



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:18 AM UTC

PDB ID : 4GTP / pdb_00004gtp
Title : FTase in complex with BMS analogue 16
Authors : Guo, Z.; Stigter, E.A.; Bon, R.S.; Waldmann, H.; Blankenfeldt, W.; Goody, R.S.
Deposited on : 2012-08-29
Resolution : 2.75 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

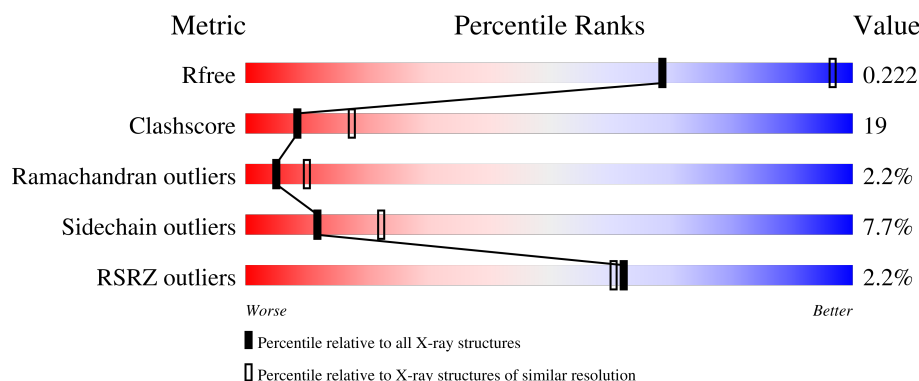
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	2% 51% 29% •• 16%
2	B	427	2% 62% 26% 5% • 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	-
5	FPP	B	502	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6072 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.

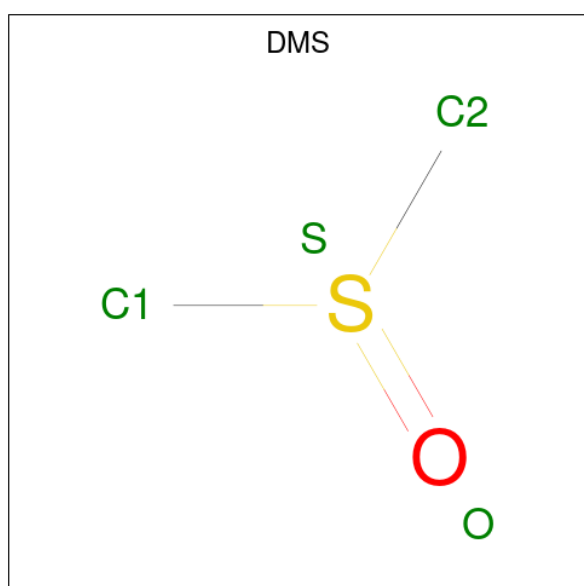
- Molecule 1 is a protein called Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2688	1712	473	498	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
			3171	2028	544	576	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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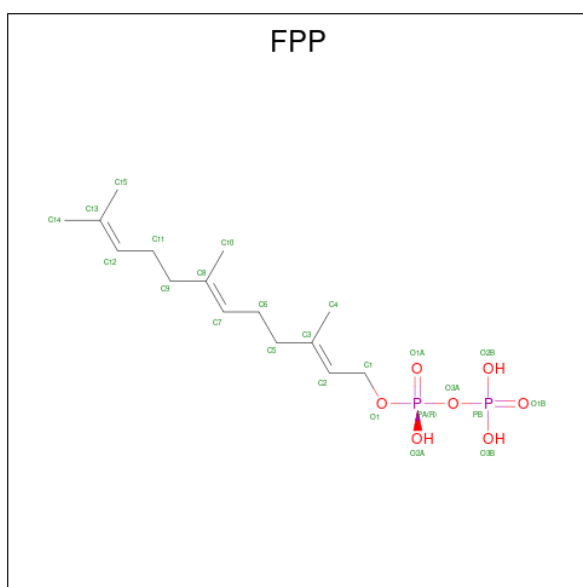
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

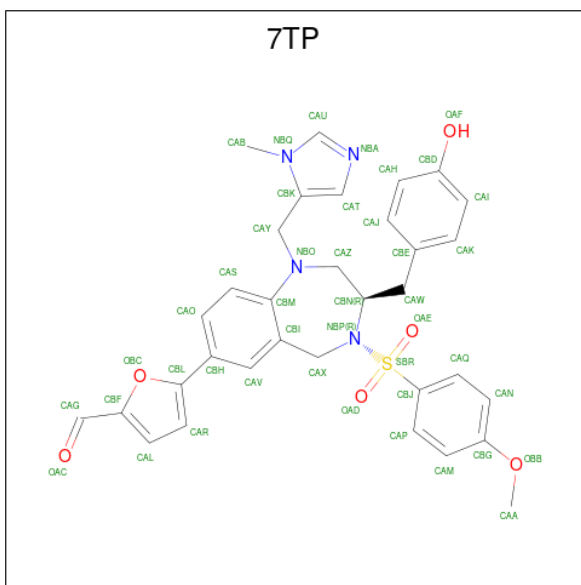
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is FARNESYL DIPHOSPHATE (CCD ID: FPP) (formula: C₁₅H₂₈O₇P₂).



