



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:18 PM UTC

PDB ID : 6B06 / pdb_00006b06
Title : Crystal structure of CfFPPS2, a lepidopteran type-II farnesyl diphosphate synthase, complexed with IPP and [2-(1-methylpyridin-2-yl)-1-phosphono-ethyl]phosphonic acid (inhibitor 1b)
Authors : Picard, M.-E.; Cusson, M.; Shi, R.
Deposited on : 2017-09-13
Resolution : 2.60 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

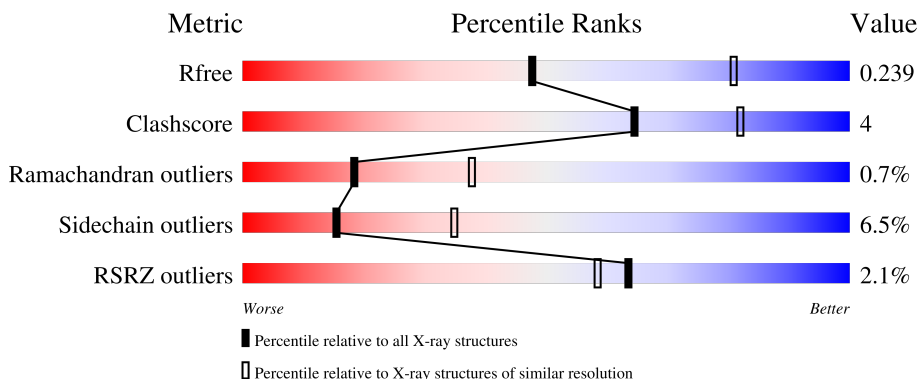
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	341	3% 85% 13% ..
1	B	341	% 85% 13% ..
1	C	341	3% 78% 17% ..

2 Entry composition [i](#)

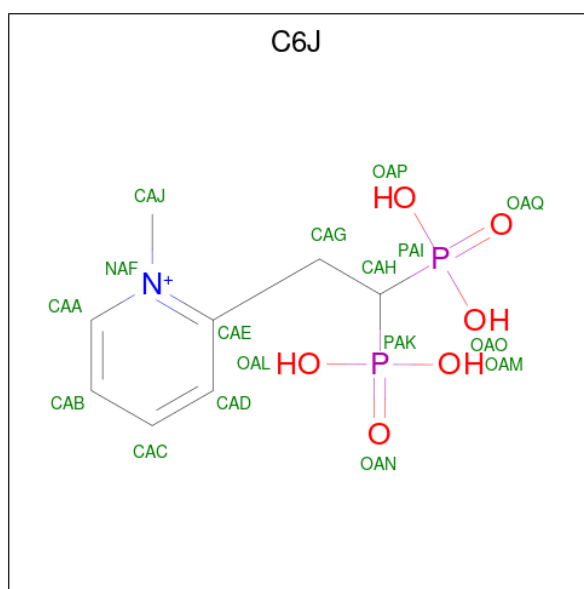
There are 5 unique types of molecules in this entry. The entry contains 8278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2715	1745	436	514	20			
1	B	338	Total	C	N	O	S	0	1	0
			2725	1751	440	514	20			
1	C	334	Total	C	N	O	S	0	0	0
			2681	1723	428	510	20			

- Molecule 2 is 2-(2,2-diphosphonoethyl)-1-methylpyridin-1-ium (CCD ID: C6J) (formula: $C_8H_{14}NO_6P_2$).

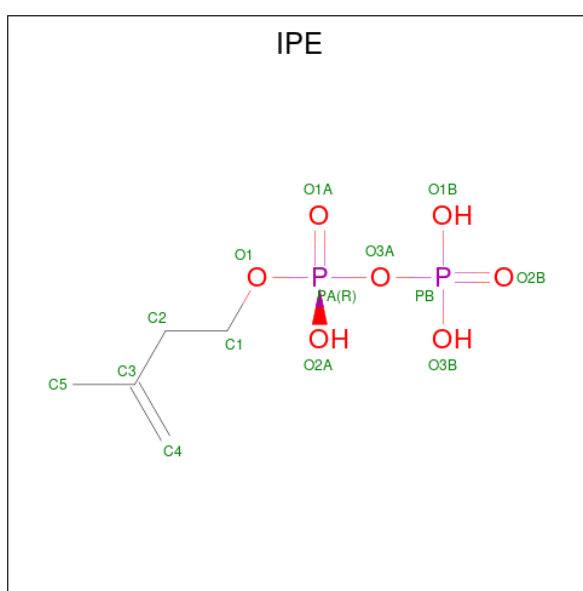


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			17	8	1	6	2		
2	B	1	Total	C	N	O	P	0	0
			17	8	1	6	2		
2	C	1	Total	C	N	O	P	0	0
			17	8	1	6	2		

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

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

- Molecule 4 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (CCD ID: IPE) (formula: $C_5H_{12}O_7P_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	26	Total	O	0	0
			26	26		

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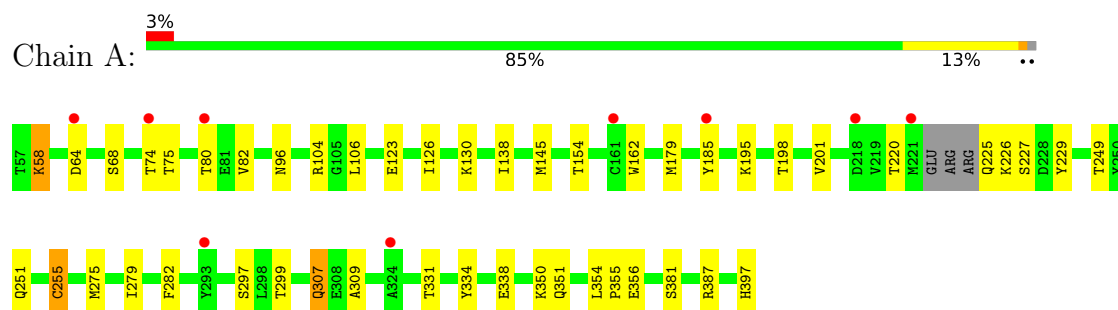
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	15	Total	O	0	0
			15	15		

