



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2016 – 10:03 PM EST

PDB ID : 5E8J  
Title : Crystal structure of mRNA cap guanine-N7 methyltransferase in complex with RAM  
Authors : Petit, P.; Cowling, V.  
Deposited on : 2015-10-14  
Resolution : 2.35 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

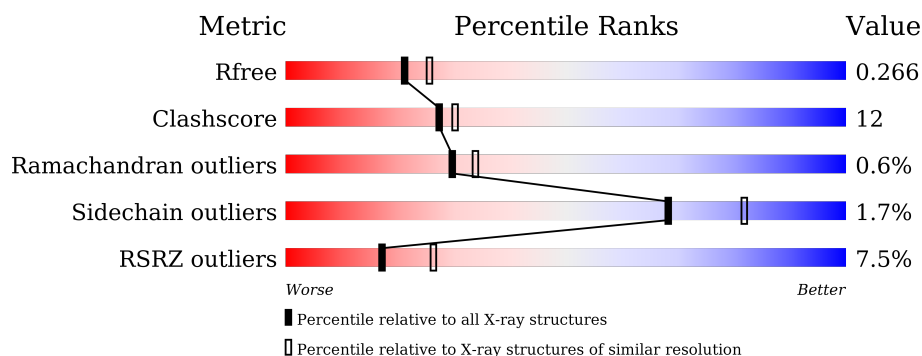
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	312	<div> <div>6%</div> <div>75%</div> <div>24%</div> <div>..</div> </div>
1	B	312	<div> <div>8%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
2	C	44	<div> <div>9%</div> <div>68%</div> <div>25%</div> <div>• 5%</div> </div>
2	D	44	<div> <div>11%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	501	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6084 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.

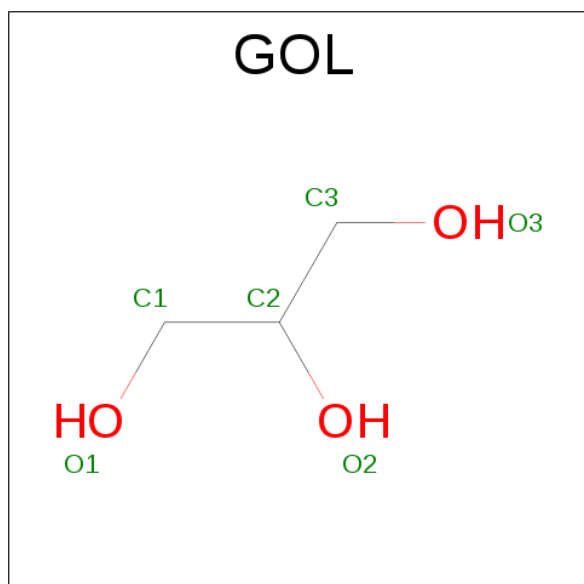
- Molecule 1 is a protein called mRNA cap guanine-N7 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2536	1628	420	469	19			
1	B	310	Total	C	N	O	S	0	0	0
			2557	1641	423	474	19			

- Molecule 2 is a protein called RNMT-activating mini protein.

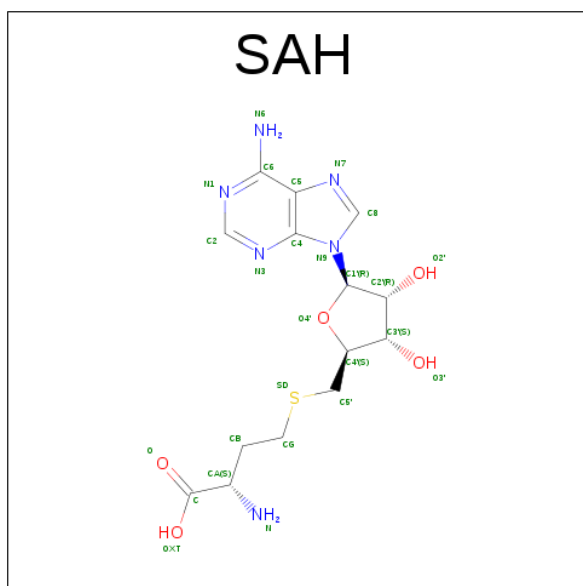
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	42	Total	C	N	O	S	0	0	0
			356	227	55	73	1			
2	D	43	Total	C	N	O	S	0	0	0
			358	228	56	73	1			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