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

- Molecule 6 is 5-{(3R)-3-(4-hydroxybenzyl)-4-[(4-methoxyphenyl)sulfonyl]-1-[(1-methyl-1H-imidazol-5-yl)methyl]-2,3,4,5-tetrahydro-1H-1,4-benzodiazepin-7-yl}furan-2-carbaldehyde (CCD ID: 7TP) (formula: C₃₃H₃₂N₄O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			44	33	4	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	57	Total O 57 57	0	0
7	B	71	Total O 71 71	0	0

CYS
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.65Å 171.65Å 70.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.75 29.91 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.91-2.75) 99.9 (29.91-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.226 (Not available) , 0.222	Depositor DCC
R_{free} test set	1557 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6072	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, FPP, 7TP, 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	1.13	1/2754 (0.0%)	1.14	7/3738 (0.2%)
2	B	1.21	6/3260 (0.2%)	1.22	15/4428 (0.3%)
All	All	1.17	7/6014 (0.1%)	1.19	22/8166 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	ILE	CA-CB	10.63	1.65	1.54
2	B	409	ILE	CA-CB	7.17	1.61	1.54
2	B	260	VAL	CA-CB	-6.96	1.46	1.54
2	B	68	VAL	CA-CB	6.19	1.62	1.54
1	A	158	ILE	CA-CB	-6.14	1.46	1.54
2	B	126	VAL	CA-CB	-5.24	1.48	1.54
2	B	348	GLY	N-CA	5.05	1.50	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	VAL	CB-CA-C	-8.13	99.55	112.16
2	B	277	VAL	CB-CA-C	-7.09	102.81	111.88
1	A	253	ARG	N-CA-C	6.97	119.77	111.33
2	B	351	LEU	N-CA-C	6.75	119.33	109.07
1	A	192	ILE	CB-CA-C	-6.71	103.38	111.97
2	B	275	GLN	N-CA-C	-6.51	104.26	111.82
2	B	116	GLU	CA-C-N	-6.43	112.41	120.51
2	B	116	GLU	C-N-CA	-6.43	112.41	120.51
2	B	277	VAL	N-CA-CB	6.18	117.37	110.51
1	A	352	ARG	CG-CD-NE	-5.53	99.84	112.00
2	B	358	ARG	CB-CA-C	-5.51	99.45	110.42
2	B	418	LYS	N-CA-C	-5.50	103.80	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	327	HIS	N-CA-C	5.48	118.49	109.72
2	B	345	CYS	CA-C-N	5.29	125.36	119.32
2	B	345	CYS	C-N-CA	5.29	125.36	119.32
1	A	168	VAL	CB-CA-C	5.19	119.14	112.14
1	A	192	ILE	N-CA-C	-5.10	105.53	110.42
2	B	171	VAL	CB-CA-C	-5.09	105.37	112.04
2	B	50	LYS	N-CA-C	5.02	117.13	111.11
1	A	83	GLY	CA-C-N	5.01	124.45	119.24
1	A	83	GLY	C-N-CA	5.01	124.45	119.24
2	B	43	VAL	N-CA-C	-5.00	105.11	110.36

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	2688	0	2614	108	0
2	B	3171	0	3098	113	0
3	A	4	0	6	1	0
3	B	12	0	18	12	0
4	B	1	0	0	0	0
5	B	24	0	25	15	0
6	B	44	0	32	6	0
7	A	57	0	0	14	0
7	B	71	0	0	12	0
All	All	6072	0	5793	223	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 19.

