



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 5AFX / pdb_00005afx
Title : T. Brucei Farnesyl Diphosphate Synthase Complexed with Bisphosphonate BPH-1238
Authors : Yang, G.; Oldfield, E.; No, J.H.
Deposited on : 2015-01-27
Resolution : 2.39 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

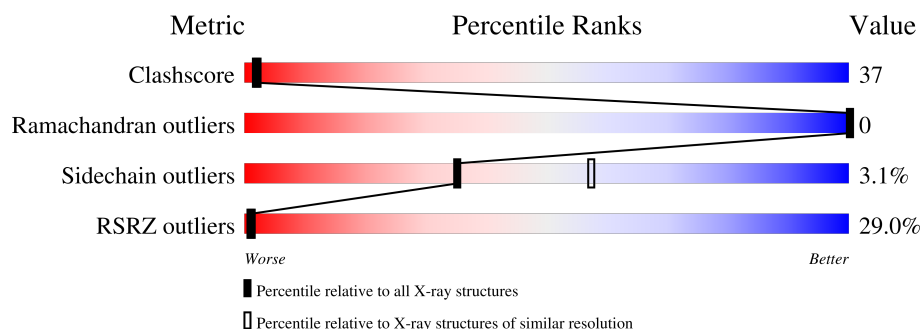
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PVZ	A	1371	-	-	X	-
3	PVZ	B	1371	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5948 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.

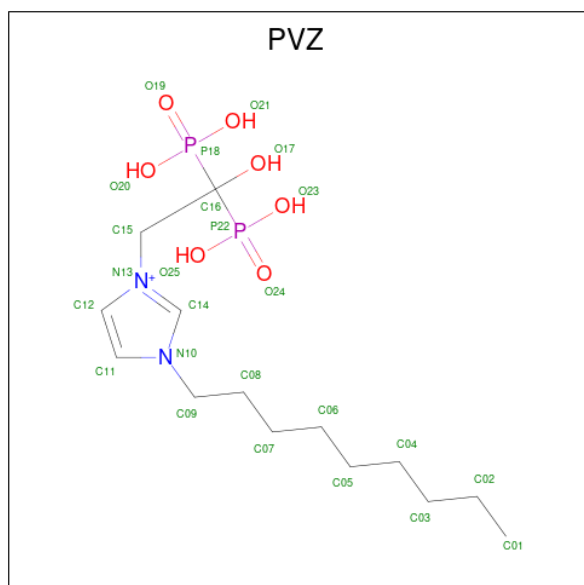
- Molecule 1 is a protein called FARNESYL PYROPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2854	1819	469	538	28			
1	B	357	Total	C	N	O	S	0	0	0
			2854	1819	469	538	28			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is [1-hydroxy-2-(1-nonyl-1H-3lambda 5 -imidazol-3-yl)ethane-1,1-diyl]bis(phosphonic acid) (CCD ID: PVZ) (formula: C₁₄H₂₉N₂O₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	14	2	7	2		
3	B	1	Total	C	N	O	P	0	0
			25	14	2	7	2		

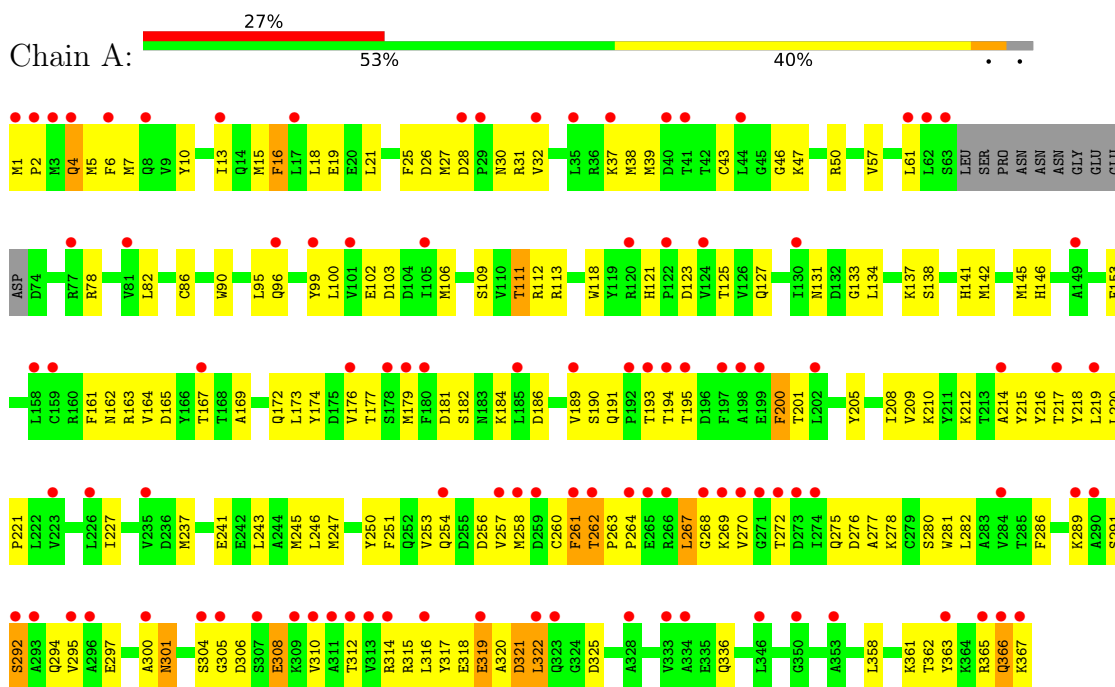
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total	O	0	0
			84	84		
4	B	100	Total	O	0	0
			100	100		

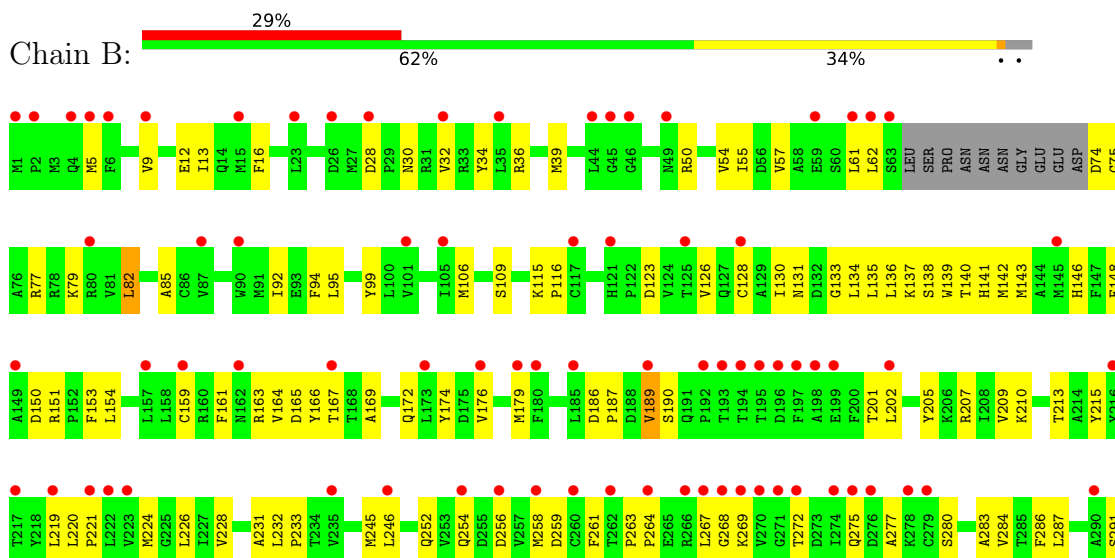
3 Residue-property plots

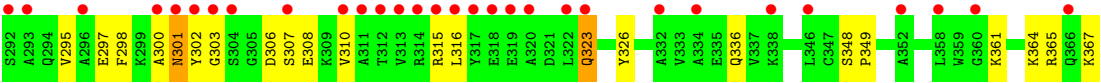
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	132.47Å 119.03Å 63.47Å 90.00° 112.47° 90.00°	Depositor
Resolution (Å)	85.34 – 2.39 85.34 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.6 (85.34-2.39) 93.0 (85.34-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.259 , 0.334 0.269 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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: MG, PVZ

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	0.71	0/2913	1.09	12/3939 (0.3%)
1	B	0.70	0/2913	0.96	2/3939 (0.1%)
All	All	0.71	0/5826	1.03	14/7878 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	PHE	N-CA-C	-12.21	91.91	110.10
1	A	261	PHE	CB-CA-C	-10.41	93.78	110.85
1	A	262	THR	N-CA-C	-8.35	94.87	109.48
1	A	191	GLN	CA-C-N	7.38	128.82	120.85
1	A	191	GLN	C-N-CA	7.38	128.82	120.85
1	A	200	PHE	CB-CA-C	7.13	121.03	109.90
1	A	321	ASP	N-CA-C	6.50	120.52	111.74
1	B	189	VAL	N-CA-C	5.89	116.49	107.77
1	A	191	GLN	CB-CA-C	-5.84	98.67	110.17
1	A	214	ALA	N-CA-C	-5.83	104.84	111.14
1	B	55	ILE	CB-CA-C	-5.63	104.68	111.88
1	A	162	ASN	N-CA-C	5.06	116.88	111.36
1	A	322	LEU	N-CA-C	5.02	117.64	111.82
1	A	292	SER	N-CA-C	5.01	117.63	111.82

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	2854	0	2808	211	0
1	B	2854	0	2808	223	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	25	0	25	19	0
3	B	25	0	25	11	0
4	A	84	0	0	90	0
4	B	100	0	0	167	0
All	All	5948	0	5666	424	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 37.

