



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 03:25 AM EDT

PDB ID : 6WW1  
Title : Crystal structure of the LmFPPS mutant E97Y  
Authors : Maheshwari, S.; Kim, Y.S.; Gabelli, S.B.  
Deposited on : 2020-05-07  
Resolution : 2.05 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](mailto: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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

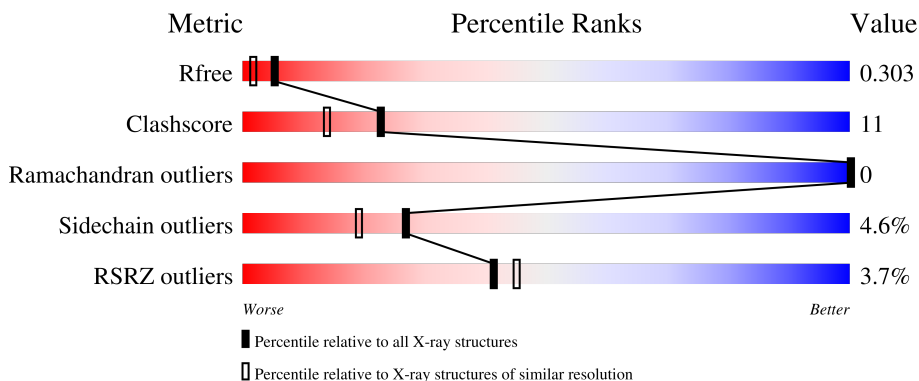
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	362	 4% 81% 17%
1	B	362	 3% 82% 16%

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
5	ACT	A	406	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6431 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
			Total	C	N	O	S			
1	A	362	2877	1843	476	534	24	0	0	0
1	B	362	2877	1843	476	534	24	0	0	0

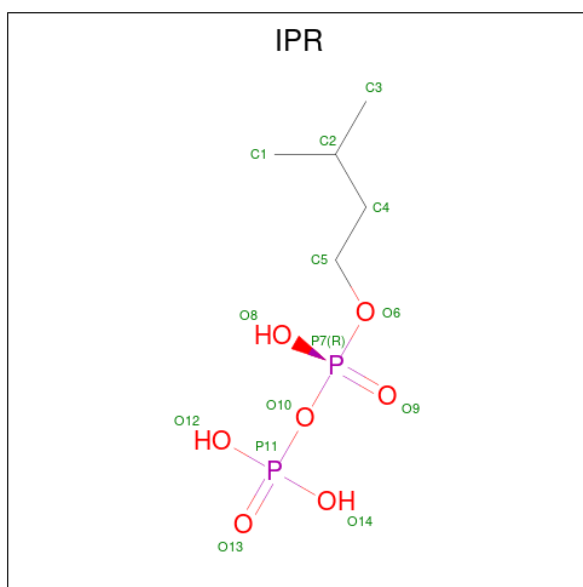
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	TYR	GLU	engineered mutation	UNP Q4QBL1
B	97	TYR	GLU	engineered mutation	UNP Q4QBL1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

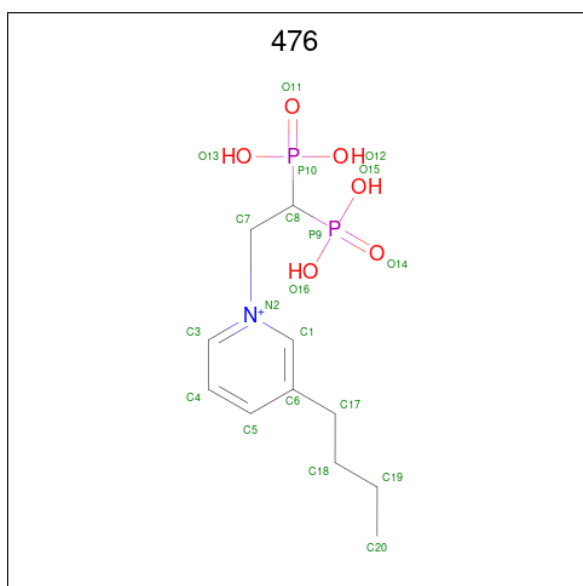
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		

- Molecule 3 is ISOPENTYL PYROPHOSPHATE (three-letter code: IPR) (formula: C<sub>5</sub>H<sub>14</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	14	5	7	2	0	0
3	B	1	14	5	7	2	0	0

- Molecule 4 is 3-butyl-1-(2,2-diphosphonoethyl)pyridinium (three-letter code: 476) (formula:  $C_{11}H_{20}NO_6P_2$ ) (labeled as "Ligand of Interest" by depositor).



