Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:04 PM EDT

PDB ID	:	2ZW9
Title	:	Crystal structure of tRNA wybutosine synthesizing enzyme TYW4
Authors	:	Suzuki, Y.; Noma, A.; Suzuki, T.; Ishitani, R.; Nureki, O.
Deposited on	:	2008-12-01
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

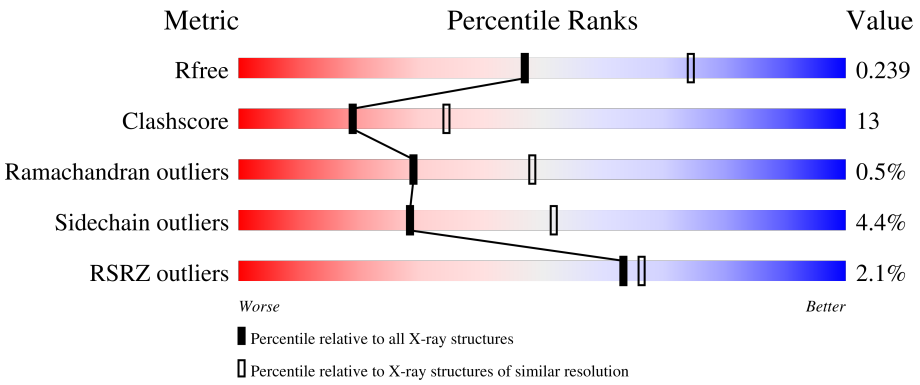
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	695	2% 68% 26% • •
1	B	695	2% 64% 29% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10810 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.

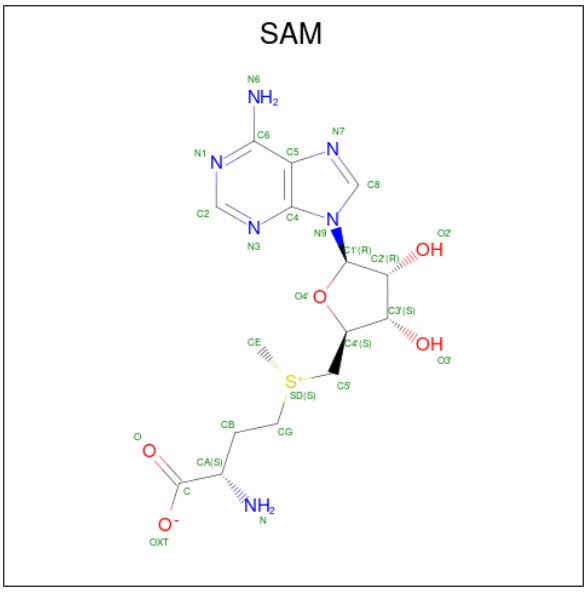
- Molecule 1 is a protein called Leucine carboxyl methyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5329	3417	891	996	25	0	0	0
1	B	664	5294	3396	880	992	26	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LEU	MET	SEE REMARK 999	UNP Q08282
B	417	LEU	MET	SEE REMARK 999	UNP Q08282

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	27	15	6	5	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	27	15	6	5	1	0	0

- Molecule 3 is water.

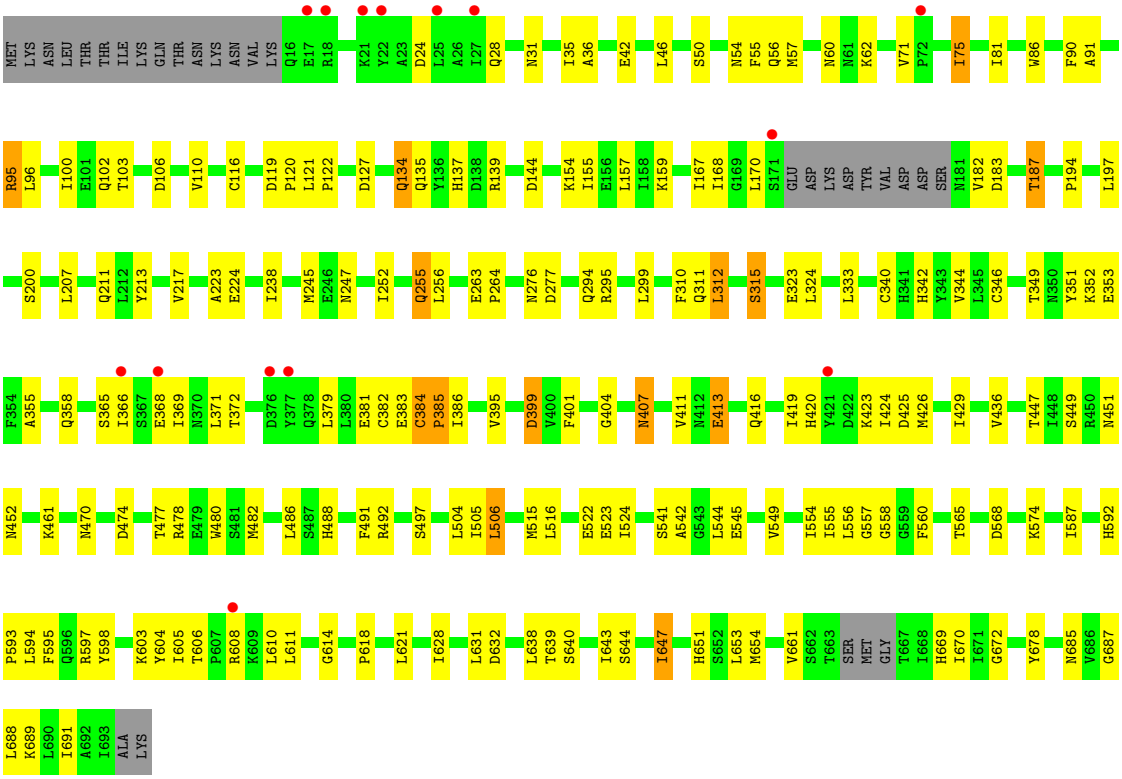
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	0	0
			Total	O		
3	B	75	75	75	0	0

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.