All (223) 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)
5:B:502:FPP:H102	3:B:504:DMS:H11	1.29	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:502:FPP:H61	3:B:504:DMS:H13	1.18	1.10
1:A:357:ARG:HD2	7:A:521:HOH:O	1.53	1.08
5:B:502:FPP:H102	3:B:504:DMS:C1	1.84	1.08
2:B:121:ILE:HA	7:B:645:HOH:O	1.53	1.07
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.40	1.02
2:B:280:ARG:HH11	2:B:289:GLN:HE21	1.10	0.99
1:A:329:ASN:HB3	1:A:332:ASP:CB	1.94	0.97
2:B:386:VAL:HG21	2:B:393:VAL:CG1	1.99	0.92
1:A:159:ILE:HG12	1:A:168:VAL:HG13	1.53	0.90
5:B:502:FPP:C10	3:B:504:DMS:C1	2.50	0.89
5:B:502:FPP:C6	3:B:504:DMS:H13	2.03	0.89
1:A:323:LEU:HD11	1:A:333:ILE:HG22	1.56	0.87
2:B:280:ARG:NH1	2:B:289:GLN:HE21	1.71	0.87
2:B:177:LEU:HD21	2:B:210:VAL:HG13	1.58	0.83
1:A:358:TYR:OH	2:B:320:ASP:OD2	1.97	0.82
2:B:150:LEU:HB2	2:B:193:MET:CE	2.09	0.82
2:B:150:LEU:HB2	2:B:193:MET:HE2	1.62	0.82
7:A:536:HOH:O	2:B:329:MET:SD	2.39	0.81
1:A:296:LEU:O	1:A:296:LEU:HD12	1.81	0.80
2:B:280:ARG:NH1	2:B:289:GLN:NE2	2.30	0.79
1:A:262:TYR:CZ	1:A:266:MET:HE3	2.18	0.78
1:A:329:ASN:CB	1:A:332:ASP:HB3	2.13	0.78
2:B:386:VAL:CG2	2:B:393:VAL:CG1	2.61	0.78
1:A:296:LEU:HD12	1:A:296:LEU:C	2.08	0.77
1:A:349:ASP:OD2	1:A:352:ARG:HD2	1.84	0.77
2:B:308:LEU:HD12	2:B:330:PHE:CD1	2.21	0.76
2:B:277:VAL:HG21	7:B:656:HOH:O	1.86	0.75
1:A:56:LEU:HD12	7:A:511:HOH:O	1.86	0.75
1:A:355:TYR:HA	7:A:536:HOH:O	1.86	0.75
2:B:308:LEU:HD12	2:B:330:PHE:HD1	1.51	0.74
5:B:502:FPP:C10	3:B:504:DMS:H11	2.11	0.73
3:A:401:DMS:H21	6:B:503:7TP:OAD	1.89	0.73
1:A:357:ARG:CD	7:A:521:HOH:O	2.20	0.73
2:B:325:MET:O	2:B:381:MET:HE2	1.88	0.73
2:B:377:GLY:HA2	2:B:382:LEU:HD23	1.69	0.73
2:B:192:LEU:HD23	2:B:199:VAL:HG12	1.70	0.73
2:B:386:VAL:CG2	2:B:393:VAL:HG12	2.19	0.72
2:B:118:ILE:HD11	7:B:643:HOH:O	1.90	0.71
2:B:386:VAL:HG22	2:B:393:VAL:HG12	1.71	0.70
2:B:95:CYS:HB2	3:B:505:DMS:H11	1.73	0.70
1:A:97:ARG:HD2	7:A:542:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:CE2	1:A:266:MET:HE3	2.27	0.70
1:A:286:ASP:HB3	7:A:506:HOH:O	1.90	0.70
1:A:166:TYR:CE2	2:B:202:ARG:NH1	2.61	0.69
1:A:255:VAL:HG13	1:A:258:ARG:HH21	1.56	0.69
2:B:27:ARG:HB3	2:B:29:GLU:OE2	1.93	0.68
1:A:198:LYS:HD3	2:B:294:LYS:HD3	1.75	0.68
1:A:152:MET:O	1:A:156:ILE:HG13	1.94	0.67
1:A:159:ILE:CG1	1:A:168:VAL:HG13	2.23	0.67
1:A:329:ASN:HB3	1:A:332:ASP:HB2	1.75	0.66
2:B:98:ALA:O	2:B:142:GLY:HA3	1.95	0.66
1:A:369:ARG:HA	1:A:369:ARG:HE	1.61	0.66
1:A:72:TRP:O	7:A:529:HOH:O	2.13	0.66
2:B:74:GLN:H	2:B:344:GLN:HE22	1.45	0.65
2:B:93:TYR:HE1	6:B:503:7TP:CAG	2.10	0.64
2:B:386:VAL:HG21	2:B:393:VAL:HG11	1.79	0.63
2:B:277:VAL:CG1	2:B:307:LEU:HD12	2.29	0.63
2:B:312:HIS:HD2	7:B:632:HOH:O	1.81	0.63
1:A:160:GLU:OE2	1:A:195:GLN:NE2	2.22	0.62
1:A:272:HIS:ND1	2:B:38:ASP:OD1	2.33	0.62
1:A:334:LEU:HD22	1:A:367:HIS:O	1.99	0.62
2:B:128:GLN:OE1	7:B:649:HOH:O	2.16	0.62
1:A:284:LEU:HD13	1:A:295:LEU:HD21	1.81	0.61
2:B:213:LEU:HD11	2:B:401:TYR:CD1	2.36	0.61
1:A:326:GLN:HE21	1:A:326:GLN:HA	1.66	0.60
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.84	0.60
1:A:262:TYR:CE2	1:A:266:MET:CE	2.85	0.60
1:A:323:LEU:CD1	1:A:333:ILE:HG22	2.29	0.60
1:A:108:GLN:HG3	7:A:525:HOH:O	2.01	0.60
1:A:166:TYR:CZ	2:B:202:ARG:NH1	2.70	0.59
1:A:281:LYS:O	1:A:285:GLN:HG2	2.02	0.59
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.84	0.59
2:B:291:ARG:HG3	2:B:294:LYS:HG3	1.82	0.59
1:A:79:PRO:HA	1:A:101:ASP:OD1	2.03	0.58
1:A:250:TYR:OH	1:A:279:TYR:OH	2.14	0.58
1:A:170:HIS:HE1	2:B:196:GLY:O	1.87	0.58
2:B:202:ARG:HG2	5:B:502:FPP:H152	1.85	0.57
1:A:369:ARG:HA	1:A:369:ARG:NE	2.19	0.57
2:B:118:ILE:CG2	2:B:122:VAL:HG23	2.34	0.57
2:B:294:LYS:HE3	5:B:502:FPP:O2B	2.05	0.57
1:A:303:GLN:HB3	1:A:304:PRO:CD	2.35	0.57
1:A:207:GLN:HE21	1:A:239:GLN:NE2	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:GLN:HG3	2:B:387:MET:SD	2.46	0.56
2:B:121:ILE:O	2:B:124:THR:HG22	2.05	0.56
2:B:308:LEU:CD1	2:B:330:PHE:HD1	2.17	0.56
2:B:277:VAL:HG11	2:B:307:LEU:HB2	1.88	0.55
2:B:348:GLY:O	2:B:358:ARG:HD3	2.07	0.55
2:B:386:VAL:HG11	2:B:393:VAL:HG13	1.89	0.54
2:B:134:GLN:HE22	2:B:173:ASN:H	1.55	0.54
1:A:326:GLN:HA	1:A:326:GLN:NE2	2.22	0.54
1:A:244:ILE:O	1:A:245:SER:C	2.49	0.54
2:B:308:LEU:HD22	2:B:329:MET:HB2	1.89	0.53
2:B:37:ASP:O	2:B:39:SER:N	2.41	0.53
1:A:159:ILE:HG12	1:A:168:VAL:CG1	2.31	0.53
2:B:64:PHE:HD1	7:B:650:HOH:O	1.92	0.53
1:A:97:ARG:CD	7:A:542:HOH:O	2.53	0.53
1:A:142:ARG:HD2	7:A:545:HOH:O	2.09	0.53
1:A:239:GLN:HE21	1:A:239:GLN:HA	1.73	0.53
2:B:73:LEU:O	2:B:75:ARG:N	2.41	0.52
1:A:129:ALA:HB2	3:B:505:DMS:H12	1.91	0.52
2:B:308:LEU:HD13	2:B:329:MET:C	2.35	0.52
1:A:296:LEU:HD11	1:A:300:LEU:HD11	1.92	0.52
1:A:198:LYS:CD	2:B:294:LYS:HD3	2.37	0.52
2:B:118:ILE:N	2:B:118:ILE:HD13	2.24	0.52
1:A:328:ASP:O	1:A:329:ASN:HB2	2.09	0.52
1:A:286:ASP:CB	7:A:506:HOH:O	2.55	0.52
2:B:118:ILE:HG22	2:B:122:VAL:HG23	1.91	0.51
2:B:277:VAL:HG13	2:B:307:LEU:HD12	1.92	0.51
1:A:87:VAL:O	1:A:88:VAL:C	2.53	0.51
1:A:223:VAL:HG13	1:A:236:VAL:CG1	2.41	0.51
2:B:180:TYR:CZ	2:B:184:LEU:HD11	2.46	0.51