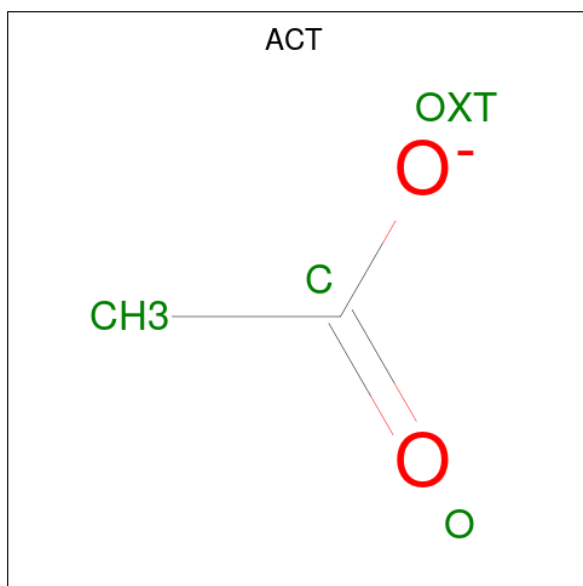
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	20	11	1	6	2	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	20	11	1	6	2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0

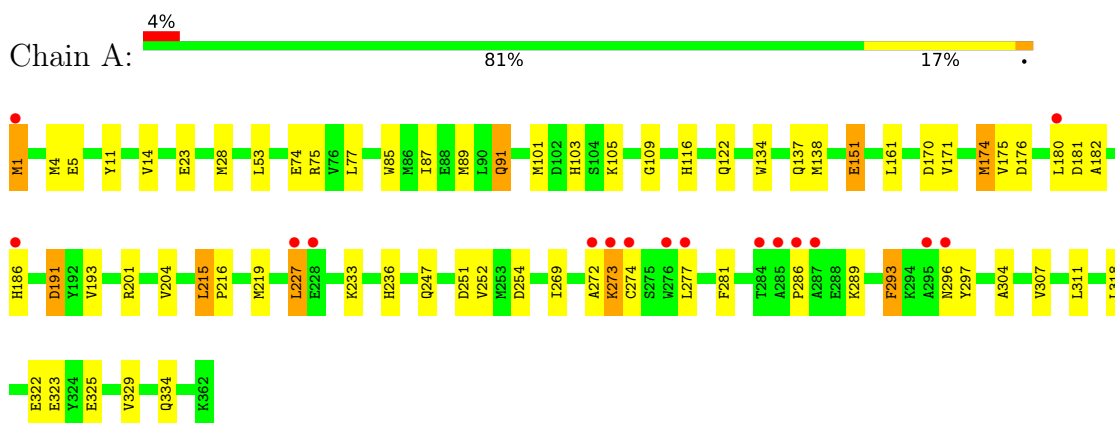
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	323	323	323	0	0
6	B	272	272	272	0	0

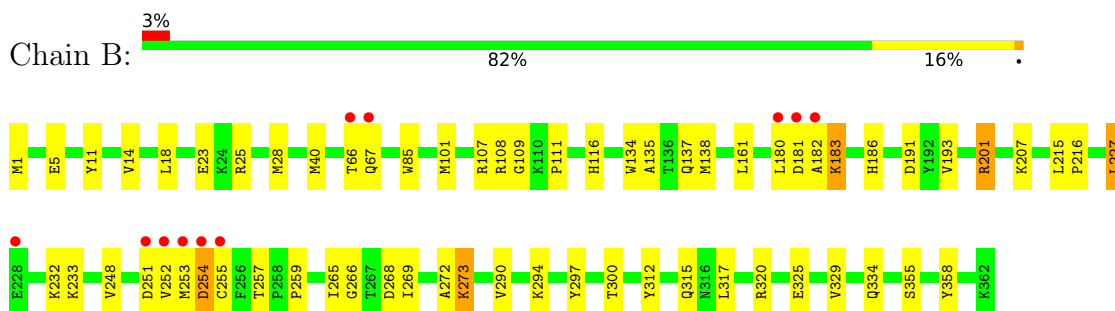
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Farnesyl pyrophosphate synthase



- Molecule 1: Farnesyl pyrophosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.70Å 86.08Å 107.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 33.59 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.1 (50.00-2.05) 88.8 (33.59-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.77 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.213 , 0.295 0.230 , 0.303	Depositor DCC
$R_{free}$ test set	2169 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7335e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, ACT, 476, IPR

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	0.88	1/2940 (0.0%)	0.88	1/3983 (0.0%)
1	B	0.86	0/2940	0.84	1/3983 (0.0%)
All	All	0.87	1/5880 (0.0%)	0.86	2/7966 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	LEU	C-N	7.86	1.49	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	LEU	C-N-CA	5.29	134.92	121.70
1	A	251	ASP	CB-CG-OD2	5.12	122.91	118.30

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	2877	0	2852	86	0
1	B	2877	0	2852	47	0
2	A	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
3	A	14	0	11	2	0
3	B	14	0	11	2	0
4	A	20	0	16	2	0
4	B	20	0	16	4	0
5	A	4	0	3	5	0
5	B	4	0	3	1	0
6	A	323	0	0	19	1
6	B	272	0	0	4	0
All	All	6431	0	5764	133	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 11.

