



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 4GTR / pdb_00004gtr
Title : FTase in complex with BMS analogue 13
Authors : Guo, Z.; Stigter, E.A.; Bon, R.S.; Waldmann, H.; Blankenfeldt, W.; Goody, R.S.
Deposited on : 2012-08-29
Resolution : 2.20 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

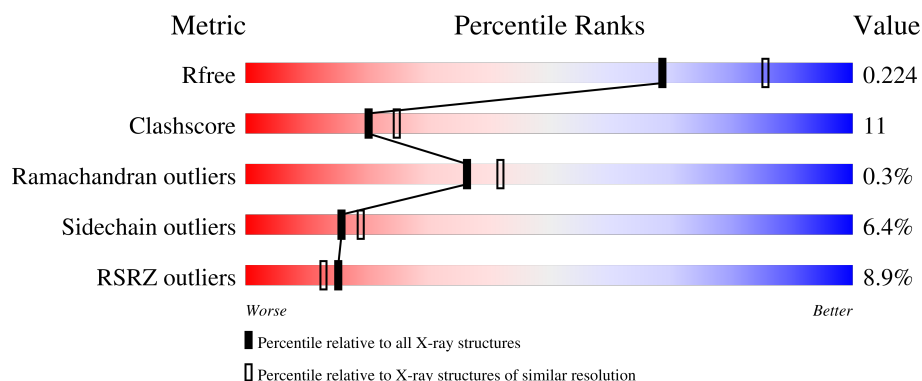
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	9% 63% 18% • 16%
2	B	427	7% 78% 15% • 6%

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	DMS	B	504	-	-	X	-
3	DMS	B	505	-	-	X	-
6	FPP	B	503	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6342 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.

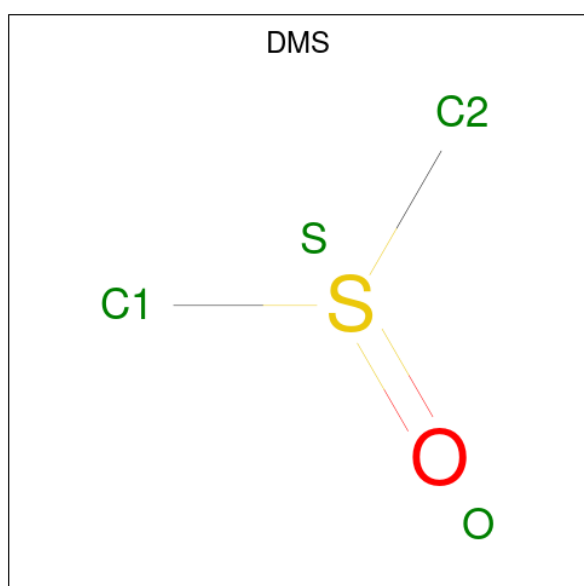
- Molecule 1 is a protein called Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	2	0
			2678	1711	469	493	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	1	0
			3176	2031	547	575	23			

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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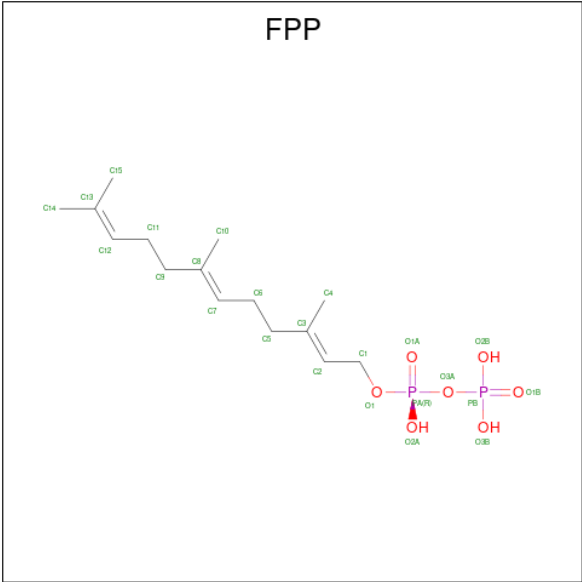
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4 | B | 1 | Total Zn
1 1 | 0 | 0 |

- # 7TR

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			46	34	6	5	1		

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- WORLD WIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			24	15	7	2		