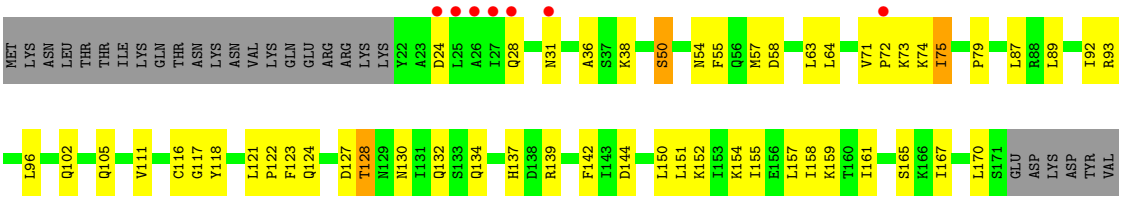
• Molecule 1: Leucine carboxyl methyltransferase 2

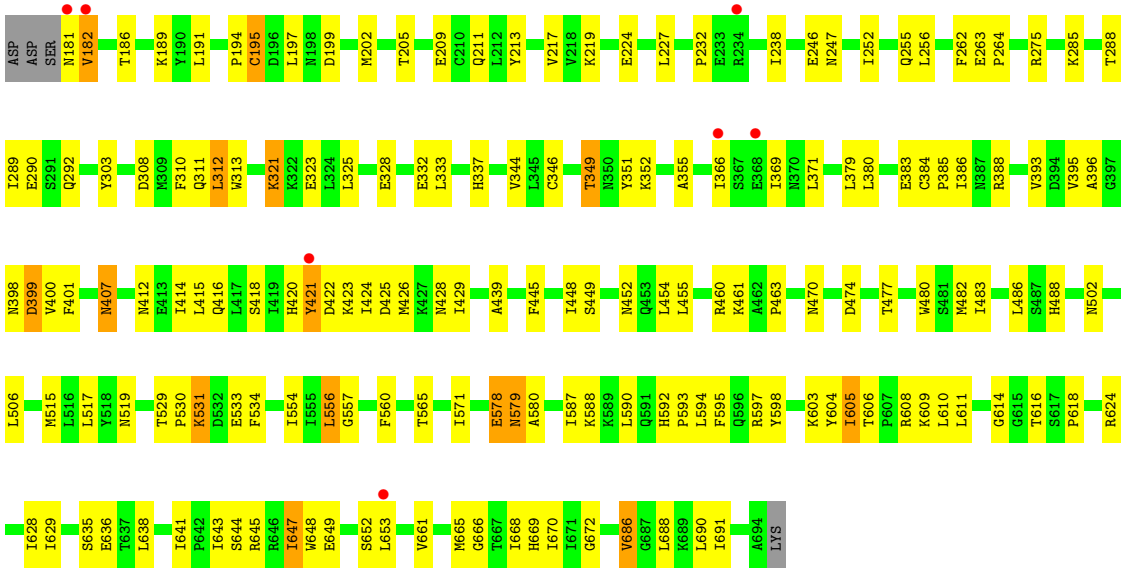
Chain A:



• Molecule 1: Leucine carboxyl methyltransferase 2

Chain B:




ASP
ASP
SER
N181
V182
T186
K189
Y190
L191
P194
C195
D196
L197
N198
D199
M202
T205
E209
C210
Q211
L212
Y213
V217
V218
K219
E224
L227
P232
E233
R234
I238
E246
N247
I252
Q255
L256
F262
E263
P264
R275
K285
T288
I289
E290
S291
Q292
Y303
D308
M309
F310
Q311
L312
W313
K321
K322
E323
L324
L325
E328
E332
L333
H337
V344
L345
C346
T349
N350
Y351
K352
A355
I366
S367
E368
I369
N370
L371
L379
L380
E383
C384
P385
I386
N387
R388
V393
D394
V395
A396
G397
N398
D399
V400
F401
N407
N412
E413
I414
L415
Q416
L417
S418
I419
H420
Y421
D422
K423
I424
D425
M426
K427
N428
I429
A439
F445
I448
S449
N452
Q453
L454
L455
R460
K461
A462
P463
N470
D474
T477
W480
S481
M482
I483
L486
S487
H488
N502
L506
M515
L516
L517
Y518
N519
T529
P530
K531
D532
E533
F534
I554
I555
L556
G557
F560
T565
I571
E578
N579
A580
I587
K588
K589
L590
Q591
H592
P593
L594
F595
Q596
R597
Y598
K603
Y604
I605
T606
P607
R608
K609
L610
L611
G614
G615
T616
S617
P618
R624
I628
I629
S635
E636
T637
L638
I641
P642
I643
S644
R645
R646
I647
W648
E649
S652
L653
V661
M665
G666
T667
I668
H669
I670
I671
G672
V686
G687
L688
K689
L690
I691
A694
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.44Å 88.63Å 256.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.50 46.32 – 2.48	Depositor EDS
% Data completeness (in resolution range)	90.0 (46.32-2.50) 90.0 (46.32-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.245 0.188 , 0.239	Depositor DCC
R_{free} test set	2600 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	0.25	0/5443	0.46	0/7359
1	B	0.24	0/5409	0.46	0/7318
All	All	0.25	0/10852	0.46	0/14677

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5329	0	5346	140	0
1	B	5294	0	5303	144	0
2	A	27	0	22	2	0
2	B	27	0	22	1	0
3	A	58	0	0	0	0
3	B	75	0	0	1	0
All	All	10810	0	10693	280	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 13.