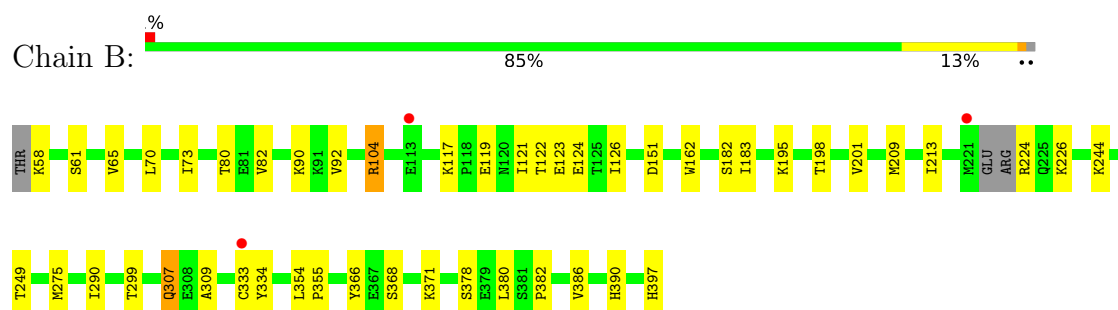
3 Residue-property plots [i](#)

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.

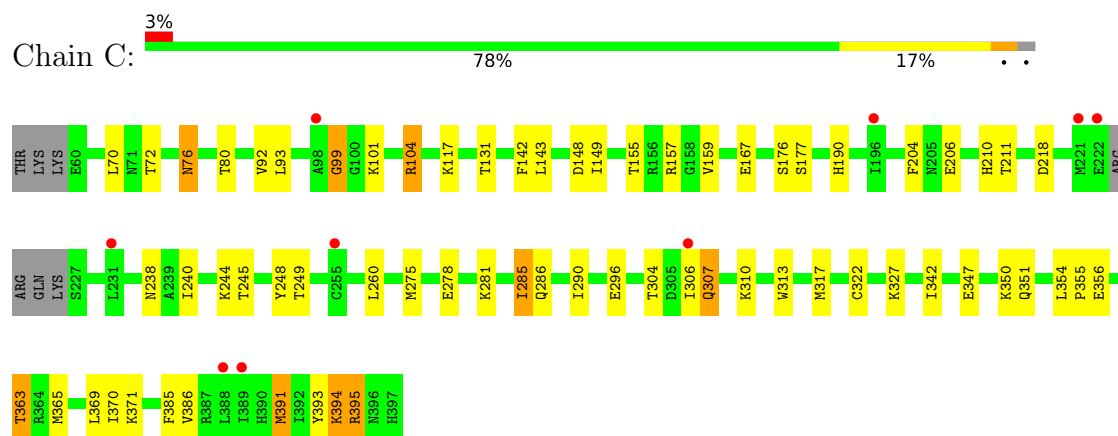
- Molecule 1: Farnesyl diphosphate synthase



- Molecule 1: Farnesyl diphosphate synthase



- Molecule 1: Farnesyl diphosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.22Å 122.65Å 68.14Å 90.00° 107.05° 90.00°	Depositor
Resolution (Å)	101.17 – 2.60 101.17 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (101.17-2.60) 99.3 (101.17-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.235 0.186 , 0.239	Depositor DCC
R_{free} test set	2258 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8278	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: IPE, C6J, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	1/2772 (0.0%)	1.08	2/3750 (0.1%)
1	B	1.07	0/2785	1.12	2/3766 (0.1%)
1	C	1.03	0/2738	1.18	5/3707 (0.1%)
All	All	1.03	1/8295 (0.0%)	1.13	9/11223 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	THR	CA-C	5.44	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	VAL	CB-CA-C	-5.94	104.37	111.97
1	B	333	CYS	N-CA-C	5.76	120.47	113.38
1	B	380	LEU	N-CA-C	5.39	119.70	113.18
1	A	75	THR	N-CA-C	5.27	118.50	111.75
1	C	356	GLU	N-CA-C	-5.25	105.20	111.03
1	C	104	ARG	CB-CA-C	-5.19	102.74	110.88
1	C	204	PHE	N-CA-C	5.10	116.65	111.14
1	C	391	MET	N-CA-C	5.08	121.63	110.80
1	A	138	ILE	N-CA-C	-5.06	105.77	110.53

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	2715	0	2709	18	0
1	B	2725	0	2723	16	0
1	C	2681	0	2661	31	0
2	A	17	0	0	2	0
2	B	17	0	0	1	0
2	C	17	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	14	0	9	1	0
4	B	14	0	9	0	0
4	C	14	0	9	1	0
5	A	14	0	0	2	0
5	B	26	0	0	1	0
5	C	15	0	0	1	0
All	All	8278	0	8120	64	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 4.

