



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:31 am BST

PDB ID : 2I19
Title : T. Brucei farnesyl diphosphate synthase complexed with bisphosphonate
Authors : Cao, R.; Mao, J.; Gao, Y.; Robinson, H.; Odeh, S.; Goddard, A.; Oldfield, E.
Deposited on : 2006-08-13
Resolution : 2.28 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

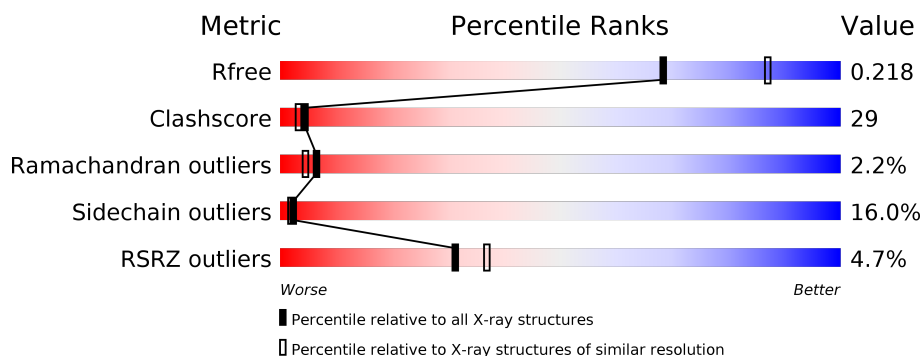
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 on 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	<div> <div>5%</div> <div> <div>42%</div> <div>43%</div> <div>9%</div> <div>6%</div> </div> </div>
1	B	390	<div> <div>3%</div> <div> <div>42%</div> <div>42%</div> <div>8%</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6230 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	367	Total	C	N	O	S	0	0	0
			2938	1865	485	560	28			
1	B	361	Total	C	N	O	S	0	0	0
			2894	1841	476	549	28			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	CLONING ARTIFACT	UNP Q86C09
A	-21	GLY	-	CLONING ARTIFACT	UNP Q86C09
A	-20	SER	-	CLONING ARTIFACT	UNP Q86C09
A	-19	SER	-	CLONING ARTIFACT	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	-	CLONING ARTIFACT	UNP Q86C09
A	-11	SER	-	CLONING ARTIFACT	UNP Q86C09
A	-10	GLY	-	CLONING ARTIFACT	UNP Q86C09
A	-9	LEU	-	CLONING ARTIFACT	UNP Q86C09
A	-8	VAL	-	CLONING ARTIFACT	UNP Q86C09
A	-7	PRO	-	CLONING ARTIFACT	UNP Q86C09
A	-6	ARG	-	CLONING ARTIFACT	UNP Q86C09
A	-5	GLY	-	CLONING ARTIFACT	UNP Q86C09
A	-4	SER	-	CLONING ARTIFACT	UNP Q86C09
A	-3	HIS	-	CLONING ARTIFACT	UNP Q86C09
A	-2	MET	-	CLONING ARTIFACT	UNP Q86C09
A	-1	ALA	-	CLONING ARTIFACT	UNP Q86C09
A	0	SER	-	CLONING ARTIFACT	UNP Q86C09
B	-22	MET	-	CLONING ARTIFACT	UNP Q86C09
B	-21	GLY	-	CLONING ARTIFACT	UNP Q86C09

Continued on next page...

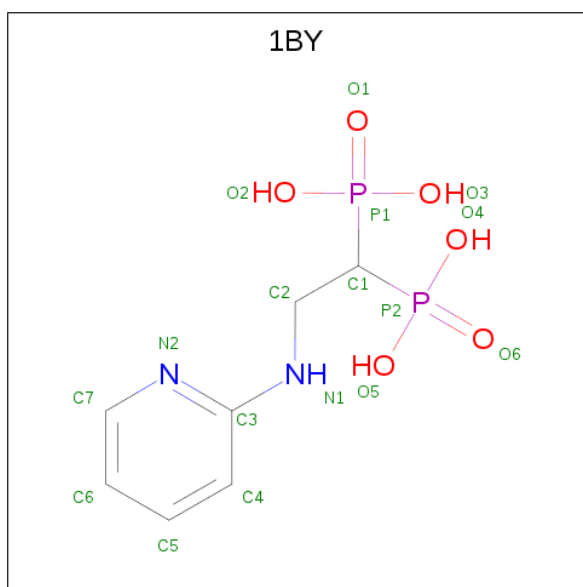
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	CLONING ARTIFACT	UNP Q86C09
B	-19	SER	-	CLONING ARTIFACT	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	-	CLONING ARTIFACT	UNP Q86C09
B	-11	SER	-	CLONING ARTIFACT	UNP Q86C09
B	-10	GLY	-	CLONING ARTIFACT	UNP Q86C09
B	-9	LEU	-	CLONING ARTIFACT	UNP Q86C09
B	-8	VAL	-	CLONING ARTIFACT	UNP Q86C09
B	-7	PRO	-	CLONING ARTIFACT	UNP Q86C09
B	-6	ARG	-	CLONING ARTIFACT	UNP Q86C09
B	-5	GLY	-	CLONING ARTIFACT	UNP Q86C09
B	-4	SER	-	CLONING ARTIFACT	UNP Q86C09
B	-3	HIS	-	CLONING ARTIFACT	UNP Q86C09
B	-2	MET	-	CLONING ARTIFACT	UNP Q86C09
B	-1	ALA	-	CLONING ARTIFACT	UNP Q86C09
B	0	SER	-	CLONING ARTIFACT	UNP Q86C09

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is [2-(PYRIDIN-2-YLAMINO)ETHANE-1,1-DIYL]BIS(PHOSPHONIC ACID) (three-letter code: 1BY) (formula: C₇H₁₂N₂O₆P₂).



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

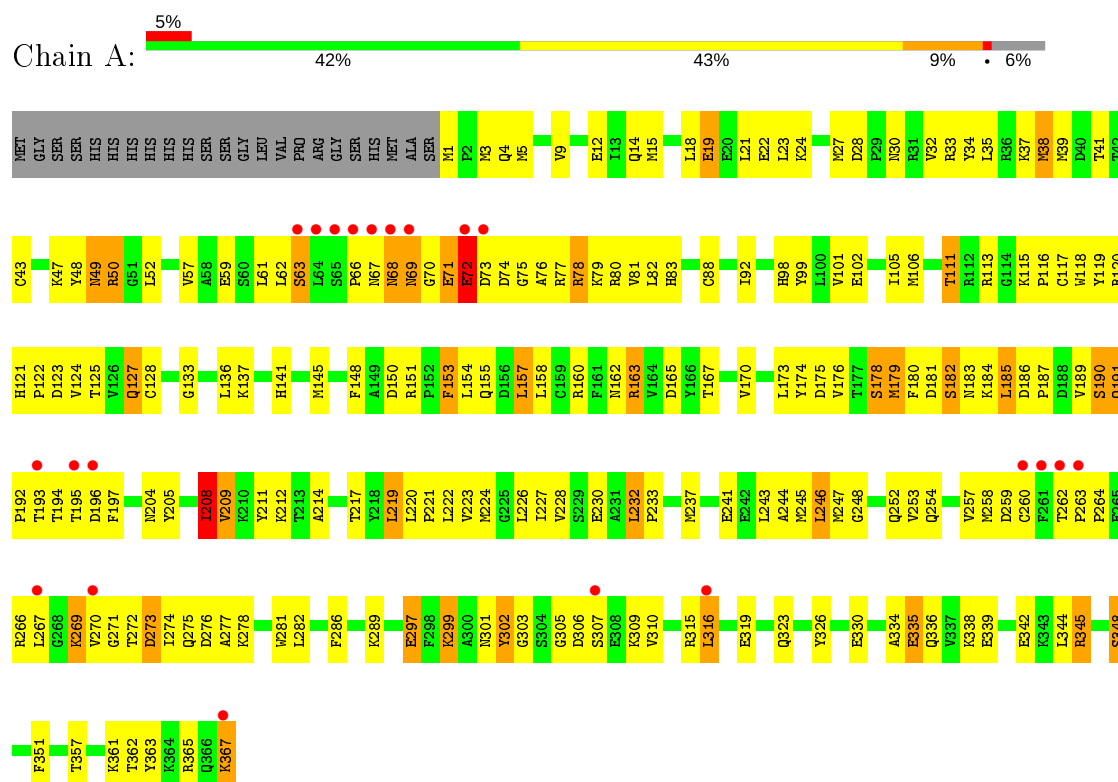
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	B	169	Total	O	0	0
			169	169		

