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:

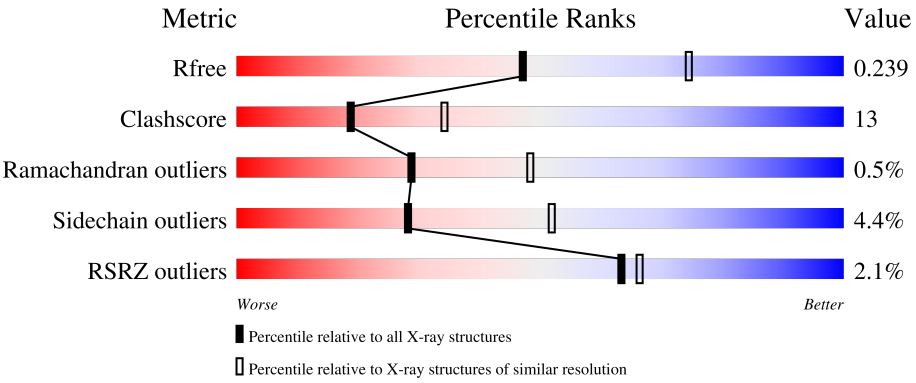
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

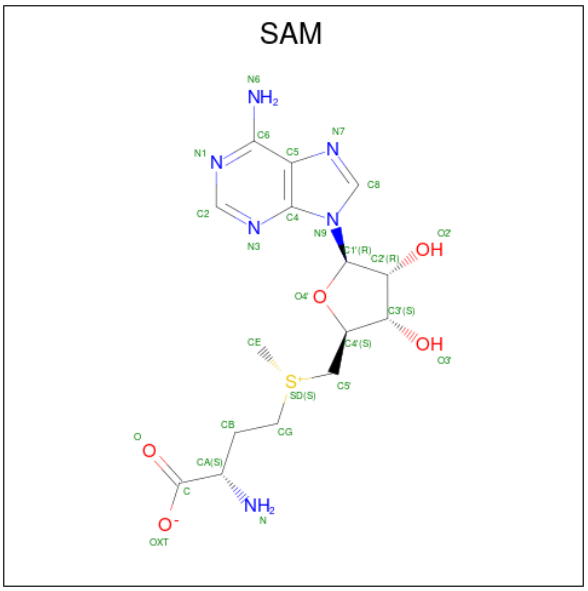
- Molecule 1 is a protein called Leucine carboxyl methyltransferase 2.

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

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
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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

- Molecule 3 is water.