All (64) 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:104:ARG:NH1	1:B:249:THR:OG1	2.19	0.75
1:C:99:GLY:O	1:C:157:ARG:NH2	2.20	0.73
1:C:143:LEU:HD22	1:C:211:THR:HG21	1.74	0.68
1:A:145:MET:HE1	1:A:179:MET:SD	2.33	0.68
1:A:201:VAL:HG11	1:B:201:VAL:HG11	1.79	0.63
1:C:347:GLU:OE1	1:C:351:GLN:NE2	2.30	0.63
1:C:317:MET:HA	1:C:317:MET:HE2	1.82	0.62
1:C:104:ARG:NH1	1:C:249:THR:HG22	2.17	0.60
1:C:285:ILE:HD13	1:C:365:MET:HE1	1.84	0.59
1:B:92:VAL:HG22	1:B:162:TRP:CZ2	2.36	0.59
1:C:238:ASN:OD1	1:C:281:LYS:NZ	2.36	0.59
1:C:245:THR:O	1:C:249:THR:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG22	1:A:130:LYS:HE3	1.87	0.56
1:C:240:ILE:HG22	1:C:244:LYS:HD3	1.87	0.55
1:A:58:LYS:HA	1:A:58:LYS:HE2	1.89	0.54
1:C:306:ILE:HD12	1:C:306:ILE:H	1.74	0.52
1:B:366:TYR:OH	1:B:390:HIS:HE1	1.93	0.51
1:A:229:TYR:CD2	1:A:331:THR:HG22	2.45	0.51
1:B:366:TYR:OH	1:B:390:HIS:CE1	2.63	0.51
1:C:72:THR:O	1:C:76:ASN:HB2	2.12	0.50
1:A:307:GLN:HG3	5:A:514:HOH:O	2.09	0.50
2:A:400:C6J:CAJ	4:A:404:IPE:C4	2.89	0.50
1:C:218:ASP:OD1	1:C:218:ASP:C	2.54	0.50
1:B:309:ALA:HA	1:B:334:TYR:CE2	2.47	0.49
1:C:70:LEU:CD2	1:C:93:LEU:HD12	2.43	0.49
1:C:206:GLU:HG2	1:C:210:HIS:CE1	2.48	0.48
1:C:310:LYS:HE3	5:C:510:HOH:O	2.13	0.47
1:C:307:GLN:HB3	1:C:342:ILE:HD11	1.96	0.47
1:C:131:THR:HG21	1:C:190:HIS:CD2	2.49	0.47
2:A:400:C6J:OAM	5:A:501:HOH:O	2.21	0.47
1:C:240:ILE:CG2	1:C:244:LYS:HD3	2.44	0.47
1:B:354:LEU:N	1:B:355:PRO:CD	2.78	0.46
1:B:121:ILE:CG2	1:B:126:ILE:HD11	2.44	0.46
1:A:299:THR:HG22	1:A:397:HIS:HA	1.97	0.46
1:C:70:LEU:HD21	1:C:93:LEU:HD12	1.97	0.46
1:C:363:THR:HG23	1:C:393:TYR:OH	2.15	0.46
1:A:225:GLN:O	1:A:227:SER:N	2.48	0.46
1:C:370:ILE:CD1	1:C:386:VAL:HG13	2.45	0.46
1:A:104:ARG:HD2	1:A:249:THR:HA	1.98	0.45
1:A:198:THR:HG22	1:B:198:THR:HG22	1.97	0.45
1:A:185:TYR:CD2	1:B:209:MET:HE2	2.52	0.44
1:B:307:GLN:HG3	5:B:525:HOH:O	2.16	0.44
1:A:275:MET:HE2	1:A:279:ILE:HD11	1.98	0.44
1:B:209:MET:O	1:B:213:ILE:HG13	2.18	0.44
1:A:354:LEU:N	1:A:355:PRO:CD	2.82	0.43
1:A:251:GLN:O	1:A:255:CYS:HB2	2.18	0.43
1:B:182:SER:O	1:B:183:ILE:C	2.61	0.43
1:C:278:GLU:HB3	1:C:369:LEU:HD21	2.01	0.43
1:A:96:ASN:HD21	1:A:162:TRP:HB2	1.84	0.42
1:B:151:ASP:OD2	2:B:400:C6J:OAL	2.37	0.42
1:C:286:GLN:HB2	1:C:395:ARG:HH21	1.85	0.42
1:C:285:ILE:HG12	1:C:313:TRP:CD1	2.55	0.42
1:C:394:LYS:O	1:C:395:ARG:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LEU:N	1:C:355:PRO:CD	2.82	0.42
1:A:279:ILE:O	1:A:282:PHE:HB3	2.20	0.42
1:A:309:ALA:HA	1:A:334:TYR:CE2	2.55	0.42
1:B:299:THR:HA	1:B:397:HIS:HB2	2.02	0.41
1:B:382:PRO:O	1:B:386:VAL:HG23	2.20	0.41
1:C:290:ILE:O	1:C:290:ILE:HG22	2.20	0.41
1:C:148:ASP:O	1:C:149:ILE:C	2.64	0.41
1:C:142:PHE:CD1	1:C:176:SER:HB2	2.56	0.41
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.92	0.41
1:C:275:MET:HG2	1:C:385:PHE:CD1	2.55	0.41
1:C:248:TYR:OH	4:C:404:IPE:H41	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/341 (98%)	315 (94%)	17 (5%)	2 (1%)	21	42
1	B	335/341 (98%)	320 (96%)	14 (4%)	1 (0%)	36	58
1	C	330/341 (97%)	299 (91%)	27 (8%)	4 (1%)	10	23
All	All	999/1023 (98%)	934 (94%)	58 (6%)	7 (1%)	18	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	226	LYS
1	C	391	MET
1	C	395	ARG
1	A	226	LYS
1	C	394	LYS
1	C	99	GLY

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Mol	Chain	Res	Type
1	A	381	SER

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	301/304 (99%)	284 (94%)	17 (6%)	19	40
1	B	302/304 (99%)	279 (92%)	23 (8%)	12	27
1	C	297/304 (98%)	279 (94%)	18 (6%)	17	37
All	All	900/912 (99%)	842 (94%)	58 (6%)	15	35

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	64	ASP
1	A	68	SER
1	A	80	THR
1	A	82	VAL
1	A	123	GLU
1	A	154	THR
1	A	195	LYS
1	A	220	THR
1	A	255	CYS
1	A	297	SER
1	A	307	GLN
1	A	338	GLU
1	A	350	LYS
1	A	351	GLN
1	A	356	GLU
1	A	387	ARG
1	B	58	LYS
1	B	61	SER
1	B	65	VAL
1	B	70	LEU

