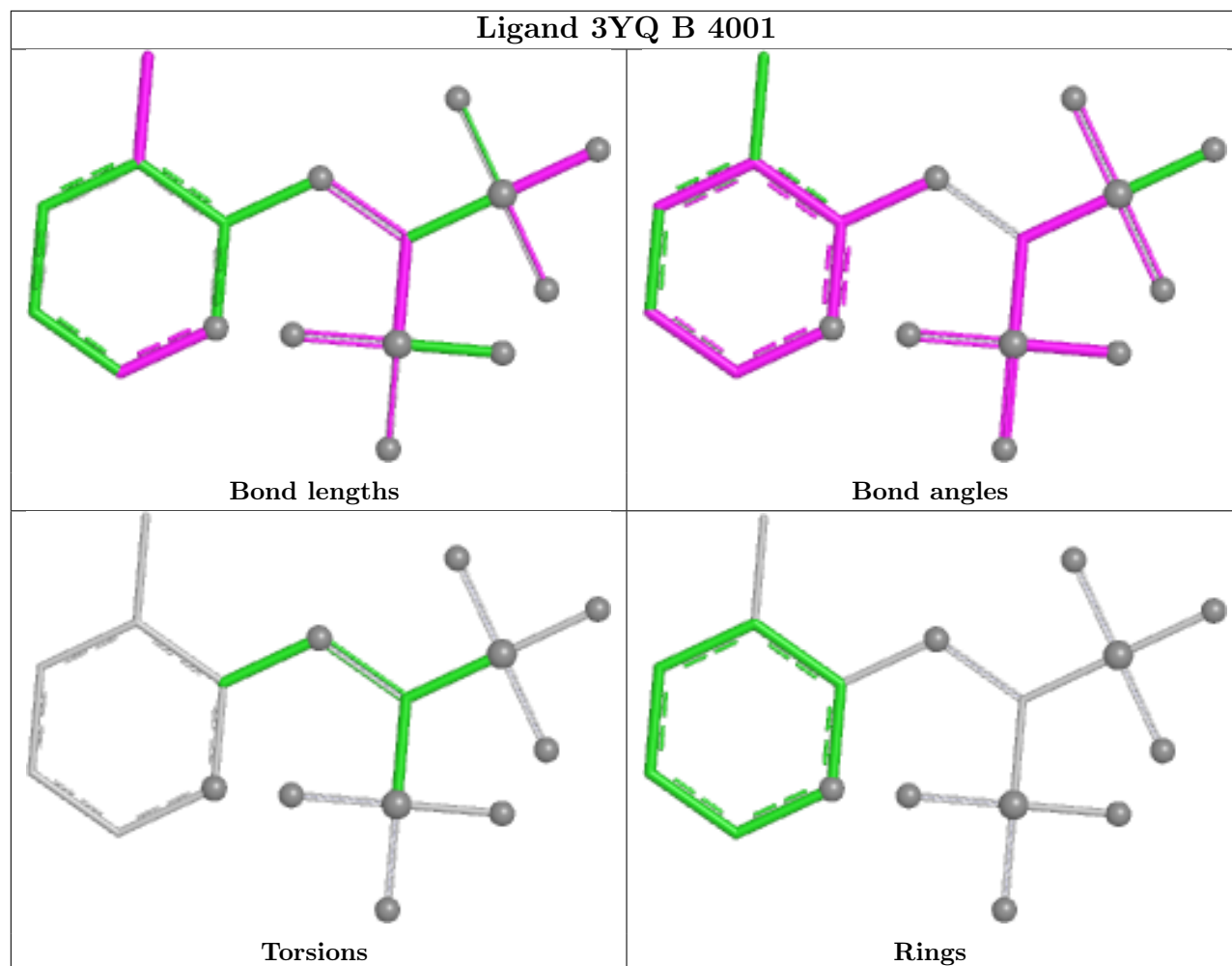
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4001	3YQ	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.