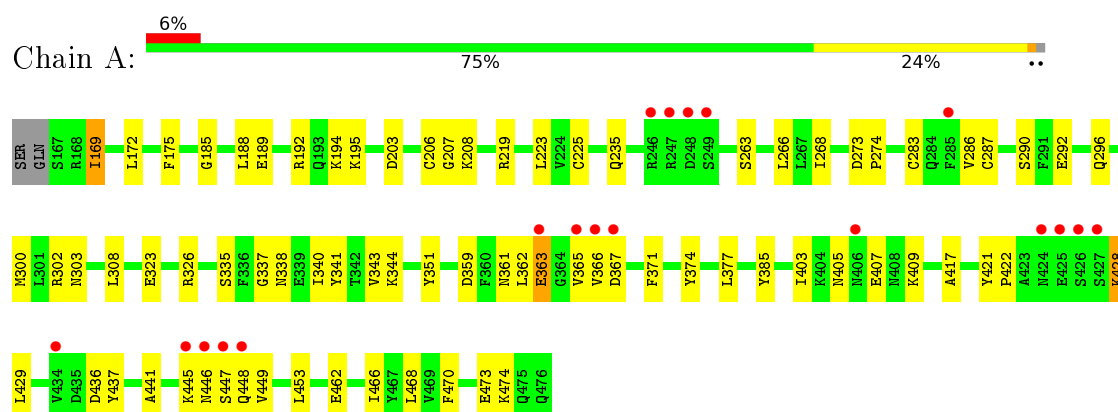
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total	O	0	0
			102	102		
5	B	78	Total	O	0	0
			78	78		
5	C	20	Total	O	0	0
			20	20		
5	D	19	Total	O	0	0
			19	19		

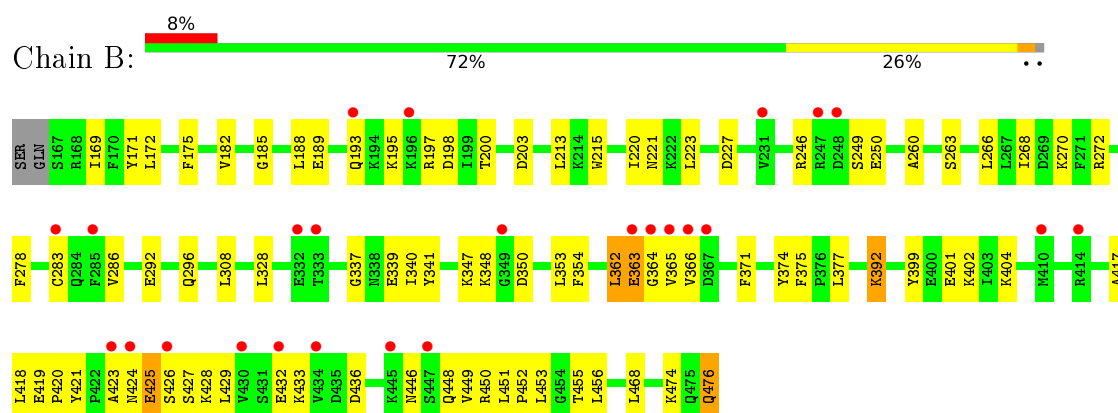
### 3 Residue-property plots

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.