All (424) 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:286:PHE:HD2	4:B:2077:HOH:O	1.10	1.29
1:B:13:ILE:HA	4:B:2003:HOH:O	1.30	1.25
1:B:323:GLN:HB3	4:B:2087:HOH:O	1.38	1.23
1:B:190:SER:HB3	4:B:2049:HOH:O	1.35	1.23
1:A:362:THR:HA	4:A:2081:HOH:O	1.31	1.22
1:A:358:LEU:HA	4:A:2078:HOH:O	1.41	1.19
1:B:267:LEU:HB2	4:B:2065:HOH:O	1.38	1.18
1:B:209:VAL:HG13	4:B:2055:HOH:O	1.45	1.16
1:A:13:ILE:HA	4:A:2005:HOH:O	1.44	1.15
1:B:150:ASP:HB2	4:B:2042:HOH:O	0.98	1.14
1:B:202:LEU:HA	4:B:2053:HOH:O	1.46	1.14
1:B:298:PHE:CZ	4:B:2076:HOH:O	2.02	1.12
1:B:36:ARG:HA	4:B:2006:HOH:O	1.47	1.11
1:B:128:CYS:SG	4:B:2009:HOH:O	2.06	1.10
1:A:26:ASP:HB2	4:A:2013:HOH:O	1.49	1.10
1:B:95:LEU:HB2	4:B:2031:HOH:O	1.50	1.10
1:B:298:PHE:HB2	4:B:2080:HOH:O	1.50	1.09
1:B:74:ASP:HA	4:B:2022:HOH:O	1.51	1.06
1:A:145:MET:HE1	1:B:159:CYS:HA	1.29	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:HB3	4:B:2030:HOH:O	1.54	1.04
1:B:220:LEU:HD23	4:B:2058:HOH:O	1.55	1.03
1:A:254:GLN:NE2	1:A:365:ARG:HG3	1.73	1.03
1:B:286:PHE:CD2	4:B:2077:HOH:O	1.87	1.03
1:B:209:VAL:HG23	4:B:2054:HOH:O	1.58	1.02
1:B:233:PRO:HD2	4:B:2059:HOH:O	1.58	1.01
1:B:297:GLU:HB3	4:B:2079:HOH:O	1.61	1.01
1:B:135:LEU:HB3	4:B:2036:HOH:O	1.60	1.00
1:B:277:ALA:HA	4:B:2072:HOH:O	1.62	0.99
1:A:306:ASP:OD1	1:A:308:GLU:HG3	1.64	0.98
1:A:318:GLU:HB3	4:A:2070:HOH:O	1.63	0.97
1:B:295:VAL:HG12	4:B:2081:HOH:O	1.64	0.97
1:A:15:MET:HG3	4:A:2007:HOH:O	1.63	0.97
1:A:106:MET:SD	4:A:2032:HOH:O	2.22	0.97
1:B:159:CYS:HB2	4:B:2044:HOH:O	1.64	0.96
1:A:262:THR:OG1	1:A:267:LEU:HD22	1.66	0.96
1:B:161:PHE:CZ	4:B:2031:HOH:O	2.17	0.96
1:A:280:SER:HB2	4:A:2060:HOH:O	1.64	0.95
1:B:228:VAL:HG21	4:B:2028:HOH:O	1.66	0.95
1:A:113:ARG:HA	4:A:2033:HOH:O	1.67	0.95
1:A:227:ILE:HG12	4:A:2041:HOH:O	1.67	0.94
1:A:121:HIS:HE1	4:A:2035:HOH:O	1.51	0.93
1:A:86:CYS:SG	4:A:2003:HOH:O	2.26	0.93
1:A:190:SER:HB3	4:A:2047:HOH:O	1.68	0.92
1:A:141:HIS:O	1:A:145:MET:HG3	1.71	0.91
1:B:137:LYS:HE3	4:B:2037:HOH:O	1.69	0.91
1:A:205:TYR:OH	1:A:256:ASP:OD2	1.90	0.90
1:B:263:PRO:HB3	4:B:2066:HOH:O	1.72	0.90
1:B:258:MET:SD	4:B:2064:HOH:O	2.29	0.89
1:A:145:MET:HE1	1:B:159:CYS:CA	2.03	0.89
1:B:172:GLN:HG3	3:B:1371:PVZ:H07A	1.55	0.89
1:A:6:PHE:HA	4:A:2003:HOH:O	1.74	0.87
1:B:82:LEU:HD22	4:B:2016:HOH:O	1.73	0.86
1:B:109:SER:HB3	4:B:2033:HOH:O	1.74	0.86
1:B:316:LEU:HD13	4:B:2080:HOH:O	1.74	0.85
1:B:92:ILE:HG23	4:B:2058:HOH:O	1.76	0.84
1:A:237:MET:HG3	4:A:2059:HOH:O	1.75	0.84
1:A:7:MET:SD	4:A:2002:HOH:O	2.34	0.84
1:A:251:PHE:CZ	4:A:2083:HOH:O	2.29	0.84
1:A:99:TYR:HE1	3:A:1371:PVZ:H01A	1.43	0.84
1:A:301:ASN:OD1	1:A:312:THR:HG21	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:NE2	1:A:365:ARG:CG	2.41	0.83
1:A:320:ALA:CB	4:A:2071:HOH:O	2.26	0.83
1:A:361:LYS:HD2	4:A:2078:HOH:O	1.78	0.83
1:B:307:SER:HB2	4:B:2082:HOH:O	1.78	0.83
1:A:264:PRO:HD2	4:A:2061:HOH:O	1.78	0.83
1:A:320:ALA:HB1	4:A:2071:HOH:O	1.77	0.82
1:A:96:GLN:NE2	1:A:216:TYR:HE1	1.77	0.82
1:A:47:LYS:HE2	4:A:2023:HOH:O	1.79	0.82
1:A:172:GLN:CG	3:A:1371:PVZ:H07A	2.10	0.82
1:A:276:ASP:HB3	1:A:278:LYS:HD3	1.62	0.81
1:A:179:MET:HE2	1:A:193:THR:HB	1.62	0.81
1:A:16:PHE:HB3	4:A:2005:HOH:O	1.79	0.81
1:A:316:LEU:HA	1:A:319:GLU:HG3	1.61	0.81
1:B:224:MET:CB	4:B:2030:HOH:O	2.19	0.81
1:A:186:ASP:O	1:B:123:ASP:CB	2.29	0.80
4:A:2037:HOH:O	1:B:106:MET:SD	2.41	0.79
1:A:241:GLU:HB2	4:A:2059:HOH:O	1.83	0.79
1:B:140:THR:HG22	4:B:2039:HOH:O	1.83	0.79
1:A:316:LEU:HD23	1:A:316:LEU:O	1.84	0.78
1:B:228:VAL:CG2	4:B:2028:HOH:O	2.28	0.78
1:B:126:VAL:HG12	4:B:2035:HOH:O	1.82	0.78
1:A:96:GLN:NE2	1:A:216:TYR:CE1	2.52	0.78
1:A:260:CYS:HG	1:A:261:PHE:HE1	1.28	0.78
1:B:50:ARG:HG3	4:B:2015:HOH:O	1.84	0.78
1:B:143:MET:HE3	4:B:2039:HOH:O	1.81	0.78
1:B:137:LYS:HE2	4:B:2038:HOH:O	1.82	0.78
4:A:2029:HOH:O	1:B:130:ILE:HD13	1.83	0.78
1:B:269:LYS:HD2	4:B:2069:HOH:O	1.84	0.77
1:B:245:MET:HE1	4:B:2056:HOH:O	1.83	0.77
1:B:79:LYS:HA	4:B:2026:HOH:O	1.84	0.77
1:A:245:MET:HE1	4:A:2055:HOH:O	1.86	0.76
1:A:300:ALA:C	1:A:301:ASN:HD22	1.94	0.76
1:B:99:TYR:CD1	3:B:1371:PVZ:H06	2.21	0.76
1:A:190:SER:CB	4:A:2047:HOH:O	2.32	0.75
1:A:278:LYS:HE2	4:A:2042:HOH:O	1.88	0.74
1:A:304:SER:HB2	4:A:2067:HOH:O	1.86	0.74
1:B:140:THR:HA	4:B:2039:HOH:O	1.86	0.74
1:A:111:THR:HG22	1:A:269:LYS:HA	1.69	0.73
1:B:75:GLY:HA3	4:B:2023:HOH:O	1.87	0.73
1:A:5:MET:HB2	4:A:2004:HOH:O	1.89	0.72
1:A:306:ASP:OD1	1:A:308:GLU:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PHE:CE2	4:A:2057:HOH:O	2.43	0.72
1:A:172:GLN:HG2	3:A:1371:PVZ:H07A	1.72	0.72
1:B:146:HIS:HD2	4:B:2041:HOH:O	1.72	0.72
1:A:251:PHE:CD2	4:A:2057:HOH:O	2.42	0.71
1:B:277:ALA:CB	4:B:2072:HOH:O	2.39	0.71