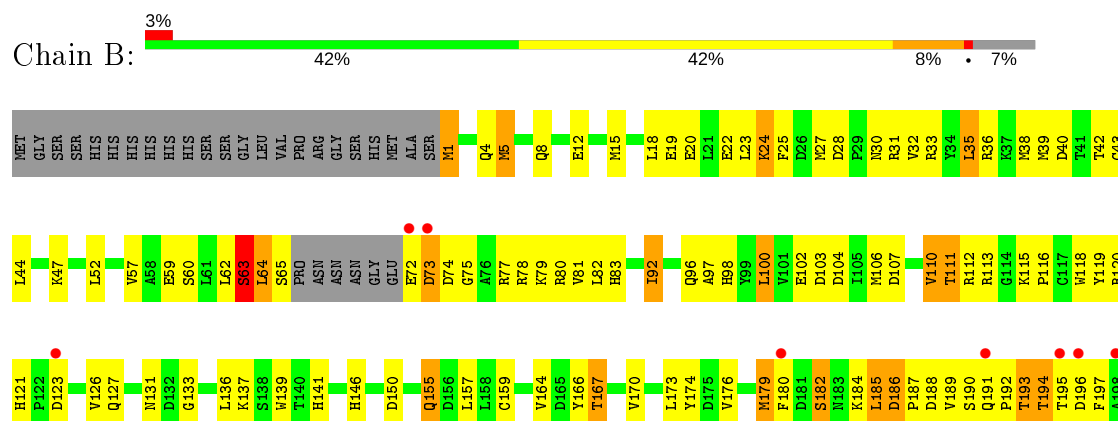
3 Residue-property plots

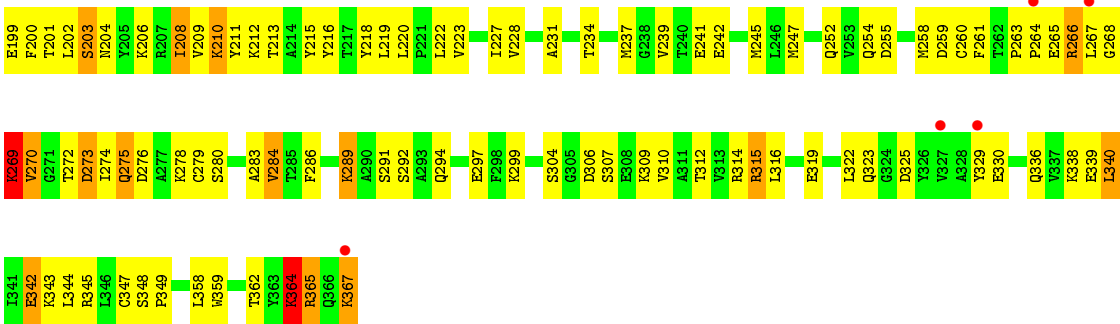
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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	133.21Å 119.55Å 62.44Å 90.00° 111.93° 90.00°	Depositor
Resolution (Å)	30.00 – 2.28 29.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.28) 85.6 (29.89-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.20Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.217 , 0.244 0.209 , 0.218	Depositor DCC
R_{free} test set	802 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.1	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	0.95	EDS
Total number of atoms	6230	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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: 1BY, 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	0.31	0/2999	0.90	2/4057 (0.0%)
1	B	0.30	0/2953	0.87	0/3992
All	All	0.31	0/5952	0.89	2/8049 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	PHE	CB-CG-CD1	5.39	124.57	120.80
1	A	208	ILE	CA-CB-CG1	5.38	121.22	111.00

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	2938	0	2882	186	0
1	B	2894	0	2847	169	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	17	0	8	1	0
3	B	17	0	8	1	0
4	A	189	0	0	21	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	169	0	0	16	0
All	All	6230	0	5745	335	1

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 29.