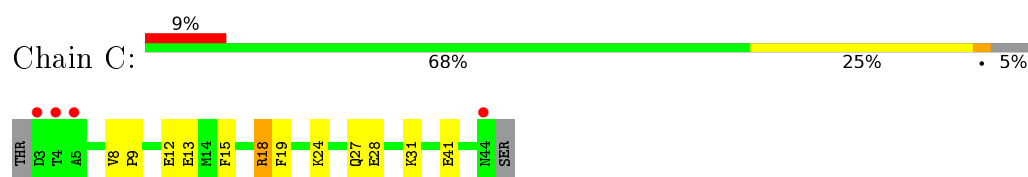
- Molecule 1: mRNA cap guanine-N7 methyltransferase



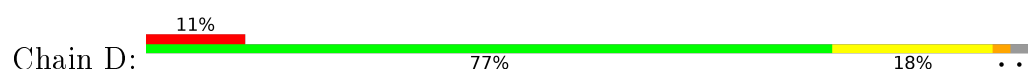
- Molecule 1: mRNA cap guanine-N7 methyltransferase

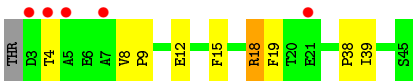


- Molecule 2: RNMT-activating mini protein



- Molecule 2: RNMT-activating mini protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.15Å 50.49Å 84.58Å 90.06° 92.41° 115.41°	Depositor
Resolution (Å)	28.16 – 2.35 28.16 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.8 (28.16-2.35) 92.4 (28.16-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.36Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.210 , 0.269 0.212 , 0.266	Depositor DCC
$R_{free}$ test set	1204 reflections (4.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.012 for k,h,-l 0.013 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6084	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.36	0/2590	0.47	0/3478
1	B	0.37	0/2611	0.46	0/3502
2	C	0.23	0/367	0.42	0/498
2	D	0.23	0/369	0.44	0/501
All	All	0.35	0/5937	0.46	0/7979

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
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	ASN	Peptide
1	A	447	SER	Peptide

### 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	2536	0	2503	55	1
1	B	2557	0	2541	69	1
2	C	356	0	324	11	0
2	D	358	0	325	10	0
3	A	6	0	8	5	0
4	A	26	0	19	1	0
4	B	26	0	19	1	0
5	A	102	0	0	0	0
5	B	78	0	0	3	0
5	C	20	0	0	2	0
5	D	19	0	0	0	0
All	All	6084	0	5739	138	1

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 12.