All (280) 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:384:CYS:SG	1:A:424:ILE:HB	1.85	1.16
1:A:461:LYS:HD3	1:B:482:MET:HE1	1.31	1.08
1:A:482:MET:HE1	1:B:461:LYS:HD3	1.42	0.99
1:B:102:GLN:HE22	1:B:355:ALA:H	1.11	0.96
1:A:71:VAL:HG11	1:A:75:ILE:HD11	1.48	0.96
1:B:606:THR:HG22	1:B:608:ARG:H	1.30	0.95
1:A:606:THR:HG22	1:A:608:ARG:H	1.32	0.92
1:A:554:ILE:HD12	1:A:610:LEU:HD22	1.55	0.87
1:B:54:ASN:HD22	1:B:57:MET:HB2	1.41	0.85
1:A:419:ILE:HA	1:A:424:ILE:HG12	1.60	0.84
1:B:395:VAL:HG12	1:B:400:VAL:HG22	1.61	0.82
1:A:654:MET:H	1:A:685:ASN:HD22	1.28	0.81
1:B:252:ILE:HG22	1:B:346:CYS:HB3	1.63	0.81
1:A:102:GLN:NE2	1:A:355:ALA:H	1.81	0.78
1:A:102:GLN:HE22	1:A:355:ALA:H	1.32	0.78
1:A:255:GLN:H	1:A:255:GLN:HE21	1.30	0.78
1:B:611:LEU:HD22	1:B:690:LEU:HD22	1.65	0.78
1:A:349:THR:HG22	1:A:351:TYR:H	1.46	0.78
1:B:134:GLN:HA	1:B:137:HIS:CD2	2.22	0.74
1:A:252:ILE:HG22	1:A:346:CYS:HB3	1.67	0.74
1:A:60:ASN:HB2	1:A:62:LYS:HG3	1.71	0.73
1:A:470:ASN:HD21	1:A:486:LEU:HG	1.52	0.73
1:A:411:VAL:HB	1:A:413:GLU:HG3	1.70	0.72
1:A:605:ILE:HD11	1:A:611:LEU:HB2	1.69	0.72
1:A:647:ILE:HD11	1:A:688:LEU:HD21	1.70	0.72
1:B:592:HIS:HD2	1:B:594:LEU:H	1.36	0.72
1:A:134:GLN:HA	1:A:137:HIS:CD2	2.27	0.70
1:B:199:ASP:OD2	1:B:202:MET:HB2	1.92	0.70
1:A:366:ILE:HD12	1:A:366:ILE:O	1.92	0.69
1:B:349:THR:HG23	1:B:351:TYR:H	1.57	0.69
1:B:102:GLN:NE2	1:B:355:ALA:H	1.89	0.68
1:B:448:ILE:HD13	1:B:455:LEU:HB2	1.75	0.68
1:B:72:PRO:C	1:B:73:LYS:HG2	2.13	0.67
1:B:154:LYS:O	1:B:158:ILE:HG13	1.95	0.67
1:A:263:GLU:HG2	1:A:264:PRO:HD2	1.77	0.67
1:A:255:GLN:H	1:A:255:GLN:NE2	1.91	0.66
1:B:421:TYR:CD1	1:B:421:TYR:N	2.61	0.66
1:B:554:ILE:HD12	1:B:610:LEU:HD22	1.75	0.66
1:B:50:SER:HB3	1:B:323:GLU:OE1	1.97	0.65
1:B:205:THR:O	1:B:209:GLU:HG3	1.96	0.65
1:A:482:MET:HE1	1:B:461:LYS:CD	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASN:ND2	1:B:118:TYR:CD1	2.65	0.64
1:A:644:SER:OG	1:A:647:ILE:HG22	1.99	0.64
1:B:38:LYS:HD3	1:B:89:LEU:HD21	1.78	0.63
1:B:54:ASN:ND2	1:B:57:MET:HB2	2.13	0.63
1:A:384:CYS:SG	1:A:424:ILE:CB	2.77	0.62
1:A:207:LEU:HB3	1:A:245:MET:HE3	1.81	0.62
1:A:407:ASN:C	1:A:407:ASN:HD22	2.02	0.61
1:B:661:VAL:HG23	1:B:669:HIS:HB2	1.82	0.61
1:A:24:ASP:O	1:A:28:GLN:HG3	2.01	0.60
1:A:379:LEU:HD21	1:A:628:ILE:HD12	1.84	0.60
1:A:592:HIS:HD2	1:A:594:LEU:HB2	1.67	0.60
1:B:58:ASP:HB3	1:B:64:LEU:HD21	1.84	0.59
1:B:127:ASP:O	1:B:137:HIS:HE1	1.84	0.59
1:B:416:GLN:HB2	1:B:429:ILE:HD11	1.84	0.59
1:A:247:ASN:HA	1:A:351:TYR:CD2	2.38	0.58
1:A:654:MET:H	1:A:685:ASN:ND2	1.97	0.58
1:A:256:LEU:HD11	1:A:344:VAL:HB	1.86	0.58
1:A:116:CYS:SG	1:A:144:ASP:HB3	2.44	0.58
1:A:264:PRO:HB3	1:A:653:LEU:O	2.03	0.58
1:B:165:SER:HB3	1:B:170:LEU:HB2	1.85	0.58
1:B:252:ILE:CG2	1:B:346:CYS:HB3	2.33	0.58
1:A:608:ARG:O	1:A:632:ASP:HA	2.03	0.58
1:B:422:ASP:OD1	1:B:423:LYS:HG2	2.04	0.58
1:A:381:GLU:OE1	1:A:651:HIS:CD2	2.57	0.58
1:A:368:GLU:O	1:A:368:GLU:HG3	2.04	0.57
1:B:157:LEU:O	1:B:161:ILE:HG13	2.04	0.57
1:A:647:ILE:CD1	1:A:688:LEU:HD21	2.34	0.57
1:B:256:LEU:HD11	1:B:344:VAL:HB	1.87	0.57
1:B:470:ASN:HD21	1:B:486:LEU:HG	1.69	0.57
1:B:592:HIS:CD2	1:B:593:PRO:HD2	2.40	0.56
1:A:447:THR:CG2	1:A:451:ASN:HA	2.36	0.56
1:A:342:HIS:CE1	1:A:621:LEU:HD11	2.41	0.56
1:B:232:PRO:HB3	1:B:285:LYS:HD3	1.88	0.56
1:B:592:HIS:CD2	1:B:594:LEU:H	2.22	0.56
1:B:606:THR:HG22	1:B:608:ARG:N	2.12	0.56
1:B:635:SER:O	1:B:636:GLU:HB2	2.05	0.55
1:A:183:ASP:O	1:A:194:PRO:HG3	2.07	0.55
1:A:554:ILE:HG13	1:A:604:TYR:OH	2.06	0.55
1:B:195:CYS:HA	1:B:202:MET:CE	2.37	0.55
1:B:560:PHE:HD1	1:B:565:THR:HB	1.70	0.55
1:B:418:SER:HB2	1:B:425:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:TYR:OH	1:B:352:LYS:HB3	2.06	0.55
1:B:414:ILE:HD11	1:B:480:TRP:CZ2	2.41	0.55
1:B:533:GLU:HG3	3:B:744:HOH:O	2.07	0.54
1:A:597:ARG:HD3	1:A:614:GLY:O	2.08	0.54
1:B:420:HIS:HE1	1:B:425:ASP:OD2	1.90	0.54
1:A:50:SER:O	1:A:54:ASN:HB2	2.08	0.54
1:A:223:ALA:HB3	1:A:252:ILE:HG13	1.90	0.54
1:B:123:PHE:HZ	1:B:158:ILE:HD13	1.71	0.54
1:A:416:GLN:HB2	1:A:429:ILE:HD11	1.89	0.54
1:A:371:LEU:HD11	1:A:594:LEU:CD1	2.38	0.54
1:A:661:VAL:HG23	1:A:669:HIS:HB2	1.89	0.54
1:A:381:GLU:OE1	1:A:651:HIS:NE2	2.41	0.54
1:A:506:LEU:HB2	1:A:544:LEU:HD22	1.90	0.54