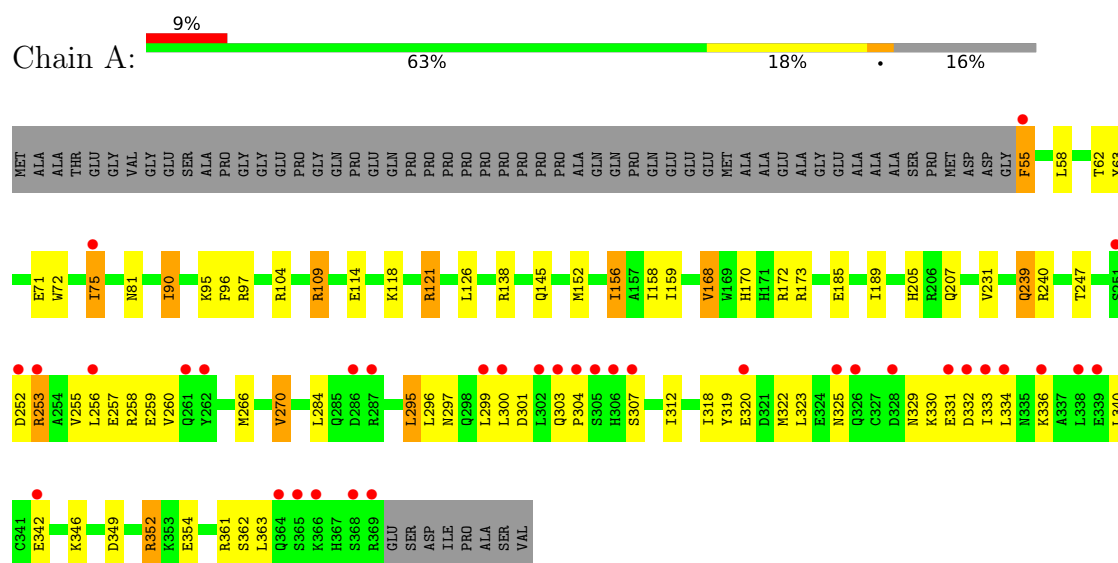
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O	0	0
			199	199		
7	B	206	Total	O	0	0
			206	206		

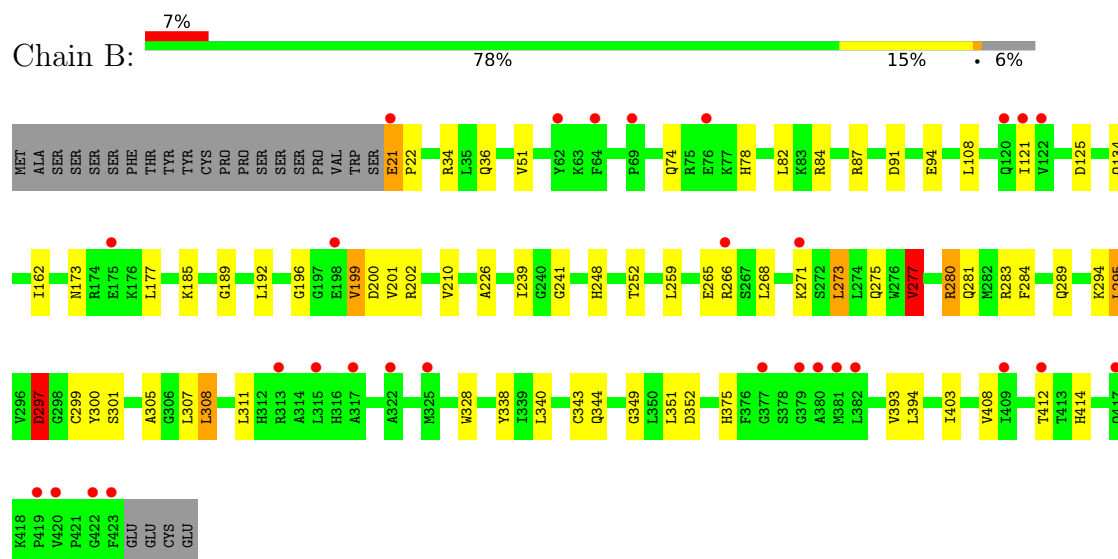
3 Residue-property plots [i](#)

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: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



- Molecule 2: Protein farnesyltransferase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	172.28Å 172.28Å 69.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.20 29.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.91-2.20) 99.9 (29.91-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.212 0.191 , 0.224	Depositor DCC
R_{free} test set	2988 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6342	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, ZN, 7TR, FPP

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	0.85	1/2750 (0.0%)	0.93	2/3735 (0.1%)
2	B	0.81	0/3266	0.92	3/4436 (0.1%)
All	All	0.83	1/6016 (0.0%)	0.92	5/8171 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	THR	CA-C	6.42	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	VAL	CB-CA-C	-7.43	102.36	111.88
1	A	252	ASP	N-CA-C	-6.91	96.09	110.80
2	B	277	VAL	N-CA-CB	5.30	116.40	110.51
1	A	158	ILE	N-CA-C	5.22	115.43	110.42
2	B	297	ASP	N-CA-C	-5.07	99.56	107.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	21	GLU	Peptide
2	B	297	ASP	Peptide