1:B:261:PHE:CD1	4:B:2088:HOH:O	2.43	0.71
1:B:275:GLN:CD	4:B:2073:HOH:O	2.32	0.71
1:B:302:TYR:CD2	4:B:2072:HOH:O	2.42	0.71
1:A:103:ASP:HB2	4:A:2028:HOH:O	1.88	0.71
1:A:306:ASP:OD1	1:A:308:GLU:CG	2.39	0.70
1:B:202:LEU:CA	4:B:2053:HOH:O	2.20	0.70
1:B:336:GLN:HG2	4:B:2094:HOH:O	1.90	0.70
1:B:115:LYS:HA	4:B:2034:HOH:O	1.91	0.70
1:B:284:VAL:HG21	4:B:2053:HOH:O	1.92	0.70
1:B:228:VAL:CB	4:B:2028:HOH:O	2.39	0.70
1:A:260:CYS:O	1:A:314:ARG:NH1	2.25	0.70
1:B:161:PHE:HZ	4:B:2031:HOH:O	1.62	0.70
1:A:46:GLY:HA2	4:A:2021:HOH:O	1.90	0.70
1:A:272:THR:HB	4:A:2062:HOH:O	1.90	0.70
1:B:361:LYS:HG3	4:B:2097:HOH:O	1.92	0.69
1:A:315:ARG:O	1:A:319:GLU:HG2	1.92	0.69
1:B:205:TYR:OH	1:B:256:ASP:OD2	2.08	0.69
1:B:365:ARG:HB3	4:B:2098:HOH:O	1.91	0.69
1:A:208:ILE:HG22	1:A:212:LYS:HD3	1.75	0.68
1:B:245:MET:CE	4:B:2056:HOH:O	2.41	0.68
1:A:169:ALA:HB2	3:A:1371:PVZ:H02A	1.74	0.67
1:A:184:LYS:HE2	4:A:2044:HOH:O	1.94	0.67
1:A:131:ASN:OD1	3:B:1371:PVZ:H03A	1.94	0.67
1:B:62:LEU:HD12	4:B:2021:HOH:O	1.95	0.67
1:B:231:ALA:HA	4:B:2059:HOH:O	1.95	0.67
1:A:123:ASP:CB	1:B:187:PRO:O	2.43	0.67
1:A:169:ALA:CB	3:A:1371:PVZ:H02A	2.25	0.67
4:A:2032:HOH:O	1:B:131:ASN:HB2	1.94	0.66
3:A:1371:PVZ:H06A	3:A:1371:PVZ:H02	1.76	0.66
1:B:231:ALA:CA	4:B:2059:HOH:O	2.43	0.66
1:A:118:TRP:CH2	4:A:2018:HOH:O	2.48	0.66
1:A:215:TYR:HA	4:A:2055:HOH:O	1.93	0.66
4:A:2029:HOH:O	1:B:130:ILE:HG21	1.95	0.66
1:B:106:MET:HE1	3:B:1371:PVZ:H04A	1.76	0.66
1:B:258:MET:HG2	4:B:2064:HOH:O	1.95	0.66
1:A:99:TYR:CE1	3:A:1371:PVZ:H01A	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ALA:CA	3:A:1371:PVZ:H02A	2.27	0.65
1:B:277:ALA:CA	4:B:2072:HOH:O	2.28	0.65
1:B:209:VAL:HG22	1:B:252:GLN:HG2	1.77	0.65
1:A:215:TYR:HD1	4:A:2056:HOH:O	1.78	0.65
1:B:146:HIS:CD2	4:B:2041:HOH:O	2.48	0.65
1:A:306:ASP:CG	1:A:308:GLU:HG3	2.20	0.65
1:B:99:TYR:HB3	3:B:1371:PVZ:H08A	1.77	0.65
1:B:150:ASP:CB	4:B:2042:HOH:O	1.81	0.65
1:A:186:ASP:CG	4:A:2046:HOH:O	2.39	0.65
1:B:172:GLN:CG	3:B:1371:PVZ:H07A	2.26	0.65
1:B:179:MET:HG3	4:B:2046:HOH:O	1.96	0.65
1:B:287:LEU:HG	4:B:2077:HOH:O	1.97	0.65
1:A:50:ARG:CZ	1:A:96:GLN:HE21	2.10	0.64
1:A:189:VAL:HB	4:A:2046:HOH:O	1.96	0.64
1:A:254:GLN:HE22	1:A:365:ARG:CG	2.10	0.64
1:B:275:GLN:CG	4:B:2073:HOH:O	2.45	0.64
1:A:169:ALA:HA	3:A:1371:PVZ:H02A	1.80	0.64
1:A:106:MET:CE	4:A:2032:HOH:O	2.41	0.64
1:A:291:SER:N	1:A:294:GLN:OE1	2.29	0.64
1:B:263:PRO:CB	4:B:2066:HOH:O	2.36	0.64
1:B:364:LYS:HA	4:B:2061:HOH:O	1.97	0.64
4:A:2037:HOH:O	1:B:106:MET:CE	2.45	0.64
1:A:263:PRO:HB3	4:A:2061:HOH:O	1.99	0.63
1:A:276:ASP:CB	1:A:278:LYS:HD3	2.27	0.63
1:B:361:LYS:CG	4:B:2097:HOH:O	2.47	0.63
1:A:306:ASP:O	1:A:310:VAL:HG23	1.98	0.63
1:B:34:TYR:CE2	4:B:2009:HOH:O	2.50	0.63
1:A:172:GLN:HG3	3:A:1371:PVZ:H07A	1.80	0.63
1:B:209:VAL:CG2	4:B:2054:HOH:O	2.29	0.62
1:B:280:SER:HB3	4:B:2071:HOH:O	1.98	0.62
1:A:258:MET:HG2	1:A:262:THR:HG21	1.81	0.62
1:B:169:ALA:HB2	3:B:1371:PVZ:H01A	1.81	0.62
1:B:367:LYS:HD2	4:B:2067:HOH:O	1.99	0.62
1:A:321:ASP:CG	1:A:321:ASP:O	2.40	0.62
1:A:179:MET:HE3	1:A:194:THR:N	2.14	0.62
4:A:2037:HOH:O	1:B:106:MET:HE1	1.98	0.62
1:A:215:TYR:HB3	4:A:2056:HOH:O	1.99	0.62
1:A:250:TYR:CG	1:A:250:TYR:O	2.53	0.62
1:A:243:LEU:HD22	1:A:247:MET:HE2	1.81	0.62
1:A:365:ARG:HD3	4:A:2081:HOH:O	2.00	0.62
1:B:163:ARG:O	1:B:167:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:MET:HE1	3:B:1371:PVZ:C04	2.29	0.61
1:B:116:PRO:HD3	4:B:2034:HOH:O	1.99	0.61
1:B:258:MET:CG	4:B:2064:HOH:O	2.45	0.61
1:A:292:SER:HB2	4:A:2066:HOH:O	2.00	0.61
1:B:231:ALA:C	4:B:2059:HOH:O	2.44	0.61
1:A:217:THR:HG21	4:A:2057:HOH:O	2.00	0.61
1:A:1:MET:SD	4:A:2001:HOH:O	2.56	0.61
1:A:18:LEU:HA	1:A:21:LEU:HD12	1.82	0.61
1:A:164:VAL:HA	1:A:167:THR:HG22	1.84	0.60
1:A:113:ARG:N	1:A:268:GLY:O	2.35	0.60
1:A:317:TYR:HB3	1:A:322:LEU:HD12	1.84	0.60
1:B:275:GLN:HG3	4:B:2073:HOH:O	2.01	0.60
1:A:31:ARG:NH1	1:B:207:ARG:HH22	1.98	0.60
1:B:39:MET:HB3	4:B:2006:HOH:O	2.01	0.59
1:B:82:LEU:HD11	4:B:2019:HOH:O	2.02	0.59
1:B:77:ARG:NE	4:B:2025:HOH:O	2.34	0.59
1:A:1:MET:O	1:A:2:PRO:C	2.41	0.59
1:A:200:PHE:O	1:A:201:THR:CG2	2.50	0.59
1:B:287:LEU:HD23	4:B:2077:HOH:O	2.02	0.59
1:B:298:PHE:CB	4:B:2080:HOH:O	2.27	0.59
1:B:95:LEU:HD22	4:B:2031:HOH:O	2.02	0.59
1:A:181:ASP:HB3	4:A:2043:HOH:O	2.04	0.58
1:B:172:GLN:HG3	3:B:1371:PVZ:C07	2.30	0.58
1:B:316:LEU:CD2	4:B:2084:HOH:O	2.51	0.58
1:A:106:MET:HE1	4:A:2032:HOH:O	2.03	0.58
1:B:79:LYS:HB3	4:B:2027:HOH:O	2.02	0.58
1:A:286:PHE:CZ	1:A:316:LEU:HD22	2.38	0.58
1:A:186:ASP:HB3	4:A:2046:HOH:O	2.04	0.58
1:B:315:ARG:CD	4:B:2086:HOH:O	2.52	0.58
1:A:113:ARG:HG2	4:A:2021:HOH:O	2.05	0.57
1:A:15:MET:O	1:A:19:GLU:HB2	2.03	0.57
1:A:16:PHE:CE2	1:A:146:HIS:CD2	2.93	0.57