1:A:54:ASN:ND2	1:A:57:MET:HB2	2.24	0.53
1:B:116:CYS:SG	1:B:144:ASP:HB3	2.48	0.53
1:B:310:PHE:CE2	1:B:618:PRO:HB3	2.44	0.53
1:B:379:LEU:O	1:B:380:LEU:HD23	2.09	0.53
1:A:211:GLN:HA	1:A:213:TYR:CE1	2.44	0.52
1:A:276:ASN:O	1:A:277:ASP:HB2	2.09	0.52
1:B:647:ILE:HD11	1:B:688:LEU:HD21	1.91	0.52
1:A:86:TRP:CH2	1:A:324:LEU:HD11	2.44	0.52
1:B:624:ARG:HG2	1:B:648:TRP:CD2	2.44	0.52
1:B:36:ALA:HB1	1:B:75:ILE:HD12	1.90	0.52
1:A:103:THR:HG22	1:A:139:ARG:HH12	1.75	0.52
1:B:578:GLU:O	1:B:580:ALA:N	2.43	0.51
1:B:445:PHE:CE2	1:B:454:LEU:HD13	2.45	0.51
1:A:386:ILE:HD11	1:A:672:GLY:HA3	1.92	0.51
1:B:421:TYR:N	1:B:421:TYR:HD1	2.08	0.51
1:B:24:ASP:O	1:B:28:GLN:HG3	2.11	0.51
1:A:295:ARG:O	1:A:299:LEU:HG	2.10	0.51
1:B:384:CYS:HB2	1:B:424:ILE:HD12	1.92	0.51
1:A:102:GLN:HE22	1:A:355:ALA:N	2.04	0.50
1:B:380:LEU:HD11	1:B:691:ILE:HD11	1.94	0.50
1:B:123:PHE:O	1:B:127:ASP:HB2	2.12	0.50
1:B:308:ASP:OD1	1:B:311:GLN:HG3	2.11	0.50
1:B:321:LYS:O	1:B:325:LEU:HG	2.12	0.50
1:B:152:LYS:HA	1:B:182:VAL:O	2.12	0.50
1:B:380:LEU:HD11	1:B:691:ILE:CD1	2.42	0.50
1:B:647:ILE:CD1	1:B:688:LEU:HD21	2.41	0.50
1:B:246:GLU:O	1:B:247:ASN:HB2	2.12	0.50
1:B:289:ILE:O	1:B:292:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HA	1:A:46:LEU:HD12	1.93	0.50
1:A:492:ARG:HD2	1:A:541:SER:OG	2.11	0.50
1:A:168:ILE:HD12	1:A:187:THR:HG21	1.94	0.50
1:A:116:CYS:O	2:A:801:SAM:HA	2.12	0.49
1:B:587:ILE:HG22	1:B:588:LYS:HB3	1.93	0.49
1:A:96:LEU:O	1:A:100:ILE:HD13	2.12	0.49
1:A:54:ASN:O	1:A:55:PHE:HB2	2.13	0.49
1:A:310:PHE:CE2	1:A:618:PRO:HB3	2.48	0.49
1:B:151:LEU:O	1:B:155:ILE:HG13	2.13	0.48
1:B:386:ILE:HD11	1:B:672:GLY:CA	2.43	0.48
1:B:127:ASP:O	1:B:137:HIS:CE1	2.65	0.48
1:B:74:LYS:C	1:B:75:ILE:HG12	2.33	0.48
1:B:186:THR:HG23	1:B:191:LEU:HD22	1.95	0.48
1:A:504:LEU:HD11	1:A:515:MET:SD	2.53	0.48
1:B:412:ASN:HB3	1:B:439:ALA:HA	1.94	0.48
1:B:155:ILE:HG22	1:B:159:LYS:HE2	1.94	0.48
1:A:670:ILE:HB	1:A:688:LEU:HB2	1.94	0.48
1:B:194:PRO:O	1:B:195:CYS:HB2	2.12	0.48
1:A:110:VAL:HG23	1:A:217:VAL:CG1	2.44	0.48
1:A:168:ILE:HG13	1:A:170:LEU:HG	1.96	0.48
1:A:197:LEU:O	1:A:238:ILE:HD11	2.14	0.47
1:A:631:LEU:HD12	1:A:632:ASP:N	2.29	0.47
1:B:502:ASN:HB3	1:B:517:LEU:HD11	1.96	0.47
1:A:119:ASP:HA	1:A:120:PRO:HD3	1.76	0.47
1:A:643:ILE:HG22	1:A:647:ILE:HG23	1.96	0.47
1:B:217:VAL:O	1:B:219:LYS:HD3	2.14	0.47
1:B:72:PRO:O	1:B:73:LYS:HG2	2.14	0.47
1:B:371:LEU:HD11	1:B:594:LEU:HD13	1.96	0.47
1:A:689:LYS:HE2	1:A:691:ILE:CG2	2.45	0.47
1:B:515:MET:HE3	1:B:530:PRO:HD3	1.97	0.47
1:B:597:ARG:HD3	1:B:614:GLY:O	2.13	0.47
1:A:349:THR:CG2	1:A:351:TYR:H	2.21	0.47
1:B:379:LEU:HD21	1:B:628:ILE:HD12	1.97	0.47
1:B:396:ALA:O	1:B:399:ASP:OD1	2.32	0.47
1:A:36:ALA:O	1:A:75:ILE:HD13	2.14	0.47
1:A:436:VAL:HG12	1:A:480:TRP:CD1	2.49	0.47
1:A:522:GLU:HB3	1:A:524:ILE:CD1	2.45	0.46
1:A:556:LEU:HD13	1:A:557:GLY:N	2.30	0.46
1:B:224:GLU:HB3	2:B:801:SAM:HN1	1.79	0.46
1:A:182:VAL:HG22	1:A:183:ASP:H	1.79	0.46
1:A:91:ALA:HA	1:A:312:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:TRP:O	1:B:321:LYS:HE2	2.15	0.46
1:A:384:CYS:HA	1:A:385:PRO:HD3	1.48	0.46
1:A:522:GLU:O	1:A:523:GLU:HB2	2.16	0.46
1:B:79:PRO:HA	1:B:328:GLU:OE1	2.16	0.46
1:A:90:PHE:HE2	1:A:312:LEU:HD22	1.80	0.46
1:A:631:LEU:HD13	1:A:638:LEU:HD23	1.98	0.46
1:B:150:LEU:HD23	1:B:150:LEU:O	2.16	0.46
1:B:641:ILE:HD13	1:B:690:LEU:HD11	1.98	0.46
1:B:31:ASN:OD1	1:B:117:GLY:HA3	2.16	0.46
1:B:127:ASP:HB2	1:B:167:ILE:HD13	1.98	0.45
1:B:644:SER:OG	1:B:647:ILE:HG22	2.16	0.45
1:B:288:THR:OG1	1:B:290:GLU:HG2	2.16	0.45
1:B:92:ILE:O	1:B:96:LEU:HG	2.17	0.45
1:B:93:ARG:HH12	1:B:124:GLN:NE2	2.15	0.45
1:B:554:ILE:HG13	1:B:604:TYR:OH	2.16	0.45
1:A:399:ASP:HB3	1:A:416:GLN:OE1	2.17	0.45
1:A:416:GLN:O	1:A:426:MET:HA	2.17	0.45
1:A:687:GLY:O	1:A:688:LEU:HD23	2.17	0.45
1:A:127:ASP:HB2	1:A:167:ILE:HD13	1.98	0.45
1:A:474:ASP:OD2	1:A:477:THR:HG23	2.17	0.45
1:A:554:ILE:HG22	1:A:555:ILE:N	2.32	0.45
1:A:542:ALA:HB2	1:A:558:GLY:HA3	1.98	0.44
1:A:654:MET:N	1:A:685:ASN:HD22	2.04	0.44
1:A:351:TYR:HD1	1:A:353:GLU:HB2	1.83	0.44
1:B:369:ILE:HD11	1:B:593:PRO:HG2	1.99	0.44
1:B:556:LEU:HD13	1:B:557:GLY:N	2.33	0.44
1:B:588:LYS:HD3	1:B:590:LEU:HD21	1.99	0.44