All (138) 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:B:340:ILE:O	1:B:363:GLU:OE1	1.82	0.97
1:B:246:ARG:HB3	1:B:249:SER:HB2	1.51	0.92
1:B:420:PRO:O	1:B:423:ALA:HB2	1.72	0.90
1:B:424:ASN:N	1:B:425:GLU:OE2	2.07	0.88
1:B:347:LYS:HE2	1:B:350:ASP:HB3	1.55	0.85
1:A:449:VAL:HG11	1:A:453:LEU:HD21	1.59	0.84
1:B:340:ILE:C	1:B:363:GLU:OE1	2.20	0.80
1:A:208:LYS:H	3:A:501:GOL:H31	1.46	0.79
1:B:266:LEU:HG	1:B:268:ILE:HG22	1.65	0.79
1:A:185:GLY:O	1:A:189:GLU:HG3	1.86	0.75
1:A:192:ARG:NH2	1:A:219:ARG:O	2.19	0.74
2:C:18:ARG:HG2	2:C:19:PHE:CD2	2.27	0.70
1:B:425:GLU:O	1:B:426:SER:HB2	1.92	0.69
1:B:195:LYS:HE3	2:C:13:GLU:OE2	1.92	0.68
1:A:351:TYR:O	2:C:18:ARG:NH1	2.27	0.67
2:C:28:GLU:OE2	2:C:31:LYS:NZ	2.28	0.67
2:C:27:GLN:NE2	5:C:102:HOH:O	2.25	0.67
1:A:169:ILE:HD11	1:A:340:ILE:HG23	1.80	0.64
1:B:392:LYS:O	1:B:392:LYS:HG2	1.97	0.64
3:A:501:GOL:H32	4:A:502:SAH:HB2	1.80	0.64
1:A:449:VAL:HG13	2:C:41:GLU:HG2	1.78	0.63
1:A:208:LYS:HD2	3:A:501:GOL:H12	1.80	0.63
1:B:347:LYS:HE2	1:B:350:ASP:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:SER:OG	1:A:344:LYS:HD3	1.99	0.62
1:A:169:ILE:HG13	1:A:172:LEU:HD23	1.82	0.62
1:B:353:LEU:HD12	2:D:12:GLU:HG3	1.80	0.62
1:A:283:CYS:SG	1:A:286:VAL:HB	2.43	0.59
1:B:375:PHE:CE2	1:B:392:LYS:HD2	2.38	0.58
1:A:266:LEU:HG	1:A:268:ILE:HG22	1.85	0.57
1:B:175:PHE:HA	1:B:417:ALA:HB1	1.87	0.57
2:D:18:ARG:HG2	2:D:19:PHE:CD2	2.39	0.57
1:B:203:ASP:HB2	1:B:223:LEU:HD11	1.87	0.57
1:B:421:TYR:O	1:B:453:LEU:N	2.32	0.56
1:A:366:VAL:HG12	1:A:367:ASP:N	2.21	0.56
1:B:185:GLY:O	1:B:189:GLU:HG3	2.06	0.56
1:B:423:ALA:HB3	1:B:429:LEU:HD23	1.88	0.56
1:B:347:LYS:CE	1:B:350:ASP:HB3	2.31	0.55
1:A:448:GLN:HG3	1:A:449:VAL:O	2.07	0.55
1:B:169:ILE:HG13	1:B:172:LEU:HD23	1.89	0.54
1:A:421:TYR:CE1	1:A:422:PRO:HG3	2.42	0.54
1:A:208:LYS:HG2	1:A:235:GLN:CD	2.29	0.54
1:A:365:VAL:HG12	1:A:366:VAL:HG23	1.89	0.54
1:A:340:ILE:O	1:A:362:LEU:HD12	2.08	0.54
1:B:476:GLN:HG3	5:B:653:HOH:O	2.09	0.53
1:B:246:ARG:NH1	1:B:250:GLU:OE1	2.42	0.53
1:A:175:PHE:HA	1:A:417:ALA:HB1	1.91	0.53
1:B:169:ILE:HG12	1:B:172:LEU:HB3	1.90	0.53
1:A:308:LEU:HB2	1:A:474:LYS:HE2	1.91	0.52
1:A:292:GLU:HB2	1:A:371:PHE:CE2	2.45	0.52
1:A:366:VAL:CG1	1:A:367:ASP:N	2.73	0.51
1:B:292:GLU:HB2	1:B:371:PHE:CE2	2.44	0.51
1:A:449:VAL:CG1	1:A:453:LEU:HD21	2.35	0.51
1:B:339:GLU:OE2	1:B:433:LYS:HD2	2.10	0.51
1:A:208:LYS:N	3:A:501:GOL:H31	2.21	0.51
1:A:169:ILE:O	1:A:169:ILE:HG23	2.13	0.49
1:B:260:ALA:HB2	1:B:270:LYS:HE2	1.94	0.49
1:B:362:LEU:O	1:B:364:GLY:N	2.46	0.49
1:B:283:CYS:SG	1:B:286:VAL:HB	2.53	0.49
1:B:362:LEU:HD13	1:B:365:VAL:HG21	1.94	0.48
2:D:15:PHE:O	2:D:18:ARG:HB2	2.13	0.48
1:B:418:LEU:CD2	1:B:456:LEU:HG	2.44	0.48
2:C:12:GLU:OE2	5:C:101:HOH:O	2.20	0.48
1:A:374:TYR:O	1:A:377:LEU:HB3	2.14	0.48
1:B:425:GLU:OE2	1:B:425:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HB2	1:B:474:LYS:HE2	1.96	0.48
1:B:337:GLY:HA2	1:B:341:TYR:CZ	2.49	0.48
2:C:24:LYS:HA	2:C:24:LYS:HD2	1.59	0.48
1:A:337:GLY:HA2	1:A:341:TYR:CZ	2.49	0.47
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.71	0.47