1:A:143:SER:C	1:A:145:GLN:H	2.19	0.51
2:B:319:GLY:O	2:B:320:ASP:C	2.53	0.51
5:B:502:FPP:H103	3:B:504:DMS:C1	2.38	0.50
2:B:311:LEU:HD12	7:B:656:HOH:O	2.11	0.50
1:A:303:GLN:HB3	1:A:304:PRO:HD3	1.93	0.50
2:B:22:PRO:HD2	7:B:602:HOH:O	2.11	0.50
5:B:502:FPP:H102	3:B:504:DMS:H13	1.82	0.50
2:B:239:ILE:HB	2:B:252:THR:HA	1.93	0.49
1:A:224:ASP:OD1	1:A:240:ARG:NH2	2.46	0.49
1:A:328:ASP:O	1:A:329:ASN:CB	2.60	0.49
2:B:74:GLN:N	2:B:344:GLN:HE22	2.09	0.49
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LYS:O	2:B:65:ASN:N	2.46	0.49
2:B:337:GLU:OE2	2:B:387:MET:HE2	2.12	0.49
2:B:37:ASP:O	2:B:38:ASP:C	2.56	0.49
2:B:312:HIS:CD2	7:B:632:HOH:O	2.61	0.49
1:A:65:LEU:HD12	1:A:67:ARG:NH1	2.28	0.49
2:B:68:VAL:HG23	2:B:69:PRO:HD2	1.95	0.48
2:B:271:LYS:NZ	7:B:635:HOH:O	2.45	0.48
1:A:207:GLN:HG2	1:A:239:GLN:HE22	1.78	0.48
2:B:117:PRO:C	2:B:118:ILE:HD13	2.38	0.48
1:A:84:PRO:HG2	7:B:649:HOH:O	2.12	0.48
2:B:200:ASP:OD1	2:B:202:ARG:HB2	2.13	0.48
2:B:251:TYR:CE2	5:B:502:FPP:H51	2.48	0.48
2:B:308:LEU:CD1	2:B:330:PHE:HB3	2.44	0.48
2:B:375:HIS:HE1	2:B:394:LEU:O	1.97	0.48
5:B:502:FPP:O1	3:B:504:DMS:O	2.32	0.48
1:A:182:PRO:HG3	1:A:213:PHE:CD2	2.49	0.48
1:A:112:ARG:O	1:A:144:LEU:HD21	2.14	0.47
2:B:157:VAL:HG21	2:B:210:VAL:HG22	1.97	0.47
1:A:368:SER:HA	7:A:528:HOH:O	2.14	0.47
2:B:277:VAL:HG13	2:B:307:LEU:CD1	2.45	0.47
2:B:409:ILE:HG22	2:B:410:GLN:N	2.29	0.47
1:A:284:LEU:HD13	1:A:295:LEU:CD2	2.45	0.47
1:A:294:ASN:O	1:A:298:GLN:HG3	2.15	0.47
1:A:144:LEU:O	1:A:145:GLN:C	2.57	0.46
1:A:323:LEU:HD21	1:A:330:LYS:O	2.16	0.46
1:A:326:GLN:HE21	1:A:326:GLN:CA	2.29	0.46
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.76	0.46
2:B:301:SER:O	2:B:305:ALA:HB3	2.15	0.46
1:A:296:LEU:C	1:A:296:LEU:CD1	2.78	0.46
2:B:55:ILE:HG22	2:B:59:PHE:CE2	2.51	0.45
1:A:311:LEU:C	1:A:311:LEU:HD23	2.41	0.45
5:B:502:FPP:C10	3:B:504:DMS:H13	2.40	0.45
1:A:338:LEU:HD23	1:A:360:GLY:HA2	1.97	0.45
1:A:172:ARG:NH1	1:A:188:PHE:CE2	2.85	0.45
1:A:240:ARG:HD3	1:A:259:GLU:OE1	2.17	0.45
1:A:357:ARG:NH2	7:B:612:HOH:O	2.49	0.45
2:B:420:VAL:O	2:B:423:PHE:HA	2.17	0.45
1:A:112:ARG:HA	1:A:140:LEU:CD2	2.47	0.44
2:B:60:SER:O	2:B:61:SER:C	2.59	0.44
2:B:100:ARG:N	2:B:101:PRO:CD	2.80	0.44
2:B:193:MET:CE	2:B:193:MET:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:HG	2:B:401:TYR:CE1	2.52	0.44
2:B:280:ARG:HH11	2:B:280:ARG:HA	1.82	0.44
1:A:182:PRO:HG3	1:A:213:PHE:CG	2.52	0.44
2:B:37:ASP:C	2:B:39:SER:N	2.75	0.44
1:A:159:ILE:O	1:A:160:GLU:C	2.56	0.44
2:B:220:ASP:O	2:B:221:LEU:C	2.60	0.44
2:B:50:LYS:O	2:B:53:GLU:HB3	2.17	0.44
1:A:258:ARG:HE	1:A:258:ARG:HB3	1.70	0.44
2:B:350:LEU:HB2	2:B:363:THR:HA	2.00	0.44
1:A:309:PRO:HA	1:A:312:ILE:HD12	1.99	0.44
2:B:45:SER:O	2:B:46:ILE:C	2.60	0.44
2:B:359:ASP:HB2	6:B:503:7TP:CBF	2.48	0.44
2:B:73:LEU:HD12	2:B:344:GLN:NE2	2.33	0.44
2:B:150:LEU:CB	2:B:193:MET:CE	2.89	0.44
1:A:78:VAL:O	1:A:104:ARG:HD2	2.18	0.43
1:A:270:VAL:HG22	2:B:40:VAL:HG21	1.99	0.43
1:A:152:MET:O	1:A:156:ILE:CG1	2.64	0.43
1:A:172:ARG:NH1	1:A:188:PHE:CD2	2.87	0.43
2:B:250:GLY:HA3	5:B:502:FPP:C8	2.48	0.43
2:B:316:HIS:C	2:B:318:GLN:H	2.27	0.43
1:A:77:PRO:HG3	1:A:102:TYR:CZ	2.54	0.43
1:A:338:LEU:HD11	1:A:364:GLN:HG3	2.01	0.43
2:B:149:HIS:ND1	2:B:152:PRO:HD2	2.33	0.43
1:A:312:ILE:CG2	1:A:340:LEU:HD22	2.47	0.43
1:A:351:ILE:HD12	1:A:351:ILE:HA	1.91	0.42
1:A:64:VAL:CG1	1:A:68:ASP:HB2	2.49	0.42
1:A:223:VAL:HG13	1:A:236:VAL:HG13	2.00	0.42
2:B:251:TYR:CZ	5:B:502:FPP:H51	2.55	0.42
1:A:284:LEU:CD1	1:A:295:LEU:HD21	2.48	0.42
2:B:227:GLU:O	2:B:231:ARG:HG3	2.20	0.42
1:A:274:GLU:HG2	1:A:278:ASN:ND2	2.35	0.41
1:A:256:LEU:O	1:A:260:VAL:HG23	2.20	0.41
1:A:311:LEU:HD23	1:A:311:LEU:O	2.19	0.41
2:B:122:VAL:O	2:B:123:ALA:C	2.62	0.41
2:B:360:PHE:CD2	6:B:503:7TP:OAC	2.73	0.41
2:B:262:LEU:O	2:B:263:LYS:HB2	2.20	0.41
2:B:63:LYS:HG2	2:B:64:PHE:N	2.34	0.41
2:B:234:ASN:OD1	2:B:234:ASN:C	2.63	0.41
1:A:85:SER:HA	1:A:86:PRO:HD3	1.87	0.41
1:A:207:GLN:HE21	1:A:239:GLN:HE22	1.67	0.41
1:A:285:GLN:O	1:A:286:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:TYR:CE1	2:B:323:LEU:HD23	2.55	0.41
2:B:282:MET:HE3	2:B:282:MET:HB3	1.98	0.41
1:A:223:VAL:HG11	1:A:240:ARG:HB2	2.03	0.41
1:A:349:ASP:OD2	1:A:352:ARG:HB2	2.21	0.41
1:A:352:ARG:O	1:A:353:LYS:C	2.64	0.41
2:B:93:TYR:CE1	6:B:503:7TP:CAG	2.99	0.41
2:B:150:LEU:HD23	2:B:150:LEU:HA	1.95	0.41
2:B:199:VAL:O	2:B:200:ASP:CB	2.68	0.41
2:B:360:PHE:HD2	6:B:503:7TP:OAC	2.03	0.41
1:A:138:ARG:NH2	7:A:513:HOH:O	2.53	0.41
1:A:146:LYS:HE3	1:A:146:LYS:HB3	1.85	0.40
2:B:82:LEU:HD11	2:B:110:SER:HB3	2.04	0.40
1:A:252:ASP:OD2	1:A:255:VAL:HG23	2.20	0.40
2:B:260:VAL:O	2:B:261:ILE:C	2.61	0.40
1:A:62:THR:HG22	1:A:62:THR:O	2.22	0.40
2:B:276:TRP:O	2:B:277:VAL:C	2.64	0.40
2:B:308:LEU:HD23	2:B:308:LEU:HA	1.81	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	313/377 (83%)	276 (88%)	34 (11%)	3 (1%)	12	24
2	B	402/427 (94%)	368 (92%)	21 (5%)	13 (3%)	3	5
All	All	715/804 (89%)	644 (90%)	55 (8%)	16 (2%)	5	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	38	ASP