1:A:31:ASN:O	1:A:35:ILE:HG22	2.18	0.44
1:A:42:GLU:HG3	1:A:46:LEU:HD12	2.00	0.44
1:A:100:ILE:HG21	1:A:135:GLN:HB3	1.99	0.44
1:A:401:PHE:HE2	1:A:429:ILE:HD11	1.83	0.44
1:B:71:VAL:HA	1:B:72:PRO:HD3	1.67	0.44
1:B:445:PHE:CZ	1:B:454:LEU:HD13	2.53	0.44
1:B:603:LYS:HD2	1:B:668:ILE:HD13	1.99	0.44
1:A:560:PHE:HD1	1:A:565:THR:HB	1.83	0.44
1:B:211:GLN:HA	1:B:213:TYR:CE1	2.53	0.44
1:A:224:GLU:HB3	2:A:801:SAM:HN1	1.83	0.44
1:A:382:CYS:O	1:A:383:GLU:C	2.55	0.44
1:A:155:ILE:HG22	1:A:159:LYS:HE2	1.99	0.43
1:B:337:HIS:HD2	1:B:616:THR:OG1	2.00	0.43
1:B:388:ARG:CZ	1:B:415:LEU:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HA	1:A:157:LEU:HD12	2.00	0.43
1:A:310:PHE:HB2	1:A:340:CYS:HB3	2.00	0.43
1:A:407:ASN:C	1:A:407:ASN:ND2	2.70	0.43
1:A:491:PHE:O	1:A:492:ARG:HB2	2.18	0.43
1:B:303:TYR:CD1	1:B:349:THR:HG22	2.53	0.43
1:B:333:LEU:HD23	1:B:598:TYR:CE1	2.53	0.43
1:B:385:PRO:O	1:B:426:MET:HE1	2.18	0.43
1:B:534:PHE:CZ	1:B:571:ILE:HD12	2.53	0.43
1:A:121:LEU:HB3	1:A:122:PRO:HD3	2.01	0.43
1:A:545:GLU:OE2	1:A:603:LYS:HG3	2.18	0.43
1:B:137:HIS:O	1:B:189:LYS:NZ	2.51	0.43
1:A:411:VAL:HB	1:A:413:GLU:CG	2.46	0.43
1:B:128:THR:HA	1:B:137:HIS:CE1	2.54	0.43
1:B:531:LYS:H	1:B:531:LYS:HG2	1.57	0.43
1:A:255:GLN:HA	1:A:342:HIS:O	2.18	0.43
1:B:474:ASP:OD2	1:B:477:THR:HG23	2.18	0.43
1:B:605:ILE:H	1:B:605:ILE:HG13	1.67	0.43
1:B:665:MET:HA	1:B:666:GLY:HA2	1.70	0.43
1:A:366:ILE:H	1:A:366:ILE:HG13	1.64	0.43
1:B:624:ARG:NH1	1:B:645:ARG:HG2	2.34	0.43
1:A:294:GLN:OE1	1:A:294:GLN:HA	2.19	0.43
1:A:50:SER:HB3	1:A:323:GLU:OE2	2.19	0.43
1:B:255:GLN:N	1:B:255:GLN:OE1	2.52	0.43
1:B:263:GLU:HG2	1:B:264:PRO:HD2	2.01	0.43
1:A:592:HIS:CD2	1:A:593:PRO:HD2	2.54	0.43
1:B:93:ARG:NH1	1:B:124:GLN:NE2	2.66	0.42
1:B:111:VAL:HB	1:B:142:PHE:CD2	2.54	0.42
1:B:595:PHE:HE2	1:B:638:LEU:HD21	1.84	0.42
1:B:643:ILE:HG23	1:B:647:ILE:HD13	2.01	0.42
1:B:197:LEU:O	1:B:238:ILE:HD11	2.19	0.42
1:A:384:CYS:SG	1:A:424:ILE:N	2.92	0.42
1:A:419:ILE:CA	1:A:424:ILE:HG12	2.40	0.42
1:B:303:TYR:CZ	1:B:352:LYS:HB3	2.54	0.42
1:B:502:ASN:OD1	1:B:519:ASN:HA	2.18	0.42
1:A:106:ASP:OD1	1:A:106:ASP:N	2.53	0.42
1:A:121:LEU:N	1:A:122:PRO:CD	2.83	0.42
1:A:371:LEU:HD11	1:A:594:LEU:HD11	2.01	0.42
1:A:488:HIS:CD2	1:B:488:HIS:CD2	3.07	0.42
1:A:333:LEU:HD23	1:A:598:TYR:CE1	2.55	0.42
1:A:382:CYS:HB2	1:A:689:LYS:HB2	2.02	0.42
1:B:54:ASN:O	1:B:55:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LYS:HE2	1:B:181:ASN:O	2.20	0.42
1:B:449:SER:O	1:B:452:ASN:HB2	2.20	0.42
1:B:54:ASN:HD21	1:B:63:LEU:HD12	1.84	0.42
1:A:404:GLY:HA2	1:A:411:VAL:O	2.20	0.41
1:A:631:LEU:HD12	1:A:632:ASP:H	1.85	0.41
1:B:371:LEU:HD11	1:B:594:LEU:CD1	2.50	0.41
1:B:262:PHE:CG	1:B:649:GLU:HG2	2.55	0.41
1:B:393:VAL:HA	1:B:401:PHE:O	2.20	0.41
1:A:95:ARG:HA	1:A:95:ARG:HD3	1.69	0.41
1:A:401:PHE:HE2	1:A:429:ILE:CD1	2.33	0.41
1:B:130:ASN:OD1	1:B:132:GLN:HB2	2.20	0.41
1:A:420:HIS:HE1	1:A:425:ASP:OD2	2.03	0.41
1:A:81:ILE:HA	1:A:678:TYR:CE1	2.55	0.41
1:A:505:ILE:HB	1:A:516:LEU:HB2	2.03	0.41
1:A:311:GLN:O	1:A:315:SER:HB3	2.21	0.41
1:A:574:LYS:HD3	1:A:587:ILE:HD11	2.02	0.41
1:B:366:ILE:O	1:B:366:ILE:HG22	2.19	0.41
1:B:460:ARG:HD2	1:B:463:PRO:HA	2.03	0.41
1:B:470:ASN:O	1:B:482:MET:HG3	2.21	0.41
1:A:255:GLN:HE21	1:A:255:GLN:N	2.07	0.41
1:A:436:VAL:HG12	1:A:480:TRP:HD1	1.86	0.41
1:A:474:ASP:O	1:A:478:ARG:N	2.53	0.41
1:A:449:SER:O	1:A:452:ASN:HB2	2.21	0.41
1:B:388:ARG:HB3	1:B:407:ASN:HB3	2.03	0.40
1:B:529:THR:HA	1:B:530:PRO:HD3	1.91	0.40
1:A:568:ASP:O	1:A:595:PHE:HB2	2.22	0.40
1:B:87:LEU:HD12	1:B:87:LEU:HA	1.93	0.40
1:A:379:LEU:CD2	1:A:628:ILE:HD12	2.48	0.40
1:A:661:VAL:CG2	1:A:669:HIS:HB2	2.51	0.40
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.85	0.40
1:B:670:ILE:HB	1:B:688:LEU:HB2	2.02	0.40
1:A:592:HIS:CD2	1:A:594:LEU:H	2.40	0.40
1:B:121:LEU:N	1:B:122:PRO:CD	2.84	0.40
1:B:652:SER:OG	1:B:686:VAL:HG23	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	660/695 (95%)	618 (94%)	40 (6%)	2 (0%)	41	61
1	B	660/695 (95%)	612 (93%)	44 (7%)	4 (1%)	25	43
All	All	1320/1390 (95%)	1230 (93%)	84 (6%)	6 (0%)	29	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	ASN
1	A	385	PRO
1	B	195	CYS
1	B	383	GLU
1	B	483	ILE
1	A	549	VAL