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	2678	0	2604	71	0
2	B	3176	0	3105	54	0
3	A	4	0	6	3	0
3	B	8	0	12	13	0
4	B	1	0	0	0	0
5	B	46	0	38	9	0
6	B	24	0	25	10	0
7	A	199	0	0	12	0
7	B	206	0	0	6	0
All	All	6342	0	5790	133	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 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:A:156:ILE:HD11	7:A:547:HOH:O	1.06	1.19
1:A:231:VAL:HG21	1:A:266:MET:HE2	1.39	1.05
1:A:318:ILE:HG22	1:A:322:MET:HE3	1.36	1.02
5:B:502:7TR:CAT	3:B:504:DMS:H13	1.95	0.96
1:A:159:ILE:HG12	1:A:168:VAL:HG13	1.50	0.94
2:B:78:HIS:HD1	2:B:349:GLY:H	1.19	0.89
6:B:503:FPP:H102	3:B:504:DMS:H23	1.57	0.86
1:A:322:MET:HE2	7:A:635:HOH:O	1.76	0.85
1:A:296:LEU:CD1	1:A:322:MET:HE1	2.06	0.85
1:A:296:LEU:HD11	1:A:322:MET:HE1	1.60	0.84
1:A:58:LEU:HD22	1:A:95:LYS:HD3	1.62	0.82
2:B:185:LYS:NZ	2:B:189:GLY:O	2.16	0.79
1:A:318:ILE:CG2	1:A:322:MET:HE3	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LEU:HD23	2:B:199:VAL:HG12	1.66	0.77
1:A:159:ILE:CG1	1:A:168:VAL:HG13	2.14	0.76
2:B:185:LYS:NZ	2:B:189:GLY:C	2.43	0.76
1:A:62:THR:HG22	1:A:62:THR:O	1.87	0.75
2:B:200:ASP:CG	7:B:695:HOH:O	2.30	0.74
5:B:502:7TR:H36	3:B:505:DMS:H22	1.68	0.73
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.69	0.73
2:B:202:ARG:HD2	6:B:503:FPP:H152	1.69	0.72
1:A:152:MET:HE1	1:A:172:ARG:NH2	2.05	0.71
1:A:118:LYS:HD3	7:A:596:HOH:O	1.93	0.68
1:A:270:VAL:HG22	1:A:270:VAL:O	1.91	0.68
2:B:200:ASP:HA	7:B:695:HOH:O	1.93	0.66
2:B:280:ARG:HH11	2:B:289:GLN:HE21	1.44	0.65
1:A:319:TYR:O	1:A:323:LEU:HG	1.96	0.65
1:A:284:LEU:HD13	1:A:295:LEU:HD21	1.78	0.65
6:B:503:FPP:C10	3:B:504:DMS:H23	2.27	0.64
1:A:159:ILE:HG12	1:A:168:VAL:CG1	2.27	0.64
2:B:280:ARG:HH11	2:B:289:GLN:NE2	1.96	0.64
1:A:320:GLU:HG3	1:A:363:LEU:HD21	1.80	0.64
1:A:156:ILE:CD1	7:A:547:HOH:O	1.88	0.63
2:B:74:GLN:H	2:B:344:GLN:HE22	1.44	0.63
2:B:185:LYS:HZ2	2:B:189:GLY:C	2.07	0.63
1:A:207:GLN:HE21	1:A:239:GLN:NE2	1.98	0.62
1:A:138:ARG:NH2	7:A:528:HOH:O	2.24	0.61
1:A:207:GLN:HE21	1:A:239:GLN:HE22	1.49	0.61
2:B:134:GLN:HE22	2:B:173:ASN:H	1.50	0.60
1:A:303:GLN:HB2	1:A:304:PRO:HD3	1.84	0.60
1:A:322:MET:O	1:A:325:ASN:O	2.21	0.59
2:B:177:LEU:HD21	2:B:210:VAL:CG1	2.32	0.59
1:A:114:GLU:OE1	7:A:549:HOH:O	2.17	0.58
1:A:231:VAL:CG2	1:A:266:MET:HE2	2.25	0.58
1:A:152:MET:O	1:A:156:ILE:HG13	2.04	0.57
1:A:284:LEU:CD1	1:A:295:LEU:HD21	2.34	0.57
1:A:239:GLN:HE21	1:A:239:GLN:HA	1.70	0.57
1:A:266:MET:HE3	1:A:266:MET:HA	1.86	0.56
1:A:72:TRP:HE3	1:A:75:ILE:HG21	1.70	0.56
2:B:201:VAL:HG23	2:B:241:GLY:O	2.06	0.56
1:A:270:VAL:O	1:A:270:VAL:CG2	2.54	0.56
6:B:503:FPP:H61	3:B:504:DMS:H22	1.86	0.56
3:A:401:DMS:H21	5:B:502:7TR:OAG	2.07	0.55
1:A:253:ARG:HH21	1:A:256:LEU:HD23	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:502:7TR:H36	3:B:505:DMS:C2	2.36	0.55
1:A:156:ILE:CD1	1:A:172:ARG:HH12	2.20	0.54
1:A:330:LYS:C	1:A:332:ASP:H	2.15	0.54
2:B:271:LYS:NZ	7:B:626:HOH:O	2.40	0.54
5:B:502:7TR:H28	3:B:505:DMS:H23	1.91	0.53
2:B:299:CYS:SG	3:B:504:DMS:H11	2.49	0.53
2:B:338:TYR:CE2	2:B:343:CYS:SG	3.02	0.53
2:B:36:GLN:NE2	7:B:773:HOH:O	2.38	0.52
1:A:253:ARG:HH21	1:A:256:LEU:CD2	2.22	0.52
1:A:170:HIS:HE1	2:B:196:GLY:O	1.93	0.52
2:B:294:LYS:HE3	6:B:503:FPP:O2B	2.10	0.52
2:B:275:GLN:OE1	7:B:806:HOH:O	2.18	0.52