All (335) 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:B:42:THR:HG22	1:B:97:ALA:HB1	1.46	0.97
1:A:232:LEU:HG	1:A:233:PRO:HD3	1.54	0.90
1:A:257:VAL:HG22	1:A:282:LEU:HD21	1.55	0.89
1:A:38:MET:HE3	1:A:136:LEU:HD11	1.59	0.82
1:B:278:LYS:HZ2	1:B:279:CYS:H	1.25	0.82
1:A:123:ASP:HB3	1:B:187:PRO:HA	1.63	0.81
1:B:364:LYS:HZ3	1:B:365:ARG:H	1.30	0.79
1:B:272:THR:HA	1:B:275:GLN:HG3	1.64	0.77
1:B:62:LEU:HD21	1:B:78:ARG:HA	1.65	0.77
1:A:204:ASN:O	1:A:208:ILE:HG23	1.84	0.77
1:B:280:SER:O	1:B:284:VAL:HG13	1.85	0.76
1:A:3:MET:HE1	4:A:5237:HOH:O	1.85	0.76
1:B:186:ASP:OD2	1:B:189:VAL:HG23	1.85	0.76
1:A:227:ILE:HA	1:A:232:LEU:HD22	1.66	0.76
1:A:362:THR:O	1:A:365:ARG:HB2	1.87	0.74
1:B:157:LEU:HD13	1:B:227:ILE:HG21	1.69	0.74
1:A:274:ILE:HB	4:A:5042:HOH:O	1.87	0.74
1:B:231:ALA:O	1:B:234:THR:HB	1.86	0.73
1:B:263:PRO:HB2	1:B:266:ARG:HB2	1.68	0.73
1:B:223:VAL:O	1:B:227:ILE:HG12	1.89	0.73
1:A:193:THR:HG22	1:A:194:THR:O	1.88	0.72
1:A:133:GLY:O	1:A:136:LEU:HB2	1.90	0.72
1:A:276:ASP:HB3	1:A:278:LYS:HE3	1.70	0.72
1:A:150:ASP:HB2	4:A:5344:HOH:O	1.90	0.72
1:A:297:GLU:OE2	4:A:5317:HOH:O	2.07	0.72
1:B:194:THR:HG23	1:B:197:PHE:H	1.55	0.71
1:B:174:TYR:HB3	1:B:208:ILE:HG22	1.72	0.71
1:A:125:THR:HG23	1:A:127:GLN:HG3	1.70	0.71
1:A:357:THR:O	1:A:361:LYS:HG2	1.91	0.71
1:B:264:PRO:HB3	1:B:270:VAL:HA	1.72	0.70
1:B:209:VAL:HG22	1:B:252:GLN:HG2	1.72	0.70
1:A:22:GLU:O	4:A:5330:HOH:O	2.10	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:GLN:HG3	4:B:5078:HOH:O	1.90	0.70
1:B:278:LYS:NZ	1:B:279:CYS:H	1.89	0.70
1:A:189:VAL:HG12	1:A:190:SER:O	1.91	0.69
1:A:232:LEU:HD23	1:A:232:LEU:H	1.56	0.69
1:B:347:CYS:O	1:B:349:PRO:HD3	1.93	0.69
1:A:148:PHE:HB2	1:A:154:LEU:HD13	1.73	0.69
1:A:174:TYR:HB3	1:A:208:ILE:HG22	1.73	0.68
1:A:259:ASP:HA	1:A:267:LEU:HD21	1.75	0.68
1:A:125:THR:HG22	1:A:128:CYS:HB2	1.74	0.68
1:A:15:MET:O	1:A:19:GLU:HB3	1.93	0.68
1:A:262:THR:HB	1:A:267:LEU:HD13	1.76	0.68
1:B:155:GLN:OE1	4:B:5300:HOH:O	2.12	0.68
1:A:307:SER:HB2	4:A:5224:HOH:O	1.93	0.67
1:B:202:LEU:O	1:B:206:LYS:HG3	1.94	0.67
1:A:243:LEU:O	1:A:247:MET:HG3	1.95	0.67
1:A:78:ARG:O	1:A:82:LEU:HG	1.94	0.67
1:A:160:ARG:HD2	1:A:227:ILE:HD11	1.78	0.66
1:B:339:GLU:OE2	4:B:5296:HOH:O	2.12	0.66
1:B:316:LEU:HA	1:B:319:GLU:HG3	1.78	0.66
1:A:214:ALA:HB2	1:A:248:GLY:HA3	1.78	0.65
1:B:180:PHE:CE2	1:B:193:THR:HG23	2.32	0.65
1:A:77:ARG:O	1:A:81:VAL:HG23	1.97	0.65
1:A:335:GLU:OE2	4:A:5356:HOH:O	2.15	0.64
1:B:266:ARG:NH2	1:B:367:LYS:HD3	2.12	0.64
1:A:237:MET:HG3	1:A:241:GLU:OE1	1.96	0.64
1:A:219:LEU:HD22	1:A:223:VAL:HG23	1.79	0.64
1:A:69:ASN:HD22	1:A:69:ASN:H	1.45	0.64
1:A:167:THR:HG22	1:B:25:PHE:HE1	1.63	0.64
1:A:68:ASN:H	1:A:68:ASN:HD22	1.46	0.64
1:B:336:GLN:O	1:B:340:LEU:HD22	1.98	0.64
1:B:179:MET:HE2	1:B:179:MET:H	1.62	0.63
1:A:187:PRO:HA	1:B:123:ASP:HB3	1.80	0.63
1:A:286:PHE:CZ	1:A:316:LEU:HD13	2.34	0.63
1:A:117:CYS:O	1:A:120:ARG:HB2	2.00	0.62
1:A:69:ASN:H	1:A:69:ASN:ND2	1.98	0.62
1:B:189:VAL:HG12	1:B:190:SER:H	1.64	0.62
1:B:316:LEU:O	1:B:319:GLU:HB2	2.00	0.62
1:A:163:ARG:NH1	4:A:5349:HOH:O	2.31	0.61
1:B:110:VAL:HA	1:B:120:ARG:HD3	1.82	0.61
1:A:167:THR:HG22	1:B:25:PHE:CE1	2.35	0.61
1:B:208:ILE:O	1:B:212:LYS:HB3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:THR:O	1:A:275:GLN:HB2	2.00	0.61
1:B:72:GLU:O	1:B:73:ASP:HB2	2.01	0.61
1:A:5:MET:O	1:A:9:VAL:HG23	2.00	0.60
1:B:22:GLU:O	4:B:5292:HOH:O	2.16	0.60
1:B:310:VAL:O	1:B:314:ARG:HG3	2.01	0.60
1:A:72:GLU:OE1	1:A:72:GLU:HA	2.00	0.60
1:A:137:LYS:HE2	1:A:165:ASP:OD1	2.02	0.59
1:A:174:TYR:HB3	1:A:208:ILE:CG2	2.32	0.59
1:B:210:LYS:HD3	1:B:211:TYR:CE1	2.37	0.59
1:A:39:MET:O	1:A:43:CYS:HB2	2.02	0.59
1:A:59:GLU:OE2	4:A:5299:HOH:O	2.15	0.59
1:A:241:GLU:O	1:A:245:MET:HG2	2.03	0.59
1:A:137:LYS:NZ	4:A:5313:HOH:O	2.30	0.58
1:A:14:GLN:O	1:A:18:LEU:HG	2.04	0.58
1:B:15:MET:O	1:B:19:GLU:HG3	2.03	0.58
1:B:364:LYS:NZ	1:B:365:ARG:H	1.99	0.58
1:A:259:ASP:OD2	1:A:273:ASP:HB2	2.04	0.58
1:B:43:CYS:O	1:B:44:LEU:HD23	2.03	0.58
1:A:281:TRP:HE3	1:A:282:LEU:HD23	1.69	0.58
1:B:274:ILE:HD13	1:B:310:VAL:HG23	1.85	0.58
1:A:28:ASP:OD2	1:A:30:ASN:HB2	2.04	0.58
1:A:181:ASP:OD1	1:A:183:ASN:HB2	2.04	0.57
1:B:201:THR:HG22	1:B:203:SER:N	2.19	0.57
1:B:18:LEU:HD11	1:B:36:ARG:HB2	1.85	0.57
1:B:272:THR:CA	1:B:275:GLN:HG3	2.35	0.57
1:B:81:VAL:HG13	1:B:228:VAL:O	2.04	0.57
1:A:196:ASP:HA	1:A:299:LYS:HE2	1.87	0.57
1:B:272:THR:HB	1:B:276:ASP:OD1	2.04	0.56
1:A:48:TYR:O	1:A:52:LEU:HG	2.05	0.56
1:B:18:LEU:CD1	1:B:36:ARG:HB2	2.35	0.56
1:B:110:VAL:HA	1:B:120:ARG:CD	2.35	0.56
1:A:123:ASP:HB2	1:B:189:VAL:O	2.04	0.56
1:A:214:ALA:CB	1:A:248:GLY:HA3	2.36	0.56
1:A:184:LYS:HE3	4:A:5063:HOH:O	2.05	0.56
1:A:178:SER:OG	1:A:208:ILE:HD12	2.06	0.56
1:A:281:TRP:CE3	1:A:282:LEU:HD23	2.41	0.56
1:A:286:PHE:CE1	1:A:316:LEU:HB2	2.41	0.56
1:A:335:GLU:O	1:A:339:GLU:HG3	2.06	0.56
1:B:28:ASP:OD1	1:B:30:ASN:HB2	2.06	0.56