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	603/630 (96%)	578 (96%)	25 (4%)	30	55
1	B	599/630 (95%)	571 (95%)	28 (5%)	26	49
All	All	1202/1260 (95%)	1149 (96%)	53 (4%)	28	52

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	75	ILE
1	A	95	ARG
1	A	134	GLN
1	A	187	THR
1	A	200	SER
1	A	255	GLN
1	A	312	LEU
1	A	315	SER
1	A	352	LYS
1	A	358	GLN
1	A	365	SER
1	A	369	ILE
1	A	372	THR
1	A	384	CYS
1	A	395	VAL
1	A	399	ASP
1	A	407	ASN
1	A	413	GLU
1	A	423	LYS
1	A	497	SER
1	A	506	LEU
1	A	639	THR
1	A	640	SER
1	A	647	ILE
1	B	50	SER
1	B	75	ILE
1	B	105	GLN
1	B	128	THR
1	B	139	ARG
1	B	182	VAL
1	B	227	LEU
1	B	275	ARG
1	B	312	LEU
1	B	321	LYS
1	B	332	GLU
1	B	349	THR
1	B	398	ASN
1	B	399	ASP
1	B	407	ASN
1	B	421	TYR
1	B	428	ASN
1	B	506	LEU

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Mol	Chain	Res	Type
1	B	531	LYS
1	B	556	LEU
1	B	578	GLU
1	B	579	ASN
1	B	605	ILE
1	B	609	LYS
1	B	629	ILE
1	B	647	ILE
1	B	653	LEU
1	B	686	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	102	GLN
1	A	105	GLN
1	A	134	GLN
1	A	137	HIS
1	A	255	GLN
1	A	297	ASN
1	A	407	ASN
1	A	420	HIS
1	A	488	HIS
1	A	592	HIS
1	A	685	ASN
1	B	54	ASN
1	B	102	GLN
1	B	105	GLN
1	B	124	GLN
1	B	132	GLN
1	B	137	HIS
1	B	297	ASN
1	B	311	GLN
1	B	337	HIS
1	B	407	ASN
1	B	416	GLN
1	B	420	HIS
1	B	488	HIS
1	B	592	HIS
1	B	685	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	SAM	A	801	-	23,29,29	1.28	3 (13%)	20,42,42	1.92	3 (15%)
2	SAM	B	801	-	23,29,29	1.24	3 (13%)	20,42,42	1.95	3 (15%)