All (133) 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:254:ASP:HB2	6:B:696:HOH:O	1.41	1.18
1:A:272:ALA:HA	1:A:297:TYR:CE2	1.80	1.17
1:A:77:LEU:HB2	6:A:552:HOH:O	1.56	1.02
1:A:236:HIS:HD2	6:A:721:HOH:O	1.50	0.92
1:A:116:HIS:HB3	1:B:182:ALA:O	1.70	0.91
1:A:272:ALA:CA	1:A:297:TYR:CE2	2.56	0.88
1:B:201:ARG:HH21	1:B:201:ARG:HG3	1.45	0.80
1:A:14:VAL:HG11	1:A:138:MET:SD	2.21	0.80
1:A:101:MET:HE1	1:A:171:VAL:HG11	1.63	0.80
1:A:89:MET:CE	1:A:134:TRP:HB2	2.13	0.78
1:A:105:LYS:HG3	6:A:811:HOH:O	1.84	0.76
1:A:181:ASP:O	1:A:186:HIS:HE1	1.69	0.76
1:B:251:ASP:OD1	6:B:501:HOH:O	2.04	0.75
1:A:296:ASN:ND2	1:A:307:VAL:HG11	2.02	0.75
1:A:233:LYS:HD2	6:A:728:HOH:O	1.86	0.74
1:A:269:ILE:H	5:A:406:ACT:H1	1.53	0.74
1:A:151:GLU:CG	6:A:650:HOH:O	2.36	0.74
3:B:404:IPR:HC2	4:B:405:476:H11	1.68	0.74
3:B:404:IPR:HC2	4:B:405:476:C3	2.18	0.73
1:B:248:VAL:O	1:B:252:VAL:HG23	1.87	0.73
1:A:325:GLU:O	1:A:329:VAL:HG23	1.88	0.72
1:A:101:MET:CE	1:A:171:VAL:HG11	2.20	0.72
1:A:286:PRO:HD2	1:A:289:LYS:HB2	1.72	0.71
1:A:89:MET:HE1	1:A:134:TRP:HB2	1.72	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:404:IPR:HC2	4:A:405:476:H11	1.73	0.69
1:A:89:MET:HE1	1:A:134:TRP:HE3	1.60	0.67
1:A:191:ASP:OD1	1:A:193:VAL:HG23	1.95	0.67
1:A:186:HIS:HD2	6:A:708:HOH:O	1.77	0.66
1:A:89:MET:CE	1:A:134:TRP:CB	2.75	0.65
1:A:181:ASP:O	1:A:186:HIS:CE1	2.49	0.64
1:A:170:ASP:OD1	1:A:273:LYS:NZ	2.30	0.64
1:B:201:ARG:HH21	1:B:201:ARG:CG	2.11	0.64
1:A:75:ARG:HD3	6:A:513:HOH:O	2.00	0.62
1:A:272:ALA:HA	1:A:297:TYR:CZ	2.32	0.62
1:A:252:VAL:HA	1:A:277:LEU:HD11	1.82	0.62
1:A:151:GLU:HG2	6:A:650:HOH:O	1.95	0.62
1:A:89:MET:HE2	1:A:134:TRP:HB2	1.81	0.61
1:A:89:MET:HE1	1:A:134:TRP:CB	2.30	0.61
1:A:227:LEU:HD22	1:A:227:LEU:O	2.00	0.61
1:B:269:ILE:H	5:B:406:ACT:H1	1.65	0.61
1:A:91:GLN:HE21	1:A:91:GLN:HA	1.67	0.60
1:A:293:PHE:HB2	1:A:311:LEU:HD13	1.85	0.59
1:A:186:HIS:CD2	6:A:708:HOH:O	2.53	0.59
1:A:174:MET:HE2	1:A:273:LYS:HE3	1.85	0.58
1:A:1:MET:HG2	1:A:1:MET:O	2.03	0.58
1:A:89:MET:HE1	1:A:134:TRP:CE3	2.39	0.57
1:B:227:LEU:HD22	1:B:227:LEU:O	2.04	0.57
1:A:272:ALA:CB	1:A:297:TYR:CD2	2.87	0.57
1:B:253:MET:O	1:B:257:THR:HB	2.04	0.57
1:A:1:MET:HB2	6:A:789:HOH:O	2.04	0.56
1:A:272:ALA:HB1	1:A:297:TYR:CD2	2.40	0.56
1:B:25:ARG:HH12	1:B:137:GLN:NE2	2.03	0.56
1:B:329:VAL:CG2	1:B:358:TYR:CE1	2.88	0.56
1:B:268:ASP:HA	1:B:273:LYS:HG3	1.87	0.56
1:B:207:LYS:O	4:B:405:476:H9	2.06	0.56
1:B:135:ALA:HA	1:B:138:MET:HE3	1.88	0.56
1:A:174:MET:CE	1:A:273:LYS:HE3	2.36	0.55
1:A:272:ALA:CB	1:A:297:TYR:CE2	2.89	0.55
1:A:204:VAL:HB	1:A:247:GLN:HG2	1.89	0.55
1:A:89:MET:HE2	1:A:134:TRP:CB	2.37	0.54
1:A:318:LEU:O	1:A:322:GLU:HG2	2.08	0.54
1:A:14:VAL:CG1	1:A:138:MET:SD	2.93	0.53
1:A:269:ILE:HG13	5:A:406:ACT:H2	1.90	0.53
1:A:161:LEU:HD22	1:B:137:GLN:HG3	1.90	0.53
1:B:25:ARG:HH12	1:B:137:GLN:HE22	1.54	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLU:HA	1:B:28:MET:HB3	1.90	0.53
