



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:31 AM GMT

PDB ID : 3B3F  
Title : The 2.2 Å crystal structure of the catalytic domain of coactivator-associated arginine methyl transferase I(CARM1,142-478), in complex with S-adenosyl homocysteine  
Authors : Troffer-Charlier, N.; Cura, V.; Hassenboehler, P.; Moras, D.; Cavarelli, J.  
Deposited on : 2007-10-22  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

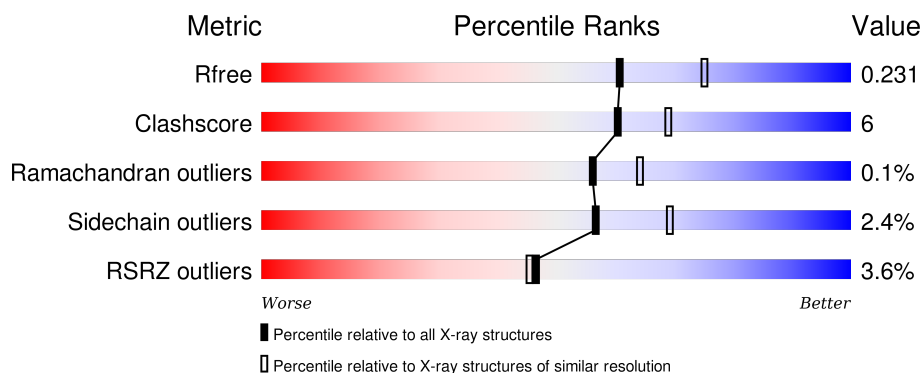
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	341	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	B	341	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	C	341	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	D	341	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

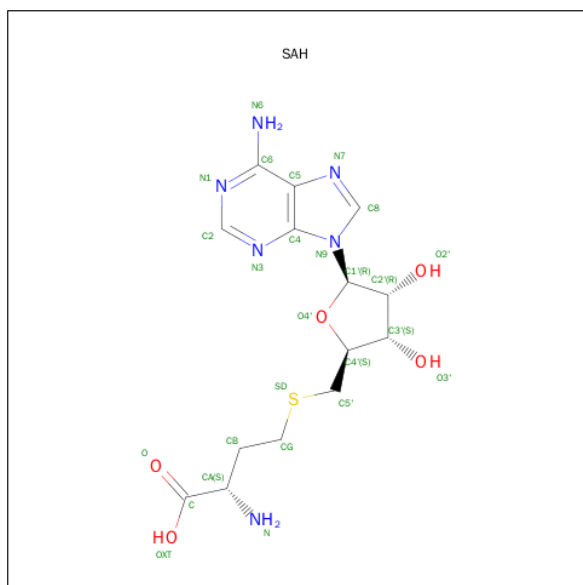
There are 3 unique types of molecules in this entry. The entry contains 11469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2701	1745	445	497	14			
1	B	337	Total	C	N	O	S	0	0	0
			2701	1745	445	497	14			
1	C	337	Total	C	N	O	S	0	0	0
			2701	1745	445	497	14			
1	D	337	Total	C	N	O	S	0	0	0
			2701	1745	445	497	14			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

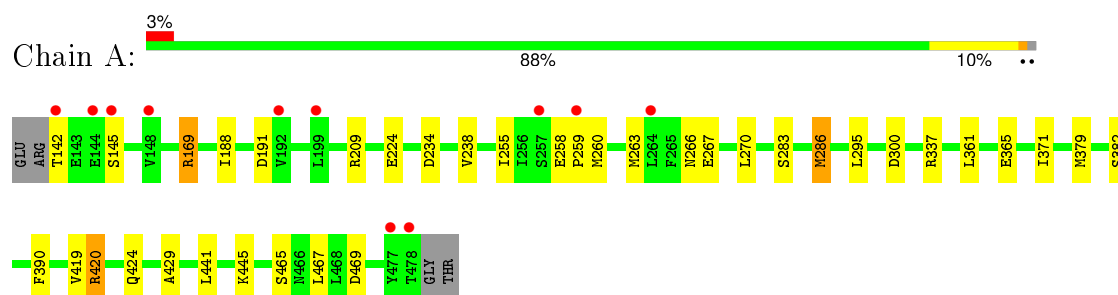
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	130	Total	O	0	0
			130	130		
3	C	130	Total	O	0	0
			130	130		
3	D	149	Total	O	0	0
			149	149		