1:A:186:ASP:O	1:B:123:ASP:HB2	2.06	0.56
1:B:247:MET:HE3	1:B:359:TRP:HE3	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:CYS:O	1:A:92:ILE:HG13	2.06	0.55
1:B:195:THR:O	1:B:299:LYS:HE2	2.05	0.55
1:A:38:MET:HE3	1:A:136:LEU:CD1	2.34	0.55
1:A:125:THR:HG21	1:A:127:GLN:HE21	1.72	0.55
1:A:125:THR:HG21	1:A:127:GLN:NE2	2.22	0.55
1:A:209:VAL:HG13	1:A:252:GLN:HG2	1.89	0.55
1:A:98:HIS:HD2	1:A:133:GLY:O	1.89	0.55
1:A:35:LEU:HD21	1:B:173:LEU:HD22	1.88	0.55
1:A:275:GLN:O	1:A:303:GLY:HA2	2.06	0.55
1:A:63:SER:O	1:A:66:PRO:HG3	2.06	0.55
1:A:227:ILE:HA	1:A:232:LEU:CD2	2.33	0.54
1:A:357:THR:O	1:A:361:LYS:HE2	2.07	0.54
1:A:119:TYR:HB3	4:A:5002:HOH:O	2.07	0.54
1:A:301:ASN:OD1	1:A:309:LYS:HG2	2.07	0.54
1:B:111:THR:HG22	1:B:269:LYS:HB3	1.89	0.54
1:A:125:THR:CG2	1:A:128:CYS:H	2.21	0.54
1:B:42:THR:HG21	1:B:136:LEU:HD11	1.89	0.54
1:A:191:GLN:HB3	1:B:123:ASP:OD1	2.08	0.54
1:B:179:MET:HB3	1:B:193:THR:HG22	1.90	0.54
1:B:155:GLN:NE2	4:B:5316:HOH:O	2.29	0.54
1:A:162:ASN:ND2	4:A:5351:HOH:O	2.40	0.53
1:B:83:HIS:HD2	4:B:5077:HOH:O	1.90	0.53
1:A:115:LYS:HG3	1:A:116:PRO:HD2	1.90	0.53
1:A:125:THR:HG22	1:A:128:CYS:CB	2.37	0.53
1:B:239:VAL:HG11	1:B:344:LEU:HG	1.90	0.53
1:A:12:GLU:OE2	1:A:83:HIS:HE1	1.90	0.53
1:A:133:GLY:HA2	1:A:136:LEU:HD12	1.91	0.53
1:B:62:LEU:O	1:B:63:SER:HB3	2.06	0.53
1:A:175:ASP:O	1:A:178:SER:HB2	2.09	0.52
1:A:21:LEU:HD22	1:A:27:MET:CE	2.39	0.52
1:A:182:SER:O	1:A:185:LEU:HB2	2.09	0.52
1:A:34:TYR:CE2	1:B:187:PRO:HG3	2.45	0.52
1:A:101:VAL:O	1:A:105:ILE:HG13	2.09	0.52
1:B:42:THR:HG21	1:B:136:LEU:CD1	2.40	0.52
1:A:230:GLU:HA	1:A:232:LEU:HD21	1.90	0.52
1:A:47:LYS:HD2	1:A:367:LYS:HE2	1.91	0.52
1:A:1:MET:O	1:A:4:GLN:HB3	2.09	0.52
1:A:150:ASP:OD2	4:A:5301:HOH:O	2.19	0.52
1:B:150:ASP:HB2	4:B:5282:HOH:O	2.09	0.52
1:B:315:ARG:HG3	1:B:316:LEU:N	2.24	0.52
1:A:224:MET:O	1:A:228:VAL:HG22	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:O	1:A:173:LEU:HB3	2.09	0.51
1:B:12:GLU:OE1	1:B:83:HIS:HE1	1.93	0.51
1:A:259:ASP:HA	1:A:267:LEU:CD2	2.40	0.51
1:A:264:PRO:HA	1:A:269:LYS:O	2.11	0.51
1:A:302:TYR:OH	4:A:5358:HOH:O	2.18	0.51
1:A:196:ASP:HA	1:A:299:LYS:CE	2.41	0.51
1:A:122:PRO:HG2	1:B:188:ASP:O	2.10	0.51
1:B:273:ASP:OD1	1:B:278:LYS:HB2	2.10	0.51
1:B:286:PHE:HB2	1:B:322:LEU:HD11	1.91	0.51
1:A:121:HIS:HB2	1:A:124:VAL:CG2	2.41	0.51
1:A:27:MET:HG2	1:A:32:VAL:HG23	1.92	0.50
1:A:191:GLN:HG2	1:B:123:ASP:OD1	2.10	0.50
1:A:1:MET:HA	1:A:4:GLN:HB3	1.93	0.50
1:A:67:ASN:O	1:A:67:ASN:OD1	2.29	0.50
1:A:105:ILE:HG12	1:A:119:TYR:CG	2.47	0.50
1:B:182:SER:OG	1:B:199:GLU:OE2	2.30	0.50
1:A:111:THR:HG23	1:A:115:LYS:H	1.76	0.50
1:A:195:THR:O	1:A:299:LYS:HG2	2.12	0.50
1:B:98:HIS:O	1:B:102:GLU:HG2	2.12	0.50
1:A:205:TYR:CZ	1:A:281:TRP:HB2	2.46	0.50
1:A:220:LEU:HB3	1:A:221:PRO:HD3	1.94	0.49
1:A:253:VAL:HG12	1:A:326:TYR:HE1	1.76	0.49
1:A:68:ASN:H	1:A:68:ASN:ND2	2.10	0.49
1:A:254:GLN:OE1	1:A:365:ARG:HD3	2.13	0.49
1:A:315:ARG:O	1:A:319:GLU:HG3	2.13	0.49
1:A:99:TYR:OH	1:A:165:ASP:OD2	2.30	0.49
1:B:146:HIS:HE1	4:B:5012:HOH:O	1.96	0.49
1:A:243:LEU:HA	1:A:246:LEU:HB2	1.94	0.49
1:B:27:MET:HG2	1:B:32:VAL:HG23	1.95	0.49
1:B:266:ARG:HH22	1:B:367:LYS:HD3	1.78	0.49
1:A:297:GLU:HA	1:A:297:GLU:OE2	2.12	0.49
1:B:278:LYS:HZ2	1:B:279:CYS:N	2.03	0.49
1:A:19:GLU:O	1:A:23:LEU:HG	2.13	0.48
1:A:271:GLY:O	1:A:275:GLN:OE1	2.31	0.48
1:B:364:LYS:HZ3	1:B:365:ARG:N	2.05	0.48
1:A:254:GLN:O	1:A:258:MET:HG3	2.13	0.48
1:B:40:ASP:O	1:B:44:LEU:HB2	2.13	0.48
1:B:64:LEU:CD1	1:B:234:THR:HG21	2.43	0.48
1:A:277:ALA:HB2	1:A:303:GLY:HA3	1.96	0.48
1:A:163:ARG:O	1:A:167:THR:HG23	2.14	0.48
1:B:119:TYR:CZ	1:B:120:ARG:HD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TYR:CE2	1:B:247:MET:HE2	2.48	0.48
1:B:364:LYS:CE	1:B:365:ARG:H	2.27	0.48
1:A:125:THR:HG23	1:A:128:CYS:H	1.79	0.48
1:A:176:VAL:HG11	1:B:127:GLN:HG3	1.95	0.48
1:A:151:ARG:HG2	1:A:153:PHE:CZ	2.49	0.47
1:A:258:MET:CE	1:A:365:ARG:HH21	2.27	0.47
1:B:289:LYS:HB2	1:B:289:LYS:HE3	1.61	0.47
1:B:309:LYS:O	1:B:312:THR:HB	2.15	0.47
4:A:5304:HOH:O	1:B:141:HIS:HE1	1.97	0.47
1:B:254:GLN:O	1:B:258:MET:HG3	2.14	0.47
1:B:31:ARG:HG3	1:B:31:ARG:HH11	1.80	0.47
1:B:362:THR:O	1:B:365:ARG:HB2	2.14	0.47
1:A:141:HIS:HE1	4:A:5304:HOH:O	1.96	0.47
1:A:148:PHE:O	1:A:151:ARG:HB2	2.15	0.47
1:B:266:ARG:HH22	1:B:367:LYS:HG3	1.80	0.47
1:A:61:LEU:CD1	1:A:226:LEU:HD23	2.45	0.47
1:A:70:GLY:O	1:A:71:GLU:O	2.32	0.47
1:B:164:VAL:HA	1:B:167:THR:HB	1.97	0.47
1:B:367:LYS:HB2	1:B:367:LYS:HE2	1.64	0.47
1:A:310:VAL:HG12	1:A:310:VAL:O	2.15	0.46
1:B:239:VAL:CG1	1:B:344:LEU:HG	2.45	0.46
1:A:305:GLY:O	1:A:306:ASP:HB2	2.15	0.46
1:A:316:LEU:HA	1:A:319:GLU:HG3	1.98	0.46
1:B:78:ARG:O	1:B:82:LEU:HG	2.15	0.46
1:A:194:THR:HG21	1:A:197:PHE:HA	1.97	0.46
1:B:112:ARG:NH2	3:B:4001:1BY:O1	2.49	0.46
1:A:155:GLN:HB2	4:A:5044:HOH:O	2.15	0.46
1:A:365:ARG:NH1	1:A:367:LYS:HD2	2.30	0.46
1:B:266:ARG:NH2	1:B:367:LYS:HG3	2.31	0.46
1:B:291:SER:OG	1:B:294:GLN:HG3	2.16	0.46