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Mol	Chain	Res	Type
2	B	63	LYS
2	B	64	PHE
2	B	74	GLN
2	B	358	ARG
2	B	378	SER
1	A	302	LEU
1	A	329	ASN
2	B	66	HIS
2	B	200	ASP
2	B	221	LEU
2	B	317	ALA
1	A	304	PRO
2	B	421	PRO
2	B	422	GLY
2	B	22	PRO

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	294/338 (87%)	269 (92%)	25 (8%)	10	18
2	B	340/363 (94%)	316 (93%)	24 (7%)	13	25
All	All	634/701 (90%)	585 (92%)	49 (8%)	12	22

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	67	ARG
1	A	71	GLU
1	A	109	ARG
1	A	121	ARG
1	A	156	ILE
1	A	168	VAL
1	A	211	GLN

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Mol	Chain	Res	Type
1	A	228	LYS
1	A	239	GLN
1	A	251	SER
1	A	257	GLU
1	A	268	LYS
1	A	281	LYS
1	A	287	ARG
1	A	296	LEU
1	A	307	SER
1	A	320	GLU
1	A	330	LYS
1	A	342	GLU
1	A	343	ILE
1	A	346	LYS
1	A	348	LYS
1	A	352	ARG
1	A	369	ARG
2	B	21	GLU
2	B	25	SER
2	B	34	ARG
2	B	39	SER
2	B	61	SER
2	B	67	LEU
2	B	68	VAL
2	B	118	ILE
2	B	193	MET
2	B	199	VAL
2	B	200	ASP
2	B	201	VAL
2	B	210	VAL
2	B	264	LYS
2	B	266	ARG
2	B	273	LEU
2	B	277	VAL
2	B	279	SER
2	B	280	ARG
2	B	325	MET
2	B	351	LEU
2	B	357	SER
2	B	372	ILE
2	B	409	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	162	GLN
1	A	170	HIS
1	A	211	GLN
1	A	218	ASN
1	A	221	GLN
1	A	239	GLN
1	A	246	ASN
1	A	294	ASN
1	A	298	GLN
1	A	326	GLN
1	A	335	ASN
2	B	30	HIS
2	B	48	GLN
2	B	74	GLN
2	B	134	GLN
2	B	170	ASN
2	B	194	HIS
2	B	275	GLN
2	B	289	GLN
2	B	332	GLN
2	B	344	GLN
2	B	375	HIS
2	B	414	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 7 ligands modelled in this entry, 1 is 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
3	DMS	B	505	-	3,3,3	2.91	1 (33%)	3,3,3	0.75	0
3	DMS	B	504	-	3,3,3	2.52	1 (33%)	3,3,3	0.78	0
3	DMS	B	506	-	3,3,3	2.69	1 (33%)	3,3,3	0.75	0
3	DMS	A	401	-	3,3,3	2.72	1 (33%)	3,3,3	1.21	1 (33%)
5	FPP	B	502	-	22,23,23	1.81	9 (40%)	27,31,31	1.52	5 (18%)
6	7TP	B	503	4	49,49,49	2.68	16 (32%)	59,71,71	3.08	25 (42%)