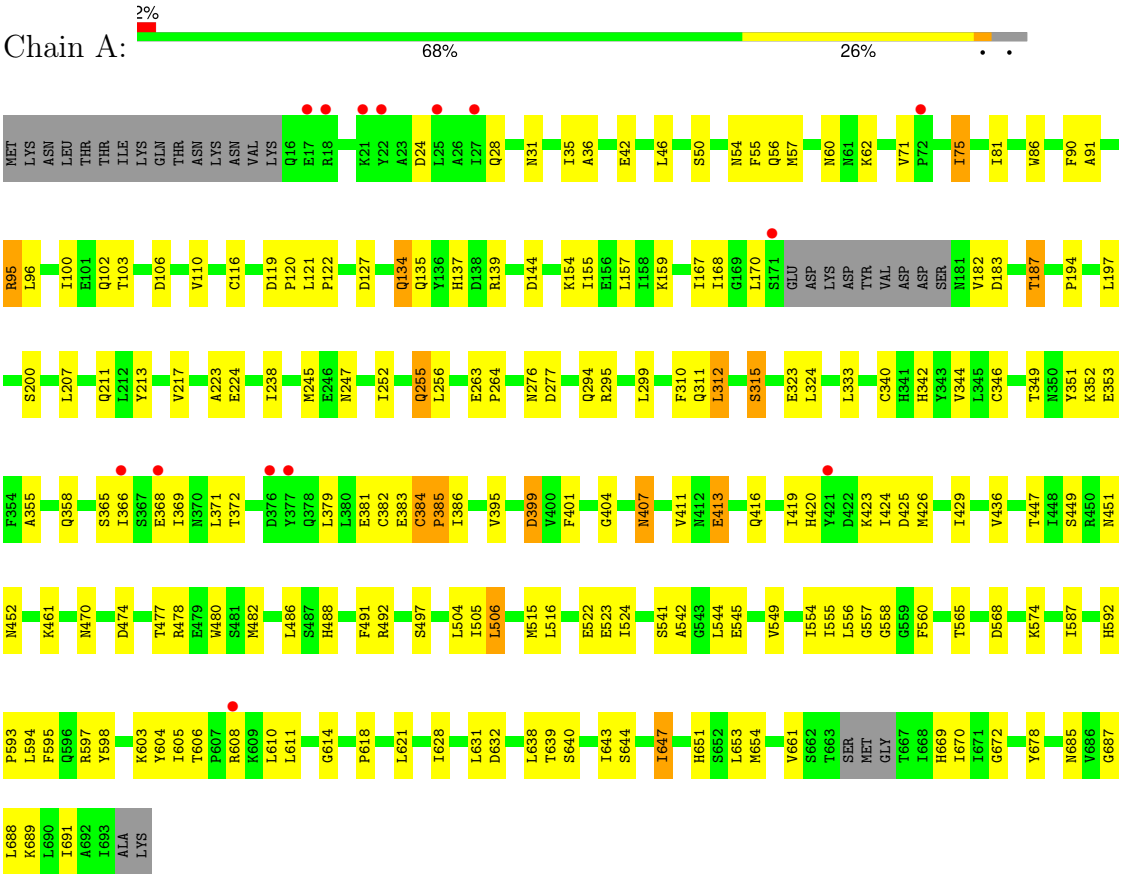
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	75	Total	O	0	0
			75	75		

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.

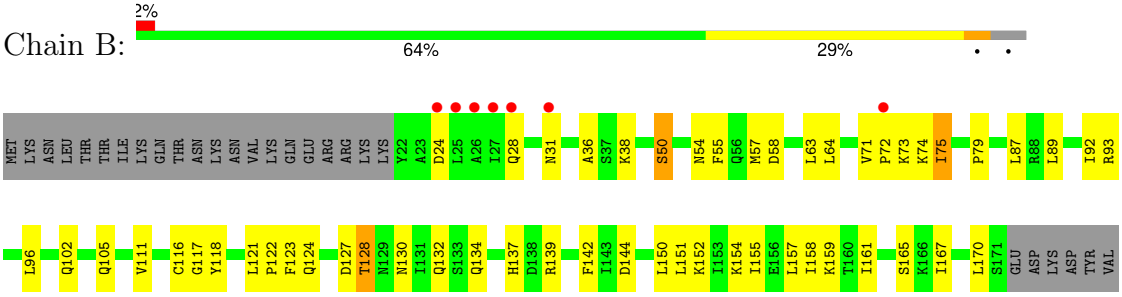
• Molecule 1: Leucine carboxyl methyltransferase 2