1:B:254:ASP:HB3	6:B:683:HOH:O	2.09	0.52
1:A:174:MET:CE	1:A:273:LYS:CE	2.89	0.51
1:A:151:GLU:HG3	6:A:650:HOH:O	2.04	0.51
1:B:252:VAL:O	1:B:252:VAL:HG12	2.10	0.51
1:B:325:GLU:O	1:B:329:VAL:HG23	2.11	0.50
1:B:329:VAL:HG21	1:B:358:TYR:CE1	2.46	0.50
1:A:5:GLU:HB2	6:A:698:HOH:O	2.11	0.50
1:B:272:ALA:HA	1:B:297:TYR:CE2	2.47	0.50
1:A:254:ASP:OD1	5:A:406:ACT:CH3	2.60	0.50
1:A:236:HIS:CD2	6:A:721:HOH:O	2.38	0.49
1:A:11:TYR:HB2	1:A:85:TRP:CZ2	2.47	0.49
1:B:273:LYS:HA	1:B:273:LYS:HE3	1.92	0.49
1:A:293:PHE:CD2	1:A:293:PHE:C	2.86	0.49
1:B:255:CYS:HG	1:B:312:TYR:HD2	1.59	0.49
1:A:252:VAL:HG22	1:A:277:LEU:HD21	1.94	0.49
1:B:201:ARG:CG	1:B:201:ARG:NH2	2.71	0.49
1:B:66:THR:HG22	1:B:67:GLN:N	2.28	0.48
1:B:268:ASP:HA	1:B:273:LYS:CG	2.43	0.48
1:A:204:VAL:HB	1:A:247:GLN:CG	2.42	0.48
1:A:1:MET:O	1:A:1:MET:CG	2.62	0.48
1:B:109:GLY:HA2	6:B:736:HOH:O	2.13	0.47
1:A:286:PRO:HD2	1:A:289:LYS:CB	2.44	0.47
3:A:404:IPR:HC2	4:A:405:476:C3	2.44	0.47
1:A:296:ASN:OD1	1:A:304:ALA:HA	2.15	0.47
1:A:1:MET:HG2	1:A:4:MET:HB2	1.97	0.46
1:B:191:ASP:OD1	1:B:193:VAL:HG23	2.15	0.46
1:B:18:LEU:HD22	1:B:134:TRP:CD1	2.51	0.46
1:A:182:ALA:O	1:B:116:HIS:HB3	2.15	0.46
1:A:176:ASP:OD1	6:A:501:HOH:O	2.21	0.46
1:A:269:ILE:H	5:A:406:ACT:CH3	2.24	0.46
1:A:175:VAL:HG11	1:A:186:HIS:HB3	1.96	0.46
1:A:272:ALA:CA	1:A:297:TYR:HE2	2.19	0.45
1:A:174:MET:HE2	1:A:273:LYS:CE	2.47	0.45
1:A:254:ASP:OD1	5:A:406:ACT:H2	2.17	0.45
1:B:290:VAL:HG12	1:B:294:LYS:HE3	2.00	0.44
1:B:254:ASP:OD2	1:B:266:GLY:HA3	2.18	0.43
1:B:111:PRO:O	1:B:116:HIS:HE1	2.02	0.43
1:B:259:PRO:HB3	1:B:265:ILE:HG12	2.00	0.43
1:A:272:ALA:HB1	1:A:297:TYR:CE2	2.54	0.43
1:A:281:PHE:CE1	1:A:311:LEU:HB3	2.54	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.61	0.43
4:B:405:476:H11	4:B:405:476:H3	1.88	0.43
1:A:75:ARG:CD	6:A:513:HOH:O	2.64	0.43
1:B:107:ARG:HG3	1:B:108:ARG:HG3	2.01	0.42
1:A:74:GLU:HA	6:A:552:HOH:O	2.19	0.42
1:A:23:GLU:HA	1:A:28:MET:HB3	2.02	0.42
1:A:103:HIS:HB3	6:A:735:HOH:O	2.18	0.42
1:A:122:GLN:NE2	1:B:101:MET:O	2.40	0.42
1:A:137:GLN:HG3	1:B:161:LEU:HD22	2.02	0.42
1:B:233:LYS:HB3	1:B:233:LYS:NZ	2.34	0.42
1:B:11:TYR:OH	1:B:40:MET:HG2	2.20	0.42
1:A:87:ILE:HD11	1:A:219:MET:SD	2.60	0.41
1:B:181:ASP:C	1:B:183:LYS:H	2.23	0.41
1:B:273:LYS:HA	1:B:273:LYS:CE	2.50	0.41
1:A:89:MET:CE	1:A:134:TRP:HB3	2.50	0.41
1:B:135:ALA:HA	1:B:138:MET:CE	2.50	0.41
1:B:320:ARG:HG2	1:B:320:ARG:HH11	1.84	0.41
1:A:91:GLN:HE21	1:A:91:GLN:CA	2.32	0.41
1:A:175:VAL:CG1	1:A:186:HIS:HB3	2.51	0.41
1:B:11:TYR:HB2	1:B:85:TRP:CZ2	2.56	0.41
1:B:201:ARG:HG3	1:B:201:ARG:NH2	2.22	0.41
1:A:269:ILE:HA	1:A:297:TYR:CE1	2.56	0.40
1:A:233:LYS:CD	6:A:728:HOH:O	2.58	0.40
1:A:215:LEU:HB3	1:A:216:PRO:HD3	2.03	0.40
1:B:215:LEU:HB3	1:B:216:PRO:HD3	2.03	0.40
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.95	0.40
1:A:109:GLY:HA2	6:A:770:HOH:O	2.21	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)
6:A:653:HOH:O	6:A:683:HOH:O[2_665]	0.40	1.80