1:A:121:ARG:CZ	7:A:598:HOH:O	2.59	0.51
2:B:277:VAL:CG1	2:B:307:LEU:HD12	2.40	0.51
1:A:62:THR:O	1:A:62:THR:CG2	2.58	0.51
2:B:280:ARG:HD3	2:B:289:GLN:HE21	1.76	0.50
1:A:121:ARG:NE	7:A:598:HOH:O	2.44	0.50
1:A:97:ARG:HD2	7:A:601:HOH:O	2.12	0.50
3:A:401:DMS:H11	5:B:502:7TR:H16	1.94	0.50
2:B:297:ASP:HB3	2:B:300:TYR:CD2	2.48	0.49
1:A:303:GLN:CB	1:A:304:PRO:HD3	2.41	0.49
1:A:72:TRP:CE3	1:A:75:ILE:HG21	2.48	0.48
2:B:177:LEU:HD21	2:B:210:VAL:HG13	1.95	0.48
2:B:185:LYS:HZ2	2:B:189:GLY:CA	2.25	0.48
2:B:78:HIS:HD1	2:B:349:GLY:N	1.99	0.48
2:B:239:ILE:HB	2:B:252:THR:HA	1.94	0.48
1:A:330:LYS:C	1:A:332:ASP:N	2.71	0.48
7:A:655:HOH:O	2:B:275:GLN:HG3	2.12	0.48
2:B:375:HIS:HE1	2:B:394:LEU:O	1.97	0.48
5:B:502:7TR:NBC	3:B:504:DMS:H13	2.25	0.48
2:B:51:VAL:HG21	2:B:295:LEU:HG	1.95	0.47
3:A:401:DMS:H11	5:B:502:7TR:CAY	2.45	0.47
1:A:334:LEU:O	1:A:334:LEU:HD12	2.14	0.47
2:B:259:LEU:HD12	2:B:268:LEU:HD11	1.96	0.47
1:A:319:TYR:CD1	1:A:333:ILE:HG23	2.48	0.47
1:A:156:ILE:HG12	1:A:172:ARG:NH1	2.29	0.46
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.50	0.46
2:B:273:LEU:HD12	2:B:273:LEU:O	2.15	0.46
1:A:172:ARG:HD3	1:A:185:GLU:OE1	2.15	0.46
1:A:352:ARG:NH2	2:B:281:GLN:O	2.48	0.46
6:B:503:FPP:C6	3:B:504:DMS:H22	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90[A]:ILE:HD11	2:B:94:GLU:HG3	1.98	0.45
2:B:308:LEU:HD13	2:B:308:LEU:HA	1.72	0.45
1:A:170:HIS:CE1	2:B:196:GLY:O	2.70	0.45
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.97	0.45
1:A:240:ARG:HD3	1:A:259:GLU:OE1	2.15	0.45
2:B:87:ARG:NH2	2:B:125:ASP:OD2	2.50	0.45
2:B:226:ALA:HA	2:B:259:LEU:HD21	1.99	0.45
2:B:393:VAL:O	2:B:393:VAL:HG13	2.17	0.44
2:B:185:LYS:NZ	2:B:189:GLY:CA	2.80	0.44
6:B:503:FPP:C10	3:B:504:DMS:C2	2.95	0.44
1:A:55:PHE:HD1	1:A:55:PHE:HA	1.75	0.44
2:B:185:LYS:NZ	2:B:189:GLY:HA2	2.33	0.44
1:A:256:LEU:O	1:A:260:VAL:HG23	2.18	0.44
1:A:75:ILE:HD11	1:A:109:ARG:HD3	2.00	0.43
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.33	0.43
1:A:299:LEU:C	1:A:301:ASP:H	2.26	0.43
1:A:303:GLN:O	1:A:307:SER:HB2	2.18	0.43
1:A:329:ASN:HB3	1:A:332:ASP:HB3	2.01	0.43
1:A:58:LEU:HD23	1:A:63:TYR:CE1	2.54	0.43
1:A:90[A]:ILE:CD1	2:B:91:ASP:HA	2.49	0.43
2:B:162:ILE:HD11	2:B:403:ILE:HG22	2.01	0.43
2:B:301:SER:O	2:B:305:ALA:HB3	2.18	0.42
1:A:296:LEU:HG	1:A:318:ILE:HG21	2.02	0.42
1:A:354:GLU:HG2	2:B:328:TRP:O	2.19	0.42
2:B:277:VAL:CG1	2:B:307:LEU:CD1	2.98	0.42
2:B:408:VAL:O	2:B:412:THR:HG23	2.19	0.42
1:A:104:ARG:NH2	7:A:548:HOH:O	2.53	0.41
2:B:294:LYS:CE	6:B:503:FPP:O2B	2.67	0.41
2:B:248:HIS:CD2	6:B:503:FPP:H42	2.56	0.41
5:B:502:7TR:H28	3:B:505:DMS:C2	2.50	0.41
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.84	0.41
1:A:349:ASP:OD1	2:B:283:ARG:NH2	2.54	0.41
6:B:503:FPP:H102	3:B:504:DMS:C2	2.40	0.41
2:B:34:ARG:HD3	2:B:284:PHE:CE1	2.56	0.41
1:A:118:LYS:HE2	7:A:653:HOH:O	2.21	0.41
1:A:58:LEU:HD23	1:A:63:TYR:CZ	2.56	0.40
2:B:22:PRO:HD2	7:B:605:HOH:O	2.21	0.40
2:B:352:ASP:OD1	2:B:352:ASP:C	2.64	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	315/377 (84%)	297 (94%)	16 (5%)	2 (1%)	21	23
2	B	402/427 (94%)	387 (96%)	15 (4%)	0	100	100
All	All	717/804 (89%)	684 (95%)	31 (4%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	LEU
1	A	331	GLU