1:A:121:HIS:HB2	1:A:124:VAL:HG23	1.98	0.46
1:A:258:MET:HA	1:A:262:THR:OG1	2.15	0.46
1:A:27:MET:SD	1:A:35:LEU:HD12	2.56	0.46
1:B:274:ILE:HG22	4:B:5324:HOH:O	2.16	0.46
1:B:179:MET:CB	1:B:193:THR:HG22	2.46	0.45
1:A:57:VAL:HG21	1:A:222:LEU:HD23	1.97	0.45
1:B:38:MET:HA	1:B:118:TRP:CH2	2.51	0.45
1:A:179:MET:O	1:A:194:THR:HB	2.17	0.45
1:A:99:TYR:HB3	3:A:3001:1BY:C5	2.47	0.45
1:B:157:LEU:HD13	1:B:227:ILE:CG2	2.43	0.45
1:B:264:PRO:HA	1:B:267:LEU:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:OE2	1:A:345:ARG:NH1	2.49	0.45
1:B:104:ASP:OD1	1:B:112:ARG:NH1	2.50	0.45
1:B:201:THR:HG23	4:B:5230:HOH:O	2.15	0.45
1:B:340:LEU:HA	1:B:343:LYS:HG3	1.98	0.45
1:A:33:ARG:NH2	1:B:185:LEU:O	2.50	0.45
1:B:209:VAL:O	1:B:213:THR:HB	2.17	0.45
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.16	0.45
1:A:186:ASP:O	4:A:5342:HOH:O	2.21	0.45
1:A:335:GLU:HG2	1:A:336:GLN:N	2.27	0.45
1:B:39:MET:HG3	1:B:139:TRP:CZ3	2.51	0.45
1:B:272:THR:O	1:B:275:GLN:HG3	2.17	0.45
1:A:148:PHE:CB	1:A:154:LEU:HD13	2.42	0.45
1:B:289:LYS:NZ	1:B:325:ASP:OD1	2.50	0.45
1:B:309:LYS:O	1:B:312:THR:N	2.50	0.45
1:A:50:ARG:NH1	1:A:217:THR:HG23	2.31	0.44
1:B:103:ASP:O	1:B:107:ASP:HB2	2.17	0.44
1:B:274:ILE:HD12	4:B:5238:HOH:O	2.17	0.44
1:A:344:LEU:HA	1:A:344:LEU:HD12	1.86	0.44
1:B:192:PRO:HA	4:B:5353:HOH:O	2.17	0.44
1:B:247:MET:HE1	1:B:359:TRP:HA	2.00	0.44
1:A:137:LYS:HE2	1:A:165:ASP:CG	2.38	0.44
1:A:194:THR:CG2	1:A:197:PHE:HA	2.48	0.44
1:A:263:PRO:O	1:A:267:LEU:N	2.50	0.44
1:B:116:PRO:O	1:B:121:HIS:HE1	2.01	0.44
1:A:123:ASP:HB3	1:B:187:PRO:CA	2.42	0.44
1:A:19:GLU:HB2	4:A:5189:HOH:O	2.18	0.44
1:A:67:ASN:HB2	1:A:69:ASN:ND2	2.33	0.44
1:B:112:ARG:O	1:B:113:ARG:HB2	2.18	0.44
1:B:167:THR:HG21	1:B:215:TYR:CG	2.53	0.44
1:A:35:LEU:HD11	1:B:173:LEU:CD2	2.48	0.44
1:B:74:ASP:HB3	1:B:75:GLY:H	1.60	0.44
1:B:19:GLU:O	1:B:23:LEU:HD23	2.17	0.44
1:B:342:GLU:OE2	1:B:345:ARG:NE	2.49	0.44
1:B:92:ILE:HD13	1:B:220:LEU:HD23	2.00	0.44
1:A:232:LEU:HD21	4:A:5314:HOH:O	2.16	0.43
1:A:106:MET:HB3	1:B:127:GLN:HB2	2.00	0.43
1:B:239:VAL:O	1:B:242:GLU:HB2	2.17	0.43
1:B:98:HIS:HD2	1:B:133:GLY:O	2.00	0.43
1:B:184:LYS:HD3	1:B:184:LYS:HA	1.80	0.43
1:B:100:LEU:HG	1:B:112:ARG:CZ	2.48	0.43
1:B:237:MET:O	1:B:241:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:HD2	1:A:319:GLU:OE1	2.18	0.43
1:B:272:THR:O	1:B:275:GLN:N	2.52	0.43
1:B:208:ILE:HG12	1:B:209:VAL:N	2.33	0.43
1:A:254:GLN:HG3	1:A:326:TYR:OH	2.18	0.43
1:B:137:LYS:NZ	4:B:5045:HOH:O	2.50	0.43
1:B:259:ASP:OD2	4:B:5298:HOH:O	2.21	0.43
1:B:39:MET:O	1:B:43:CYS:HB2	2.18	0.43
1:A:41:THR:O	1:A:113:ARG:NH2	2.50	0.43
1:A:115:LYS:CG	1:A:116:PRO:HD2	2.49	0.43
1:A:49:ASN:HA	1:A:49:ASN:HD22	1.49	0.43
1:B:102:GLU:O	1:B:106:MET:HG3	2.19	0.43
1:B:273:ASP:N	4:B:5298:HOH:O	2.51	0.43
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.78	0.43
1:B:180:PHE:CZ	1:B:193:THR:HG23	2.54	0.42
1:B:201:THR:HG22	1:B:204:ASN:H	1.83	0.42
1:A:189:VAL:O	1:B:123:ASP:HB2	2.18	0.42
1:B:166:TYR:O	1:B:170:VAL:HG23	2.19	0.42
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.79	0.42
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.85	0.42
1:A:334:ALA:HB2	1:A:363:TYR:CE1	2.54	0.42
1:A:211:TYR:OH	1:B:25:PHE:HA	2.20	0.42
1:B:323:GLN:HG2	1:B:323:GLN:H	1.65	0.42
1:B:260:CYS:HB3	1:B:261:PHE:CD1	2.55	0.42
1:B:316:LEU:HA	1:B:319:GLU:CG	2.47	0.42
1:B:5:MET:O	1:B:8:GLN:HB2	2.19	0.42
1:B:219:LEU:HD12	1:B:219:LEU:O	2.19	0.41
1:A:145:MET:SD	1:A:154:LEU:HD21	2.60	0.41
1:B:57:VAL:HG21	1:B:222:LEU:HD23	2.02	0.41
1:B:247:MET:CE	1:B:359:TRP:HA	2.50	0.41
1:B:315:ARG:O	1:B:319:GLU:HG3	2.20	0.41
1:B:20:GLU:HG3	1:B:24:LYS:HD3	2.02	0.41
1:B:189:VAL:HG12	1:B:190:SER:N	2.32	0.41
1:A:102:GLU:O	1:A:106:MET:HG3	2.20	0.41
1:A:123:ASP:N	1:B:189:VAL:O	2.54	0.41
1:B:259:ASP:OD2	1:B:273:ASP:HB2	2.21	0.41
1:A:118:TRP:HA	1:A:121:HIS:CD2	2.55	0.41
1:B:112:ARG:HD2	1:B:112:ARG:HH11	1.71	0.41
1:A:253:VAL:HG12	1:A:326:TYR:CE1	2.55	0.41
1:A:68:ASN:ND2	1:A:68:ASN:N	2.69	0.41
1:B:1:MET:O	1:B:4:GLN:HB3	2.21	0.41
1:B:200:PHE:HD2	1:B:283:ALA:HB1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HE1	1:A:365:ARG:HH21	1.85	0.41
1:A:123:ASP:HA	1:B:191:GLN:HG2	2.03	0.41
1:A:277:ALA:HA	1:A:302:TYR:CE2	2.56	0.41
1:A:348:SER:HB2	1:A:351:PHE:HB3	2.03	0.41
1:B:272:THR:O	1:B:276:ASP:N	2.49	0.41
1:A:174:TYR:HB3	1:A:208:ILE:CB	2.52	0.40
1:A:361:LYS:HA	1:A:361:LYS:HD3	1.66	0.40
1:B:131:ASN:HB3	4:B:5184:HOH:O	2.20	0.40
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.91	0.40
1:A:243:LEU:HD12	1:A:244:ALA:N	2.36	0.40
1:A:62:LEU:O	1:A:66:PRO:HB3	2.20	0.40
1:B:96:GLN:HG3	1:B:216:TYR:CE1	2.56	0.40
1:A:257:VAL:HG22	1:A:282:LEU:CD2	2.40	0.40
1:B:268:GLY:O	1:B:269:LYS:HB3	2.21	0.40
1:B:274:ILE:CD1	1:B:310:VAL:HG23	2.50	0.40
1:A:316:LEU:HG	1:A:316:LEU:H	1.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:GLU:OE1	4:A:5290:HOH:O[4_546]	2.06	0.14