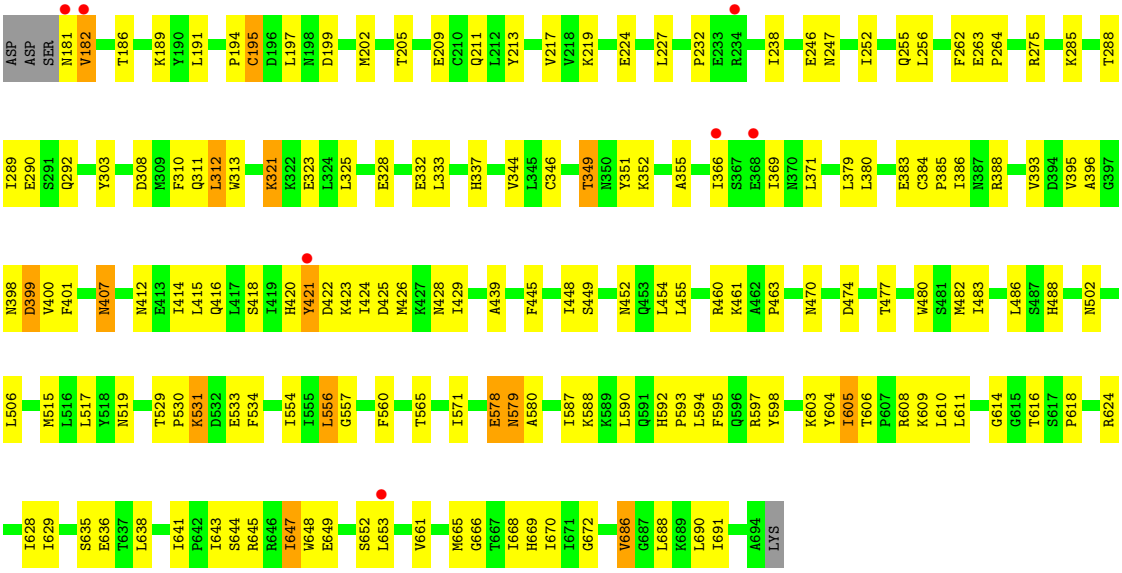
Chain A:



• 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

5.1 Standard geometry

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

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.

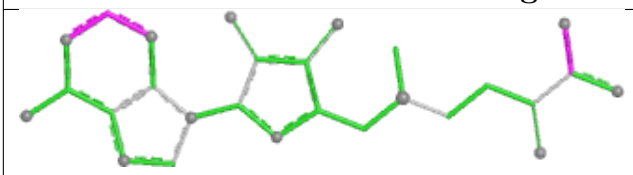
2 monomers are involved in 3 short contacts:

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

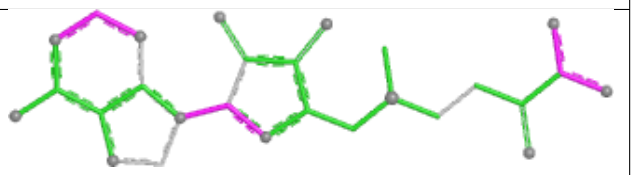
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