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
2	SAM	A	801	-	-	1/13/33/33	0/3/3/3
2	SAM	B	801	-	-	2/13/33/33	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SAM	C2-N3	4.15	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SAM	C2-N3	4.00	1.38	1.32
2	A	801	SAM	C2-N1	2.68	1.38	1.33
2	B	801	SAM	C2-N1	2.62	1.38	1.33
2	A	801	SAM	OXT-C	-2.14	1.23	1.30
2	B	801	SAM	OXT-C	-2.13	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	SAM	N3-C2-N1	-6.49	119.87	128.67
2	B	801	SAM	N3-C2-N1	-6.31	120.10	128.67
2	B	801	SAM	O4'-C1'-N9	3.69	113.64	108.75
2	A	801	SAM	O4'-C1'-N9	3.11	112.86	108.75
2	B	801	SAM	OXT-C-O	-3.02	117.24	124.08
2	A	801	SAM	OXT-C-O	-2.80	117.74	124.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	SAM	CB-CG-SD-C5'
2	B	801	SAM	CB-CG-SD-CE
2	A	801	SAM	CB-CG-SD-C5'

There are no ring outliers.

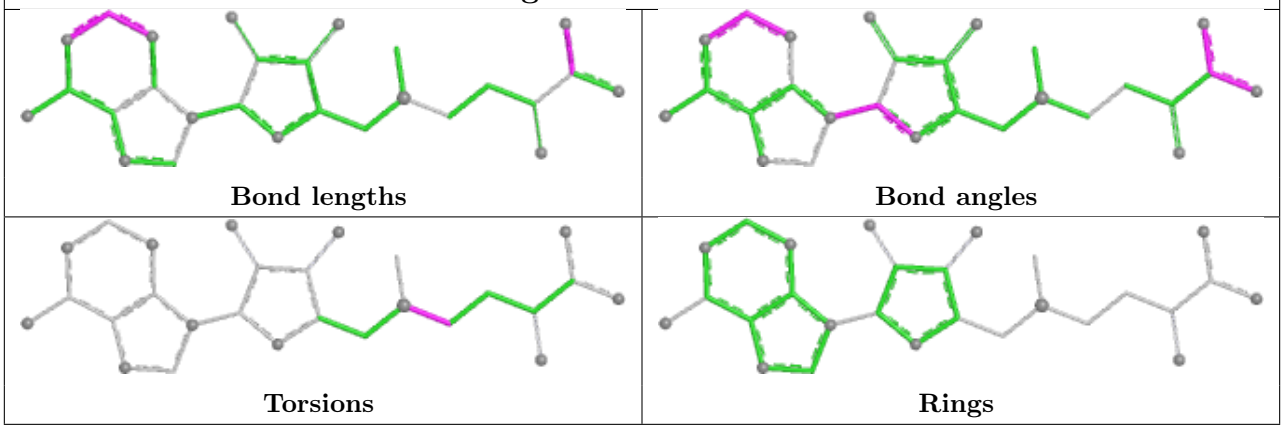
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SAM	2	0
2	B	801	SAM	1	0

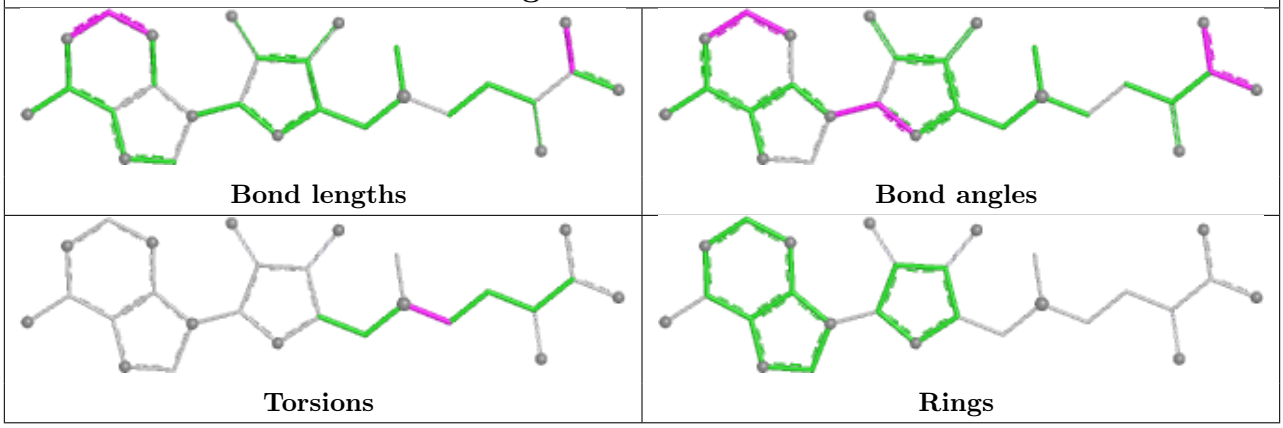
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand SAM A 801



