Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:58 PM GMT

PDB ID	:	4GTR
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

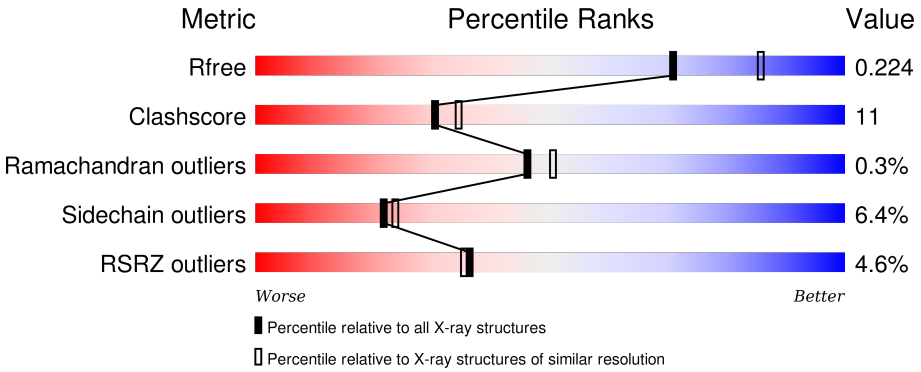
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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 <=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	5%, 64%, 15%, •, 16%
2	B	427	3%, 78%, 14%, •, 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	X

2 Entry composition

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.

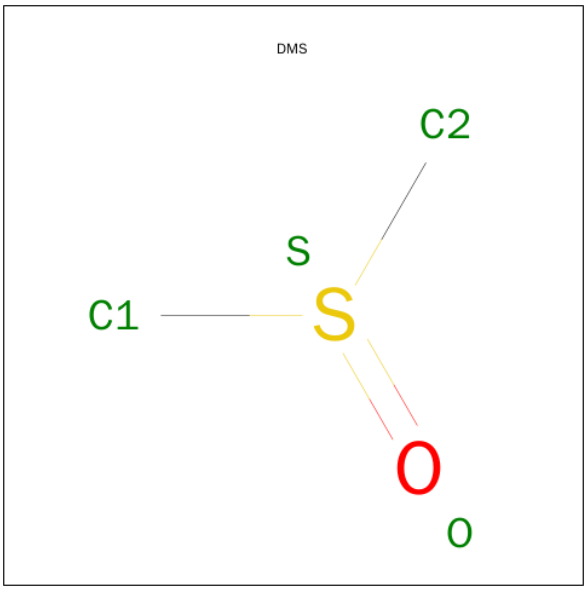
- Molecule 1 is a protein called Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

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

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

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

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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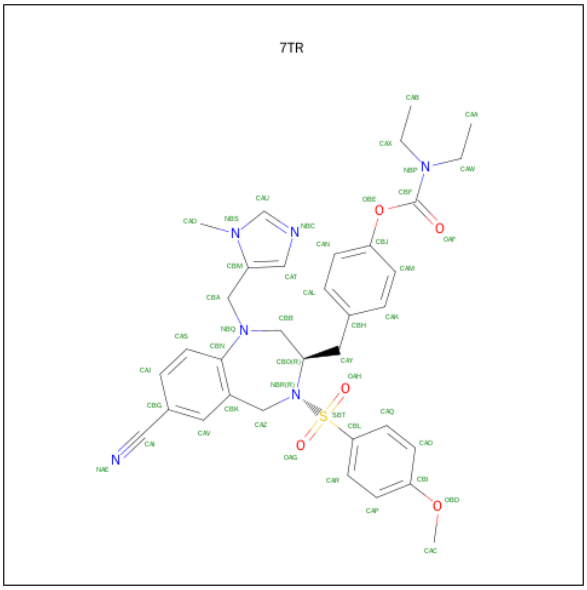
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O S 4 2 1 1	0	0