## 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	360/362 (99%)	346 (96%)	14 (4%)	0	100	100
1	B	360/362 (99%)	355 (99%)	5 (1%)	0	100	100
All	All	720/724 (99%)	701 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	303/303 (100%)	290 (96%)	13 (4%)	29	22
1	B	303/303 (100%)	288 (95%)	15 (5%)	24	16
All	All	606/606 (100%)	578 (95%)	28 (5%)	27	19

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	91	GLN
1	A	151	GLU
1	A	174	MET
1	A	180	LEU
1	A	191	ASP
1	A	201	ARG
1	A	227	LEU
1	A	273	LYS
1	A	274	CYS
1	A	293	PHE
1	A	323	GLU
1	A	334	GLN
1	B	1	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	5	GLU
1	B	14	VAL
1	B	183	LYS
1	B	186	HIS
1	B	201	ARG
1	B	227	LEU
1	B	232	LYS
1	B	254	ASP
1	B	273	LYS
1	B	300	THR
1	B	315	GLN
1	B	317	LEU
1	B	334	GLN
1	B	355	SER

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

Mol	Chain	Res	Type
1	A	91	GLN
1	A	103	HIS
1	A	186	HIS
1	A	236	HIS
1	A	315	GLN
1	A	334	GLN
1	B	31	HIS
1	B	137	GLN
1	B	200	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
5	ACT	B	406	-	3,3,3	0.85	0	3,3,3	0.17	0
4	476	B	405	2	19,20,20	1.19	1 (5%)	25,29,29	2.52	10 (40%)
5	ACT	A	406	-	3,3,3	0.76	0	3,3,3	0.76	0
3	IPR	B	404	-	11,13,13	0.54	0	16,19,19	0.97	1 (6%)
4	476	A	405	2	19,20,20	1.58	5 (26%)	25,29,29	2.30	9 (36%)
3	IPR	A	404	-	11,13,13	0.51	0	16,19,19	1.44	4 (25%)

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
4	476	B	405	2	-	3/18/20/20	0/1/1/1
4	476	A	405	2	-	5/18/20/20	0/1/1/1
3	IPR	A	404	-	-	3/13/13/13	-
3	IPR	B	404	-	-	1/13/13/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	476	P9-O15	-3.08	1.50	1.54
4	A	405	476	P10-O13	-3.08	1.50	1.54
4	A	405	476	P10-O12	-2.38	1.51	1.54
4	A	405	476	P9-O14	2.19	1.53	1.49
4	A	405	476	C3-C4	2.09	1.43	1.38
4	B	405	476	P9-O15	-2.05	1.51	1.54

All (24) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	476	C6-C1-N2	-5.31	117.70	121.03
4	A	405	476	C6-C1-N2	4.79	124.03	121.03
4	A	405	476	C7-N2-C1	-4.37	113.42	120.17
4	A	405	476	O16-P9-O15	4.29	119.16	107.64
4	B	405	476	O11-P10-C8	-4.26	100.21	112.29
4	A	405	476	O12-P10-O13	4.11	118.69	107.64
4	A	405	476	C7-N2-C3	4.09	126.83	120.25
4	B	405	476	O16-P9-O15	4.08	118.60	107.64
4	B	405	476	C19-C18-C17	-3.74	96.37	113.98
4	B	405	476	C1-C6-C5	3.60	122.46	117.57
4	B	405	476	C17-C6-C5	-3.58	112.18	121.23
4	B	405	476	O12-P10-O13	3.35	116.65	107.64
4	B	405	476	O16-P9-O14	-3.26	105.27	113.45
4	A	405	476	O14-P9-C8	-2.97	103.85	112.29
3	B	404	IPR	O12-P11-O14	2.95	118.92	107.64
3	A	404	IPR	O6-C5-C4	-2.91	99.11	109.09
4	A	405	476	O11-P10-C8	-2.87	104.15	112.29
4	B	405	476	O14-P9-C8	-2.70	104.63	112.29
3	A	404	IPR	O10-P11-O13	-2.65	96.49	111.19
4	A	405	476	O16-P9-O14	-2.59	106.93	113.45
3	A	404	IPR	O12-P11-O10	2.51	113.04	104.64
3	A	404	IPR	O12-P11-O14	2.48	117.11	107.64
4	B	405	476	C4-C5-C6	-2.33	117.05	120.63
4	A	405	476	C17-C6-C5	2.00	126.29	121.23

There are no chirality outliers.

