



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:15 am GMT

PDB ID : 4GTP
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

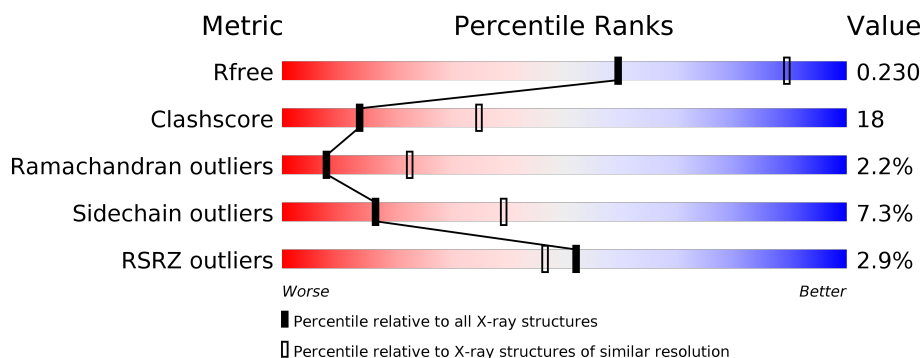
1 Overall quality at a glance

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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>•</div> <div>16%</div> </div> </div>
2	B	427	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>24%</div> <div>• •</div> <div>6%</div> </div> </div>

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
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.

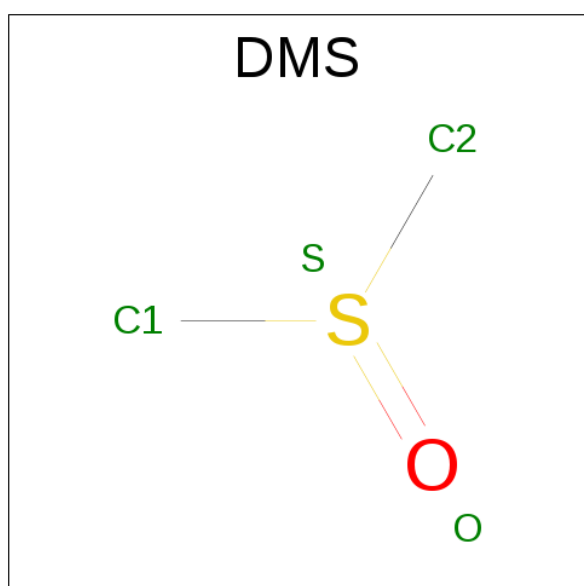
- Molecule 1 is a protein called Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

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 (three-letter code: 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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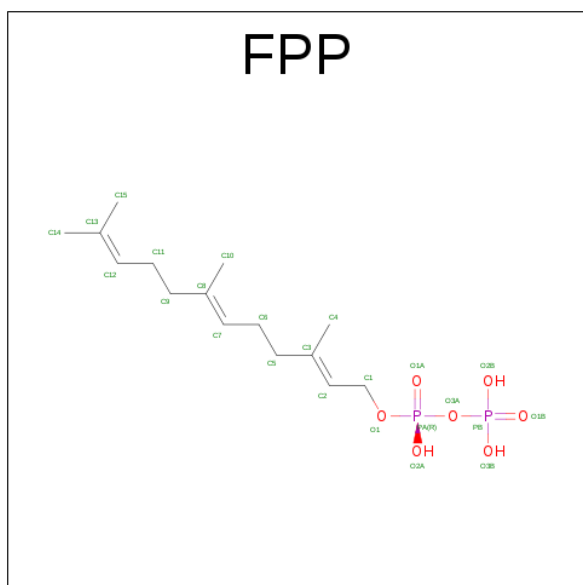
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 1	S 1	0	0
3	B	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