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Mol	Chain	Res	Type
1	B	73	ILE
1	B	80	THR
1	B	82	VAL
1	B	90	LYS
1	B	104	ARG
1	B	117	LYS
1	B	119	GLU
1	B	122	THR
1	B	123	GLU
1	B	124	GLU
1	B	195	LYS
1	B	224	ARG
1	B	244	LYS
1	B	275	MET
1	B	290	ILE
1	B	307	GLN
1	B	368	SER
1	B	371	LYS
1	B	378	SER
1	C	76	ASN
1	C	80	THR
1	C	101	LYS
1	C	117	LYS
1	C	155	THR
1	C	159	VAL
1	C	167	GLU
1	C	177	SER
1	C	260	LEU
1	C	285	ILE
1	C	296	GLU
1	C	304	THR
1	C	307	GLN
1	C	322	CYS
1	C	327	LYS
1	C	350	LYS
1	C	363	THR
1	C	371	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN

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Mol	Chain	Res	Type
1	A	96	ASN
1	A	188	HIS
1	A	216	HIS
1	A	251	GLN
1	A	269	HIS
1	A	284	GLN
1	A	307	GLN
1	A	372	GLN
1	A	390	HIS
1	B	96	ASN
1	B	164	GLN
1	B	199	ASN
1	B	216	HIS
1	B	284	GLN
1	B	390	HIS
1	C	190	HIS
1	C	210	HIS
1	C	372	GLN
1	C	397	HIS

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 15 ligands modelled in this entry, 9 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	$\# Z > 2$
2	C6J	B	400	3	16,17,17	3.42	8 (50%)	20,26,26	2.62	9 (45%)
4	IPE	C	404	-	12,13,13	1.79	1 (8%)	16,19,19	0.99	0
4	IPE	A	404	-	12,13,13	1.14	1 (8%)	16,19,19	1.23	2 (12%)
2	C6J	A	400	3	16,17,17	4.20	6 (37%)	20,26,26	2.88	10 (50%)
4	IPE	B	404	-	12,13,13	0.91	1 (8%)	16,19,19	1.29	2 (12%)
2	C6J	C	400	3	16,17,17	2.96	9 (56%)	20,26,26	2.27	6 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C6J	B	400	3	-	2/16/16/16	0/1/1/1
4	IPE	C	404	-	-	5/13/13/13	-
4	IPE	A	404	-	-	3/13/13/13	-
2	C6J	A	400	3	-	2/16/16/16	0/1/1/1
4	IPE	B	404	-	-	2/13/13/13	-
2	C6J	C	400	3	-	2/16/16/16	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	C6J	PAK-OAN	10.47	1.67	1.49
2	A	400	C6J	PAI-OAQ	7.90	1.62	1.49
2	A	400	C6J	PAK-OAM	-7.35	1.43	1.54
2	B	400	C6J	PAK-OAN	7.28	1.61	1.49
2	C	400	C6J	PAI-OAO	6.62	1.65	1.54
4	C	404	IPE	PA-O3A	5.84	1.65	1.59
2	B	400	C6J	PAK-OAM	-5.44	1.46	1.54
2	A	400	C6J	PAI-OAO	5.24	1.63	1.54
2	B	400	C6J	PAI-CAH	5.00	1.88	1.81
2	C	400	C6J	PAK-OAL	4.87	1.62	1.54
2	B	400	C6J	PAK-OAL	4.60	1.62	1.54
2	B	400	C6J	CAG-CAE	-4.42	1.42	1.50
2	C	400	C6J	PAK-CAH	-4.28	1.76	1.81
2	B	400	C6J	PAI-OAP	3.85	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	C6J	PAK-OAM	3.75	1.60	1.54
4	A	404	IPE	PA-O3A	3.63	1.63	1.59
2	C	400	C6J	PAI-CAH	3.63	1.86	1.81
2	A	400	C6J	PAI-OAP	-3.49	1.49	1.54
2	A	400	C6J	CAG-CAE	-3.42	1.44	1.50
2	B	400	C6J	CAA-NAF	3.29	1.42	1.36
2	C	400	C6J	CAG-CAE	-2.94	1.45	1.50
2	C	400	C6J	CAA-NAF	2.70	1.41	1.36
2	B	400	C6J	PAI-OAO	2.31	1.58	1.54
2	C	400	C6J	PAI-OAP	2.27	1.58	1.54
2	C	400	C6J	PAK-OAN	-2.18	1.46	1.49
4	B	404	IPE	PA-O3A	2.00	1.61	1.59