1:A:16:PHE:CE2	1:A:146:HIS:CG	2.92	0.57
1:B:228:VAL:HB	4:B:2028:HOH:O	2.02	0.57
1:A:366:GLN:HB2	4:A:2084:HOH:O	2.04	0.57
1:A:305:GLY:O	1:A:306:ASP:C	2.49	0.56
1:A:78:ARG:O	1:A:82:LEU:HG	2.04	0.56
1:A:262:THR:HG1	1:A:267:LEU:HD22	1.69	0.56
1:A:320:ALA:HB3	4:A:2071:HOH:O	1.98	0.56
1:B:261:PHE:CG	4:B:2088:HOH:O	2.57	0.56
1:B:315:ARG:HB2	4:B:2083:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLN:HB2	4:A:2062:HOH:O	2.06	0.56
1:A:286:PHE:CE1	1:A:316:LEU:HD22	2.40	0.56
1:B:205:TYR:CB	4:B:2053:HOH:O	2.54	0.56
1:A:272:THR:CB	4:A:2062:HOH:O	2.51	0.55
1:B:151:ARG:HG2	1:B:153:PHE:CZ	2.40	0.55
1:B:220:LEU:HB3	1:B:221:PRO:HD3	1.86	0.55
1:B:82:LEU:HA	4:B:2016:HOH:O	2.05	0.55
1:A:200:PHE:O	1:A:201:THR:HG23	2.06	0.55
1:B:316:LEU:CA	4:B:2084:HOH:O	2.55	0.55
1:B:315:ARG:HG2	4:B:2086:HOH:O	2.07	0.55
1:A:123:ASP:CB	1:B:186:ASP:O	2.54	0.55
1:B:291:SER:O	1:B:295:VAL:HG23	2.07	0.55
1:B:310:VAL:HG22	4:B:2073:HOH:O	2.06	0.54
1:B:139:TRP:CE2	4:B:2036:HOH:O	2.60	0.54
1:A:26:ASP:CB	4:A:2013:HOH:O	2.26	0.54
1:A:145:MET:CE	1:B:159:CYS:HA	2.19	0.54
1:B:133:GLY:O	1:B:136:LEU:HB2	2.07	0.54
1:B:336:GLN:CG	4:B:2094:HOH:O	2.50	0.54
1:A:125:THR:HB	1:A:127:GLN:CD	2.33	0.54
1:B:148:PHE:HB2	1:B:154:LEU:HD13	1.89	0.54
1:B:246:LEU:HD21	1:B:336:GLN:HB3	1.89	0.54
1:B:287:LEU:CG	4:B:2077:HOH:O	2.53	0.54
1:A:218:TYR:CE1	1:A:358:LEU:HD11	2.43	0.54
1:A:289:LYS:NZ	1:A:325:ASP:OD1	2.41	0.54
1:B:85:ALA:N	4:B:2028:HOH:O	2.41	0.54
1:B:62:LEU:CD1	4:B:2021:HOH:O	2.55	0.53
1:A:118:TRP:HH2	4:A:2018:HOH:O	1.90	0.53
1:B:57:VAL:HG12	1:B:61:LEU:HD12	1.90	0.53
1:B:287:LEU:CD2	4:B:2077:HOH:O	2.56	0.53
1:A:365:ARG:HB3	4:A:2080:HOH:O	2.08	0.53
1:A:78:ARG:HD2	4:A:2025:HOH:O	2.08	0.53
1:B:264:PRO:HD2	4:B:2066:HOH:O	2.08	0.53
1:A:269:LYS:NZ	3:A:1371:PVZ:O23	2.39	0.53
1:A:1:MET:O	1:A:4:GLN:N	2.42	0.53
1:B:215:TYR:HB3	4:B:2057:HOH:O	2.07	0.53
1:A:145:MET:HE1	1:B:159:CYS:CB	2.38	0.53
1:A:301:ASN:HD22	1:A:301:ASN:N	2.07	0.52
1:A:57:VAL:HG12	1:A:61:LEU:HD12	1.92	0.52
1:B:205:TYR:HB3	4:B:2053:HOH:O	2.09	0.52
1:B:283:ALA:HA	4:B:2076:HOH:O	2.09	0.52
1:B:316:LEU:CB	4:B:2084:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASP:O	1:B:32:VAL:HG23	2.10	0.52
1:B:316:LEU:HD22	4:B:2084:HOH:O	2.09	0.52
1:B:298:PHE:CE1	4:B:2076:HOH:O	2.45	0.52
1:B:365:ARG:CB	4:B:2098:HOH:O	2.54	0.52
1:A:179:MET:HG3	1:A:179:MET:O	2.11	0.51
1:B:269:LYS:HG3	4:B:2068:HOH:O	2.09	0.51
1:B:161:PHE:CD2	4:B:2040:HOH:O	2.64	0.51
1:B:137:LYS:HZ1	1:B:165:ASP:CG	2.18	0.51
1:B:141:HIS:CD2	4:B:2040:HOH:O	2.63	0.51
1:B:306:ASP:O	1:B:310:VAL:HG23	2.11	0.51
1:A:254:GLN:NE2	1:A:365:ARG:O	2.44	0.51
3:A:1371:PVZ:H03	1:B:134:LEU:HD13	1.92	0.51
1:A:363:TYR:CD2	4:A:2079:HOH:O	2.54	0.51
1:A:257:VAL:HG22	1:A:282:LEU:HD21	1.92	0.51
1:A:127:GLN:OE1	1:A:127:GLN:N	2.30	0.50
3:A:1371:PVZ:C03	1:B:134:LEU:HD13	2.41	0.50
1:A:37:LYS:C	4:A:2018:HOH:O	2.54	0.50
1:B:140:THR:CA	4:B:2039:HOH:O	2.51	0.50
1:B:264:PRO:CD	4:B:2066:HOH:O	2.60	0.50
1:A:27:MET:HG2	1:A:32:VAL:HG23	1.94	0.50
1:B:140:THR:CG2	4:B:2039:HOH:O	2.48	0.50
1:A:246:LEU:HD21	1:A:336:GLN:HB3	1.93	0.49
1:A:179:MET:HE2	1:A:193:THR:CB	2.39	0.49
1:A:260:CYS:SG	1:A:261:PHE:CE1	2.94	0.49
1:B:36:ARG:NH2	4:B:2011:HOH:O	2.38	0.49
1:B:215:TYR:HD1	4:B:2057:HOH:O	1.94	0.49
1:B:77:ARG:HB3	4:B:2024:HOH:O	2.11	0.49
3:A:1371:PVZ:H08	4:A:2028:HOH:O	2.11	0.49
1:B:202:LEU:N	4:B:2053:HOH:O	2.39	0.49
1:A:137:LYS:CE	1:A:165:ASP:OD2	2.61	0.49
1:B:179:MET:CG	4:B:2046:HOH:O	2.58	0.49
1:B:259:ASP:HB2	4:B:2062:HOH:O	2.12	0.49
1:A:174:TYR:HB3	1:A:208:ILE:HG12	1.95	0.48
1:A:245:MET:CE	4:A:2055:HOH:O	2.54	0.48
1:A:256:ASP:HB3	4:A:2060:HOH:O	2.12	0.48
1:A:260:CYS:SG	1:A:261:PHE:HE1	2.32	0.48
1:B:303:GLY:N	4:B:2072:HOH:O	2.46	0.48
1:A:219:LEU:HD21	1:A:237:MET:CE	2.43	0.48
1:B:5:MET:SD	1:B:82:LEU:HD12	2.53	0.48
1:A:102:GLU:OE2	1:A:133:GLY:HA3	2.13	0.48
1:A:142:MET:HE2	1:B:166:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HB3	1:A:262:THR:OG1	2.13	0.48
1:A:26:ASP:CG	4:A:2013:HOH:O	2.52	0.48
1:A:38:MET:N	4:A:2018:HOH:O	2.46	0.48
1:B:277:ALA:HB2	4:B:2072:HOH:O	2.07	0.48
1:B:54:VAL:HG13	4:B:2030:HOH:O	2.13	0.48
1:A:106:MET:HE1	3:A:1371:PVZ:H05	1.96	0.48
1:B:315:ARG:CG	4:B:2086:HOH:O	2.61	0.48
1:B:137:LYS:CE	4:B:2037:HOH:O	2.42	0.48
1:A:39:MET:O	1:A:43:CYS:HB2	2.14	0.48
1:A:47:LYS:CE	4:A:2023:HOH:O	2.51	0.48
1:B:367:LYS:CD	4:B:2067:HOH:O	2.58	0.48
1:A:190:SER:C	4:A:2047:HOH:O	2.55	0.47
1:B:264:PRO:O	1:B:268:GLY:N	2.46	0.47
1:B:232:LEU:N	1:B:233:PRO:HD2	2.29	0.47
1:A:258:MET:HG2	1:A:262:THR:CG2	2.42	0.47
1:A:25:PHE:O	1:B:174:TYR:OH	2.28	0.47
1:A:264:PRO:HB3	1:A:269:LYS:O	2.15	0.47
