



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:50 PM UTC

PDB ID : 4GTO / pdb_00004gto
Title : FTase in complex with BMS analogue 14
Authors : Guo, Z.; Stigter, E.A.; Bon, R.S.; Waldmann, H.; Blankenfeldt, W.; Goody, R.S.
Deposited on : 2012-08-29
Resolution : 2.15 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

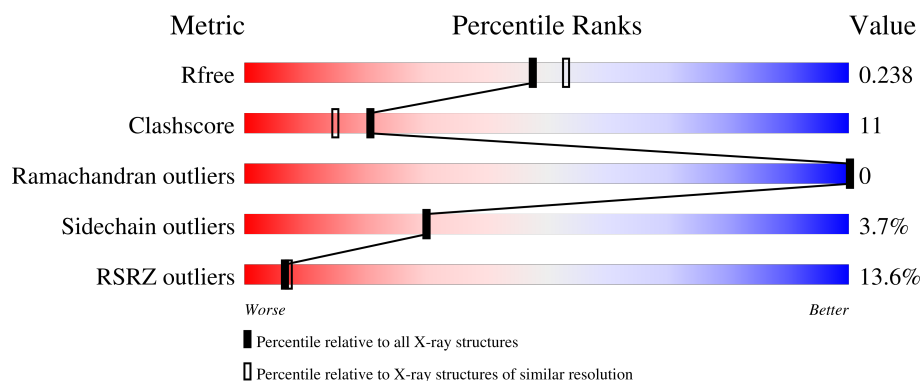
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	377	15% 68% 14% • 16%
2	B	427	10% 79% 15% • 5%

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
6	DMS	B	504	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6507 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 Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	3	0
			2707	1725	476	501	5			

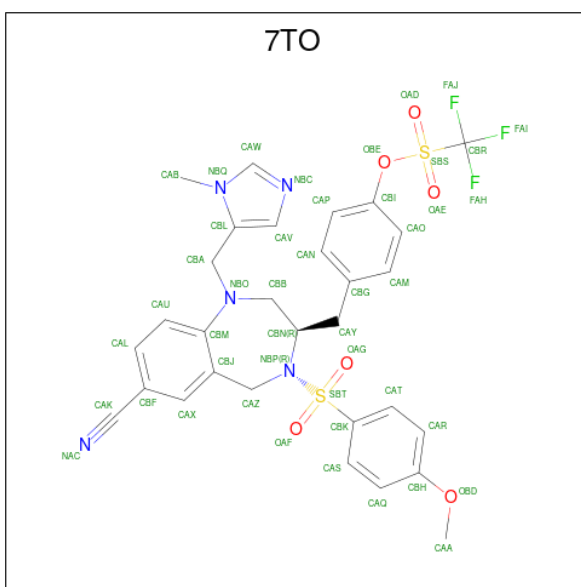
- Molecule 2 is a protein called Protein farnesyltransferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	2	0
			3173	2024	547	578	24			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

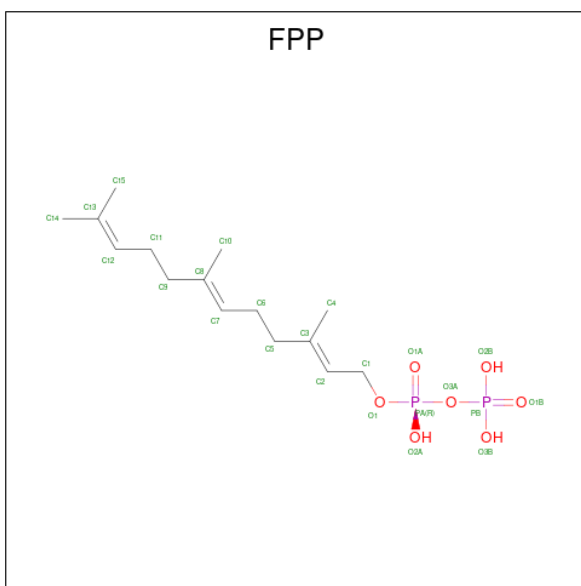
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 4-({(3R)-7-cyano-4-[(4-methoxyphenyl)sulfonyl]-1-[(1-methyl-1H-imidazol-5-yl)methyl]-2,3,4,5-tetrahydro-1H-1,4-benzodiazepin-3-yl)methyl)phenyl trifluoromethanesulfonate (CCD ID: 7TO) (formula: C₃₀H₂₈F₃N₅O₆S₂).