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

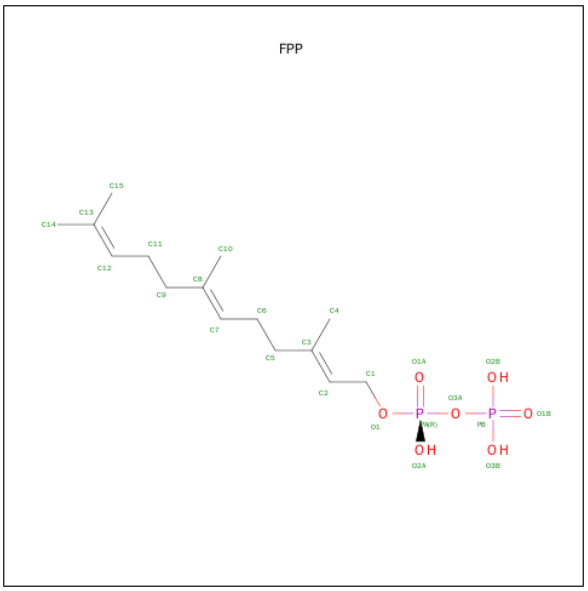
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is 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 DIETHYLCARBAMATE (three-letter code: 7TR) (formula: $C_{34}H_{38}N_6O_5S$).



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

- Molecule 6 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: $C_{15}H_{28}O_7P_2$).



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

- Molecule 7 is water.

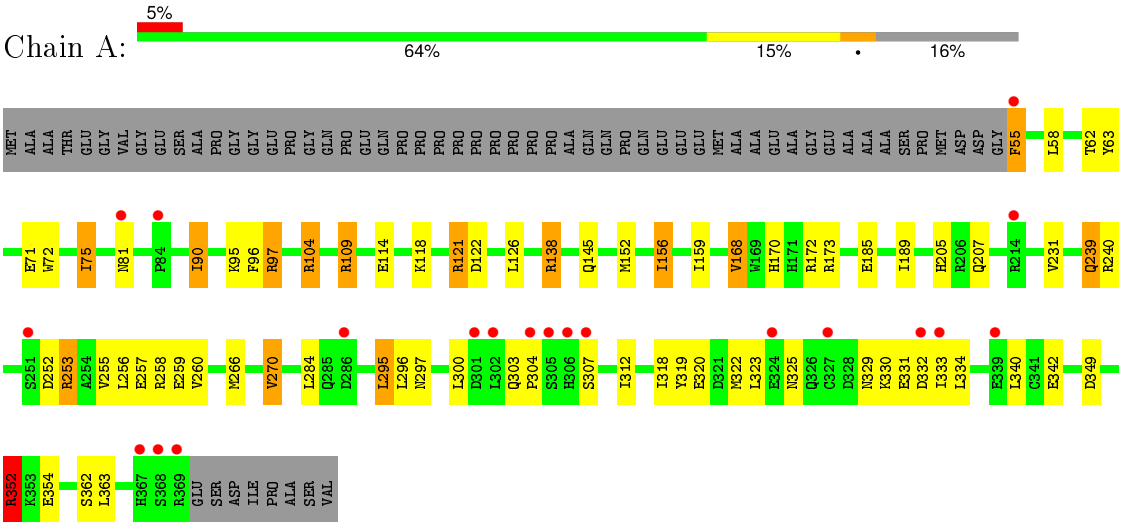
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	199	Total O 199 199	0	0
7	B	206	Total O 206 206	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

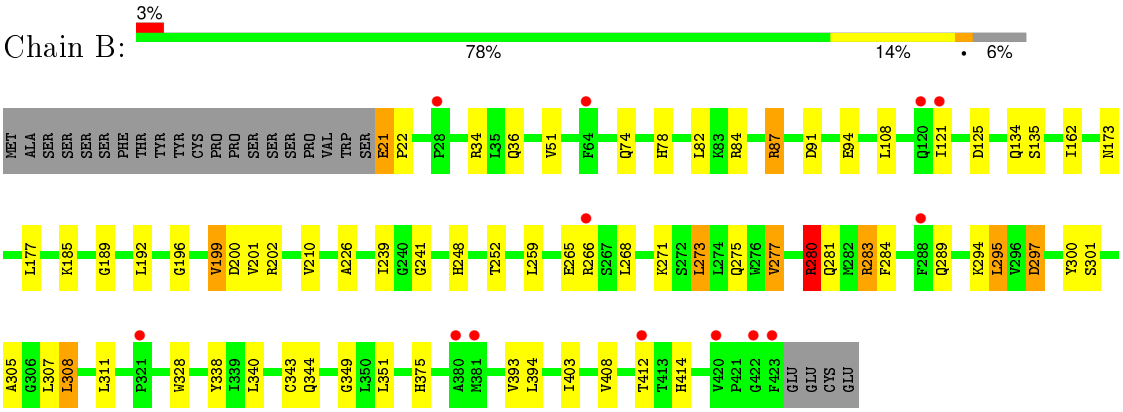
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain A:



- Molecule 2: Protein farnesyltransferase subunit beta

Chain B:



4 Data and refinement statistics (i)

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 29.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.91-2.20) 100.0 (29.84-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [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 (5.24%)	DCC
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.7	EDS
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 60003 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 7TR, DMS, ZN, 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	0.69	0/2750	0.78	9/3735 (0.2%)
2	B	0.65	0/3266	0.72	2/4436 (0.0%)
All	All	0.67	0/6016	0.75	11/8171 (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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ARG	NE-CZ-NH2	-9.57	115.52	120.30
2	B	280	ARG	NE-CZ-NH1	8.41	124.51	120.30
2	B	280	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	A	352	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	352	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	138	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	104	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	104	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	252	ASP	N-CA-C	-5.52	96.09	111.00
1	A	122	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	97	ARG	NE-CZ-NH1	5.09	122.84	120.30

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 (i)

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	72	0
2	B	3176	0	3105	52	0
3	A	4	0	6	1	0
3	B	8	0	12	11	0
4	B	1	0	0	0	0
5	B	46	0	38	9	0
6	B	24	0	25	7	0
7	A	199	0	0	11	0
7	B	206	0	0	6	0
All	All	6342	0	5790	129	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 (129) 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: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:H22	1.53	0.88
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
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
1:A:62:THR:HG22	1:A:62:THR:O	1.87	0.75
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
2:B:185:LYS:NZ	2:B:189:GLY:C	2.43	0.71
1:A:270:VAL:O	1:A:270:VAL:HG22	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:ASP:CG	7:B:695:HOH:O	2.30	0.69
1:A:118:LYS:HD3	7:A:596:HOH:O	1.93	0.68
6:B:503:FPP:C10	3:B:504:DMS:H22	2.23	0.67
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
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
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:318:ILE:HG22	1:A:322:MET:CE	2.32	0.59
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:231:VAL:HG21	1:A:266:MET:CE	2.32	0.59
1:A:296:LEU:CD1	1:A:322:MET:HE1	2.33	0.58
1:A:114:GLU:OE1	7:A:549:HOH:O	2.17	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:HA	1:A:239:GLN:HE21	1.70	0.57
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
2:B:185:LYS:HZ2	2:B:189:GLY:C	2.09	0.56
1:A:270:VAL:CG2	1:A:270:VAL:O	2.54	0.56
1:A:231:VAL:HG21	1:A:266:MET:HE2	1.88	0.55
3:A:401:DMS:H23	5:B:502:7TR:H17	1.87	0.55
5:B:502:7TR:H36	3:B:505:DMS:C2	2.36	0.55
1:A:296:LEU:HD12	1:A:322:MET:HE1	1.88	0.55
1:A:253:ARG:HH21	1:A:256:LEU:HD23	1.72	0.55
1:A:156:ILE:CD1	1:A:172:ARG:HH12	2.20	0.54
2:B:271:LYS:NZ	7:B:626:HOH:O	2.40	0.54
5:B:502:7TR:NBC	3:B:504:DMS:H13	2.24	0.53
1:A:318:ILE:HG22	1:A:322:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:318:ILE:CG2	1:A:322:MET:HE2	2.41	0.51
2:B:277:VAL:CG1	2:B:307:LEU:HD12	2.40	0.51
1:A:62:THR:CG2	1:A:62:THR:O	2.58	0.51
5:B:502:7TR:H36	3:B:505:DMS:H21	1.93	0.50
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
1:A:330:LYS:C	1:A:332:ASP:H	2.15	0.49
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
5:B:502:7TR:CAT	3:B:504:DMS:C1	2.91	0.49
2:B:177:LEU:HD21	2:B:210:VAL:HG13	1.95	0.48
1:A:72:TRP:CE3	1:A:75:ILE:HG21	2.48	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
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
2:B:51:VAL:HG21	2:B:295:LEU:HG	1.95	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:O	2:B:273:LEU:HD12	2.15	0.46
2:B:185:LYS:HZ1	2:B:189:GLY:HA2	1.81	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
1:A:318:ILE:HG22	1:A:322:MET:HE3	1.98	0.46
2:B:308:LEU:HD13	2:B:308:LEU:HA	1.72	0.45
1:A:90[A]:ILE:HD11	2:B:94:GLU:HG3	1.98	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
2:B:226:ALA:HA	2:B:259:LEU:HD21	1.99	0.45
2:B:87:ARG:NH2	2:B:125:ASP:OD2	2.50	0.45
1:A:240:ARG:HD3	1:A:259:GLU:OE1	2.15	0.45
1:A:152:MET:HE1	1:A:172:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:VAL:O	2:B:393:VAL:HG13	2.17	0.44
6:B:503:FPP:C10	3:B:504:DMS:C2	2.95	0.44
2:B:185:LYS:NZ	2:B:189:GLY:CA	2.80	0.44
2:B:185:LYS:NZ	2:B:189:GLY:HA2	2.33	0.44
1:A:55:PHE:HA	1:A:55:PHE:HD1	1.75	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:330:LYS:C	1:A:332:ASP:N	2.71	0.43
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.33	0.43
1:A:303:GLN:O	1:A:307:SER:HB2	2.18	0.43
1:A:296:LEU:CD1	1:A:322:MET:CE	2.95	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
5:B:502:7TR:CAT	3:B:504:DMS:H12	2.48	0.43
1:A:318:ILE:CG2	1:A:322:MET:CE	2.97	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
5:B:502:7TR:CAT	3:B:504:DMS:H13	2.49	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
5:B:502:7TR:H36	3:B:505:DMS:H23	2.01	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
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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	315/377 (84%)	297 (94%)	16 (5%)	2 (1%)	30 29
2	B	402/427 (94%)	387 (96%)	15 (4%)	0	100 100
All	All	717/804 (89%)	684 (95%)	31 (4%)	2 (0%)	46 50