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	C6J	CAJ-NAF-CAE	7.17	130.61	120.96
2	B	400	C6J	CAJ-NAF-CAE	5.72	128.65	120.96
2	A	400	C6J	CAJ-NAF-CAA	-5.10	107.82	118.19
2	C	400	C6J	CAE-CAG-CAH	4.79	123.42	112.51
2	B	400	C6J	CAJ-NAF-CAA	-4.68	108.67	118.19
2	C	400	C6J	CAJ-NAF-CAE	4.62	127.18	120.96
2	A	400	C6J	CAG-CAE-CAD	-4.26	111.83	120.79
2	C	400	C6J	CAG-CAE-CAD	-4.20	111.95	120.79
2	B	400	C6J	CAC-CAD-CAE	4.05	124.00	119.19
2	A	400	C6J	OAN-PAK-CAH	-3.97	101.01	112.29
2	A	400	C6J	CAC-CAD-CAE	3.92	123.84	119.19
2	B	400	C6J	CAG-CAE-CAD	-3.76	112.89	120.79
2	C	400	C6J	CAJ-NAF-CAA	-3.41	111.24	118.19
2	B	400	C6J	OAL-PAK-OAN	-3.31	105.15	113.45
2	C	400	C6J	CAC-CAD-CAE	3.28	123.08	119.19
2	B	400	C6J	CAE-CAG-CAH	2.94	119.20	112.51
2	B	400	C6J	CAA-CAB-CAC	-2.92	114.90	118.88
2	A	400	C6J	OAQ-PAI-CAH	-2.79	104.37	112.29
2	B	400	C6J	OAM-PAK-CAH	2.67	115.25	106.88
2	A	400	C6J	OAM-PAK-CAH	2.63	115.12	106.88
4	A	404	IPE	O2A-PA-O1A	2.46	123.88	112.44
4	A	404	IPE	O3A-PB-O2B	-2.32	98.83	111.04
2	B	400	C6J	OAP-PAI-OAO	-2.28	101.41	107.58
4	B	404	IPE	O3B-PB-O3A	2.27	112.24	104.64
2	A	400	C6J	OAL-PAK-OAN	-2.22	107.88	113.45
2	C	400	C6J	OAM-PAK-OAN	-2.21	107.90	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	C6J	OAP-PAI-OAO	2.12	113.33	107.58
4	B	404	IPE	C5-C3-C2	2.07	120.65	114.96
2	A	400	C6J	OAO-PAI-OAQ	-2.02	108.39	113.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	C6J	CAD-CAE-CAG-CAH
2	A	400	C6J	NAF-CAE-CAG-CAH
2	B	400	C6J	CAD-CAE-CAG-CAH
2	B	400	C6J	NAF-CAE-CAG-CAH
2	C	400	C6J	CAD-CAE-CAG-CAH
2	C	400	C6J	NAF-CAE-CAG-CAH
4	C	404	IPE	PA-O3A-PB-O1B
4	C	404	IPE	PA-O3A-PB-O3B
4	B	404	IPE	C1-O1-PA-O1A
4	C	404	IPE	C1-O1-PA-O1A
4	A	404	IPE	PA-O3A-PB-O2B
4	C	404	IPE	PA-O3A-PB-O2B
4	A	404	IPE	PB-O3A-PA-O1A
4	B	404	IPE	PB-O3A-PA-O2A
4	C	404	IPE	C1-C2-C3-C4
4	A	404	IPE	C1-C2-C3-C5

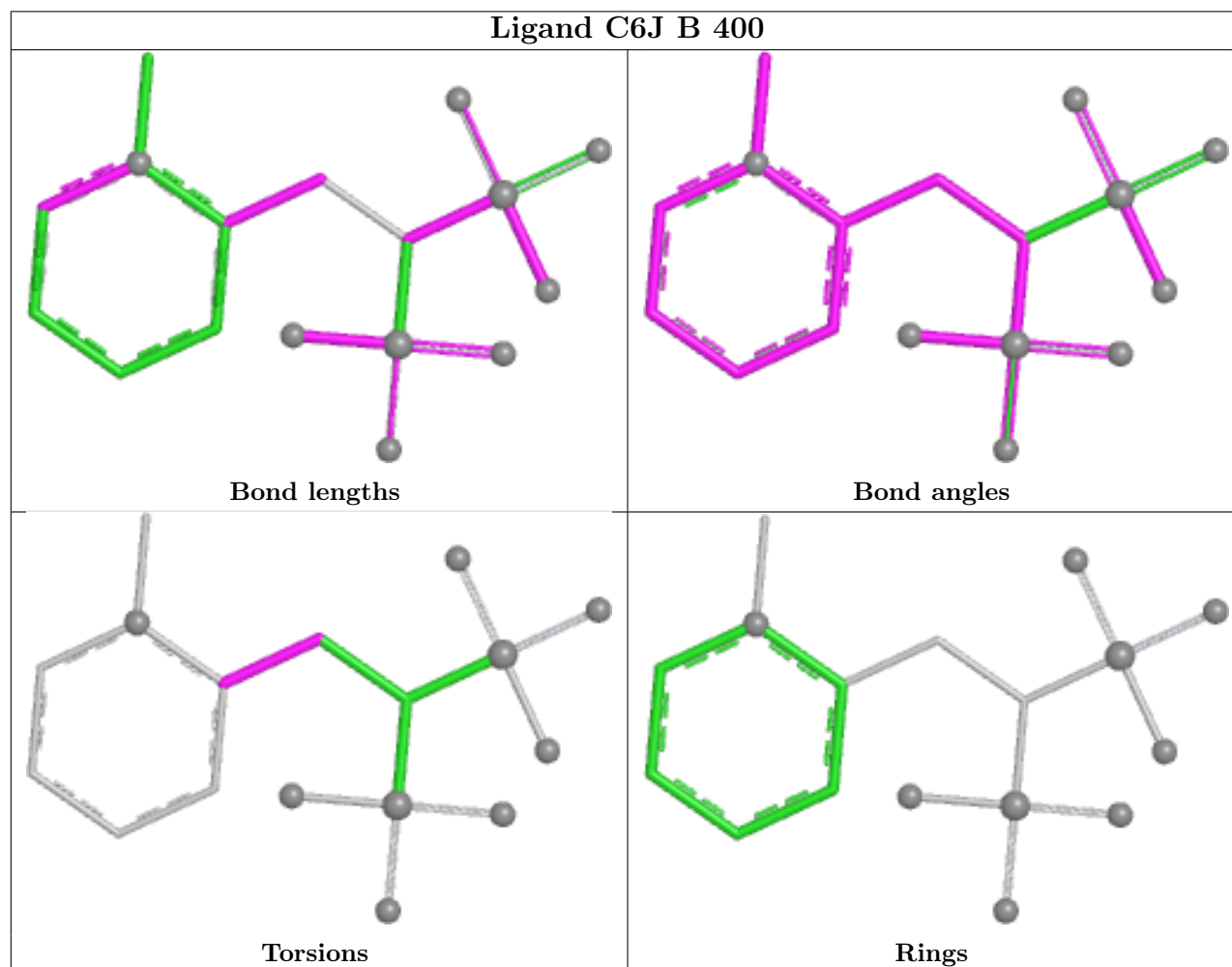
There are no ring outliers.