All (12) torsion outliers are listed below:

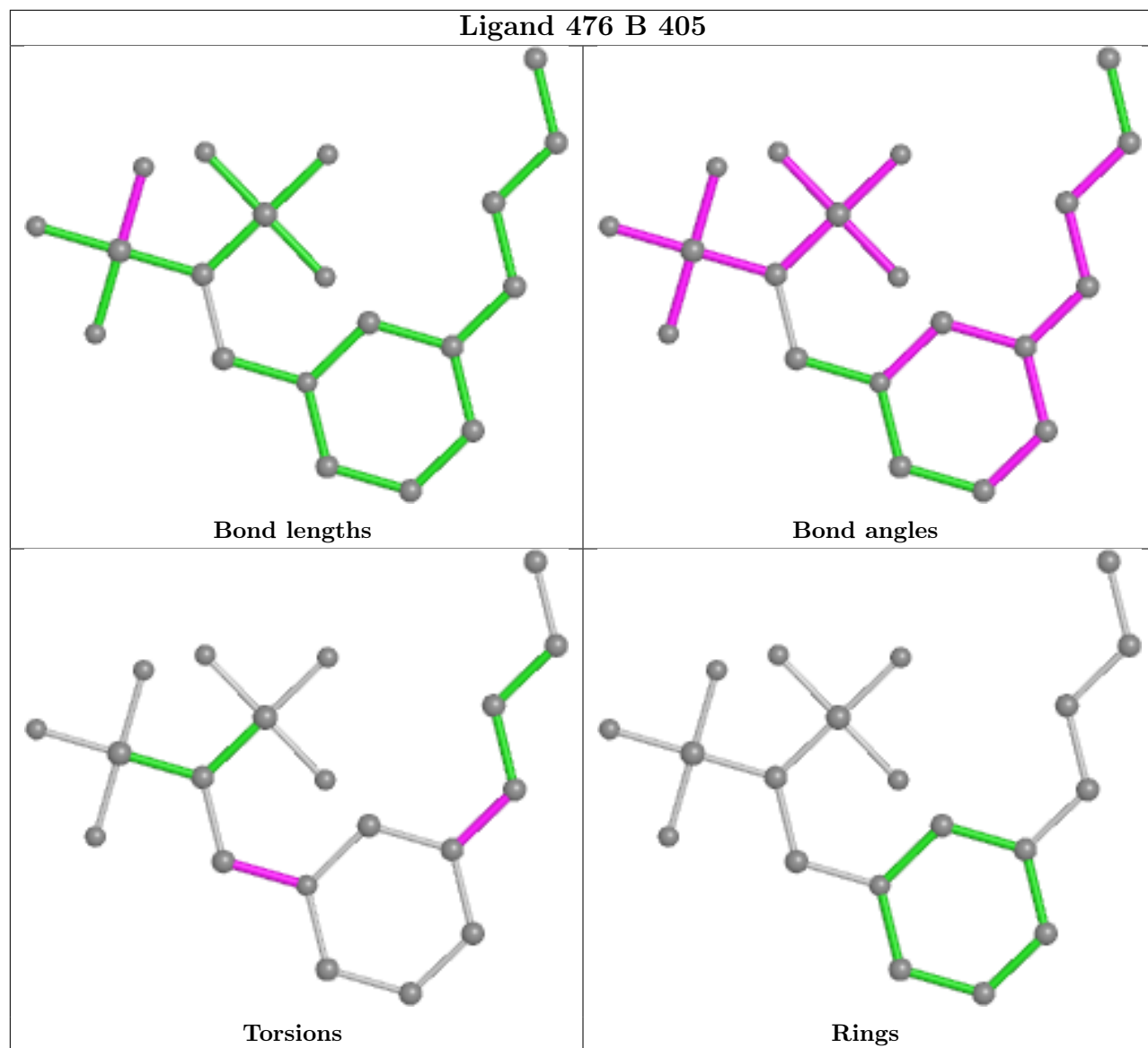
Mol	Chain	Res	Type	Atoms
4	A	405	476	C8-C7-N2-C1
4	A	405	476	C8-C7-N2-C3
4	B	405	476	C8-C7-N2-C1
4	B	405	476	C8-C7-N2-C3
3	A	404	IPR	C3-C2-C4-C5
3	A	404	IPR	C1-C2-C4-C5
4	A	405	476	C17-C18-C19-C20
3	A	404	IPR	C2-C4-C5-O6
4	A	405	476	C18-C17-C6-C1
3	B	404	IPR	C1-C2-C4-C5
4	B	405	476	C18-C17-C6-C5
4	A	405	476	C18-C17-C6-C5