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	270 (93%)	21 (7%)	18 18
2	B	341/363 (94%)	321 (94%)	20 (6%)	24 27
All	All	632/701 (90%)	591 (94%)	41 (6%)	22 23

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	342	GLU
1	A	352	ARG
1	A	362	SER
2	B	21	GLU
2	B	82	LEU
2	B	84	ARG
2	B	87	ARG
2	B	108	LEU
2	B	121	ILE
2	B	135	SER
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	283	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	221	GLN
1	A	239	GLN
1	A	246	ASN
1	A	294	ASN
1	A	335	ASN
2	B	30	HIS
2	B	134	GLN
2	B	186	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 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	$\#\|Z\| > 2$
3	DMS	A	401	-	3,3,3	2.60	1 (33%)	3,3,3	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	7TR	B	502	4	46,50,50	1.72	6 (13%)	57,71,71	2.09	9 (15%)
6	FPP	B	503	-	21,23,23	2.19	9 (42%)	27,31,31	1.49	5 (18%)
3	DMS	B	504	-	3,3,3	2.57	1 (33%)	3,3,3	0.79	0
3	DMS	B	505	-	3,3,3	2.56	1 (33%)	3,3,3	0.92	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	7TR	B	502	4	-	0/36/52/52	0/4/5/5
6	FPP	B	503	-	-	0/25/25/25	0/0/0/0
3	DMS	B	504	-	-	0/0/0/0	0/0/0/0
3	DMS	B	505	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	503	FPP	C11-C12	-4.26	1.38	1.50
6	B	503	FPP	C6-C7	-3.80	1.39	1.50
5	B	502	7TR	CBN-NBQ	-3.70	1.36	1.43
6	B	503	FPP	O1-C1	-2.79	1.39	1.43
6	B	503	FPP	C1-C2	-2.77	1.39	1.49
6	B	503	FPP	PB-O2B	2.17	1.62	1.54
5	B	502	7TR	CBL-SBT	2.18	1.79	1.76
5	B	502	7TR	CBB-NBQ	2.33	1.49	1.46
5	B	502	7TR	SBT-NBR	2.40	1.66	1.63
6	B	503	FPP	C12-C13	2.60	1.40	1.32
6	B	503	FPP	C2-C3	2.76	1.38	1.33
6	B	503	FPP	C7-C8	2.84	1.38	1.33
6	B	503	FPP	PB-O1B	3.83	1.63	1.51
3	B	505	DMS	O-S	4.27	1.79	1.50
3	B	504	DMS	O-S	4.37	1.80	1.50
3	A	401	DMS	O-S	4.38	1.80	1.50
5	B	502	7TR	OAH-SBT	5.29	1.50	1.43
5	B	502	7TR	OAG-SBT	6.69	1.52	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	502	7TR	CAZ-CBK-CAV	-7.18	109.71	119.28
5	B	502	7TR	OAH-SBT-OAG	-6.64	108.01	119.47
5	B	502	7TR	NBC-CAU-NBS	-4.53	106.15	112.28
5	B	502	7TR	CAC-OBD-CBI	-4.46	107.09	117.51