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	365/390 (94%)	336 (92%)	18 (5%)	11 (3%)	4	2
1	B	357/390 (92%)	331 (93%)	21 (6%)	5 (1%)	11	10
All	All	722/780 (93%)	667 (92%)	39 (5%)	16 (2%)	6	4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	B	63	SER
1	B	73	ASP
1	B	269	LYS
1	A	76	ALA
1	A	63	SER
1	A	73	ASP
1	A	208	ILE
1	A	302	TYR
1	A	72	GLU
1	A	209	VAL
1	A	273	ASP
1	B	364	LYS
1	A	192	PRO
1	A	75	GLY
1	B	270	VAL

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	321/340 (94%)	276 (86%)	45 (14%)	3	3
1	B	316/340 (93%)	259 (82%)	57 (18%)	1	1
All	All	637/680 (94%)	535 (84%)	102 (16%)	2	2

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	24	LYS
1	A	37	LYS
1	A	38	MET
1	A	49	ASN
1	A	50	ARG
1	A	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	ASN
1	A	72	GLU
1	A	74	ASP
1	A	78	ARG
1	A	79	LYS
1	A	80	ARG
1	A	111	THR
1	A	127	GLN
1	A	157	LEU
1	A	158	LEU
1	A	163	ARG
1	A	178	SER
1	A	179	MET
1	A	180	PHE
1	A	182	SER
1	A	185	LEU
1	A	190	SER
1	A	191	GLN
1	A	208	ILE
1	A	212	LYS
1	A	219	LEU
1	A	232	LEU
1	A	246	LEU
1	A	260	CYS
1	A	266	ARG
1	A	269	LYS
1	A	270	VAL
1	A	289	LYS
1	A	297	GLU
1	A	299	LYS
1	A	316	LEU
1	A	323	GLN
1	A	330	GLU
1	A	335	GLU
1	A	338	LYS
1	A	345	ARG
1	A	348	SER
1	A	367	LYS
1	B	1	MET
1	B	5	MET
1	B	24	LYS
1	B	33	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	35	LEU
1	B	47	LYS
1	B	60	SER
1	B	63	SER
1	B	64	LEU
1	B	65	SER
1	B	77	ARG
1	B	79	LYS
1	B	92	ILE
1	B	100	LEU
1	B	110	VAL
1	B	111	THR
1	B	115	LYS
1	B	126	VAL
1	B	155	GLN
1	B	159	CYS
1	B	167	THR
1	B	176	VAL
1	B	179	MET
1	B	182	SER
1	B	185	LEU
1	B	186	ASP
1	B	193	THR
1	B	194	THR
1	B	196	ASP
1	B	203	SER
1	B	208	ILE
1	B	210	LYS
1	B	245	MET
1	B	255	ASP
1	B	265	GLU
1	B	266	ARG
1	B	269	LYS
1	B	273	ASP
1	B	275	GLN
1	B	284	VAL
1	B	289	LYS
1	B	292	SER
1	B	297	GLU
1	B	304	SER
1	B	306	ASP
1	B	307	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	315	ARG
1	B	329	TYR
1	B	330	GLU
1	B	338	LYS
1	B	340	LEU
1	B	342	GLU
1	B	348	SER
1	B	358	LEU
1	B	364	LYS
1	B	365	ARG
1	B	367	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	68	ASN
1	A	69	ASN
1	A	83	HIS
1	A	98	HIS
1	A	108	ASN
1	A	121	HIS
1	A	141	HIS
1	A	162	ASN
1	A	191	GLN
1	A	204	ASN
1	A	252	GLN
1	B	4	GLN
1	B	49	ASN
1	B	83	HIS
1	B	96	GLN
1	B	98	HIS
1	B	141	HIS
1	B	191	GLN
1	B	204	ASN
1	B	336	GLN
1	B	366	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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$
3	1BY	B	4001	2	16,17,17	2.85	10 (62%)	22,25,25	2.26	7 (31%)
3	1BY	A	3001	2	16,17,17	2.95	10 (62%)	22,25,25	1.88	4 (18%)