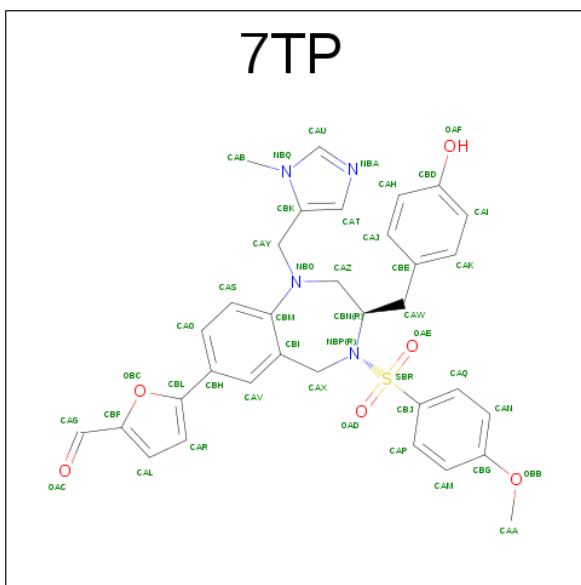
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: $C_{15}H_{28}O_7P_2$).



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 (three-letter code: 7TP) (formula: $C_{33}H_{32}N_4O_6S$).



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

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 29.71 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.91-2.75) 100.0 (29.71-2.75)	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 0.185 , 0.230	Depositor DCC
R_{free} test set	1557 reflections (5.32%)	DCC
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 , 45.0	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	0.94	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: 7TP, ZN, DMS, 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	0.94	1/2754 (0.0%)	0.92	7/3738 (0.2%)
2	B	0.96	2/3260 (0.1%)	0.94	3/4428 (0.1%)
All	All	0.95	3/6014 (0.0%)	0.93	10/8166 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	364	CYS	CB-SG	-6.89	1.70	1.82
2	B	76	GLU	CB-CG	5.60	1.62	1.52
1	A	341	CYS	CB-SG	-5.44	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	173	ARG	NE-CZ-NH2	-6.41	117.10	120.30
2	B	201	VAL	CB-CA-C	-6.24	99.55	111.40
1	A	291	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	138	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	352	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	352	ARG	CG-CD-NE	-5.70	99.84	111.80
2	B	358	ARG	CB-CA-C	-5.47	99.45	110.40
1	A	291	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	B	193	MET	CG-SD-CE	5.06	108.30	100.20

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	104	0
2	B	3171	0	3098	104	0
3	A	4	0	6	0	0
3	B	12	0	18	10	0
4	B	1	0	0	0	0
5	B	24	0	25	15	0
6	B	44	0	32	5	0
7	A	57	0	0	14	0
7	B	71	0	0	11	0
All	All	6072	0	5793	209	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 18.