5	B	502	7TR	CAY-CBO-NBR	-3.13	108.19	112.87
6	B	503	FPP	C4-C3-C2	-2.69	118.22	123.50
6	B	503	FPP	C9-C8-C7	-2.14	116.98	121.05
6	B	503	FPP	O3B-PB-O2B	2.26	115.97	107.38
5	B	502	7TR	CBJ-OBE-CBF	3.64	123.76	117.30
6	B	503	FPP	C4-C3-C5	3.68	121.03	115.41
5	B	502	7TR	CAZ-CBK-CBN	3.75	128.26	122.44
6	B	503	FPP	C10-C8-C9	3.76	121.15	115.41
5	B	502	7TR	CAV-CBK-CBN	3.82	122.03	118.93
5	B	502	7TR	CBL-SBT-NBR	4.55	114.81	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	DMS	1	0
5	B	502	7TR	9	0
6	B	503	FPP	7	0
3	B	504	DMS	7	0
3	B	505	DMS	4	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

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, 95^{th} 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%)	0.10	20 (6%)	23	23	30, 53, 88, 100	0
2	B	403/427 (94%)	0.07	13 (3%)	51	50	30, 49, 75, 94	0
All	All	718/804 (89%)	0.08	33 (4%)	36	35	30, 51, 81, 100	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	64	PHE	6.1
1	A	302	LEU	6.1
1	A	305	SER	5.1
1	A	306	HIS	5.1
1	A	333	ILE	4.4
2	B	423	PHE	4.0
1	A	55	PHE	3.8
1	A	339	GLU	3.6
1	A	304	PRO	3.4
1	A	369	ARG	3.3
1	A	368	SER	3.3
1	A	301	ASP	3.2
1	A	84	PRO	2.9
1	A	327	CYS	2.9
2	B	412	THR	2.8
1	A	307	SER	2.7
2	B	420	VAL	2.7
1	A	367	HIS	2.6
2	B	381	MET	2.5
2	B	422	GLY	2.5
1	A	81	ASN	2.5
1	A	286	ASP	2.4
2	B	120	GLN	2.4
2	B	266	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	28	PRO	2.4
2	B	380	ALA	2.3
2	B	288	PHE	2.3
1	A	324	GLU	2.2
1	A	251	SER	2.2
1	A	214	ARG	2.2
2	B	321	PRO	2.2
1	A	332	ASP	2.1
2	B	121	ILE	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 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, 95^{th} 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	0.94	0.25	8.58	79,88,91,95	0
6	FPP	B	503	24/24	0.96	0.18	1.89	34,45,49,51	0
5	7TR	B	502	46/46	0.91	0.14	0.26	33,37,54,61	0
4	ZN	B	501	1/1	1.00	0.08	-1.62	36,36,36,36	0
3	DMS	A	401	4/4	0.98	0.24	-	71,76,76,90	0
3	DMS	B	504	4/4	0.98	0.26	-	62,69,69,75	0

6.5 Other polymers (i)

There are no such residues in this entry.