1:B:130:ILE:HD12	4:B:2035:HOH:O	2.13	0.47
1:A:251:PHE:CE1	4:A:2083:HOH:O	2.59	0.47
1:A:253:VAL:HG13	1:A:281:TRP:CG	2.50	0.47
1:A:186:ASP:CB	4:A:2046:HOH:O	2.58	0.47
1:A:210:LYS:NZ	4:A:2053:HOH:O	2.34	0.47
1:A:106:MET:HE1	3:A:1371:PVZ:C05	2.44	0.47
1:A:125:THR:HB	4:A:2036:HOH:O	2.15	0.47
1:B:54:VAL:CG1	4:B:2030:HOH:O	2.63	0.47
1:B:205:TYR:HB2	4:B:2053:HOH:O	2.15	0.47
1:B:364:LYS:HE2	4:B:2091:HOH:O	2.15	0.47
1:A:16:PHE:HE2	1:A:146:HIS:CD2	2.33	0.47
1:A:254:GLN:NE2	1:A:365:ARG:HG2	2.29	0.47
1:B:300:ALA:C	1:B:301:ASN:HD22	2.23	0.47
1:A:173:LEU:O	1:A:177:THR:HG23	2.14	0.47
1:B:364:LYS:HG2	4:B:2091:HOH:O	2.15	0.47
1:A:99:TYR:HB3	3:A:1371:PVZ:H08A	1.96	0.46
1:B:75:GLY:CA	4:B:2023:HOH:O	2.57	0.46
1:B:61:LEU:HD13	1:B:226:LEU:HD23	1.98	0.46
1:B:213:THR:HB	4:B:2055:HOH:O	2.15	0.46
1:B:301:ASN:HD22	1:B:301:ASN:N	2.13	0.46
3:A:1371:PVZ:H06A	3:A:1371:PVZ:C02	2.37	0.46
1:B:36:ARG:NH2	4:B:2010:HOH:O	2.48	0.46
1:B:139:TRP:CH2	4:B:2036:HOH:O	2.69	0.46
1:B:316:LEU:HB3	4:B:2084:HOH:O	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	4:A:2001:HOH:O	2.15	0.46
1:A:145:MET:CE	4:B:2044:HOH:O	2.63	0.46
3:B:1371:PVZ:P22	4:B:2069:HOH:O	2.73	0.46
1:B:254:GLN:HG2	1:B:326:TYR:OH	2.16	0.45
1:B:303:GLY:CA	4:B:2072:HOH:O	2.64	0.45
1:A:182:SER:O	1:B:30:ASN:CB	2.65	0.45
1:A:264:PRO:HB3	1:A:270:VAL:HG22	1.99	0.45
1:B:130:ILE:CD1	4:B:2035:HOH:O	2.64	0.45
1:B:316:LEU:HA	4:B:2084:HOH:O	2.16	0.45
1:A:254:GLN:CD	1:A:365:ARG:CG	2.89	0.45
1:B:263:PRO:CA	4:B:2066:HOH:O	2.62	0.45
1:A:163:ARG:NH1	1:B:142:MET:HE1	2.32	0.44
1:A:182:SER:O	1:B:30:ASN:HB3	2.17	0.44
1:A:220:LEU:HB3	1:A:221:PRO:HD3	1.98	0.44
1:A:131:ASN:HA	1:A:134:LEU:HD12	1.98	0.44
1:A:362:THR:CA	4:A:2081:HOH:O	2.16	0.44
1:B:272:THR:HB	4:B:2070:HOH:O	2.17	0.44
1:A:47:LYS:HB2	1:A:367:LYS:NZ	2.33	0.44
1:A:306:ASP:OD1	1:A:306:ASP:C	2.61	0.44
1:B:82:LEU:HD13	4:B:2016:HOH:O	2.16	0.44
1:B:190:SER:CB	4:B:2049:HOH:O	2.18	0.44
3:B:1371:PVZ:H14	3:B:1371:PVZ:H08	1.84	0.44
1:B:164:VAL:HG22	4:B:2057:HOH:O	2.18	0.44
1:B:275:GLN:HB2	4:B:2070:HOH:O	2.17	0.44
1:B:348:SER:CB	4:B:2095:HOH:O	2.66	0.44
1:B:161:PHE:CE1	4:B:2031:HOH:O	2.60	0.43
1:A:179:MET:SD	1:A:277:ALA:HB1	2.58	0.43
1:A:251:PHE:CE2	1:A:365:ARG:CZ	3.01	0.43
1:B:209:VAL:O	1:B:210:LYS:C	2.61	0.43
1:A:209:VAL:O	1:A:210:LYS:C	2.62	0.43
1:A:264:PRO:O	1:A:268:GLY:N	2.51	0.43
1:A:286:PHE:CE1	1:A:316:LEU:CD2	3.00	0.43
1:B:298:PHE:CA	4:B:2080:HOH:O	2.60	0.43
1:B:16:PHE:CD1	1:B:146:HIS:CE1	3.07	0.43
1:A:153:PHE:CD1	1:A:153:PHE:C	2.96	0.43
1:A:260:CYS:C	1:A:261:PHE:HD1	2.27	0.43
1:A:317:TYR:CB	1:A:322:LEU:HD12	2.49	0.43
1:B:77:ARG:CG	4:B:2024:HOH:O	2.66	0.43
1:A:215:TYR:CD1	4:A:2056:HOH:O	2.56	0.43
1:B:30:ASN:HA	4:B:2008:HOH:O	2.18	0.42
1:A:179:MET:HE3	1:A:194:THR:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD22	1:A:161:PHE:CZ	2.54	0.42
1:A:181:ASP:CB	4:A:2043:HOH:O	2.66	0.42
1:A:123:ASP:CB	1:B:189:VAL:O	2.68	0.42
1:A:291:SER:O	1:A:295:VAL:HG23	2.19	0.42
1:A:164:VAL:HG22	4:A:2056:HOH:O	2.19	0.42
1:B:16:PHE:CZ	1:B:146:HIS:HB2	2.55	0.42
1:B:275:GLN:N	4:B:2073:HOH:O	2.53	0.42
1:A:316:LEU:HD23	1:A:316:LEU:C	2.43	0.42
1:A:278:LYS:CE	4:A:2042:HOH:O	2.59	0.42
1:B:94:PHE:HB2	4:B:2039:HOH:O	2.19	0.42
1:B:349:PRO:HD2	4:B:2096:HOH:O	2.20	0.42
1:A:125:THR:HG22	4:A:2036:HOH:O	2.19	0.41
1:B:295:VAL:C	4:B:2081:HOH:O	2.63	0.41
1:A:264:PRO:CD	4:A:2061:HOH:O	2.51	0.41
1:B:228:VAL:HB	4:B:2029:HOH:O	2.20	0.41
1:B:348:SER:HB2	4:B:2095:HOH:O	2.20	0.41
1:B:164:VAL:HG11	1:B:220:LEU:HD22	2.02	0.41
1:B:201:THR:C	4:B:2053:HOH:O	2.63	0.41
1:A:100:LEU:HD22	1:A:112:ARG:NH2	2.36	0.41
1:A:142:MET:HE1	1:B:163:ARG:NH1	2.36	0.41
1:B:252:GLN:HB2	4:B:2055:HOH:O	2.20	0.41
1:A:47:LYS:CD	4:A:2023:HOH:O	2.68	0.41
1:B:126:VAL:C	4:B:2035:HOH:O	2.63	0.41
1:A:28:ASP:O	1:A:32:VAL:HG23	2.20	0.41
1:A:112:ARG:NH1	3:A:1371:PVZ:O25	2.37	0.41
1:A:121:HIS:CE1	4:A:2035:HOH:O	2.42	0.41
1:B:77:ARG:CB	4:B:2024:HOH:O	2.67	0.41
1:B:306:ASP:OD1	1:B:308:GLU:HG2	2.21	0.41
1:B:28:ASP:OD2	1:B:30:ASN:HB2	2.20	0.41
1:B:215:TYR:CB	4:B:2057:HOH:O	2.68	0.41
1:A:30:ASN:N	4:A:2015:HOH:O	2.53	0.40
1:A:314:ARG:O	1:A:315:ARG:C	2.64	0.40
1:A:184:LYS:HG3	4:A:2043:HOH:O	2.21	0.40
1:B:9:VAL:HA	1:B:12:GLU:HB2	2.04	0.40
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.56	0.40
1:A:250:TYR:O	1:A:250:TYR:CD2	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/367 (96%)	343 (97%)	10 (3%)	0	100	100
1	B	353/367 (96%)	341 (97%)	12 (3%)	0	100	100
All	All	706/734 (96%)	684 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	310/321 (97%)	297 (96%)	13 (4%)	26	45
1	B	310/321 (97%)	304 (98%)	6 (2%)	50	71
All	All	620/642 (97%)	601 (97%)	19 (3%)	35	57