All (209) 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: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
5:B:502:FPP:H102	3:B:504:DMS:H13	1.39	1.03
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
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
1:A:250:TYR:HH	1:A:279:TYR:HH	1.25	0.84
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
5:B:502:FPP:H61	3:B:504:DMS:H13	1.61	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	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
5:B:502:FPP:H61	3:B:504:DMS:C1	2.15	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
1:A:357:ARG:CD	7:A:521:HOH:O	2.20	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
1:A:296:LEU:HD12	1:A:296:LEU:C	2.08	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
1:A:97:ARG:HD2	7:A:542:HOH:O	1.92	0.70
5:B:502:FPP:H102	3:B:504:DMS:H11	1.70	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
1:A:262:TYR:CE2	1:A:266:MET:HE2	2.28	0.68
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
5:B:502:FPP:C10	3:B:504:DMS:H13	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:502:FPP:C10	3:B:504:DMS:H11	2.29	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: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
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:NE2	1:A:326:GLN:HA	2.22	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:142:ARG:HD2	7:A:545:HOH:O	2.09	0.53
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.73	0.53
1:A:97:ARG:CD	7:A:542:HOH:O	2.53	0.53
2:B:73:LEU:O	2:B:75:ARG:N	2.41	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:HD13	2:B:118:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
2:B:63:LYS:O	2:B:65:ASN:N	2.46	0.49
1:A:244:ILE:O	1:A:245:SER:C	2.49	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
1:A:207:GLN:HG2	1:A:239:GLN:HE22	1.78	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:193:MET:HE3	2:B:193:MET:HA	1.95	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
2:B:308:LEU:HD13	2:B:329:MET:C	2.35	0.47
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
2:B:277:VAL:HG13	2:B:307:LEU:CD1	2.45	0.47
1:A:368:SER:HA	7:A:528:HOH:O	2.14	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:87:VAL:O	1:A:88:VAL:C	2.53	0.47
1:A:326:GLN:CA	1:A:326:GLN:HE21	2.29	0.46
1:A:323:LEU:HD21	1:A:330:LYS:O	2.16	0.46
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:SER:O	2:B:305:ALA:HB3	2.15	0.46
2:B:319:GLY:O	2:B:320:ASP:C	2.53	0.46
2:B:325:MET:O	2:B:381:MET:HE2	2.15	0.46
2:B:337:GLU:OE2	2:B:387:MET:HE2	2.15	0.46
1:A:143:SER:C	1:A:145:GLN:H	2.19	0.45
2:B:55:ILE:HG22	2:B:59:PHE:CE2	2.51	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: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
2:B:280:ARG:HA	2:B:280:ARG:HH11	1.82	0.44
2:B:213:LEU:HG	2:B:401:TYR:CE1	2.52	0.44
1:A:182:PRO:HG3	1:A:213:PHE:CG	2.52	0.44
2:B:381:MET:HE1	2:B:382:LEU:O	2.17	0.44
2:B:50:LYS:O	2:B:53:GLU:HB3	2.17	0.44
1:A:258:ARG:HB3	1:A:258:ARG:HE	1.70	0.44
2:B:37:ASP:O	2:B:38:ASP:C	2.56	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:359:ASP:HB2	6:B:503:7TP:CBF	2.48	0.44
2:B:150:LEU:CB	2:B:193:MET:CE	2.89	0.44
2:B:73:LEU:HD12	2:B:344:GLN:NE2	2.33	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
2:B:117:PRO:C	2:B:118:ILE:HD13	2.38	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
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:HA	1:A:351:ILE:HD12	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
1:A:159:ILE:O	1:A:160:GLU:C	2.56	0.42
2:B:251:TYR:CZ	5:B:502:FPP:H51	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:O	1:A:145:GLN:C	2.57	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:O	1:A:311:LEU:HD23	2.19	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
1:A:207:GLN:HE21	1:A:239:GLN:HE22	1.67	0.41
1:A:85:SER:HA	1:A:86:PRO:HD3	1.87	0.41
1:A:358:TYR:CE1	2:B:323:LEU:HD23	2.55	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
2:B:93:TYR:CE1	6:B:503:7TP:CAG	2.99	0.41
2:B:360:PHE:HD2	6:B:503:7TP:OAC	2.03	0.41
2:B:150:LEU:HA	2:B:150:LEU:HD23	1.95	0.41
2:B:199:VAL:O	2:B:200:ASP:CB	2.68	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
1:A:296:LEU:C	1:A:296:LEU:CD1	2.78	0.40
1:A:62:THR:HG22	1:A:62:THR:O	2.22	0.40
2:B:308:LEU:HD23	2:B:308:LEU:HA	1.81	0.40
1:A:311:LEU:HD23	1:A:311:LEU:C	2.41	0.40
2:B:37:ASP:C	2:B:39:SER:N	2.75	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%)	18	46
2	B	402/427 (94%)	368 (92%)	21 (5%)	13 (3%)	5	13
All	All	715/804 (89%)	644 (90%)	55 (8%)	16 (2%)	8	22

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	38	ASP
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%)	271 (92%)	23 (8%)	15	36
2	B	340/363 (94%)	317 (93%)	23 (7%)	18	43
All	All	634/701 (90%)	588 (93%)	46 (7%)	16	39