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
5	FPP	B	502	-	-	5/25/25/25	-
6	7TP	B	503	4	-	7/28/44/44	0/5/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	503	7TP	OAE-SBR	11.43	1.55	1.43
6	B	503	7TP	CBM-NBO	-6.78	1.31	1.43
6	B	503	7TP	CBH-CBL	-5.44	1.35	1.48
3	B	505	DMS	O-S	4.79	1.81	1.50
3	A	401	DMS	O-S	4.54	1.80	1.50
3	B	506	DMS	O-S	4.37	1.79	1.50
3	B	504	DMS	O-S	4.27	1.78	1.50
6	B	503	7TP	OAD-SBR	4.07	1.47	1.43
6	B	503	7TP	CBJ-SBR	3.27	1.80	1.76
6	B	503	7TP	OBC-CBF	-3.26	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	503	7TP	CAB-NBQ	3.10	1.52	1.46
6	B	503	7TP	SBR-NBP	3.10	1.67	1.63
5	B	502	FPP	C1-C2	-3.04	1.40	1.49
6	B	503	7TP	CAV-CBI	-2.97	1.34	1.39
5	B	502	FPP	C2-C3	2.89	1.39	1.33
5	B	502	FPP	C12-C13	2.71	1.40	1.32
5	B	502	FPP	O1-C1	2.70	1.48	1.44
6	B	503	7TP	CAG-CBF	2.65	1.49	1.44
6	B	503	7TP	CAW-CBN	2.65	1.57	1.53
5	B	502	FPP	C6-C7	-2.63	1.42	1.50
5	B	502	FPP	C11-C12	-2.57	1.42	1.50
6	B	503	7TP	OBC-CBL	-2.55	1.34	1.38
6	B	503	7TP	CBK-NBQ	-2.53	1.33	1.38
6	B	503	7TP	CAT-NBA	-2.47	1.33	1.37
5	B	502	FPP	C7-C8	2.38	1.38	1.33
5	B	502	FPP	PB-O3B	-2.36	1.46	1.54
6	B	503	7TP	CAL-CAR	-2.08	1.32	1.39
6	B	503	7TP	OBB-CAA	2.07	1.48	1.42
5	B	502	FPP	C5-C6	2.05	1.60	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	7TP	CAX-CBI-CAV	-9.05	107.22	119.17
6	B	503	7TP	NBQ-CAU-NBA	-7.34	108.57	112.94
6	B	503	7TP	OAE-SBR-CBJ	6.74	116.48	108.10
6	B	503	7TP	CAX-CBI-CBM	6.18	131.94	122.45
6	B	503	7TP	OBC-CBL-CBH	5.52	123.27	116.73
6	B	503	7TP	OAE-SBR-OAD	-5.12	111.59	119.59
6	B	503	7TP	OBC-CBF-CAG	4.90	124.84	118.33
6	B	503	7TP	CAO-CBH-CAV	4.88	124.89	119.25
6	B	503	7TP	CBJ-SBR-NBP	4.86	115.84	107.36
5	B	502	FPP	C10-C8-C9	4.65	123.30	115.23
6	B	503	7TP	OBC-CBL-CAR	4.61	112.92	109.39
6	B	503	7TP	OAE-SBR-NBP	-4.04	99.90	106.97
6	B	503	7TP	CBL-OBC-CBF	-3.96	101.86	107.04
6	B	503	7TP	CBH-CAV-CBI	-3.84	115.72	121.47
6	B	503	7TP	CAQ-CBJ-SBR	3.64	123.35	119.73
6	B	503	7TP	CAS-CBM-NBO	-3.51	112.69	118.33
6	B	503	7TP	CBH-CBL-CAR	-3.31	123.45	132.99
6	B	503	7TP	CAZ-CBN-NBP	3.03	118.18	112.15
6	B	503	7TP	CAW-CBN-NBP	-2.96	107.79	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	7TP	CAV-CBH-CBL	-2.88	115.59	120.25
6	B	503	7TP	CAL-CBF-CAG	-2.84	122.14	131.53
6	B	503	7TP	CAP-CBJ-CAQ	-2.49	117.22	120.47
6	B	503	7TP	OAD-SBR-CBJ	-2.35	105.19	108.10
5	B	502	FPP	O3A-PB-O1B	-2.30	98.91	111.04
5	B	502	FPP	C10-C8-C7	-2.14	118.14	123.63
5	B	502	FPP	O3B-PB-O2B	2.10	115.67	107.80
3	A	401	DMS	C2-S-C1	2.04	108.87	98.42
6	B	503	7TP	CAQ-CAN-CBG	2.03	122.05	119.73
6	B	503	7TP	CAV-CBI-CBM	2.02	120.84	118.95
5	B	502	FPP	C6-C5-C3	2.01	119.83	113.19
6	B	503	7TP	CAJ-CAH-CBD	-2.00	117.76	119.88