Ligand 3YQ A 3001





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	358/390 (91%)	0.13	3 (0%) 82 80	25, 47, 78, 92	0
1	B	359/390 (92%)	0.07	6 (1%) 69 65	24, 44, 78, 104	0
All	All	717/780 (91%)	0.10	9 (1%) 75 71	24, 45, 78, 104	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	THR	2.8
1	B	194	THR	2.6
1	A	270	VAL	2.4
1	A	198	ALA	2.3
1	B	248	GLY	2.2
1	B	367	LYS	2.2
1	B	308	GLU	2.1
1	B	1	MET	2.1
1	B	270	VAL	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.

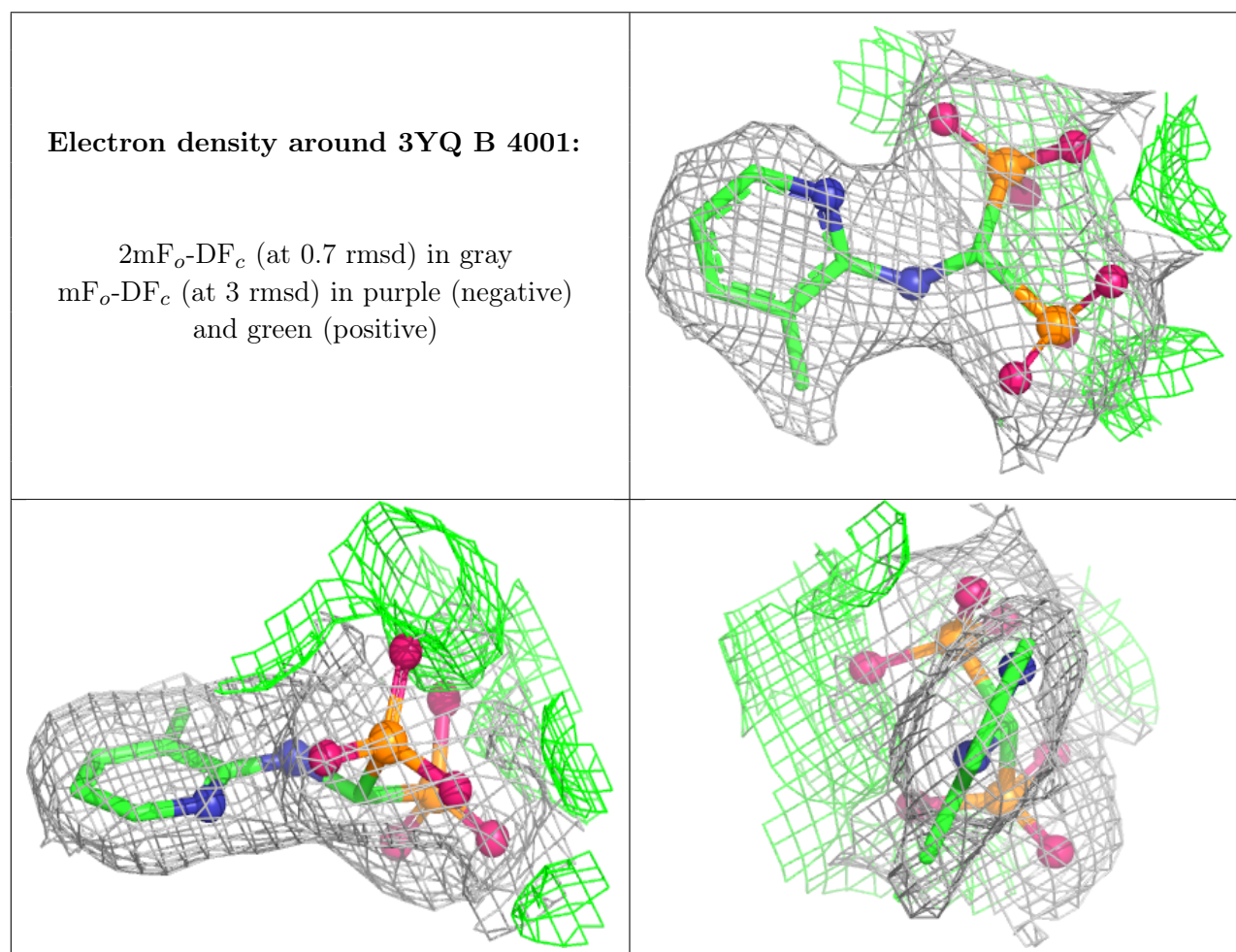