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	291/338 (86%)	267 (92%)	24 (8%)	10	12
2	B	341/363 (94%)	324 (95%)	17 (5%)	22	28
All	All	632/701 (90%)	591 (94%)	41 (6%)	16	18

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	71	GLU
1	A	75	ILE
1	A	81	ASN

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Mol	Chain	Res	Type
1	A	90[A]	ILE
1	A	90[B]	ILE
1	A	109	ARG
1	A	121	ARG
1	A	145	GLN
1	A	156	ILE
1	A	168	VAL
1	A	173	ARG
1	A	239	GLN
1	A	253	ARG
1	A	257	GLU
1	A	270	VAL
1	A	295	LEU
1	A	297	ASN
1	A	336	LYS
1	A	342	GLU
1	A	346	LYS
1	A	352	ARG
1	A	361	ARG
1	A	362	SER
2	B	21	GLU
2	B	82	LEU
2	B	84	ARG
2	B	108	LEU
2	B	121	ILE
2	B	199	VAL
2	B	265	GLU
2	B	266	ARG
2	B	273	LEU
2	B	277	VAL
2	B	280	ARG
2	B	295	LEU
2	B	308	LEU
2	B	311	LEU
2	B	340	LEU
2	B	351	LEU
2	B	414	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN

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Mol	Chain	Res	Type
1	A	170	HIS
1	A	211	GLN
1	A	221	GLN
1	A	239	GLN
1	A	294	ASN
1	A	303	GLN
1	A	335	ASN
2	B	30	HIS
2	B	65	ASN
2	B	128	GLN
2	B	134	GLN
2	B	289	GLN
2	B	332	GLN
2	B	344	GLN
2	B	375	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	7TR	B	502	4	50,50,50	1.97	9 (18%)	59,71,71	2.67	15 (25%)
3	DMS	B	504	-	3,3,3	2.67	1 (33%)	3,3,3	0.82	0
6	FPP	B	503	-	22,23,23	2.10	9 (40%)	27,31,31	1.52	6 (22%)
3	DMS	A	401	-	3,3,3	2.70	1 (33%)	3,3,3	0.43	0
3	DMS	B	505	-	3,3,3	2.66	1 (33%)	3,3,3	1.01	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
6	FPP	B	503	-	-	4/25/25/25	-
5	7TR	B	502	4	-	2/36/52/52	0/4/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	7TR	OAG-SBT	7.99	1.52	1.43
5	B	502	7TR	OAH-SBT	6.33	1.50	1.43
3	A	401	DMS	O-S	4.56	1.80	1.50
3	B	504	DMS	O-S	4.56	1.80	1.50
3	B	505	DMS	O-S	4.44	1.79	1.50
6	B	503	FPP	PB-O1B	4.27	1.63	1.50
6	B	503	FPP	C11-C12	-3.94	1.38	1.50
5	B	502	7TR	CBN-NBQ	-3.84	1.36	1.43
6	B	503	FPP	C6-C7	-3.51	1.39	1.50
6	B	503	FPP	C1-C2	-3.31	1.39	1.49
5	B	502	7TR	CBA-CBM	3.26	1.54	1.50
6	B	503	FPP	C12-C13	2.60	1.40	1.32
6	B	503	FPP	O1-C1	-2.59	1.39	1.44
5	B	502	7TR	CAT-CBM	-2.54	1.33	1.36
5	B	502	7TR	CBL-SBT	2.43	1.79	1.76
6	B	503	FPP	C7-C8	2.37	1.38	1.33
6	B	503	FPP	C2-C3	2.30	1.38	1.33
5	B	502	7TR	SBT-NBR	2.27	1.66	1.63
5	B	502	7TR	OAF-CBF	2.08	1.24	1.21
6	B	503	FPP	PB-O2B	2.08	1.62	1.54
5	B	502	7TR	CBM-NBS	-2.05	1.34	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	7TR	NBS-CAU-NBC	-11.41	106.15	112.94
5	B	502	7TR	OAH-SBT-OAG	-7.42	108.01	119.59
5	B	502	7TR	CAZ-CBK-CAV	-7.16	109.71	119.17
5	B	502	7TR	CAC-OB-D-CBI	-4.86	107.09	117.50
5	B	502	7TR	CBL-SBT-NBR	4.27	114.81	107.36
5	B	502	7TR	CBO-NBR-SBT	-4.05	109.52	119.05
5	B	502	7TR	CAZ-CBK-CBN	3.78	128.26	122.45
5	B	502	7TR	OBE-CBF-NBP	3.67	115.19	110.75
5	B	502	7TR	CBJ-OBE-CBF	3.55	123.76	117.19
6	B	503	FPP	C10-C8-C9	3.41	121.15	115.23
6	B	503	FPP	C4-C3-C5	3.34	121.03	115.23
5	B	502	7TR	CAV-CBK-CBN	3.29	122.03	118.95
5	B	502	7TR	CBB-NBQ-CBN	2.93	123.53	116.96
5	B	502	7TR	CBK-CBN-NBQ	2.90	125.62	123.79
5	B	502	7TR	CAY-CBO-NBR	-2.70	108.19	112.46
5	B	502	7TR	CAT-NBC-CAU	2.60	108.64	105.24
6	B	503	FPP	O2A-PA-O3A	2.48	113.99	107.27
6	B	503	FPP	O3A-PA-O1A	-2.32	103.73	110.70
6	B	503	FPP	O3B-PB-O2B	2.18	115.97	107.80
6	B	503	FPP	C4-C3-C2	-2.11	118.22	123.63
5	B	502	7TR	CBB-CBO-NBR	2.06	116.25	112.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