4 monomers are involved in 4 short contacts:

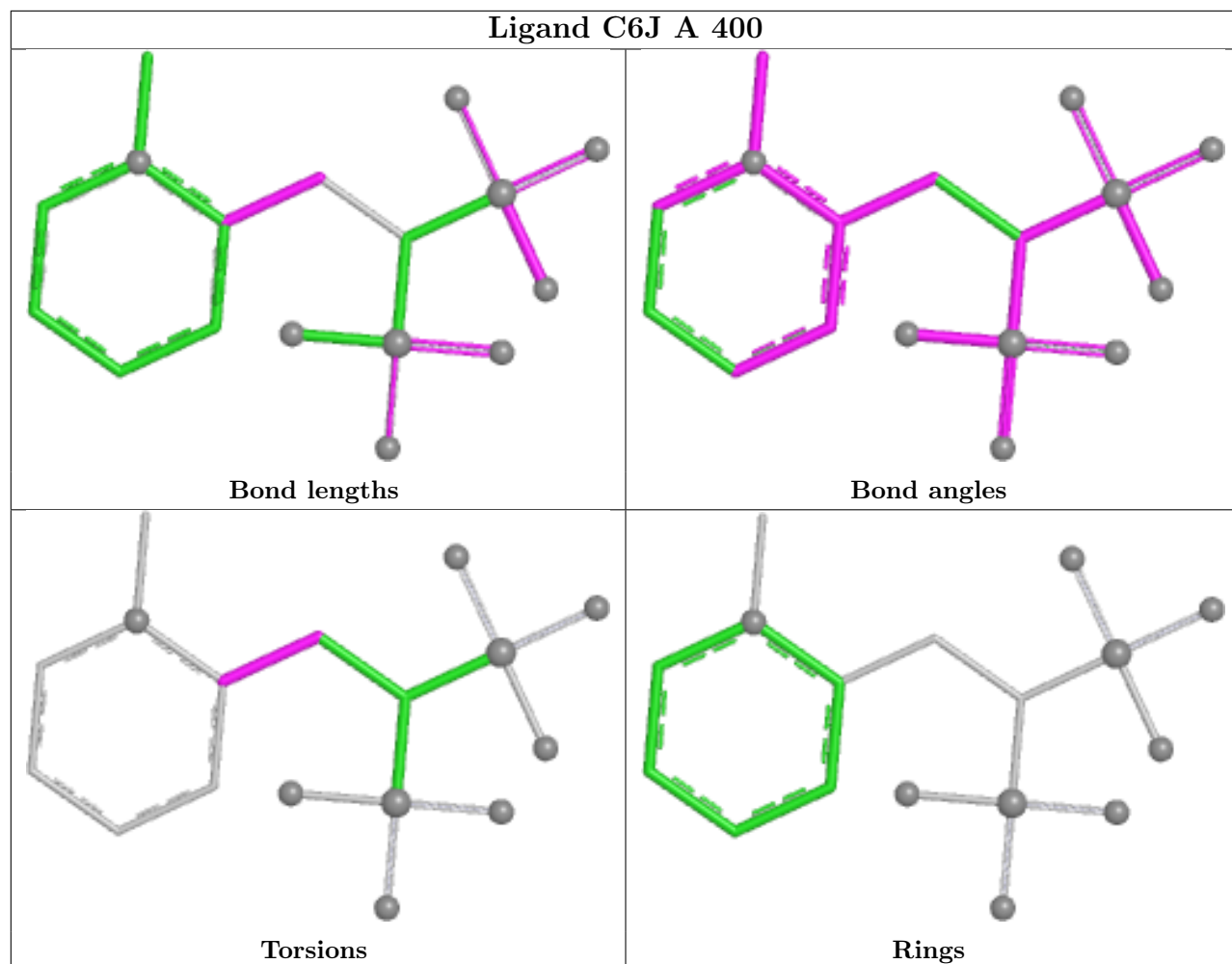
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	C6J	1	0
4	C	404	IPE	1	0
4	A	404	IPE	1	0
2	A	400	C6J	2	0