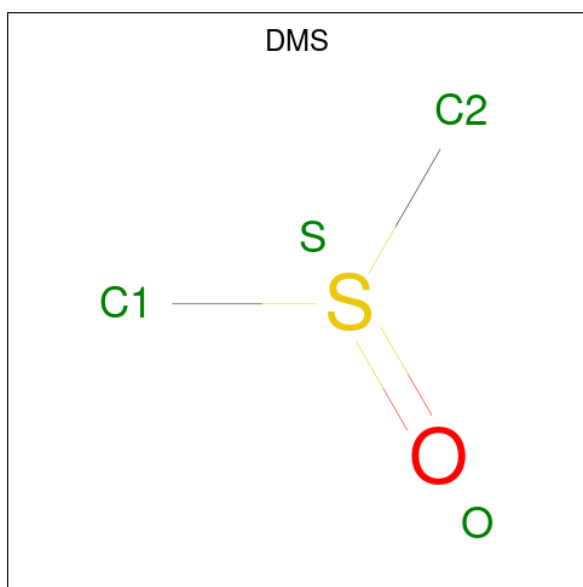
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	S	0	0
			46	30	3	5	6	2		

- Molecule 5 is FARNESYL DIPHOSPHATE (CCD ID: FPP) (formula: $\text{C}_{15}\text{H}_{28}\text{O}_7\text{P}_2$).



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

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	268	Total	O	0	0
			268	268		
7	B	294	Total	O	0	0
			294	294		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	172.70Å 172.70Å 69.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.15 29.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.91-2.15) 99.0 (29.91-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.225 0.205 , 0.238	Depositor DCC
R_{free} test set	3225 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6507	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: DMS, 7TO, FPP, ZN

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	1/2782 (0.0%)	0.94	9/3776 (0.2%)
2	B	0.65	0/3264	0.84	0/4437
All	All	0.68	1/6046 (0.0%)	0.89	9/8213 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	HIS	CG-ND1	-6.30	1.31	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ASP	N-CA-C	12.20	126.28	111.40
1	A	329	ASN	N-CA-C	10.69	126.14	111.39
1	A	332	ASP	N-CA-CB	-8.91	96.94	110.13
1	A	331	GLU	CB-CA-C	8.43	127.19	110.42
1	A	328	ASP	CB-CA-C	8.36	126.81	109.68
1	A	328	ASP	N-CA-C	-6.51	101.94	110.53
1	A	291	ARG	N-CA-C	-5.53	106.37	113.23
1	A	83	GLY	CA-C-N	5.06	125.09	119.32
1	A	83	GLY	C-N-CA	5.06	125.09	119.32