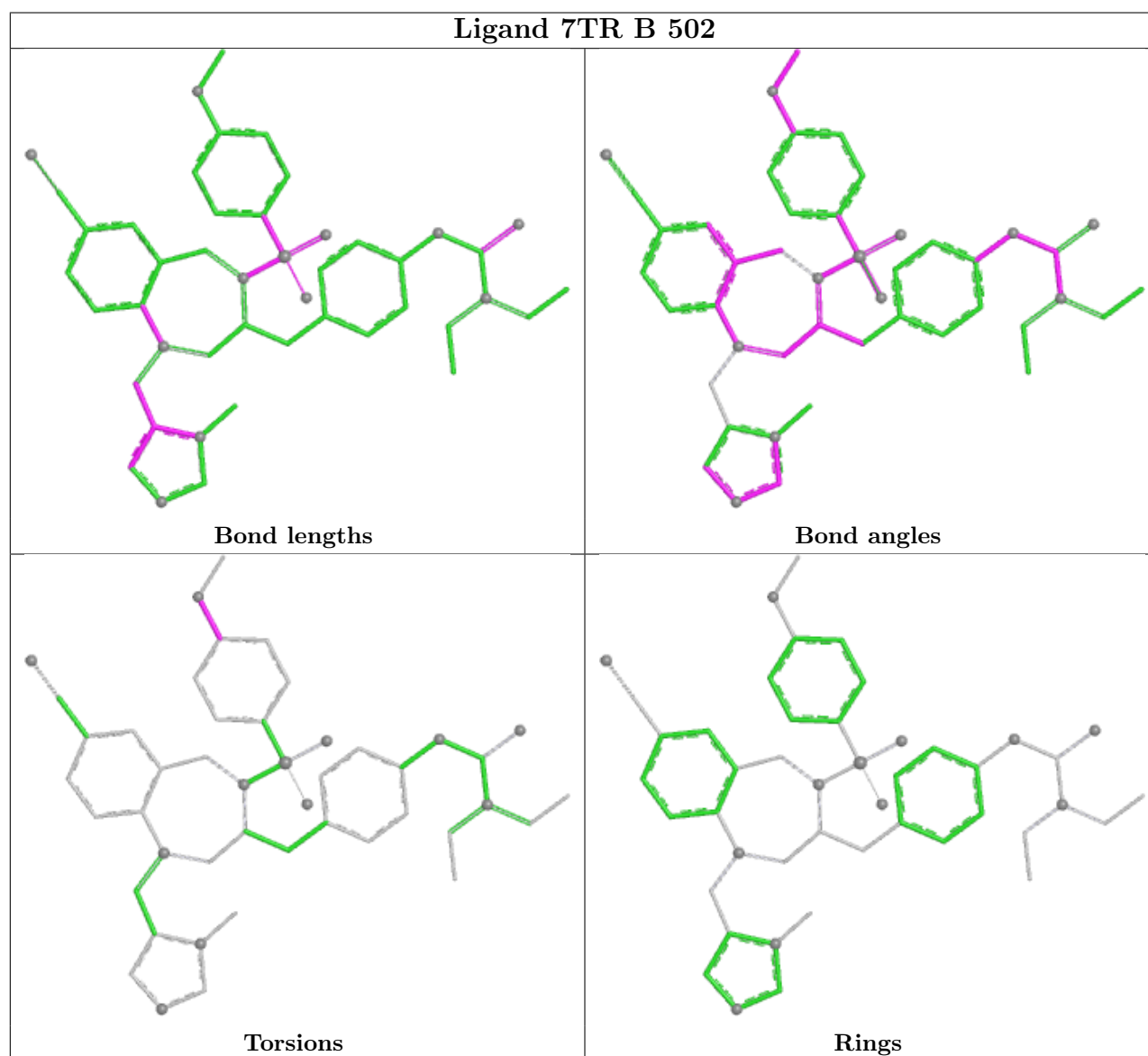
Mol	Chain	Res	Type	Atoms
5	B	502	7TR	CAO-CBI-OB-D-CAC
5	B	502	7TR	CAP-CBI-OB-D-CAC
6	B	503	FPP	C4-C3-C5-C6
6	B	503	FPP	C2-C3-C5-C6
6	B	503	FPP	PB-O3A-PA-O1A
6	B	503	FPP	PB-O3A-PA-O2A