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	16	PHE
1	A	109	SER
1	A	111	THR
1	A	138	SER
1	A	176	VAL
1	A	195	THR
1	A	267	LEU

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Mol	Chain	Res	Type
1	A	297	GLU
1	A	301	ASN
1	A	308	GLU
1	A	319	GLU
1	A	366	GLN
1	B	82	LEU
1	B	138	SER
1	B	176	VAL
1	B	219	LEU
1	B	301	ASN
1	B	323	GLN

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	96	GLN
1	A	146	HIS
1	A	162	ASN
1	A	191	GLN
1	A	254	GLN
1	B	146	HIS
1	B	162	ASN
1	B	301	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	PVZ	A	1371	2	24,25,25	1.61	2 (8%)	33,36,36	1.27	5 (15%)
3	PVZ	B	1371	2	24,25,25	1.50	2 (8%)	33,36,36	1.14	2 (6%)

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	PVZ	A	1371	2	-	13/32/32/32	0/1/1/1
3	PVZ	B	1371	2	-	10/32/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1371	PVZ	P22-C16	-5.63	1.81	1.85
3	B	1371	PVZ	P22-C16	-5.53	1.81	1.85
3	A	1371	PVZ	O17-C16	-2.51	1.41	1.44
3	B	1371	PVZ	P18-O19	2.14	1.53	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1371	PVZ	P22-C16-P18	-4.04	105.48	112.72
3	A	1371	PVZ	C15-N13-C12	3.09	129.74	126.70
3	B	1371	PVZ	C15-N13-C12	2.91	129.55	126.70
3	A	1371	PVZ	O24-P22-C16	2.57	116.41	109.82
3	A	1371	PVZ	P22-C16-P18	-2.54	108.17	112.72
3	A	1371	PVZ	O20-P18-C16	-2.44	100.81	106.19
3	A	1371	PVZ	C15-N13-C14	-2.20	121.82	124.69

There are no chirality outliers.

All (23) torsion outliers are listed below:

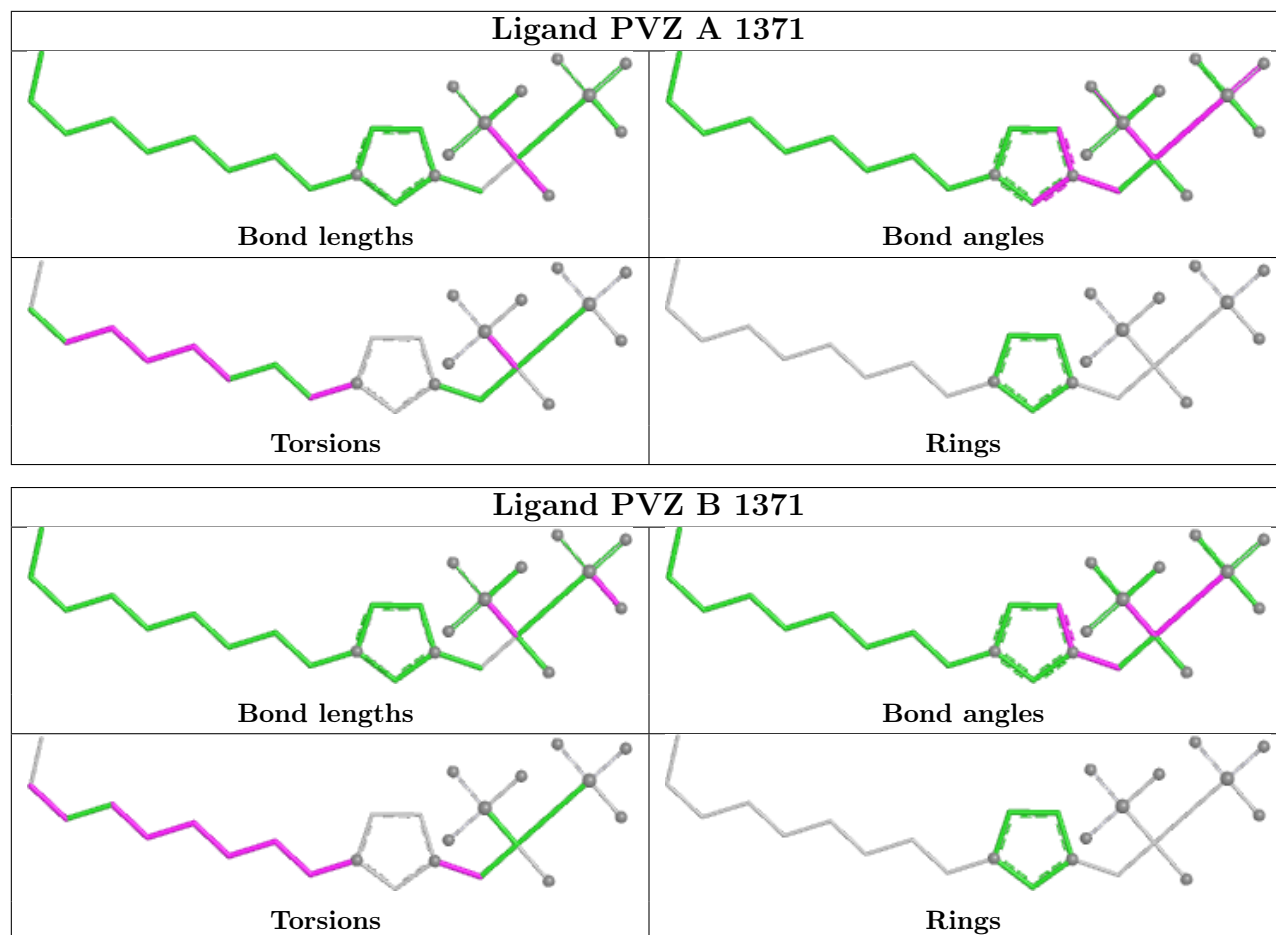
Mol	Chain	Res	Type	Atoms
3	A	1371	PVZ	C15-C16-P22-O23
3	A	1371	PVZ	C15-C16-P22-O24
3	A	1371	PVZ	O17-C16-P22-O23
3	A	1371	PVZ	O17-C16-P22-O24
3	B	1371	PVZ	C16-C15-N13-C12
3	B	1371	PVZ	C16-C15-N13-C14
3	B	1371	PVZ	C03-C04-C05-C06
3	A	1371	PVZ	C05-C06-C07-C08
3	B	1371	PVZ	C04-C05-C06-C07
3	A	1371	PVZ	C04-C05-C06-C07
3	B	1371	PVZ	C06-C07-C08-C09
3	A	1371	PVZ	C03-C04-C05-C06
3	B	1371	PVZ	C05-C06-C07-C08
3	A	1371	PVZ	C02-C03-C04-C05
3	B	1371	PVZ	C01-C02-C03-C04
3	B	1371	PVZ	C08-C09-N10-C14
3	A	1371	PVZ	C08-C09-N10-C14
3	A	1371	PVZ	C15-C16-P22-O25
3	A	1371	PVZ	C08-C09-N10-C11
3	B	1371	PVZ	C08-C09-N10-C11
3	B	1371	PVZ	C07-C08-C09-N10
3	A	1371	PVZ	P18-C16-P22-O23
3	A	1371	PVZ	P18-C16-P22-O24