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	2707	0	2631	63	1
2	B	3173	0	3081	64	0
3	B	1	0	0	0	0
4	B	46	0	28	2	0
5	B	14	0	6	2	0
6	B	4	0	6	6	0
7	A	268	0	0	27	0
7	B	294	0	0	23	1
All	All	6507	0	5752	130	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 (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:SER:CB	1:A:370:GLU:OE2	1.85	1.23
1:A:368:SER:HB3	1:A:370:GLU:OE2	1.38	1.21
1:A:335:ASN:HB3	7:A:616:HOH:O	1.42	1.17
2:B:150:LEU:HB2	2:B:193[A]:MET:HE3	1.34	1.09
1:A:231:VAL:HG21	1:A:266:MET:HE2	1.35	1.07
2:B:66:HIS:HD2	7:B:820:HOH:O	1.40	1.03
2:B:66:HIS:CD2	7:B:820:HOH:O	2.16	0.97
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.32	0.94
1:A:211:GLN:OE1	7:A:451:HOH:O	1.86	0.93
6:B:504:DMS:H22	7:B:873:HOH:O	1.68	0.92
2:B:190:SER:HB2	2:B:199:VAL:HG11	1.53	0.90
1:A:368:SER:HB2	1:A:370:GLU:OE2	1.71	0.87
1:A:330:LYS:HD2	7:A:456:HOH:O	1.76	0.85
6:B:504:DMS:C2	7:B:873:HOH:O	2.24	0.81
1:A:152:MET:O	1:A:156:ILE:HG13	1.80	0.81
2:B:150:LEU:CB	2:B:193[A]:MET:HE3	2.10	0.81
2:B:118:ILE:HD11	7:B:717:HOH:O	1.82	0.78
2:B:93:TYR:CZ	6:B:504:DMS:H13	2.20	0.76
1:A:211:GLN:HG3	7:A:543:HOH:O	1.85	0.76
1:A:335:ASN:CG	7:A:572:HOH:O	2.28	0.75
1:A:156:ILE:HG12	1:A:172:ARG:NH1	2.02	0.74
1:A:335:ASN:CB	7:A:572:HOH:O	2.36	0.73
1:A:335:ASN:ND2	7:A:572:HOH:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:LYS:HD3	2:B:346:PRO:O	1.89	0.71
1:A:334:LEU:O	1:A:338:LEU:HG	1.91	0.70
1:A:302:LEU:HD23	7:A:621:HOH:O	1.91	0.70
1:A:156:ILE:CG1	1:A:172:ARG:HH12	2.05	0.70
2:B:93:TYR:CE1	7:B:757:HOH:O	2.44	0.70
2:B:70:ARG:HB3	7:B:764:HOH:O	1.91	0.69
1:A:265:GLU:HG3	7:A:554:HOH:O	1.92	0.67
1:A:214:ARG:HH11	1:A:214:ARG:HG2	1.59	0.67
4:B:502:7TO:H2	7:B:873:HOH:O	1.93	0.67
2:B:77:LYS:CD	2:B:346:PRO:O	2.43	0.66
1:A:326:GLN:HG2	7:A:561:HOH:O	1.96	0.66
1:A:368:SER:HB3	1:A:370:GLU:CD	2.19	0.66
2:B:202:ARG:NH2	7:B:688:HOH:O	2.28	0.65
1:A:287:ARG:HA	7:A:580:HOH:O	1.96	0.65
2:B:150:LEU:HB2	2:B:193[A]:MET:CE	2.20	0.64
2:B:190:SER:HB2	2:B:199:VAL:CG1	2.25	0.64
2:B:150:LEU:CB	2:B:193[A]:MET:CE	2.74	0.63
1:A:200:TYR:HB3	5:B:503:FPP:H42	1.82	0.61
1:A:109:ARG:NH1	7:A:634:HOH:O	2.33	0.61
1:A:150:GLU:HG2	7:A:648:HOH:O	2.01	0.60
2:B:151:ALA:N	2:B:193[A]:MET:HE2	2.17	0.60
2:B:201:VAL:HG11	2:B:251:TYR:HB3	1.83	0.60
1:A:81:ASN:HB3	7:A:425:HOH:O	2.03	0.58
2:B:301:SER:O	2:B:305:ALA:HB3	2.02	0.58
2:B:409:ILE:HG22	7:B:721:HOH:O	2.03	0.57
1:A:335:ASN:HB2	7:A:572:HOH:O	2.01	0.57
1:A:251:SER:HB2	7:A:620:HOH:O	2.05	0.57
4:B:502:7TO:CAA	7:B:873:HOH:O	2.52	0.57
2:B:70:ARG:HG3	7:B:611:HOH:O	2.05	0.57
2:B:93:TYR:CE2	6:B:504:DMS:H13	2.40	0.55
2:B:83:LYS:HE2	7:B:830:HOH:O	2.06	0.54
1:A:214:ARG:HG2	1:A:214:ARG:NH1	2.22	0.54
2:B:70:ARG:HD2	7:B:824:HOH:O	2.07	0.54
2:B:226:ALA:HA	2:B:259:LEU:HD21	1.89	0.53
1:A:335:ASN:CB	7:A:616:HOH:O	2.22	0.53
2:B:190:SER:CB	2:B:199:VAL:HG11	2.33	0.53
1:A:54:GLY:HA3	1:A:121:ARG:CZ	2.38	0.53
2:B:149:HIS:CE1	2:B:193[A]:MET:HG3	2.44	0.52
2:B:355:GLY:N	7:B:780:HOH:O	2.37	0.52
1:A:97[B]:ARG:NH2	7:A:510:HOH:O	2.42	0.52
1:A:368:SER:C	1:A:370:GLU:HG2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.92	0.51
2:B:93:TYR:HE1	7:B:757:HOH:O	1.88	0.51
1:A:231:VAL:CG2	1:A:266:MET:HE2	2.23	0.51
1:A:329:ASN:O	1:A:332:ASP:HB3	2.10	0.51
1:A:328:ASP:HB2	7:A:562:HOH:O	2.11	0.50
1:A:334:LEU:HD13	1:A:367:HIS:HB2	1.94	0.50
2:B:312:HIS:CE1	7:B:701:HOH:O	2.65	0.49
2:B:176:LYS:NZ	2:B:179:GLN:OE1	2.40	0.49
2:B:70:ARG:CB	7:B:764:HOH:O	2.57	0.49
2:B:262:LEU:C	2:B:263:LYS:HZ2	2.21	0.49
7:A:546:HOH:O	2:B:275:GLN:HG3	2.12	0.48
1:A:142:ARG:HD2	1:A:178:TRP:CZ2	2.48	0.48
2:B:56:GLN:NE2	7:B:818:HOH:O	2.41	0.48
1:A:307:SER:OG	1:A:312:ILE:HD11	2.13	0.48
2:B:93:TYR:CE2	6:B:504:DMS:C1	2.96	0.48
1:A:286:ASP:HB2	7:A:521:HOH:O	2.13	0.48
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.96	0.47
1:A:167[B]:GLN:H	1:A:167[B]:GLN:CD	2.22	0.47
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.97	0.47
2:B:291:ARG:NH2	5:B:503:FPP:O2A	2.46	0.47
2:B:408:VAL:O	2:B:412:THR:HG23	2.15	0.47
2:B:151:ALA:H	2:B:193[A]:MET:HE2	1.78	0.47
2:B:201:VAL:HG13	2:B:251:TYR:HD2	1.80	0.46
1:A:302:LEU:CD2	7:A:621:HOH:O	2.57	0.46
2:B:338:TYR:CE2	2:B:343:CYS:SG	3.08	0.46
1:A:167[A]:GLN:NE2	7:A:565:HOH:O	2.48	0.46
1:A:265:GLU:CG	7:A:554:HOH:O	2.60	0.46
1:A:121:ARG:HD3	7:A:460:HOH:O	2.15	0.46
2:B:351:LEU:HD23	2:B:358:ARG:HA	1.97	0.46
2:B:83:LYS:CE	7:B:830:HOH:O	2.63	0.45
2:B:151:ALA:HB3	2:B:152:PRO:CD	2.47	0.45
2:B:336:GLN:HG2	2:B:370:LEU:HD12	1.98	0.45
1:A:272:HIS:ND1	2:B:38:ASP:OD1	2.44	0.45
1:A:296:LEU:HD22	1:A:322:MET:HE1	1.97	0.45
1:A:156:ILE:CD1	1:A:172:ARG:HH12	2.28	0.45
1:A:166:TYR:HE2	7:A:565:HOH:O	1.99	0.45
1:A:330:LYS:O	1:A:331:GLU:C	2.58	0.45
2:B:93:TYR:OH	6:B:504:DMS:H13	2.15	0.45
1:A:105:ALA:O	1:A:109:ARG:HG3	2.17	0.45
2:B:191:PHE:C	2:B:199:VAL:HG22	2.41	0.44
2:B:266:ARG:HG2	7:B:659:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:HE3	1:A:266:MET:HA	2.00	0.44
1:A:255:VAL:HG13	1:A:258:ARG:HH21	1.83	0.43
2:B:118:ILE:O	2:B:119:PRO:C	2.60	0.43
2:B:150:LEU:HD21	2:B:181:LEU:CD2	2.49	0.43
2:B:353:LYS:HB2	2:B:354:PRO:HD2	1.99	0.43
2:B:84:ARG:HH11	2:B:84:ARG:HG3	1.84	0.43
2:B:21:GLU:OE2	2:B:22:PRO:HD2	2.19	0.43
1:A:297:ASN:N	1:A:297:ASN:ND2	2.67	0.42
2:B:217:ILE:HB	7:B:790:HOH:O	2.19	0.42
1:A:152:MET:O	1:A:156:ILE:CG1	2.62	0.42
2:B:308:LEU:HD13	2:B:308:LEU:HA	1.86	0.42
2:B:66:HIS:O	2:B:67:LEU:HD23	2.19	0.42
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.85	0.42
2:B:239:ILE:HB	2:B:252:THR:HA	2.01	0.42
2:B:53:GLU:OE2	7:B:702:HOH:O	2.21	0.42
1:A:334:LEU:CD1	1:A:363:LEU:HB3	2.50	0.41
2:B:192:LEU:HD22	2:B:197:GLY:O	2.19	0.41
1:A:112:ARG:HA	1:A:140:LEU:CD2	2.50	0.41
2:B:191:PHE:O	2:B:199:VAL:HG22	2.20	0.41
1:A:369:ARG:C	1:A:370:GLU:HG2	2.45	0.41
2:B:350:LEU:HB2	2:B:363:THR:HA	2.02	0.41
1:A:217:ASP:HB2	7:A:555:HOH:O	2.21	0.41
2:B:352:ASP:OD1	2:B:352:ASP:C	2.64	0.41
2:B:264:LYS:O	2:B:265:GLU:C	2.64	0.40
2:B:353:LYS:HB2	2:B:354:PRO:CD	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASP:OD2	7:B:820:HOH:O[1_556]	2.11	0.09