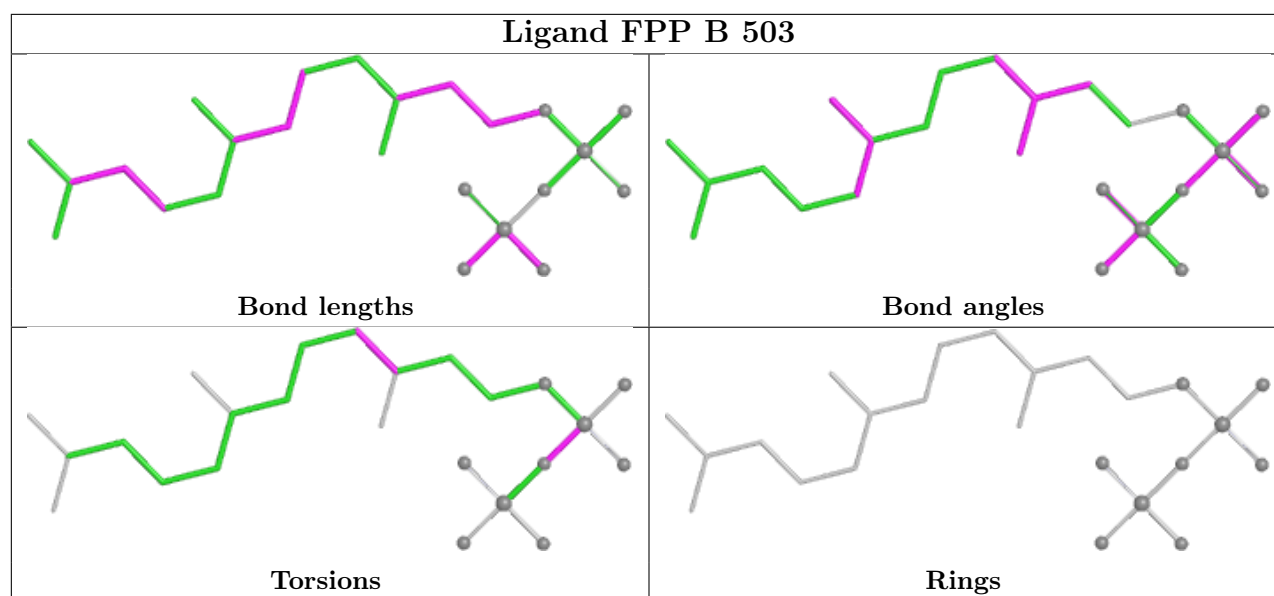
There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	7TR	9	0
3	B	504	DMS	9	0
6	B	503	FPP	10	0
3	A	401	DMS	3	0
3	B	505	DMS	4	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	315/377 (83%)	0.59	35 (11%) 10 8	26, 53, 88, 100	2 (0%)
2	B	403/427 (94%)	0.31	29 (7%) 21 18	27, 49, 75, 94	1 (0%)
All	All	718/804 (89%)	0.44	64 (8%) 15 13	26, 51, 81, 100	3 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	LEU	5.3
2	B	64	PHE	5.0
1	A	369	ARG	4.9
2	B	423	PHE	4.7
1	A	331	GLU	4.6
2	B	121	ILE	4.2
1	A	55	PHE	4.2
1	A	328	ASP	4.1
1	A	306	HIS	3.4
1	A	299	LEU	3.3
1	A	305	SER	3.3
1	A	307	SER	3.2
1	A	253	ARG	3.2
1	A	304	PRO	3.1
1	A	333	ILE	3.0
2	B	380	ALA	2.9
1	A	252	ASP	2.8
1	A	286	ASP	2.8
2	B	409	ILE	2.7
1	A	342	GLU	2.7
2	B	377	GLY	2.6
2	B	313	ARG	2.6
2	B	120	GLN	2.5
2	B	381	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.5
2	B	266	ARG	2.5
1	A	364	GLN	2.5
2	B	315	LEU	2.4
2	B	382	LEU	2.4
1	A	287	ARG	2.4
2	B	122	VAL	2.4
2	B	322	ALA	2.4
1	A	339	GLU	2.4
1	A	261	GLN	2.4
1	A	366	LYS	2.3
1	A	75	ILE	2.3
1	A	334	LEU	2.3
2	B	317	ALA	2.3
2	B	76	GLU	2.3
1	A	300	LEU	2.3
2	B	69	PRO	2.3
1	A	338	LEU	2.3
2	B	325	MET	2.3
1	A	325	ASN	2.2
2	B	422	GLY	2.2
1	A	320	GLU	2.2
2	B	198	GLU	2.2
2	B	412	THR	2.2
2	B	419	PRO	2.2
2	B	175	GLU	2.2
1	A	332	ASP	2.2
2	B	62	TYR	2.1
2	B	417	GLN	2.1
1	A	365	SER	2.1
1	A	368	SER	2.1
2	B	271	LYS	2.1
2	B	420	VAL	2.1
2	B	21	GLU	2.1
1	A	303	GLN	2.1
2	B	379	GLY	2.1
1	A	256	LEU	2.1
1	A	326	GLN	2.1
1	A	336	LYS	2.0
1	A	251	SER	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](#)