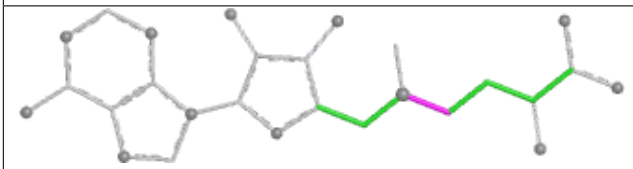
Ligand SAM A 801



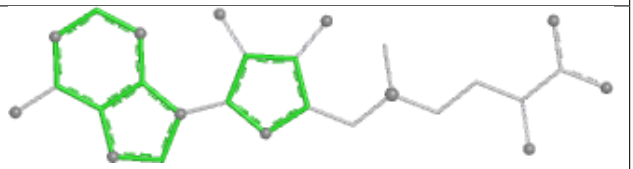
Bond lengths



Bond angles

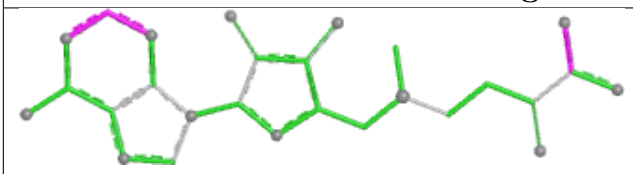


Torsions

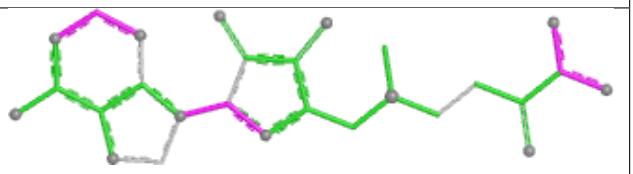


Rings

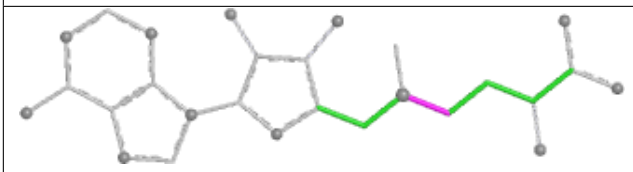
Ligand SAM B 801



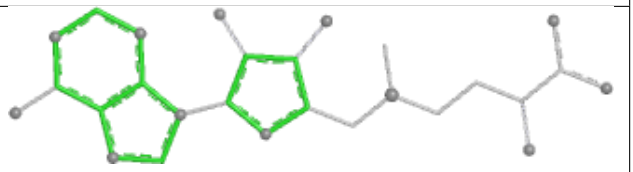
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	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)

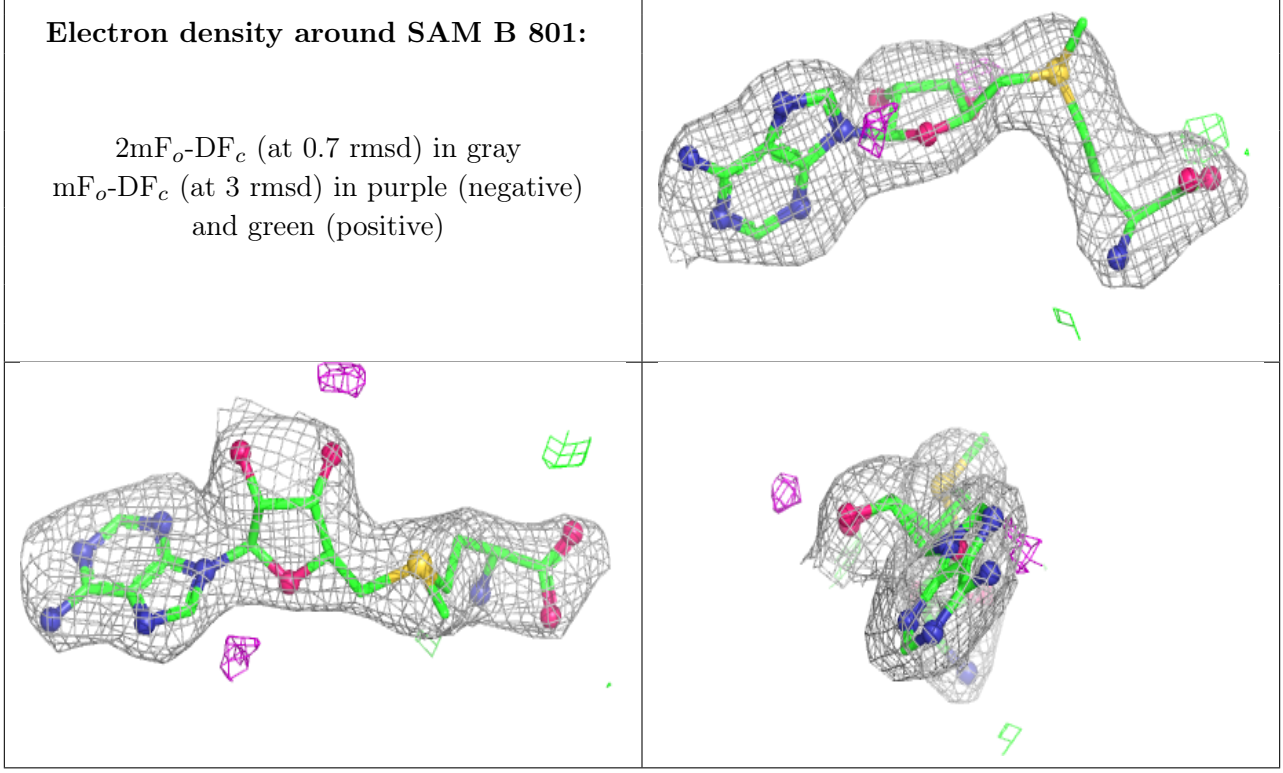
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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.