All (46) 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
1	A	228	LYS
1	A	239	GLN
1	A	251	SER
1	A	257	GLU
1	A	268	LYS
1	A	287	ARG
1	A	291	ARG
1	A	296	LEU
1	A	307	SER
1	A	320	GLU
1	A	342	GLU
1	A	343	ILE
1	A	348	LYS
1	A	362	SER
1	A	369	ARG
2	B	21	GLU
2	B	25	SER
2	B	39	SER
2	B	61	SER
2	B	67	LEU
2	B	68	VAL
2	B	112	GLU
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	271	LYS
2	B	273	LEU
2	B	277	VAL
2	B	279	SER
2	B	280	ARG
2	B	325	MET

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Mol	Chain	Res	Type
2	B	357	SER
2	B	409	ILE
2	B	418	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	162	GLN
1	A	170	HIS
1	A	218	ASN
1	A	221	GLN
1	A	239	GLN
1	A	294	ASN
1	A	298	GLN
1	A	326	GLN
1	A	335	ASN
2	B	30	HIS
2	B	134	GLN
2	B	170	ASN
2	B	194	HIS
2	B	275	GLN
2	B	289	GLN
2	B	344	GLN
2	B	375	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 carbohydrates 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	A	401	-	3,3,3	2.65	1 (33%)	3,3,3	1.19	1 (33%)
5	FPP	B	502	-	22,23,23	1.83	9 (40%)	24,31,31	1.49	4 (16%)
6	7TP	B	503	4	41,49,49	2.55	10 (24%)	53,71,71	3.24	20 (37%)
3	DMS	B	504	-	3,3,3	2.46	1 (33%)	3,3,3	0.76	0
3	DMS	B	505	-	3,3,3	2.83	1 (33%)	3,3,3	0.71	0
3	DMS	B	506	-	3,3,3	2.62	1 (33%)	3,3,3	0.70	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
3	DMS	A	401	-	-	0/0/0/0	0/0/0/0
5	FPP	B	502	-	-	0/25/25/25	0/0/0/0
6	7TP	B	503	4	-	0/24/44/44	0/4/6/6
3	DMS	B	504	-	-	0/0/0/0	0/0/0/0
3	DMS	B	505	-	-	0/0/0/0	0/0/0/0
3	DMS	B	506	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	503	7TP	CBM-NBO	-6.82	1.31	1.43
6	B	503	7TP	CBH-CBL	-6.09	1.35	1.46
5	B	502	FPP	C1-C2	-2.75	1.40	1.49
6	B	503	7TP	CAV-CBI	-2.67	1.34	1.39
5	B	502	FPP	C6-C7	-2.33	1.42	1.50
5	B	502	FPP	C11-C12	-2.27	1.42	1.50
5	B	502	FPP	PB-O3A	-2.14	1.56	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	FPP	PB-O3B	-2.14	1.46	1.54
6	B	503	7TP	CBK-NBQ	-2.00	1.33	1.38
5	B	502	FPP	C7-C8	2.23	1.38	1.33
6	B	503	7TP	CAB-NBQ	2.49	1.52	1.47
6	B	503	7TP	CAW-CBN	2.63	1.57	1.53
5	B	502	FPP	C2-C3	2.70	1.39	1.33
5	B	502	FPP	C12-C13	2.82	1.40	1.32
6	B	503	7TP	CBJ-SBR	3.03	1.80	1.76
6	B	503	7TP	SBR-NBP	3.10	1.67	1.63
6	B	503	7TP	OAD-SBR	3.49	1.47	1.43
5	B	502	FPP	O1-C1	3.79	1.48	1.43
3	B	504	DMS	O-S	4.15	1.78	1.50
3	B	506	DMS	O-S	4.25	1.79	1.50
3	A	401	DMS	O-S	4.41	1.80	1.50
3	B	505	DMS	O-S	4.66	1.81	1.50
6	B	503	7TP	OAE-SBR	9.89	1.55	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	7TP	OAC-CAG-CBF	-11.13	114.69	124.32
6	B	503	7TP	CAX-CBI-CAV	-9.31	107.22	119.20
6	B	503	7TP	CAR-CBL-CBH	-5.82	123.45	128.78
6	B	503	7TP	OAD-SBR-OAE	-4.68	111.59	119.46
6	B	503	7TP	CBH-CAV-CBI	-4.18	115.72	121.98
6	B	503	7TP	CAV-CBH-CBL	-3.74	115.59	120.44
6	B	503	7TP	OAE-SBR-NBP	-3.69	99.90	106.97
6	B	503	7TP	CAS-CBM-NBO	-3.33	112.69	118.29
6	B	503	7TP	CAW-CBN-NBP	-3.32	107.79	112.73
6	B	503	7TP	CAX-NBP-SBR	-3.02	112.87	118.41
6	B	503	7TP	CAP-CBJ-CAQ	-2.24	117.22	120.43
6	B	503	7TP	OAD-SBR-CBJ	-2.16	105.19	108.00
5	B	502	FPP	C10-C8-C7	-2.08	118.14	123.69
5	B	502	FPP	O3A-PB-O1B	-2.04	98.91	111.44
3	A	401	DMS	C2-S-C1	2.01	108.87	98.44
5	B	502	FPP	C6-C5-C3	2.04	119.83	112.93
6	B	503	7TP	CAV-CBI-CBM	2.14	120.84	118.95
6	B	503	7TP	CAB-NBQ-CBK	2.41	127.64	124.44
6	B	503	7TP	CAZ-CBN-NBP	2.92	118.18	112.42
6	B	503	7TP	CAQ-CBJ-SBR	3.28	123.35	119.78
5	B	502	FPP	C10-C8-C9	4.61	123.30	115.29
6	B	503	7TP	CBJ-SBR-NBP	4.85	115.84	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	7TP	CAO-CBH-CAV	5.21	124.89	118.16
6	B	503	7TP	CAX-CBI-CBM	6.46	131.94	122.43
6	B	503	7TP	OAE-SBR-CBJ	6.51	116.48	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	FPP	15	0
6	B	503	7TP	5	0
3	B	504	DMS	10	0