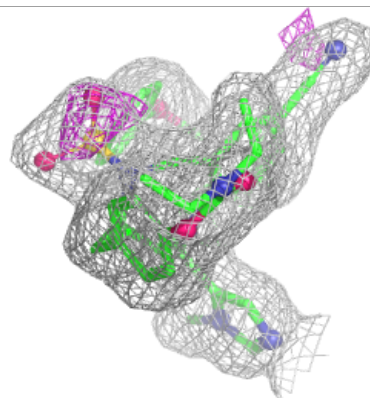
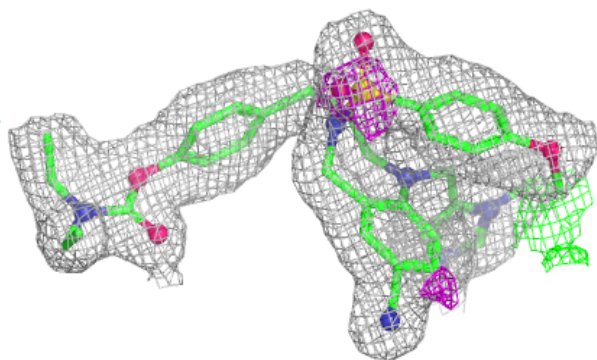
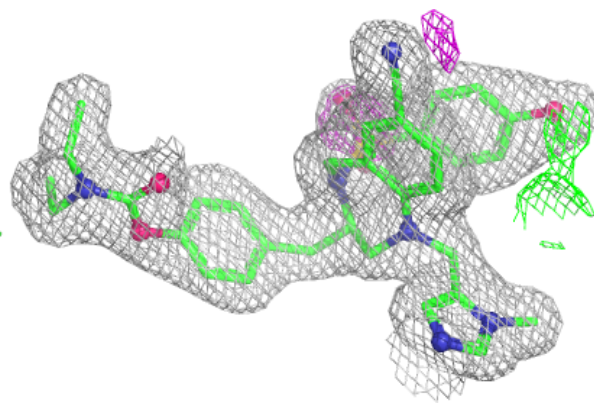
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	DMS	B	505	4/4	0.92	0.28	79,88,91,95	0
3	DMS	B	504	4/4	0.96	0.16	62,69,69,75	0
3	DMS	A	401	4/4	0.96	0.14	71,76,76,90	0
5	7TR	B	502	46/46	0.96	0.08	33,37,54,61	0
6	FPP	B	503	24/24	0.97	0.10	34,45,49,51	0
4	ZN	B	501	1/1	1.00	0.02	36,36,36,36	0

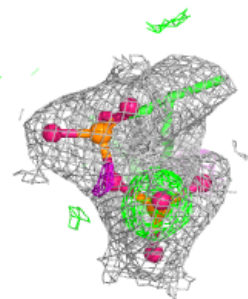
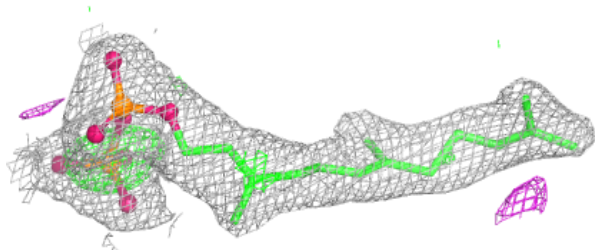
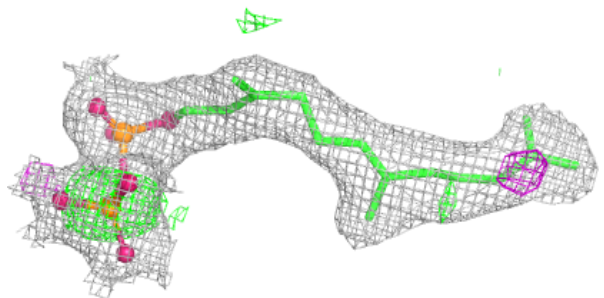
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7TR 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)

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.