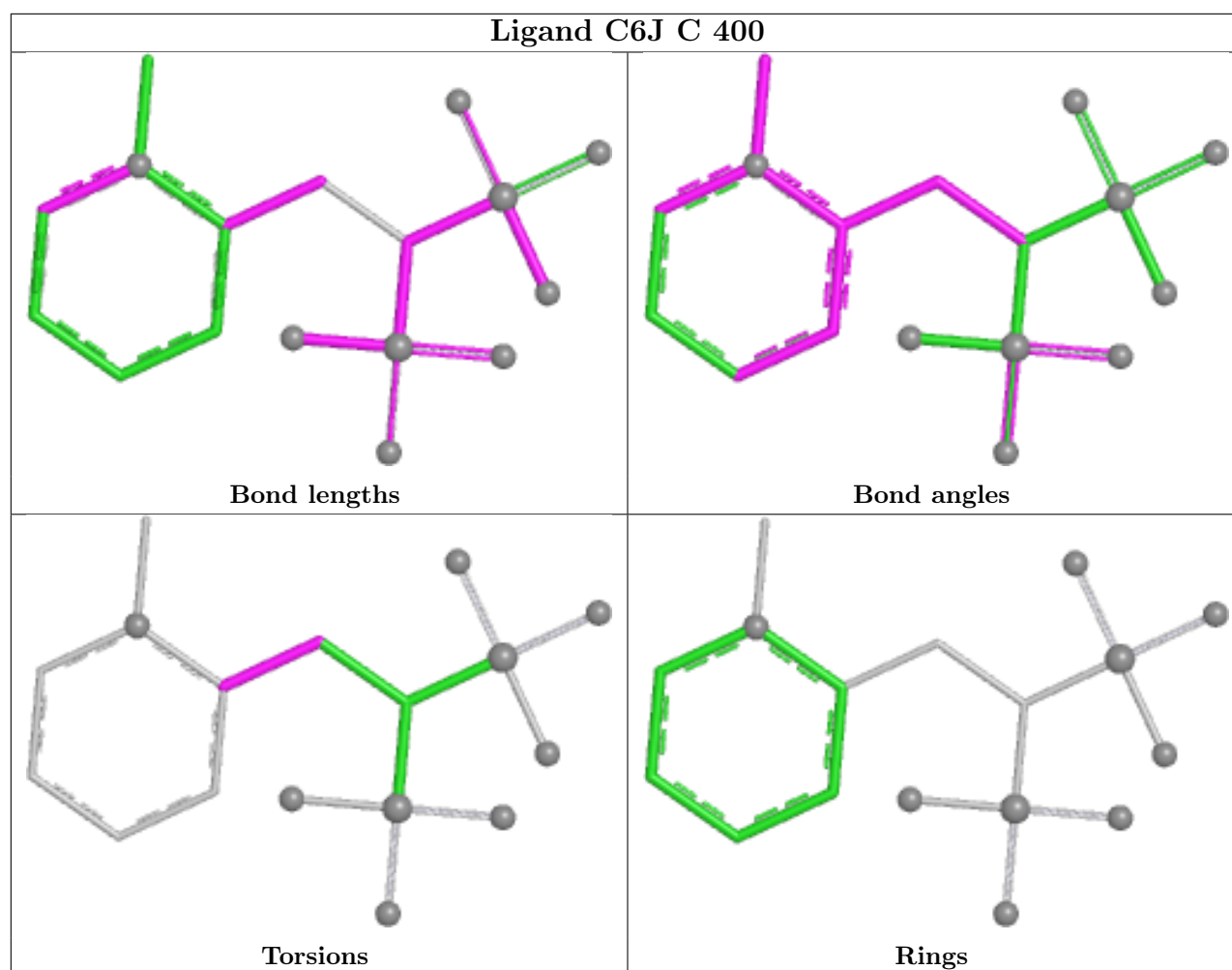
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand C6J A 400





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	338/341 (99%)	0.00	9 (2%)	56	50	48, 68, 101, 126	0
1	B	338/341 (99%)	-0.14	3 (0%)	81	78	37, 63, 98, 122	1 (0%)
1	C	334/341 (97%)	0.14	9 (2%)	56	50	43, 71, 113, 126	0
All	All	1010/1023 (98%)	0.00	21 (2%)	63	58	37, 68, 106, 126	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	ILE	4.2
1	A	218	ASP	3.3
1	B	221	MET	3.2
1	C	255	CYS	3.0
1	C	196	ILE	3.0
1	C	389	ILE	2.9
1	A	161	CYS	2.8
1	C	388	LEU	2.6
1	A	324	ALA	2.6
1	C	222	GLU	2.5
1	A	221	MET	2.5
1	C	221	MET	2.5
1	B	333	CYS	2.4
1	A	185	TYR	2.4
1	C	98	ALA	2.2
1	B	113	GLU	2.1
1	A	64	ASP	2.1
1	A	80	THR	2.1
1	C	231	LEU	2.1
1	A	74	THR	2.0
1	A	293	TYR	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](#)

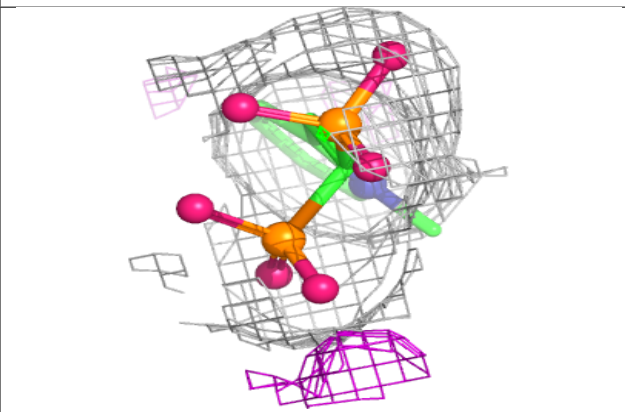
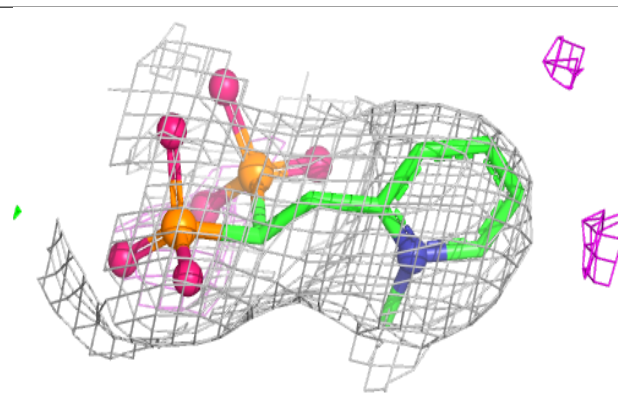
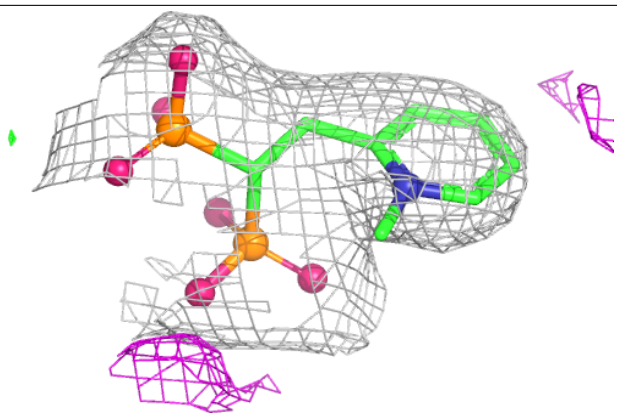
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	IPE	C	404	14/14	0.87	0.16	89,98,111,112	0
4	IPE	A	404	14/14	0.91	0.12	76,83,95,97	0
4	IPE	B	404	14/14	0.97	0.09	55,62,70,70	0
3	MG	A	402	1/1	0.97	0.08	49,49,49,49	0
2	C6J	A	400	17/17	0.98	0.07	43,57,77,96	0
2	C6J	C	400	17/17	0.98	0.08	36,67,98,116	0
3	MG	C	401	1/1	0.99	0.04	63,63,63,63	0
3	MG	A	401	1/1	0.99	0.03	49,49,49,49	0
2	C6J	B	400	17/17	0.99	0.06	37,43,70,96	0
3	MG	A	403	1/1	0.99	0.04	63,63,63,63	0
3	MG	C	402	1/1	1.00	0.03	56,56,56,56	0
3	MG	C	403	1/1	1.00	0.02	71,71,71,71	0
3	MG	B	402	1/1	1.00	0.04	45,45,45,45	0
3	MG	B	403	1/1	1.00	0.03	39,39,39,39	0
3	MG	B	401	1/1	1.00	0.01	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.