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	318/377 (84%)	305 (96%)	13 (4%)	0	100	100
2	B	406/427 (95%)	400 (98%)	6 (2%)	0	100	100
All	All	724/804 (90%)	705 (97%)	19 (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	295/338 (87%)	282 (96%)	13 (4%)	25	23
2	B	338/363 (93%)	327 (97%)	11 (3%)	33	34
All	All	633/701 (90%)	609 (96%)	24 (4%)	30	29

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	85	SER
1	A	121	ARG
1	A	156	ILE
1	A	212	GLU
1	A	255	VAL
1	A	281[A]	LYS
1	A	281[B]	LYS
1	A	297	ASN
1	A	302	LEU
1	A	328	ASP
1	A	335	ASN
1	A	369	ARG
2	B	20	SER
2	B	50	LYS

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Mol	Chain	Res	Type
2	B	57	GLU
2	B	68	VAL
2	B	83	LYS
2	B	121	ILE
2	B	263	LYS
2	B	273	LEU
2	B	308	LEU
2	B	313	ARG
2	B	409	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
2	B	30	HIS
2	B	56	GLN
2	B	65	ASN
2	B	332	GLN

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
6	DMS	B	504	-	3,3,3	2.71	1 (33%)	3,3,3	0.57	0
4	7TO	B	502	3	50,50,50	2.09	12 (24%)	63,75,75	2.40	19 (30%)
5	FPP	B	503	-	12,13,23	1.91	4 (33%)	15,19,31	0.82	0