6.4 Ligands [i](#)

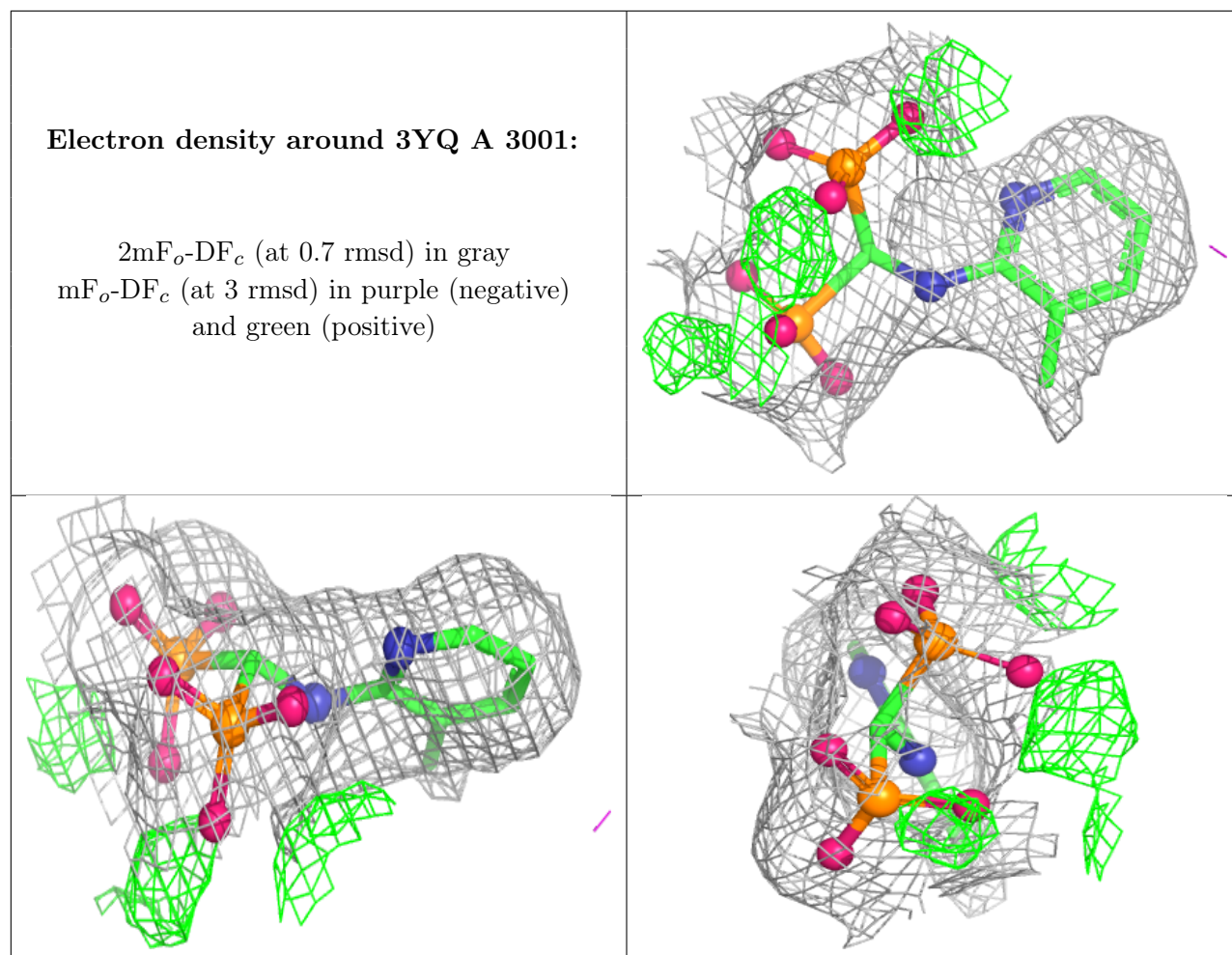
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	MG	B	4002	1/1	0.77	0.25	47,47,47,47	0
3	MG	B	4003	1/1	0.81	0.24	43,43,43,43	0
3	MG	A	3002	1/1	0.83	0.23	51,51,51,51	0
3	MG	B	4004	1/1	0.88	0.18	33,33,33,33	0
3	MG	A	3004	1/1	0.93	0.15	36,36,36,36	0
2	3YQ	B	4001	17/17	0.95	0.08	27,33,38,39	0
2	3YQ	A	3001	17/17	0.96	0.07	28,34,39,39	0
3	MG	A	3003	1/1	0.98	0.05	34,34,34,34	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.