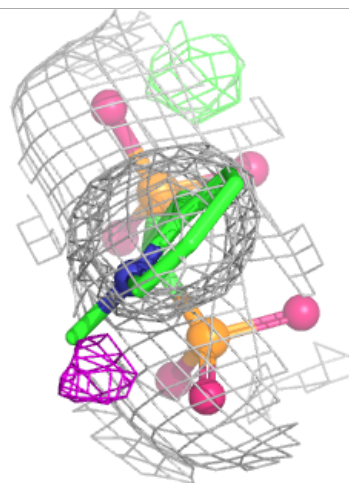
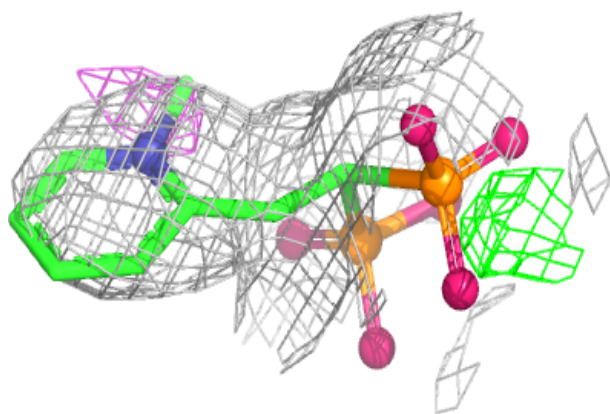
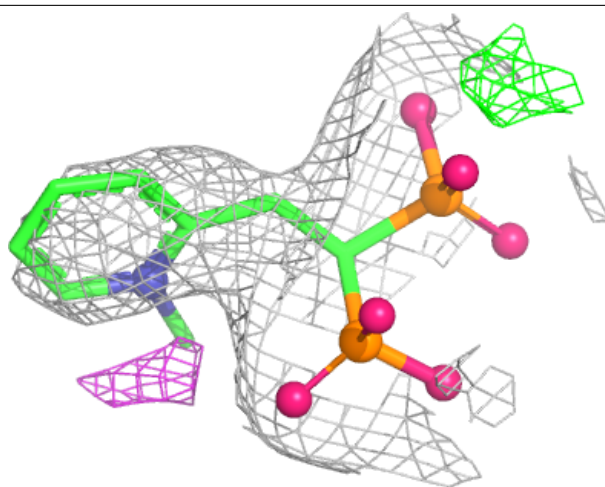
Electron density around C6J A 400:

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



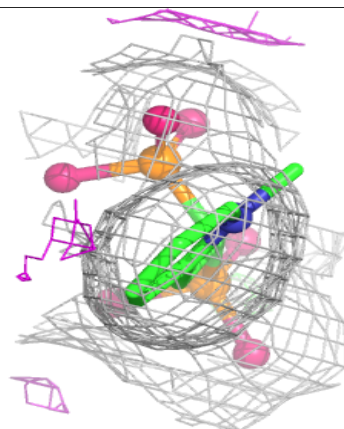
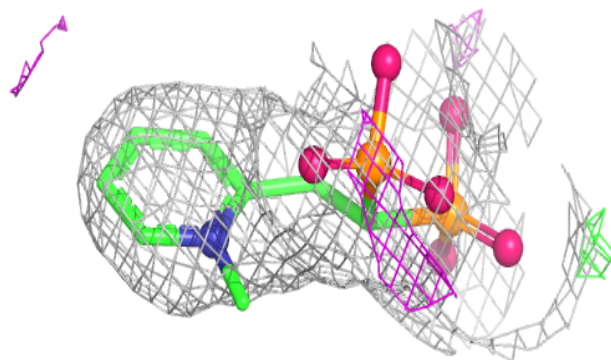
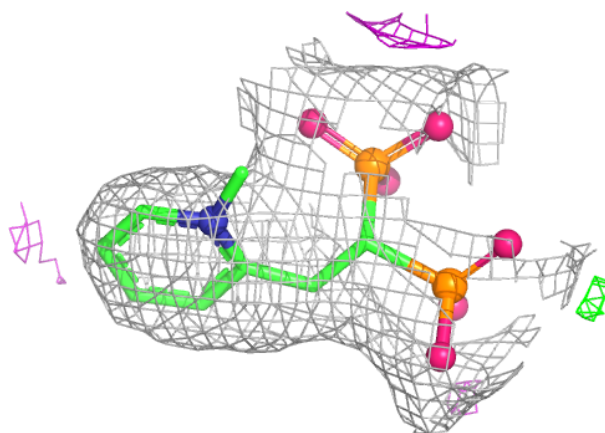
Electron density around C6J C 400:

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



Electron density around C6J B 400:

$2mF_o-DF_c$ (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.