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	7TO	B	502	3	-	1/38/54/54	0/4/5/5
5	FPP	B	503	-	-	1/13/13/25	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	7TO	OAF-SBT	6.62	1.50	1.43
4	B	502	7TO	OAG-SBT	6.51	1.50	1.43
4	B	502	7TO	SBT-NBP	5.24	1.71	1.63
4	B	502	7TO	CBM-NBO	-4.94	1.34	1.43
6	B	504	DMS	O-S	4.56	1.80	1.50
5	B	503	FPP	PA-O3A	3.50	1.63	1.59
4	B	502	7TO	CBA-CBL	3.15	1.54	1.50
5	B	503	FPP	C1-C2	-3.14	1.40	1.49
4	B	502	7TO	CBL-NBQ	-2.74	1.33	1.38
5	B	503	FPP	PB-O2B	2.51	1.64	1.54
4	B	502	7TO	CBB-CBN	2.40	1.55	1.52
4	B	502	7TO	OBE-SBS	-2.31	1.51	1.57
4	B	502	7TO	CAV-NBC	-2.30	1.33	1.37
5	B	503	FPP	C2-C3	2.29	1.39	1.32
4	B	502	7TO	CAB-NBQ	2.12	1.50	1.46
4	B	502	7TO	OAE-SBS	2.06	1.50	1.43
4	B	502	7TO	OAD-SBS	2.03	1.50	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	7TO	NBQ-CAW-NBC	-9.92	107.04	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	7TO	OAG-SBT-OAF	-7.00	108.67	119.59
4	B	502	7TO	CBK-SBT-NBP	5.78	117.45	107.36
4	B	502	7TO	CAZ-CBJ-CAX	-5.39	112.05	119.17
4	B	502	7TO	CBG-CAY-CBN	3.92	120.79	113.22
4	B	502	7TO	OBE-SBS-CBR	3.89	109.93	99.20
4	B	502	7TO	CAS-CBK-SBT	3.10	122.81	119.73
4	B	502	7TO	CBJ-CBM-NBO	2.99	125.68	123.79
4	B	502	7TO	CAA-OB-DBH	-2.95	111.18	117.50
4	B	502	7TO	OAE-SBS-OAD	-2.89	107.19	117.10
4	B	502	7TO	CAZ-CBJ-CBM	2.82	126.79	122.45
4	B	502	7TO	CBN-NBP-SBT	-2.44	113.29	119.05
4	B	502	7TO	CAX-CBJ-CBM	2.36	121.16	118.95
4	B	502	7TO	CBB-CBN-NBP	2.30	116.74	112.15
4	B	502	7TO	CBB-NBO-CBM	2.30	122.11	116.96
4	B	502	7TO	CAV-NBC-CAW	2.27	108.21	105.24
4	B	502	7TO	CAO-CBI-CAP	-2.26	116.86	120.16
4	B	502	7TO	CAT-CBK-SBT	-2.20	117.55	119.73
4	B	502	7TO	CAU-CBM-NBO	-2.08	114.99	118.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	FPP	PB-O3A-PA-O2A
4	B	502	7TO	CAZ-NBP-SBT-OAG