1:B:455:THR:HG22	2:D:39:ILE:HA	1.97	0.47
1:B:450:ARG:NH1	5:B:608:HOH:O	2.47	0.47
1:B:374:TYR:O	1:B:377:LEU:HB3	2.14	0.47
2:D:8:VAL:N	2:D:9:PRO:HD2	2.28	0.47
1:A:203:ASP:HB2	1:A:223:LEU:HD11	1.96	0.47
1:A:207:GLY:HA3	3:A:501:GOL:H31	1.95	0.47
1:B:169:ILE:CG1	1:B:172:LEU:HD23	2.44	0.46
1:A:302:ARG:HB2	1:A:385:TYR:OH	2.16	0.46
1:A:421:TYR:O	1:A:453:LEU:N	2.40	0.46
1:B:197:ARG:NH1	1:B:198:ASP:O	2.48	0.46
1:B:399:TYR:CZ	2:D:38:PRO:HB3	2.50	0.46
1:B:227:ASP:OD1	4:B:501:SAH:O2'	2.31	0.46
1:B:246:ARG:CB	1:B:249:SER:HB2	2.33	0.46
1:B:451:LEU:HB3	1:B:452:PRO:HA	1.98	0.46
1:A:219:ARG:O	1:A:219:ARG:HG2	2.17	0.45
1:A:263:SER:HB2	1:A:296:GLN:HB3	1.98	0.45
1:A:266:LEU:HD12	1:A:303:ASN:OD1	2.16	0.45
1:A:287:CYS:HG	1:A:470:PHE:HZ	1.63	0.45
1:B:449:VAL:HG11	1:B:453:LEU:HD21	1.97	0.45
1:B:292:GLU:HG3	1:B:371:PHE:CZ	2.51	0.45
1:B:328:LEU:O	1:B:348:LYS:HE3	2.17	0.45
2:C:8:VAL:N	2:C:9:PRO:HD2	2.32	0.45
1:B:263:SER:O	1:B:296:GLN:HA	2.17	0.44
1:B:272:ARG:NH1	5:B:610:HOH:O	2.49	0.44
1:A:338:ASN:ND2	1:A:462:GLU:OE1	2.49	0.44
1:A:468:LEU:HD12	1:A:468:LEU:C	2.37	0.44
1:B:468:LEU:HD12	1:B:468:LEU:C	2.37	0.44
1:B:215:TRP:HB3	1:B:220:ILE:CD1	2.48	0.44
1:B:169:ILE:HD11	1:B:172:LEU:HD23	2.00	0.44
1:A:208:LYS:HD3	1:A:235:GLN:NE2	2.33	0.43
1:A:429:LEU:HD13	1:A:437:TYR:CD2	2.54	0.43
1:A:403:ILE:HD11	1:A:409:LYS:HG3	1.99	0.43
1:A:263:SER:O	1:A:296:GLN:HA	2.18	0.43
1:B:455:THR:HG22	2:D:39:ILE:HG12	2.01	0.43
1:B:246:ARG:NH1	1:B:249:SER:HB3	2.34	0.43
1:B:198:ASP:HA	1:B:221:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:ARG:HG2	2:D:19:PHE:HD2	1.80	0.43
1:A:448:GLN:NE2	1:A:449:VAL:O	2.52	0.43
1:B:189:GLU:O	1:B:193:GLN:HG3	2.19	0.43
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.89	0.42
1:B:425:GLU:CD	1:B:425:GLU:N	2.73	0.42
1:B:171:TYR:CD2	1:B:419:GLU:HB3	2.53	0.42
1:A:441:ALA:O	1:A:445:LYS:HG3	2.19	0.42
1:A:273:ASP:HA	1:A:274:PRO:HD2	1.87	0.42
1:B:169:ILE:HG12	1:B:169:ILE:O	2.20	0.42
1:B:425:GLU:H	1:B:425:GLU:CD	2.23	0.42
1:B:249:SER:HB3	1:B:250:GLU:H	1.61	0.42
1:A:206:CYS:SG	1:A:225:CYS:HB3	2.60	0.42
1:A:428:LYS:HB3	1:A:428:LYS:HE3	1.63	0.42
2:C:15:PHE:O	2:C:18:ARG:HB2	2.20	0.41
1:A:323:GLU:OE1	1:A:326:ARG:NH1	2.52	0.41
2:C:18:ARG:HG2	2:C:19:PHE:HD2	1.78	0.41
1:A:343:VAL:HA	1:A:359:ASP:O	2.19	0.41
1:B:200:THR:HG22	1:B:278:PHE:HD1	1.85	0.41
2:D:4:THR:HG23	2:D:8:VAL:CG2	2.50	0.41
1:B:420:PRO:HA	1:B:453:LEU:O	2.21	0.41
1:A:290:SER:HB3	1:A:300:MET:SD	2.61	0.41
1:A:341:TYR:HA	1:A:361:ASN:O	2.20	0.41
1:B:446:ASN:OD1	1:B:448:GLN:HG3	2.20	0.41
1:B:354:PHE:CE1	1:B:377:LEU:HD21	2.55	0.41
1:B:427:SER:OG	1:B:428:LYS:N	2.54	0.41
1:A:405:ASN:OD1	1:A:407:GLU:HB2	2.21	0.40
1:A:194:LYS:NZ	1:A:473:GLU:OE2	2.54	0.40
1:A:188:LEU:HA	1:A:188:LEU:HD23	1.90	0.40
1:B:401:GLU:HA	1:B:404:LYS:HE2	2.03	0.40
1:A:195:LYS:HA	1:A:195:LYS:HD2	1.85	0.40
1:B:182:VAL:HG11	1:B:402:LYS:HG3	2.03	0.40
1:B:399:TYR:CE2	2:D:38:PRO:HB3	2.56	0.40
1:A:292:GLU:HG3	1:A:371:PHE:CZ	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:NE2	1:B:432:GLU:OE1[1_544]	2.07	0.13