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	1BY	B	4001	2	-	1/15/17/17	0/1/1/1
3	1BY	A	3001	2	-	1/15/17/17	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	1BY	C3-N2	6.04	1.45	1.34
3	B	4001	1BY	C3-N2	5.73	1.45	1.34
3	B	4001	1BY	C5-C4	3.93	1.47	1.38
3	A	3001	1BY	C5-C4	3.90	1.47	1.38
3	B	4001	1BY	P1-O2	-3.77	1.48	1.54
3	A	3001	1BY	P2-O4	-3.62	1.49	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	1BY	P1-O3	-3.58	1.49	1.54
3	B	4001	1BY	P1-O3	-3.46	1.49	1.54
3	A	3001	1BY	P1-O2	-3.41	1.49	1.54
3	A	3001	1BY	C6-C7	3.33	1.47	1.37
3	B	4001	1BY	C7-N2	-3.32	1.27	1.34
3	B	4001	1BY	P2-O4	-3.18	1.49	1.54
3	A	3001	1BY	C7-N2	-3.17	1.28	1.34
3	B	4001	1BY	C6-C7	3.14	1.46	1.37
3	A	3001	1BY	C3-N1	-3.01	1.31	1.36
3	A	3001	1BY	P2-O5	-2.89	1.50	1.54
3	B	4001	1BY	P2-O5	-2.81	1.50	1.54
3	B	4001	1BY	C3-N1	-2.72	1.32	1.36
3	A	3001	1BY	C4-C3	-2.37	1.34	1.39
3	B	4001	1BY	C4-C3	-2.33	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4001	1BY	N1-C3-N2	5.68	125.53	116.95
3	A	3001	1BY	N1-C3-N2	4.84	124.25	116.95
3	B	4001	1BY	C7-N2-C3	4.36	123.41	117.22
3	B	4001	1BY	C4-C3-N2	-3.67	116.83	122.57
3	A	3001	1BY	C7-N2-C3	3.50	122.18	117.22
3	A	3001	1BY	C4-C3-N2	-3.20	117.58	122.57
3	B	4001	1BY	O3-P1-O1	-2.78	106.47	113.45
3	B	4001	1BY	C2-N1-C3	-2.43	118.91	123.36
3	B	4001	1BY	O4-P2-O6	-2.33	107.59	113.45
3	A	3001	1BY	C5-C4-C3	2.31	121.39	117.73
3	B	4001	1BY	C5-C4-C3	2.05	120.99	117.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

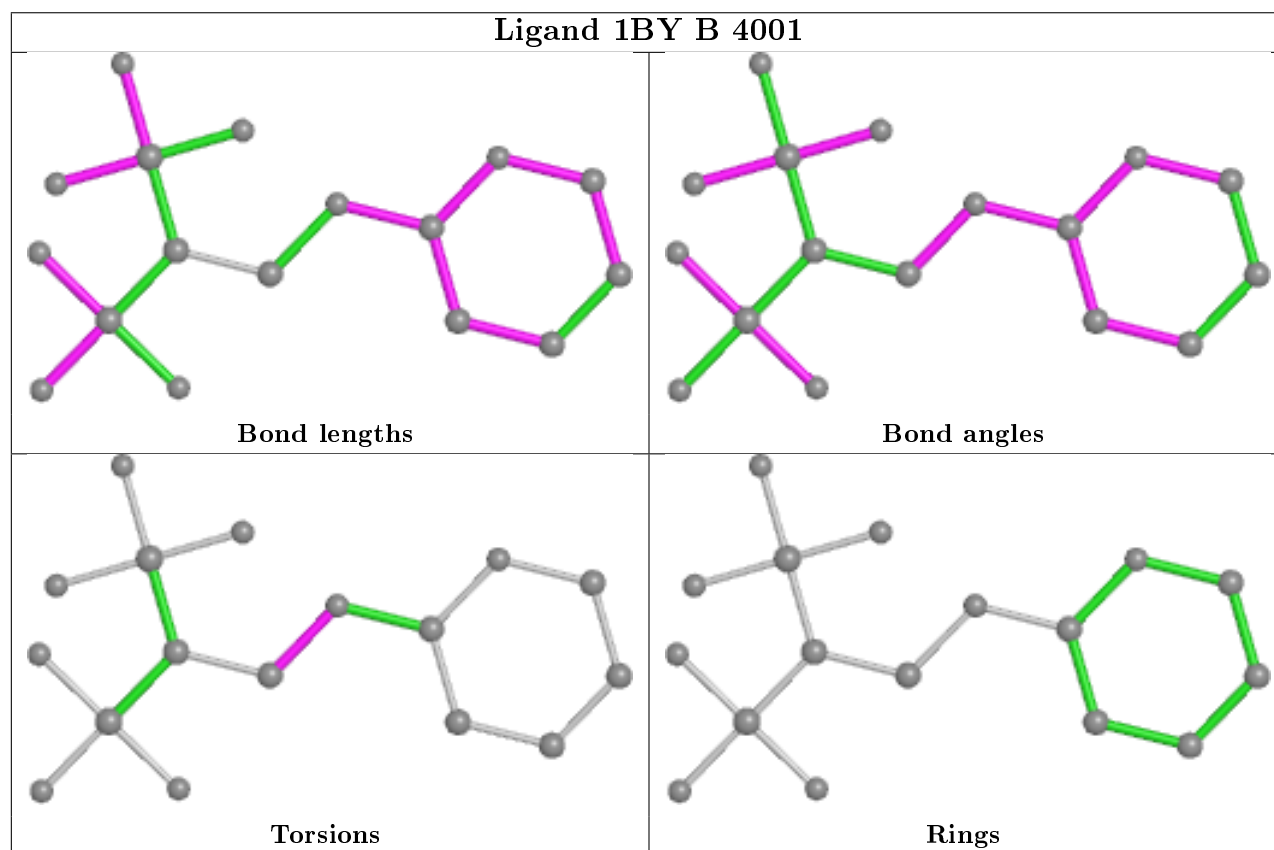
Mol	Chain	Res	Type	Atoms
3	B	4001	1BY	C1-C2-N1-C3
3	A	3001	1BY	C1-C2-N1-C3