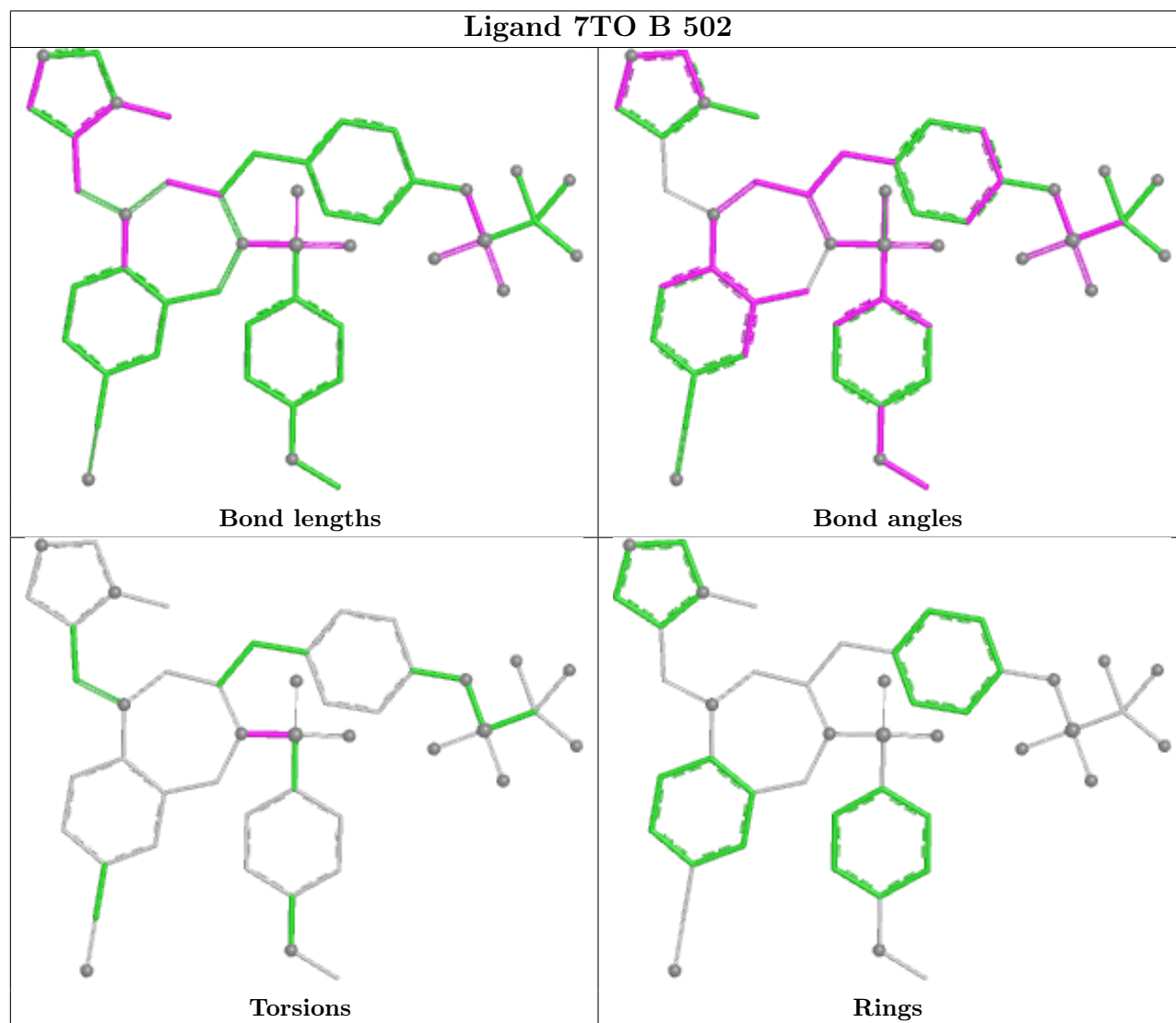
There are no ring outliers.