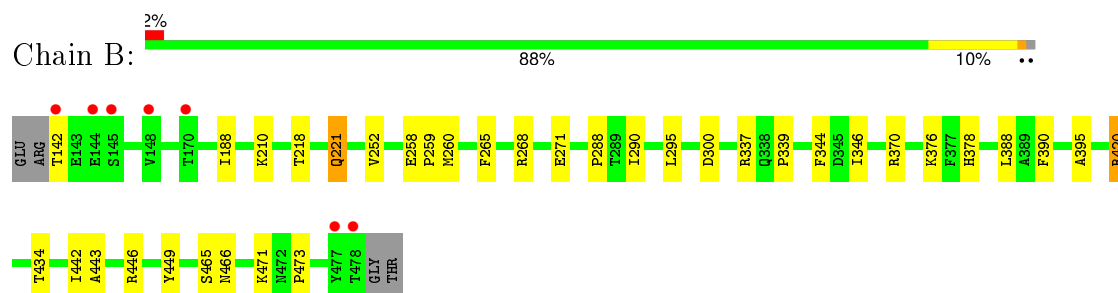
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

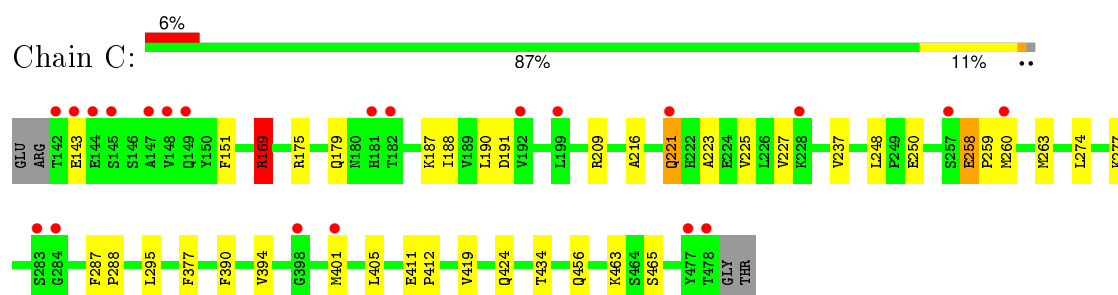
#### • Molecule 1: Histone-arginine methyltransferase CARM1



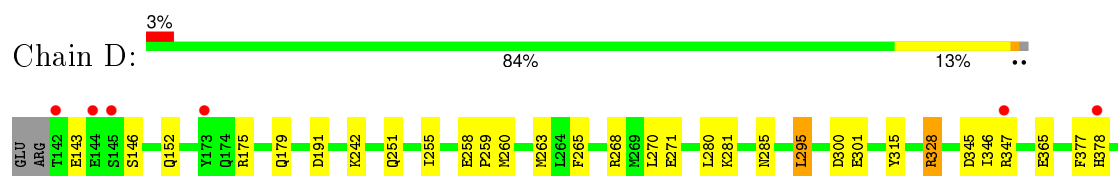
#### • Molecule 1: Histone-arginine methyltransferase CARM1



#### • Molecule 1: Histone-arginine methyltransferase CARM1



#### • Molecule 1: Histone-arginine methyltransferase CARM1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.82Å 98.69Å 206.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 2.20 29.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.85-2.20) 99.4 (29.85-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.182 , 0.234 0.181 , 0.231	Depositor DCC
$R_{free}$ test set	3864 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 78026 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.77 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.1686e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/2770	0.74	5/3755 (0.1%)
1	B	0.63	0/2770	0.68	2/3755 (0.1%)
1	C	0.64	0/2770	0.70	3/3755 (0.1%)
1	D	0.67	0/2770	0.68	3/3755 (0.1%)
All	All	0.65	0/11080	0.70	13/15020 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	A	420	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	420	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	420	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	C	169	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	169	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	D	420	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	B	420	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	420	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	191	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	169	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	191	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	191	ASP	CB-CG-OD1	5.03	122.82	118.30

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	2701	0	2652	27	0
1	B	2701	0	2652	29	0
1	C	2701	0	2652	30	0
1	D	2701	0	2652	33	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
2	C	26	0	19	2	0
2	D	26	0	19	1	0
3	A	152	0	0	4	0
3	B	130	0	0	6	0
3	C	130	0	0	1	0
3	D	149	0	0	6	0
All	All	11469	0	10684	120	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 6.