## 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	308/312 (99%)	297 (96%)	10 (3%)	1 (0%)	46	55
1	B	308/312 (99%)	293 (95%)	14 (4%)	1 (0%)	46	55
2	C	40/44 (91%)	39 (98%)	0	1 (2%)	7	4
2	D	41/44 (93%)	40 (98%)	0	1 (2%)	7	5
All	All	697/712 (98%)	669 (96%)	24 (3%)	4 (1%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	GLU
1	B	363	GLU
2	D	18	ARG
2	C	18	ARG

### 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	277/285 (97%)	272 (98%)	5 (2%)	66	81
1	B	282/285 (99%)	276 (98%)	6 (2%)	61	76
2	C	39/41 (95%)	39 (100%)	0	100	100
2	D	39/41 (95%)	39 (100%)	0	100	100
All	All	637/652 (98%)	626 (98%)	11 (2%)	68	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ILE
1	A	363	GLU
1	A	428	LYS
1	A	436	ASP
1	A	466	ILE
1	B	362	LEU
1	B	366	VAL
1	B	392	LYS
1	B	425	GLU
1	B	436	ASP
1	B	476	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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
3	GOL	A	501	-	5,5,5	0.34	0	5,5,5	0.20	0
4	SAH	A	502	-	22,28,28	4.96	7 (31%)	18,40,40	2.72	4 (22%)
4	SAH	B	501	-	22,28,28	4.98	7 (31%)	18,40,40	2.74	3 (16%)