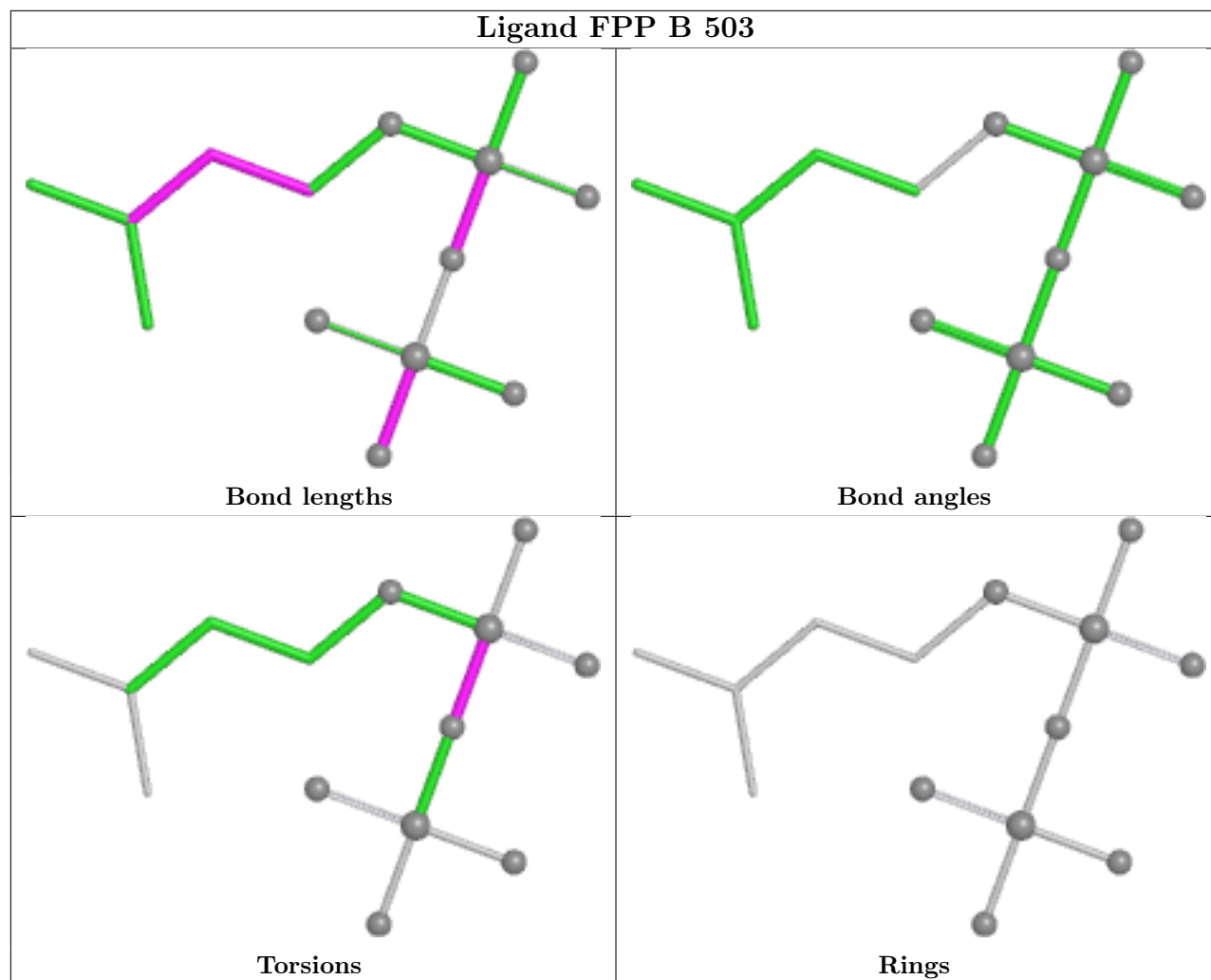
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	504	DMS	6	0
4	B	502	7TO	2	0
5	B	503	FPP	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, 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	317/377 (84%)	0.80	56 (17%)	4 4	15, 48, 88, 104	3 (0%)
2	B	406/427 (95%)	0.48	42 (10%)	12 13	19, 42, 76, 96	2 (0%)
All	All	723/804 (89%)	0.62	98 (13%)	7 7	15, 45, 83, 104	5 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	ARG	6.7
1	A	334	LEU	6.0
2	B	423	PHE	5.9
1	A	55	PHE	5.6
1	A	54	GLY	5.1
2	B	19	TRP	4.9
2	B	18	VAL	4.7
1	A	333	ILE	4.2
1	A	370	GLU	4.2
1	A	331	GLU	4.2
2	B	422	GLY	4.1
2	B	409	ILE	4.1
2	B	137	ASP	3.7
2	B	416	LEU	3.4
2	B	420	VAL	3.3
2	B	64	PHE	3.2
1	A	253	ARG	3.2
2	B	68	VAL	3.2
1	A	214	ARG	3.2
1	A	291	ARG	3.2
1	A	142	ARG	3.1
1	A	335	ASN	3.1
1	A	300	LEU	3.1
1	A	302	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	323	LEU	3.1
2	B	315	LEU	3.1
2	B	65	ASN	3.0
1	A	366	LYS	3.0
1	A	365	SER	2.9
1	A	337	ALA	2.9
2	B	121	ILE	2.9
1	A	289	LEU	2.9
2	B	20	SER	2.9
2	B	268	LEU	2.8
1	A	368	SER	2.8
2	B	325	MET	2.8
2	B	170	ASN	2.7
1	A	288	GLY	2.7
1	A	297	ASN	2.7
1	A	339	GLU	2.7
2	B	355	GLY	2.7
1	A	364	GLN	2.6
1	A	325	ASN	2.6
1	A	255	VAL	2.6
2	B	419	PRO	2.6
1	A	166	TYR	2.6
1	A	260	VAL	2.6
2	B	381	MET	2.6
1	A	336	LYS	2.6
1	A	307	SER	2.6
2	B	317	ALA	2.6
1	A	269	LEU	2.6
1	A	254	ALA	2.5
2	B	412	THR	2.5
1	A	299	LEU	2.5
2	B	323	LEU	2.5
1	A	357	ARG	2.5
1	A	328	ASP	2.5
2	B	417	GLN	2.5
2	B	53	GLU	2.4
1	A	310	TYR	2.4
1	A	367	HIS	2.4
2	B	377	GLY	2.4
1	A	85	SER	2.4
1	A	62	THR	2.4
1	A	329	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	319	GLY	2.4
1	A	327	CYS	2.4
2	B	321	PRO	2.3
2	B	380	ALA	2.3
2	B	40	VAL	2.3
1	A	251	SER	2.2
2	B	218	THR	2.2
2	B	219	PRO	2.2
2	B	272	SER	2.2
1	A	363	LEU	2.2
1	A	287	ARG	2.2
1	A	304	PRO	2.2
2	B	411	ALA	2.2
2	B	62	TYR	2.2
1	A	330	LYS	2.2
1	A	286	ASP	2.2
1	A	94	GLU	2.1
2	B	322	ALA	2.1
1	A	338	LEU	2.1
1	A	359	ILE	2.1
2	B	118	ILE	2.1
1	A	56	LEU	2.1
2	B	382	LEU	2.1
1	A	320	GLU	2.1
1	A	261	GLN	2.1
1	A	346	LYS	2.1
2	B	413	THR	2.1
2	B	216	ILE	2.1
2	B	123	ALA	2.1
2	B	69	PRO	2.0
1	A	292	TYR	2.0
1	A	225	GLN	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 ⓘ