Ligand SAM B 801



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	666/695 (95%)	0.05	14 (2%)	63	66	39, 61, 94, 127	0
1	B	664/695 (95%)	-0.04	14 (2%)	63	66	37, 61, 93, 131	0
All	All	1330/1390 (95%)	0.01	28 (2%)	63	66	37, 61, 94, 131	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	PRO	6.2
1	A	366	ILE	4.9
1	A	421	TYR	4.4
1	B	366	ILE	4.3
1	A	368	GLU	4.1
1	B	181	ASN	3.6
1	A	171	SER	3.3
1	A	17	GLU	3.2
1	B	182	VAL	3.1
1	B	368	GLU	3.0
1	B	25	LEU	3.0
1	A	25	LEU	2.9
1	A	21	LYS	2.9
1	B	421	TYR	2.6
1	A	376	ASP	2.6
1	B	26	ALA	2.6
1	A	22	TYR	2.5
1	A	72	PRO	2.5
1	B	24	ASP	2.5
1	A	608	ARG	2.4
1	A	377	TYR	2.4
1	B	28	GLN	2.4
1	B	234	ARG	2.2
1	B	31	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	18	ARG	2.2
1	B	27	ILE	2.2
1	A	27	ILE	2.1
1	B	653	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

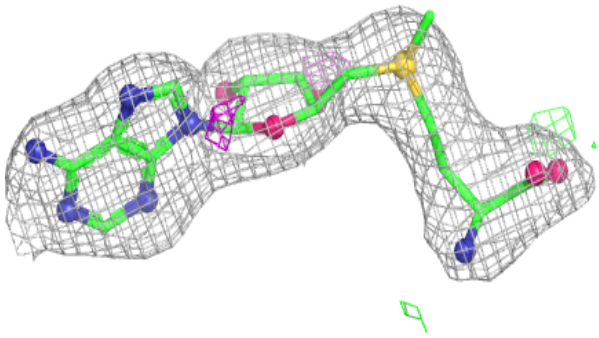
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

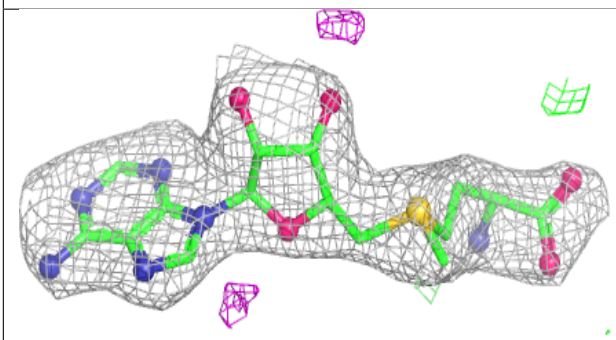
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAM	B	801	27/27	0.95	0.14	62,72,79,89	0
2	SAM	A	801	27/27	0.96	0.13	52,64,78,82	0

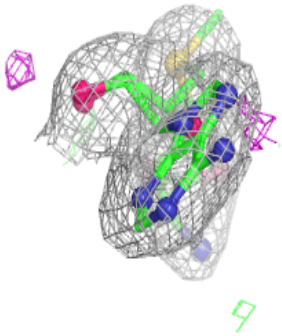
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM B 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

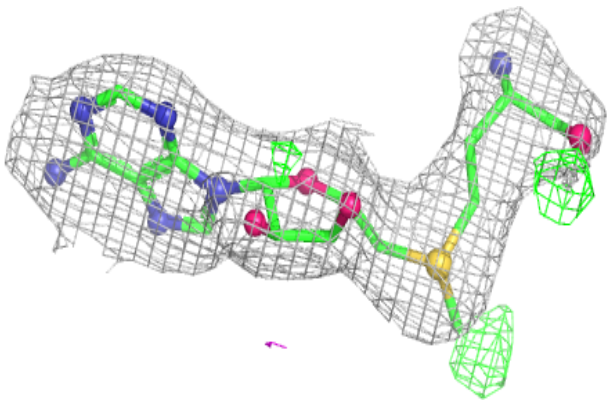


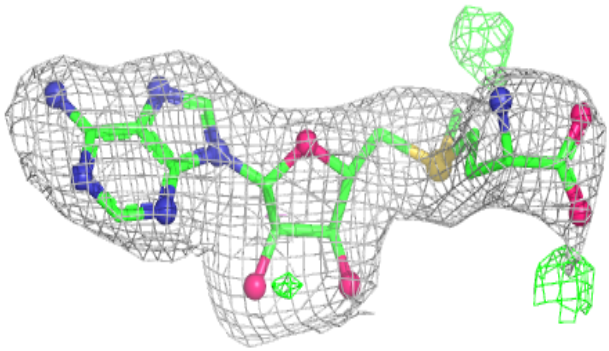


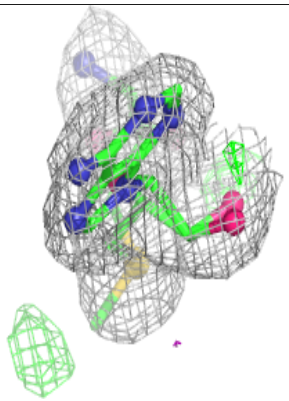


Electron density around SAM A 801:

$2mF_o$-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.