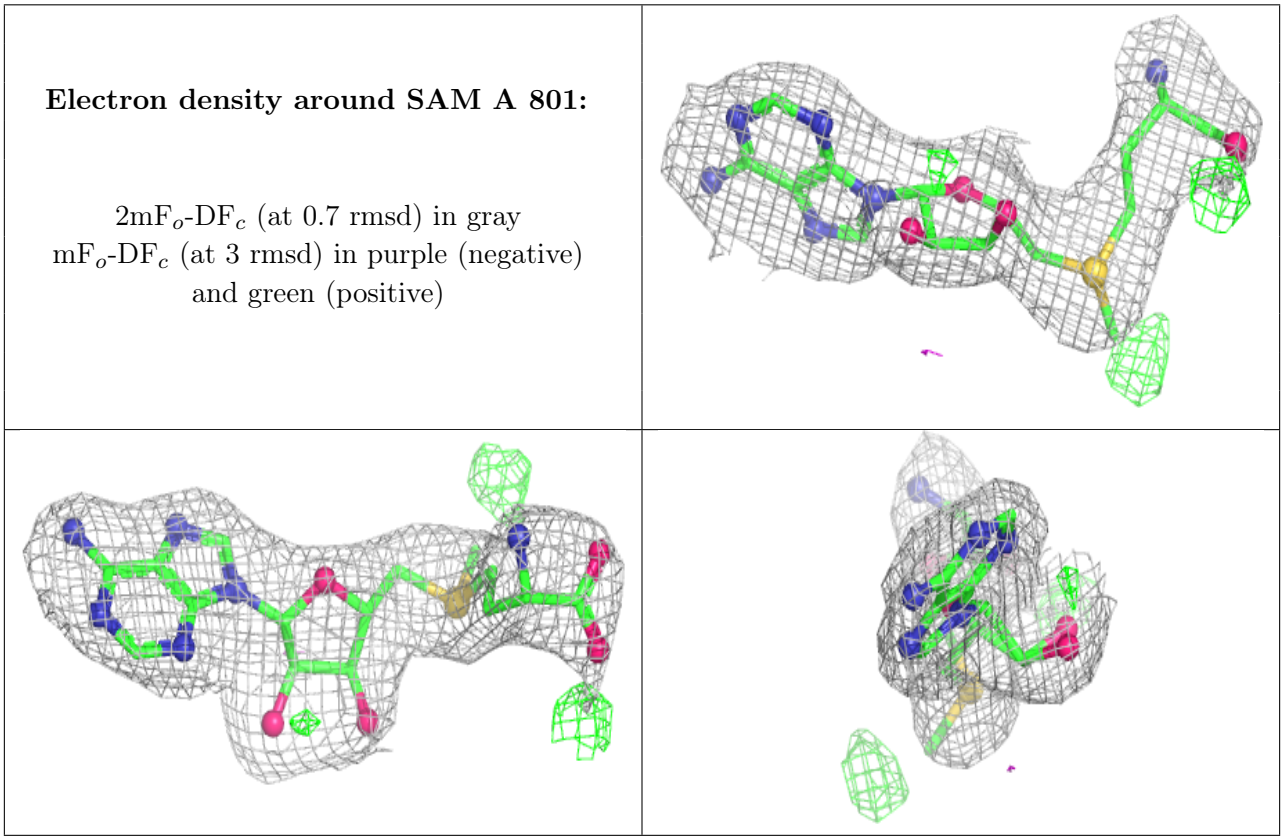
Electron density around SAM B 801:

$2mF_o$-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.