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	GOL	A	501	-	-	0/4/4/4	0/0/0/0
4	SAH	A	502	-	-	0/7/31/31	0/3/3/3
4	SAH	B	501	-	-	0/7/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	SAH	C2'-C1'	-14.67	1.30	1.53
4	A	502	SAH	C2'-C1'	-14.55	1.30	1.53
4	B	501	SAH	O4'-C4'	-7.49	1.27	1.45
4	A	502	SAH	O4'-C4'	-7.28	1.28	1.45
4	B	501	SAH	O3'-C3'	-2.44	1.37	1.43
4	A	502	SAH	O3'-C3'	-2.42	1.37	1.43
4	B	501	SAH	C5'-C4'	2.47	1.59	1.52
4	A	502	SAH	C5'-C4'	2.48	1.59	1.52
4	B	501	SAH	C5'-SD	2.71	1.86	1.81
4	A	502	SAH	C5'-SD	2.74	1.86	1.81
4	A	502	SAH	O2'-C2'	4.23	1.52	1.43
4	B	501	SAH	O2'-C2'	4.27	1.53	1.43
4	B	501	SAH	O4'-C1'	14.85	1.62	1.41
4	A	502	SAH	O4'-C1'	14.95	1.62	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	SAH	N3-C2-N1	-10.11	120.93	128.87
4	B	501	SAH	N3-C2-N1	-9.98	121.03	128.87
4	B	501	SAH	C4'-O4'-C1'	-3.88	105.53	109.64
4	A	502	SAH	C4'-O4'-C1'	-3.36	106.09	109.64
4	A	502	SAH	C1'-N9-C4	-2.04	124.53	126.81
4	A	502	SAH	C5'-SD-CG	2.10	108.79	102.42
4	B	501	SAH	C5'-SD-CG	2.57	110.22	102.42



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GOL	5	0
4	A	502	SAH	1	0
4	B	501	SAH	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	310/312 (99%)	0.41	19 (6%) 25 37	11, 22, 45, 58	0
1	B	310/312 (99%)	0.46	25 (8%) 15 23	11, 23, 46, 56	0
2	C	42/44 (95%)	0.30	4 (9%) 10 17	16, 25, 39, 49	0
2	D	43/44 (97%)	0.53	5 (11%) 6 11	17, 26, 41, 53	0
All	All	705/712 (99%)	0.43	53 (7%) 17 26	11, 23, 46, 58	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	5	ALA	6.8
1	A	365	VAL	5.8
1	B	423	ALA	5.0
1	A	425	GLU	4.8
1	B	424	ASN	4.7
1	B	332	GLU	4.4
1	B	365	VAL	4.4
1	A	247	ARG	4.4
1	A	246	ARG	4.2
1	A	249	SER	4.0
1	B	364	GLY	3.8
1	A	367	ASP	3.8
1	A	424	ASN	3.6
2	C	5	ALA	3.5
1	A	446	ASN	3.5
2	D	3	ASP	3.5
1	A	426	SER	3.1
1	A	434	VAL	3.1
1	B	363	GLU	3.1
1	B	430	VAL	3.0
1	A	366	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	333	THR	3.0
1	B	366	VAL	2.9
1	B	432	GLU	2.8
1	B	367	ASP	2.8
1	B	445	LYS	2.7
1	A	447	SER	2.7
1	B	283	CYS	2.6
1	A	427	SER	2.6
1	B	349	GLY	2.6
2	C	3	ASP	2.6
1	B	447	SER	2.5
1	B	410	MET	2.5
1	A	406	ASN	2.4
1	A	285	PHE	2.4
2	D	21	GLU	2.4
2	D	7	ALA	2.4
1	B	196	LYS	2.3
1	B	414	ARG	2.3
2	C	4	THR	2.2
1	B	248	ASP	2.2
1	B	426	SER	2.2
2	C	44	ASN	2.2
1	B	247	ARG	2.2
1	A	445	LYS	2.2
1	B	193	GLN	2.2
2	D	4	THR	2.1
1	A	363	GLU	2.1
1	A	248	ASP	2.1
1	B	434	VAL	2.1
1	A	448	GLN	2.1
1	B	231	VAL	2.1
1	B	285	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	A	501	6/6	0.76	0.24	4.47	35,42,45,47	0
4	SAH	B	501	26/26	0.89	0.16	0.32	15,25,30,34	0
4	SAH	A	502	26/26	0.93	0.14	-0.37	15,16,23,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.