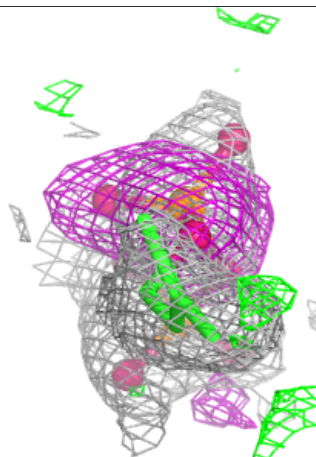
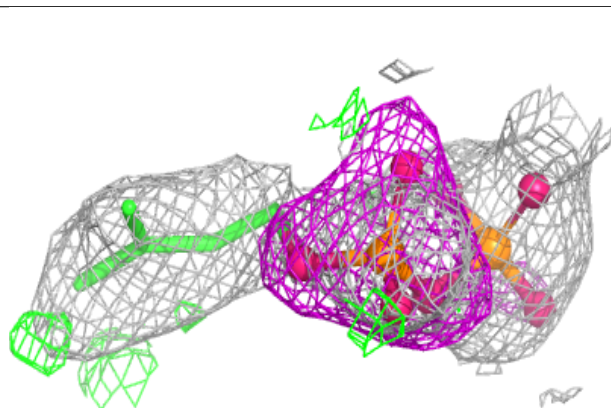
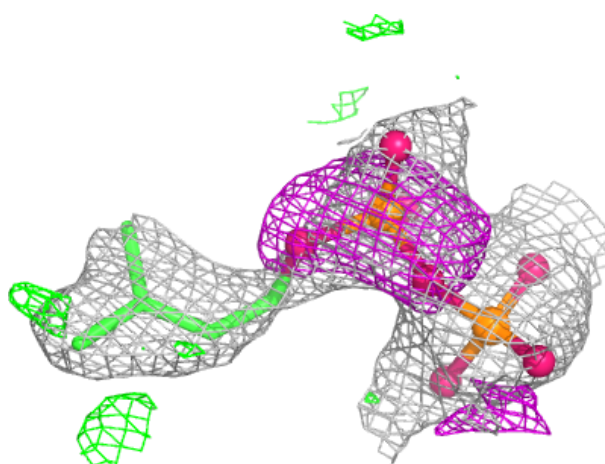
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FPP	B	503	14/24	0.79	0.23	49,62,79,80	0
6	DMS	B	504	4/4	0.88	0.22	78,78,78,78	0
4	7TO	B	502	46/46	0.90	0.14	32,59,95,100	0
3	ZN	B	501	1/1	1.00	0.01	31,31,31,31	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.

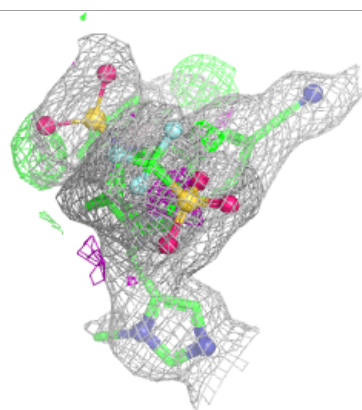
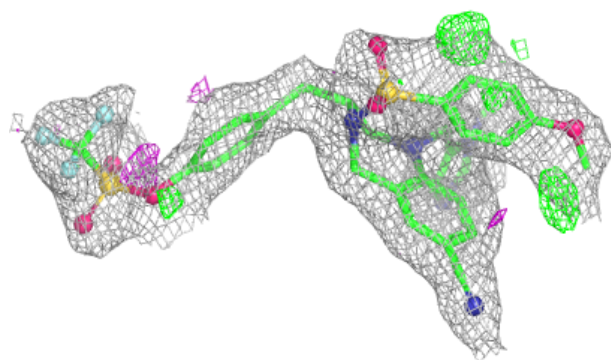
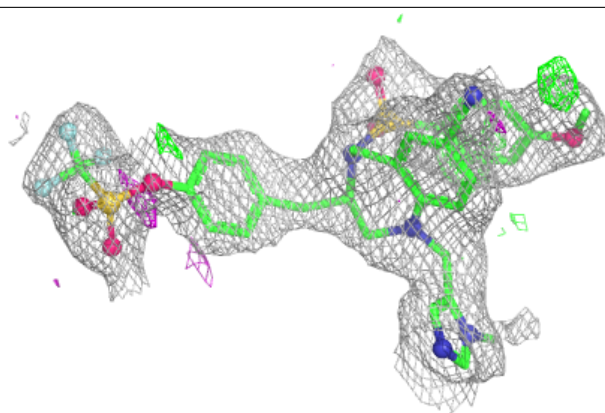
Electron density around FPP B 503:

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 7TO B 502:

$2mF_o - DF_c$ (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.