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%)	-0.20	8 (2%) 58 52	23, 51, 83, 106	0
2	B	403/427 (94%)	-0.08	13 (3%) 48 42	25, 46, 77, 107	0
All	All	718/804 (89%)	-0.13	21 (2%) 52 46	23, 49, 81, 107	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	64	PHE	7.7
1	A	331	GLU	4.7
2	B	65	ASN	4.5
1	A	305	SER	4.4
2	B	381	MET	4.2
2	B	66	HIS	3.6
1	A	330	LYS	3.4
2	B	21	GLU	3.2
1	A	55	PHE	2.8
2	B	69	PRO	2.6
1	A	326	GLN	2.5
2	B	423	PHE	2.4
2	B	67	LEU	2.2
2	B	68	VAL	2.1
1	A	302	LEU	2.1
2	B	380	ALA	2.1
1	A	304	PRO	2.1
2	B	413	THR	2.1
2	B	63	LYS	2.1
1	A	306	HIS	2.0
2	B	70	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	DMS	B	505	4/4	0.89	0.25	10.04	77,78,80,83	0
5	FPP	B	502	24/24	0.98	0.18	0.93	26,40,44,45	0
3	DMS	B	506	4/4	0.94	0.19	0.85	60,62,63,66	0
6	7TP	B	503	44/44	0.95	0.17	0.62	37,46,72,87	0
3	DMS	B	504	4/4	0.98	0.17	0.48	69,69,74,74	0
4	ZN	B	501	1/1	1.00	0.09	-2.36	36,36,36,36	0
3	DMS	A	401	4/4	0.95	0.18	-	63,64,65,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.