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1371	PVZ	19	0
3	B	1371	PVZ	11	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	357/367 (97%)	1.54	100 (28%)  	45, 66, 107, 139	0
1	B	357/367 (97%)	1.62	107 (29%)  	40, 68, 105, 125	0
All	All	714/734 (97%)	1.58	207 (28%)  	40, 67, 107, 139	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ILE	8.6
1	B	272	THR	7.5
1	A	180	PHE	6.6
1	B	180	PHE	6.5
1	B	311	ALA	6.2
1	B	274	ILE	5.6
1	B	268	GLY	5.5
1	B	270	VAL	5.4
1	B	262	THR	5.1
1	B	179	MET	5.0
1	A	44	LEU	5.0
1	A	311	ALA	5.0
1	A	198	ALA	5.0
1	A	193	THR	4.9
1	B	310	VAL	4.8
1	B	303	GLY	4.7
1	A	62	LEU	4.7
1	A	270	VAL	4.6
1	A	304	SER	4.6
1	A	269	LYS	4.5
1	B	334	ALA	4.5
1	A	310	VAL	4.5
1	A	266	ARG	4.5
1	B	44	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	266	ARG	4.4
1	A	195	THR	4.3
1	A	262	THR	4.3
1	A	268	GLY	4.3
1	B	193	THR	4.2
1	A	273	ASP	4.2
1	A	292	SER	4.1
1	B	318	GLU	4.1
1	A	293	ALA	4.1
1	B	292	SER	4.1
1	B	62	LEU	4.0
1	B	23	LEU	4.0
1	A	295	VAL	4.0
1	A	272	THR	3.9
1	B	63	SER	3.9
1	B	312	THR	3.9
1	A	101	VAL	3.9
1	B	346	LEU	3.9
1	B	2	PRO	3.9
1	B	202	LEU	3.8
1	A	313	VAL	3.8
1	B	1	MET	3.8
1	B	338	LYS	3.8
1	B	101	VAL	3.7
1	B	45	GLY	3.6
1	A	32	VAL	3.5
1	A	179	MET	3.5
1	B	267	LEU	3.5
1	B	217	THR	3.4
1	B	300	ALA	3.4
1	B	149	ALA	3.4
1	A	13	ILE	3.4
1	B	194	THR	3.4
1	B	276	ASP	3.4
1	A	271	GLY	3.3
1	A	8	GLN	3.3
1	A	192	PRO	3.2
1	B	264	PRO	3.2
1	A	312	THR	3.2
1	A	334	ALA	3.2
1	B	198	ALA	3.2
1	A	159	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	319	GLU	3.2
1	A	366	GLN	3.2
1	A	2	PRO	3.1
1	A	96	GLN	3.1
1	B	304	SER	3.0
1	A	300	ALA	3.0
1	B	313	VAL	3.0
1	B	117	CYS	3.0
1	A	81	VAL	2.9
1	B	32	VAL	2.9
1	B	235	VAL	2.9
1	A	217	THR	2.9
1	A	176	VAL	2.9
1	A	63	SER	2.9
1	B	307	SER	2.9
1	A	17	LEU	2.9
1	A	124	VAL	2.9
1	A	284	VAL	2.9
1	B	159	CYS	2.9
1	A	167	THR	2.9
1	A	296	ALA	2.8
1	B	360	GLY	2.8
1	B	323	GLN	2.8
1	A	4	GLN	2.8
1	A	99	TYR	2.8
1	A	37	LYS	2.8
1	A	289	LYS	2.8
1	A	223	VAL	2.8
1	A	77	ARG	2.8
1	B	192	PRO	2.8
1	A	149	ALA	2.8
1	B	293	ALA	2.8
1	B	9	VAL	2.8
1	B	254	GLN	2.7
1	A	235	VAL	2.7
1	A	333	VAL	2.7
1	B	269	LYS	2.7
1	A	178	SER	2.7
1	A	316	LEU	2.7
1	B	49	ASN	2.7
1	A	197	PHE	2.6
1	B	197	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	167	THR	2.6
1	B	315	ARG	2.6
1	B	46	GLY	2.6
1	B	278	LYS	2.6
1	A	264	PRO	2.6
1	B	189	VAL	2.6
1	A	254	GLN	2.6
1	A	323	GLN	2.6
1	B	222	LEU	2.6
1	B	223	VAL	2.6
1	B	322	LEU	2.5
1	B	128	CYS	2.5
1	A	194	THR	2.5
1	B	105	ILE	2.5
1	B	302	TYR	2.5
1	A	258	MET	2.5
1	B	28	ASP	2.5
1	B	290	ALA	2.5
1	B	296	ALA	2.5
1	B	301	ASN	2.5
1	A	61	LEU	2.5
1	A	185	LEU	2.5
1	B	219	LEU	2.5
1	A	290	ALA	2.5
1	A	305	GLY	2.5
1	B	279	CYS	2.5
1	A	41	THR	2.5
1	B	6	PHE	2.5
1	A	199	GLU	2.4
1	B	366	GLN	2.4
1	A	29	PRO	2.4
1	A	309	LYS	2.4
1	B	162	ASN	2.4
1	B	332	ALA	2.4
1	B	195	THR	2.4
1	A	6	PHE	2.4
1	B	5	MET	2.4
1	A	158	LEU	2.4
1	A	120	ARG	2.4
1	A	365	ARG	2.4
1	B	176	VAL	2.4
1	A	363	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	367	LYS	2.3
1	A	353	ALA	2.3
1	B	352	ALA	2.3
1	A	307	SER	2.3
1	A	314	ARG	2.3
1	A	261	PHE	2.3
1	B	199	GLU	2.3
1	B	316	LEU	2.3
1	B	358	LEU	2.3
1	A	259	ASP	2.3
1	B	317	TYR	2.3
1	A	130	ILE	2.3
1	B	35	LEU	2.3
1	B	157	LEU	2.3
1	A	319	GLU	2.3
1	B	87	VAL	2.3
1	A	28	ASP	2.2
1	B	26	ASP	2.2
1	B	221	PRO	2.2
1	A	350	GLY	2.2
1	A	328	ALA	2.2
1	B	173	LEU	2.2
1	B	185	LEU	2.2
1	B	260	CYS	2.2
1	B	271	GLY	2.2
1	B	121	HIS	2.2
1	B	216	TYR	2.2
1	A	322	LEU	2.2
1	B	59	GLU	2.2
1	B	314	ARG	2.1
1	A	202	LEU	2.1
1	B	61	LEU	2.1
1	A	1	MET	2.1
1	A	189	VAL	2.1
1	A	214	ALA	2.1
1	A	3	MET	2.1
1	B	15	MET	2.1
1	B	145	MET	2.1
1	B	258	MET	2.1
1	A	40	ASP	2.1
1	B	256	ASP	2.1
1	B	90	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	35	LEU	2.1
1	A	226	LEU	2.1
1	A	265	GLU	2.1
1	B	246	LEU	2.1
1	B	196	ASP	2.1
1	B	4	GLN	2.1
1	B	320	ALA	2.1
1	A	257	VAL	2.1
1	A	105	ILE	2.0
1	A	122	PRO	2.0
1	B	80	ARG	2.0
1	B	125	THR	2.0
1	B	275	GLN	2.0
1	A	219	LEU	2.0
1	A	346	LEU	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](#)