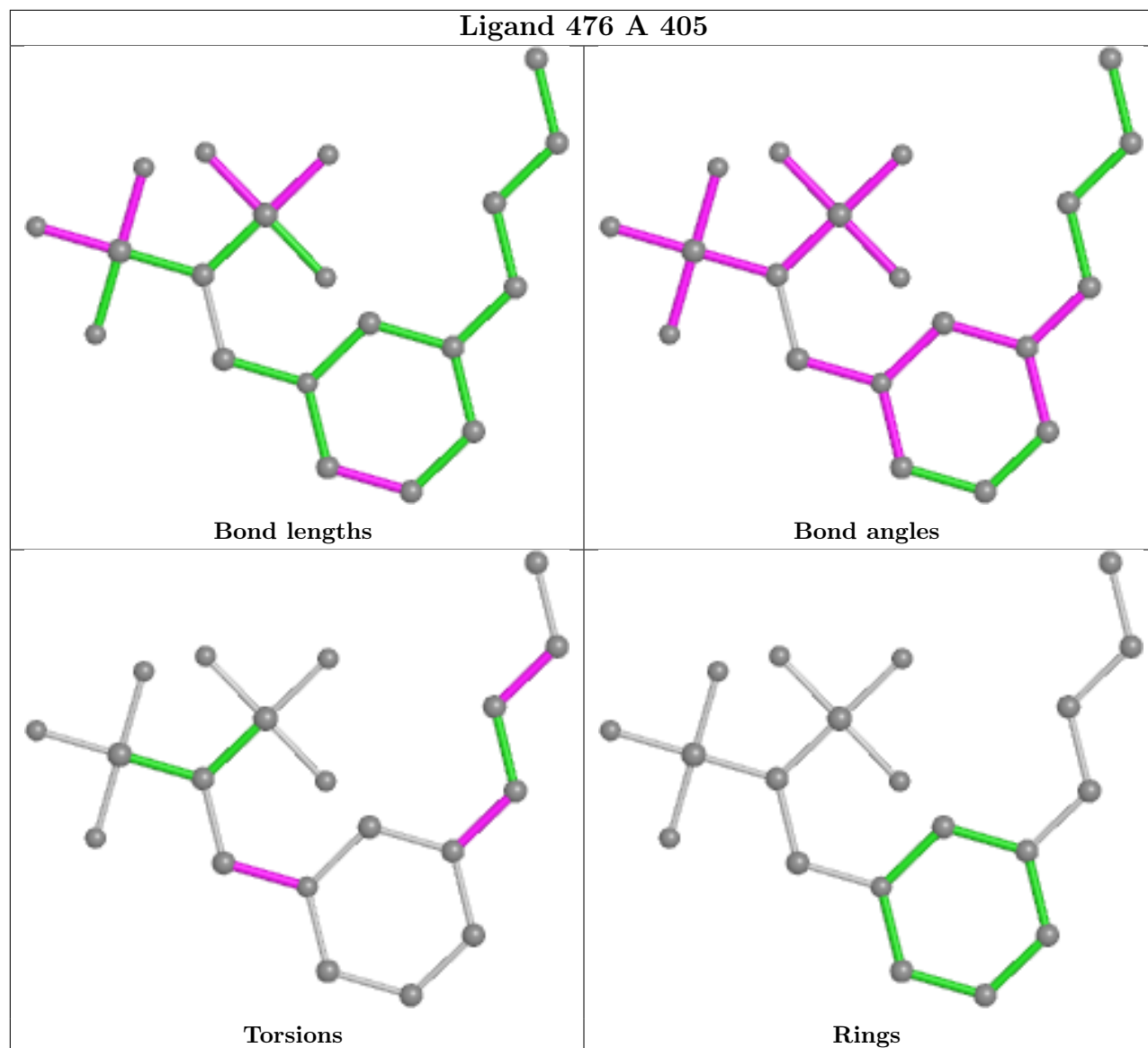
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	406	ACT	1	0
4	B	405	476	4	0
5	A	406	ACT	5	0
3	B	404	IPR	2	0
4	A	405	476	2	0
3	A	404	IPR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	362/362 (100%)	0.07	16 (4%) 34 37	9, 16, 29, 42	0
1	B	362/362 (100%)	-0.05	11 (3%) 50 54	8, 16, 32, 51	0
All	All	724/724 (100%)	0.01	27 (3%) 41 45	8, 16, 30, 51	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	VAL	6.6
1	B	255	CYS	4.9
1	B	67	GLN	4.4
1	A	180	LEU	4.2
1	A	286	PRO	4.1
1	A	277	LEU	3.8
1	A	1	MET	3.5
1	A	276	TRP	3.4
1	A	228	GLU	3.2
1	B	182	ALA	3.2
1	A	296	ASN	3.1
1	A	295	ALA	3.1
1	B	181	ASP	2.9
1	A	274	CYS	2.9
1	B	228	GLU	2.9
1	A	287	ALA	2.8
1	A	284	THR	2.7
1	B	251	ASP	2.4
1	B	254	ASP	2.4
1	A	273	LYS	2.4
1	B	66	THR	2.4
1	A	272	ALA	2.3
1	A	285	ALA	2.3
1	B	253	MET	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	227	LEU	2.2
1	B	180	LEU	2.2
1	A	186	HIS	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