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	502	FPP	C1-O1-PA-O2A
5	B	502	FPP	C1-O1-PA-O3A
6	B	503	7TP	CAX-NBP-SBR-OAE
6	B	503	7TP	OAC-CAG-CBF-OBC
6	B	503	7TP	OAC-CAG-CBF-CAL
6	B	503	7TP	CAV-CBH-CBL-CAR
6	B	503	7TP	CAO-CBH-CBL-CAR
6	B	503	7TP	CAV-CBH-CBL-OBC
6	B	503	7TP	CAO-CBH-CBL-OBC
5	B	502	FPP	C1-O1-PA-O1A
5	B	502	FPP	PB-O3A-PA-O2A
5	B	502	FPP	PB-O3A-PA-O1A

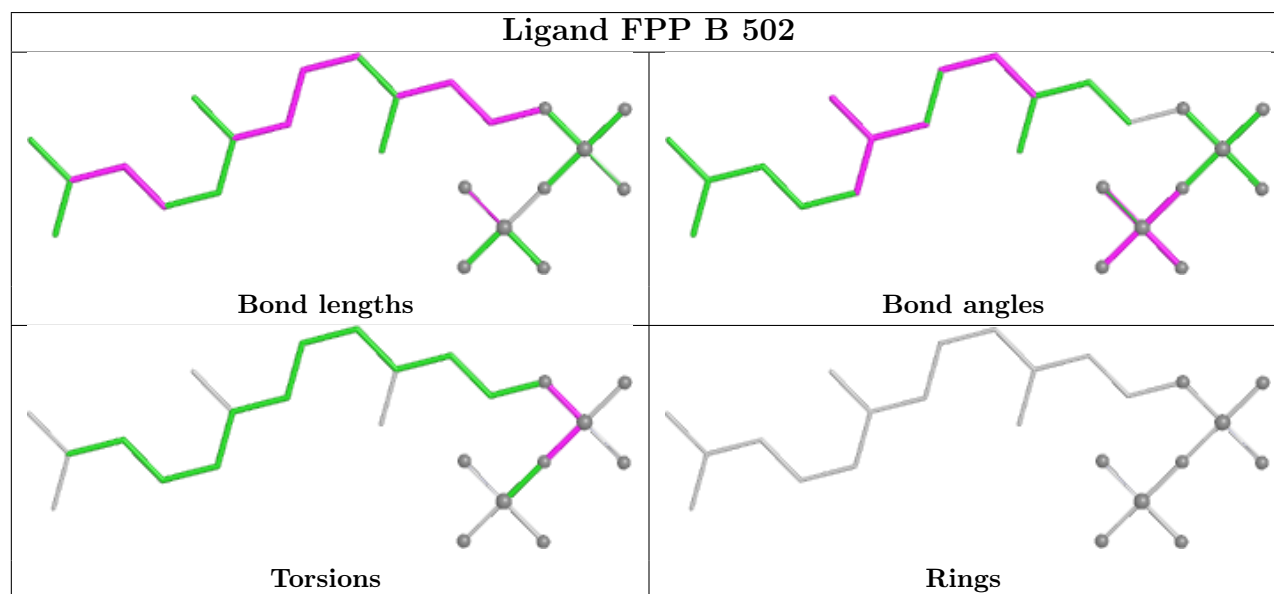
There are no ring outliers.

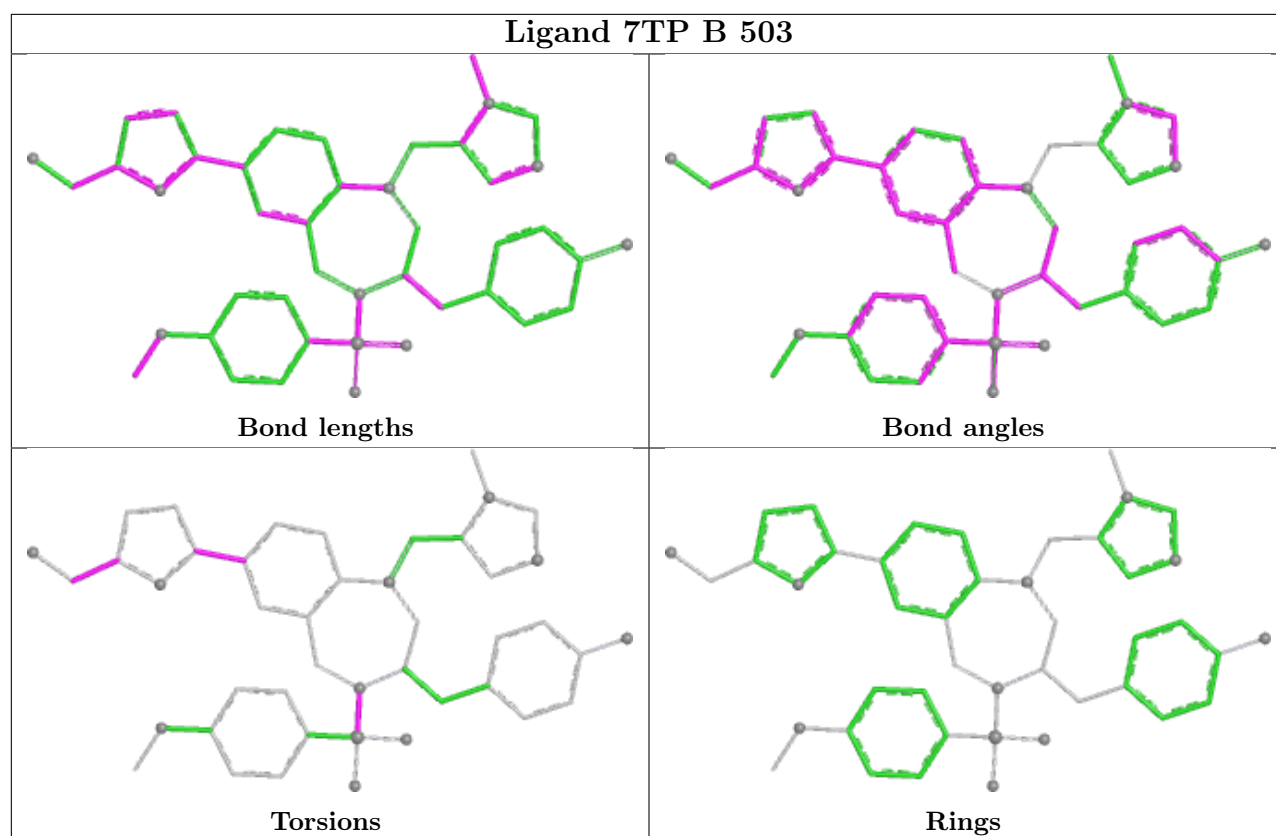
5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	505	DMS	2	0
3	B	504	DMS	10	0
3	A	401	DMS	1	0
5	B	502	FPP	15	0
6	B	503	7TP	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.14	7 (2%) 62 60	23, 51, 83, 106	0
2	B	403/427 (94%)	-0.26	9 (2%) 62 60	20, 46, 77, 107	1 (0%)
All	All	718/804 (89%)	-0.21	16 (2%) 62 60	20, 49, 81, 107	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	GLU	4.4
2	B	64	PHE	4.3
2	B	62	TYR	4.3
1	A	302	LEU	3.5
2	B	423	PHE	3.4
1	A	330	LYS	3.3
2	B	69	PRO	3.1
1	A	369	ARG	2.9
2	B	67	LEU	2.6
1	A	55	PHE	2.6
2	B	66	HIS	2.5
2	B	68	VAL	2.5
2	B	65	ASN	2.4
1	A	304	PRO	2.3
2	B	121	ILE	2.2
1	A	307	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