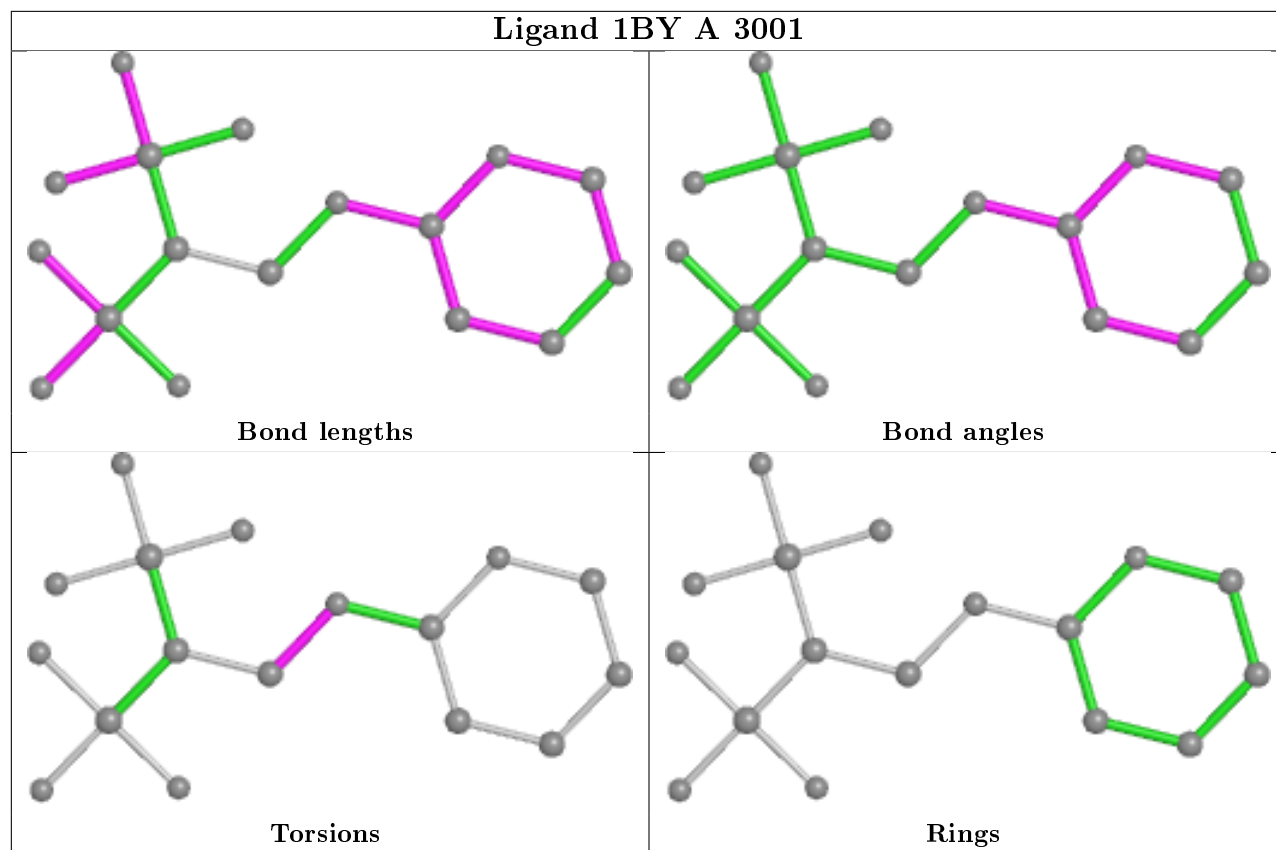
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4001	1BY	1	0
3	A	3001	1BY	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	367/390 (94%)	0.16	21 (5%)	23 28	14, 31, 69, 94	0
1	B	361/390 (92%)	0.06	13 (3%)	42 48	14, 30, 60, 86	0
All	All	728/780 (93%)	0.11	34 (4%)	31 37	14, 31, 63, 94	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	7.2
1	A	65	SER	5.2
1	B	196	ASP	4.9
1	A	196	ASP	4.4
1	A	68	ASN	4.2
1	A	267	LEU	4.1
1	B	73	ASP	4.1
1	A	270	VAL	4.1
1	B	191	GLN	4.1
1	A	193	THR	3.9
1	B	72	GLU	3.9
1	A	66	PRO	3.7
1	A	63	SER	3.6
1	A	67	ASN	3.4
1	B	123	ASP	3.4
1	B	267	LEU	3.4
1	A	367	LYS	3.3
1	B	367	LYS	3.3
1	A	73	ASP	3.2
1	A	72	GLU	3.1
1	A	263	PRO	3.0
1	B	195	THR	3.0
1	A	260	CYS	2.9
1	B	327	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	180	PHE	2.5
1	A	195	THR	2.4
1	A	262	THR	2.4
1	B	329	TYR	2.3
1	A	69	ASN	2.3
1	A	261	PHE	2.2
1	A	307	SER	2.2
1	A	316	LEU	2.1
1	B	198	ALA	2.1
1	B	264	PRO	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

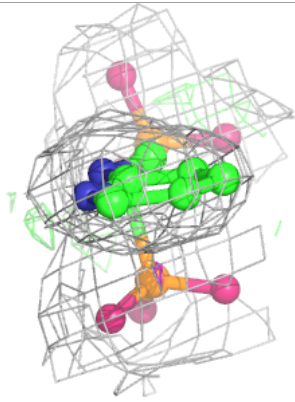
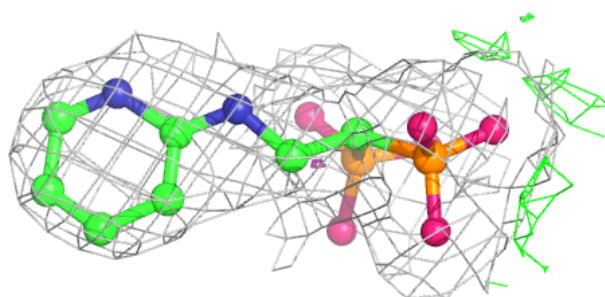
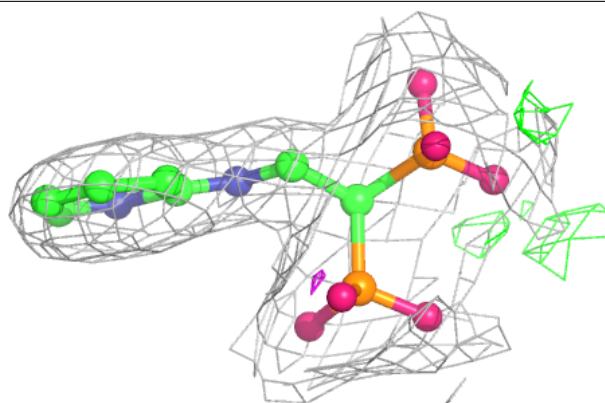
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	4003	1/1	0.90	0.39	33,33,33,33	0
2	MG	A	3003	1/1	0.90	0.15	21,21,21,21	0
2	MG	A	3002	1/1	0.91	0.14	25,25,25,25	0
2	MG	A	3004	1/1	0.95	0.20	29,29,29,29	0
3	1BY	B	4001	17/17	0.96	0.18	25,30,36,38	0
3	1BY	A	3001	17/17	0.96	0.15	30,35,40,41	0
2	MG	B	4004	1/1	0.97	0.27	23,23,23,23	0
2	MG	B	4002	1/1	0.98	0.26	27,27,27,27	0

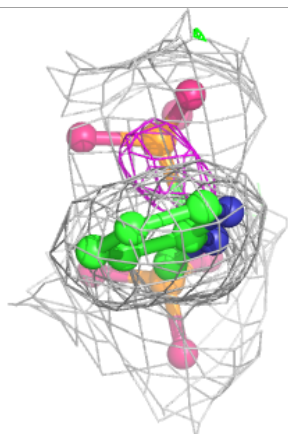
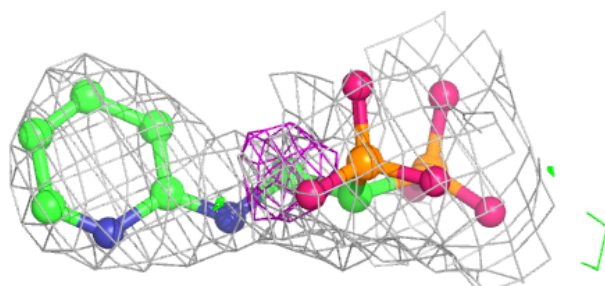
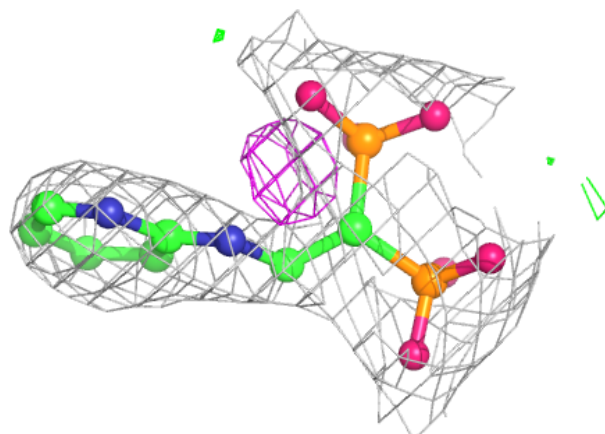
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1BY B 4001:

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

**Electron density around 1BY A 3001:**

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



6.5 Other polymers

There are no such residues in this entry.