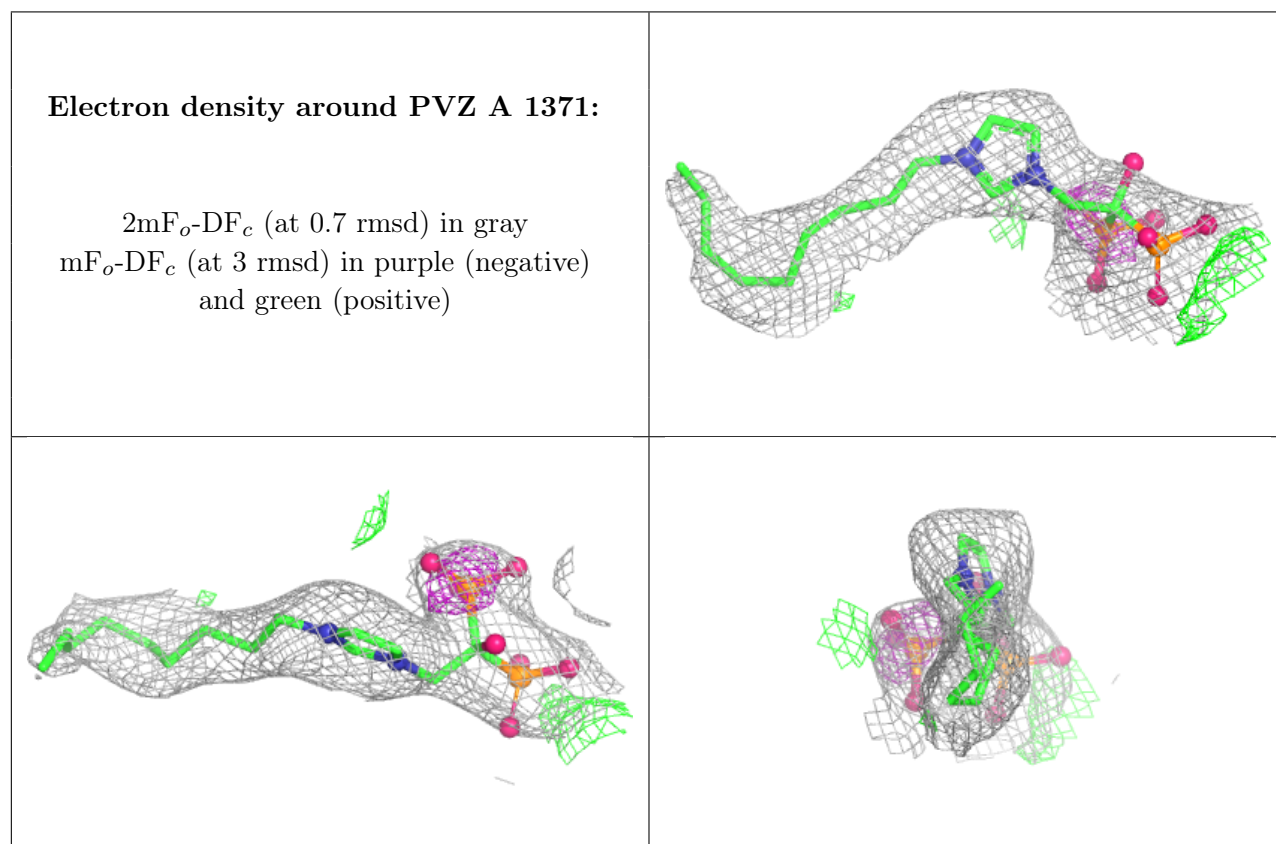
There are no oligosaccharides in this entry.

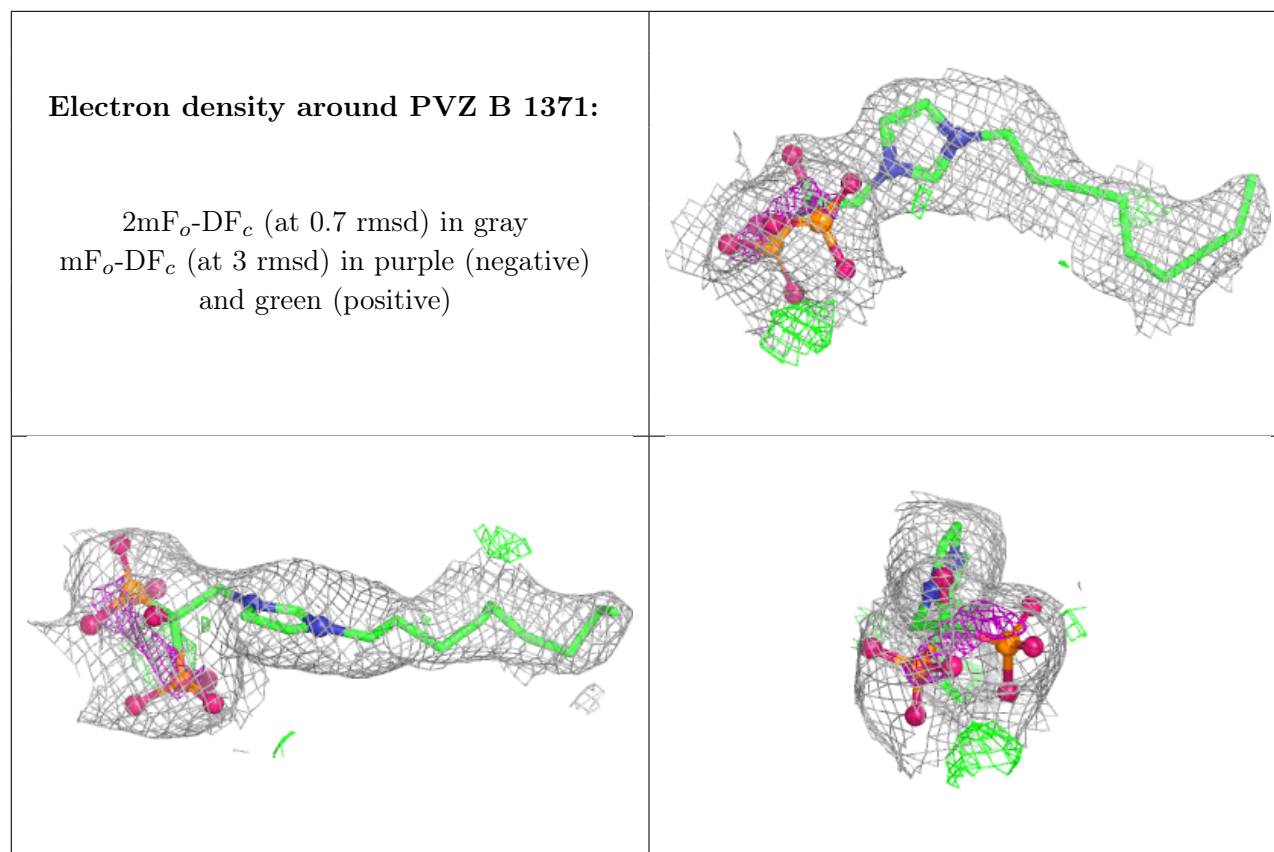
6.4 Ligands [i](#)

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	MG	B	1369	1/1	0.70	0.29	64,64,64,64	0
2	MG	A	1369	1/1	0.73	0.17	57,57,57,57	0
3	PVZ	A	1371	25/25	0.84	0.16	53,60,70,75	0
2	MG	A	1368	1/1	0.85	0.17	55,55,55,55	0
3	PVZ	B	1371	25/25	0.86	0.15	51,66,73,77	0
2	MG	B	1368	1/1	0.87	0.11	75,75,75,75	0
2	MG	A	1370	1/1	0.89	0.11	54,54,54,54	0
2	MG	B	1370	1/1	0.96	0.07	44,44,44,44	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.