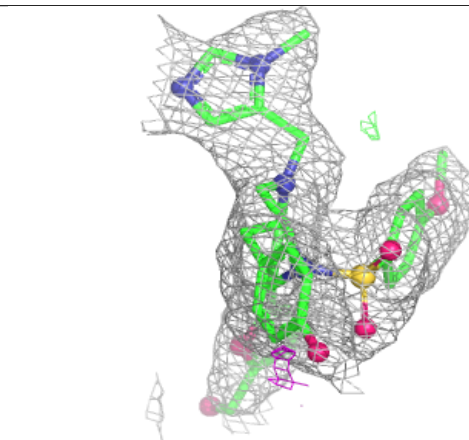
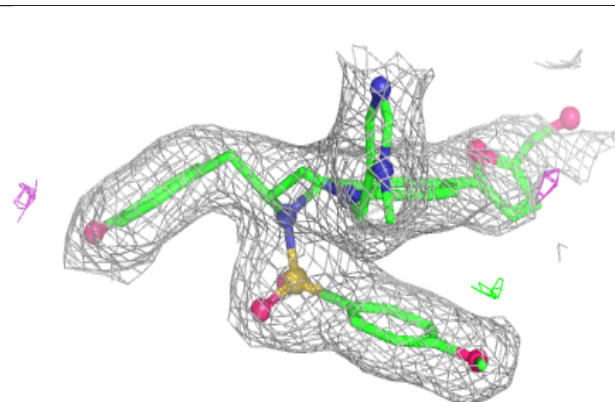
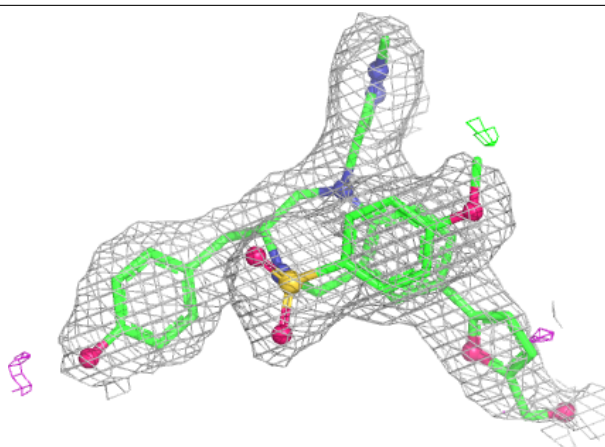
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.85	0.23	77,78,80,83	0
3	DMS	B	506	4/4	0.94	0.15	60,62,63,66	0
3	DMS	A	401	4/4	0.96	0.13	63,64,65,70	0
6	7TP	B	503	44/44	0.96	0.09	37,46,72,87	0
5	FPP	B	502	24/24	0.98	0.07	26,40,44,45	0
3	DMS	B	504	4/4	0.98	0.11	69,69,74,74	0
4	ZN	B	501	1/1	1.00	0.01	36,36,36,36	0

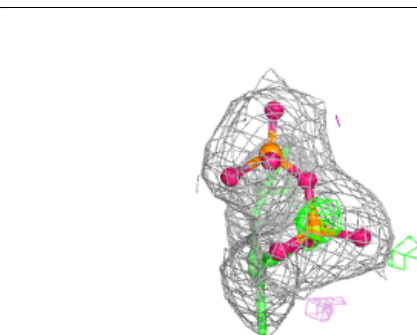
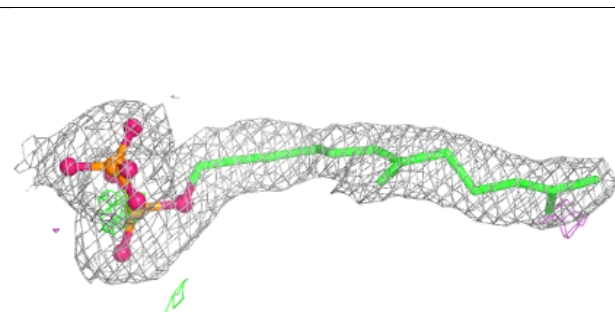
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7TP 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 FPP 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.