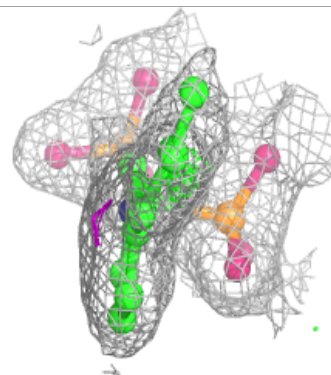
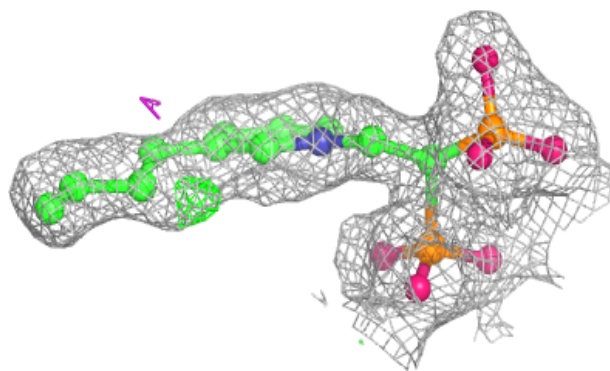
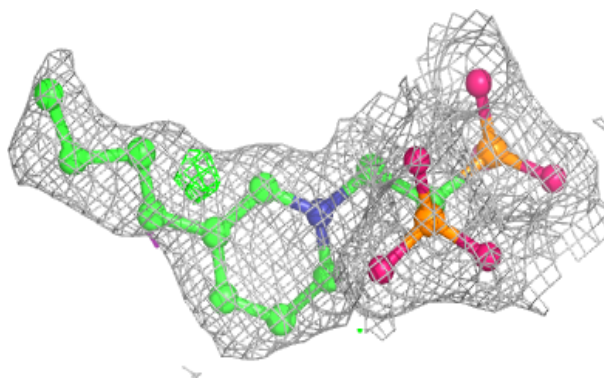
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACT	B	406	4/4	0.87	0.16	19,20,21,22	0
5	ACT	A	406	4/4	0.88	0.19	14,17,17,17	0
2	CA	A	401	1/1	0.97	0.10	13,13,13,13	0
4	476	B	405	20/20	0.97	0.13	11,14,16,17	0
4	476	A	405	20/20	0.98	0.13	10,13,15,16	0
2	CA	A	403	1/1	0.98	0.07	14,14,14,14	0
3	IPR	A	404	14/14	0.98	0.12	11,12,13,14	0
3	IPR	B	404	14/14	0.98	0.11	12,14,15,16	0
2	CA	B	401	1/1	0.99	0.03	14,14,14,14	0
2	CA	B	402	1/1	0.99	0.06	21,21,21,21	0
2	CA	A	402	1/1	1.00	0.06	20,20,20,20	0
2	CA	B	403	1/1	1.00	0.06	13,13,13,13	0

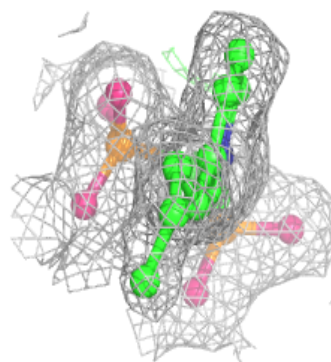
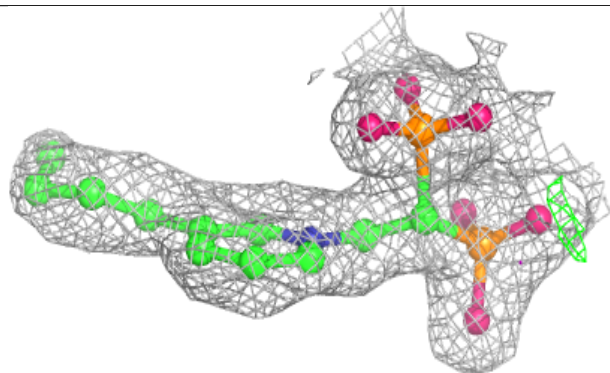
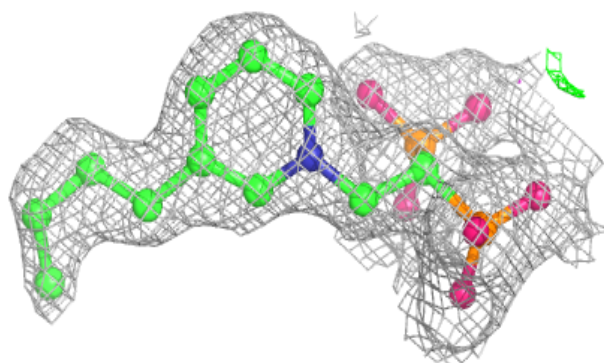
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 476 B 405:**

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

**Electron density around 476 A 405:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.