All (120) 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:260:MET:CE	1:B:288:PRO:HG3	1.85	1.07
1:B:260:MET:HE1	1:B:288:PRO:HG3	1.43	0.96
1:D:263:MET:HE3	1:D:419:VAL:HG11	1.54	0.87
1:C:169:ARG:HH22	2:C:481:SAH:C	1.88	0.87
1:B:268:ARG:HD2	1:B:271:GLU:OE2	1.74	0.86
1:A:255:ILE:HB	1:A:286:MET:CE	2.08	0.84
1:D:179:GLN:HG2	1:D:401:MET:SD	2.21	0.81
1:B:221:GLN:HG3	3:B:565:HOH:O	1.81	0.79
1:B:260:MET:HE3	1:B:288:PRO:HG3	1.62	0.79
1:B:378:HIS:HB3	3:B:593:HOH:O	1.84	0.76
1:D:263:MET:CE	1:D:419:VAL:HG11	2.14	0.76
1:C:288:PRO:HB2	1:C:394:VAL:HG22	1.70	0.74
1:C:411:GLU:HG3	1:C:412:PRO:HD2	1.69	0.73
1:B:268:ARG:CD	1:B:271:GLU:OE2	2.35	0.73
1:B:295:LEU:HD11	1:B:388:LEU:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:LYS:HE2	1:B:434:THR:HG21	1.72	0.71
1:C:188:ILE:HD11	1:C:209:ARG:HH21	1.57	0.70
1:D:301:GLU:HG2	1:D:386:HIS:CE1	2.27	0.70
1:B:295:LEU:HD13	1:B:390:PHE:CE2	2.26	0.70
1:B:218:THR:O	1:B:221:GLN:HG2	1.92	0.69
1:C:169:ARG:NH2	1:C:258:GLU:HG2	2.07	0.69
1:D:476:ARG:O	1:D:477:TYR:HB3	1.93	0.69
1:C:295:LEU:HD13	1:C:390:PHE:CE2	2.28	0.68
1:D:476:ARG:O	1:D:477:TYR:CB	2.42	0.68
1:C:258:GLU:HG3	1:C:258:GLU:O	1.92	0.67
1:A:169:ARG:HH22	2:A:481:SAH:C	2.07	0.67
1:C:169:ARG:HH21	1:C:258:GLU:HG2	1.60	0.66
1:B:300:ASP:OD2	1:B:420:ARG:NH2	2.28	0.66
1:A:424:GLN:HG3	1:A:465:SER:O	1.96	0.66
1:D:315:TYR:HB2	1:D:328:ARG:HG3	1.79	0.65
1:C:175:ARG:HD3	3:C:602:HOH:O	1.96	0.65
1:A:224:GLU:HG2	1:A:238:VAL:HB	1.80	0.64
1:A:255:ILE:HB	1:A:286:MET:HE2	1.80	0.64
1:D:420:ARG:HD3	3:D:543:HOH:O	1.98	0.64
1:A:420:ARG:CD	3:A:538:HOH:O	2.46	0.63
1:B:420:ARG:HD3	3:B:538:HOH:O	2.00	0.61
1:D:268:ARG:HD2	1:D:271:GLU:OE2	2.00	0.60
1:A:420:ARG:HD3	3:A:538:HOH:O	2.00	0.60
1:A:188:ILE:HD11	1:A:209:ARG:NH1	2.16	0.60
1:D:285:ASN:HB2	3:D:499:HOH:O	2.01	0.60
1:C:288:PRO:CB	1:C:394:VAL:HG22	2.33	0.59
1:B:376:LYS:HG3	1:B:434:THR:CG2	2.33	0.58
1:C:424:GLN:HG3	1:C:465:SER:O	2.04	0.57
1:D:179:GLN:CG	1:D:401:MET:SD	2.92	0.57
1:C:221:GLN:O	1:C:225:VAL:HG23	2.04	0.57
1:A:300:ASP:OD2	1:A:420:ARG:NH2	2.34	0.57
1:C:169:ARG:NH2	2:C:481:SAH:O	2.37	0.56
1:A:295:LEU:HG	1:A:390:PHE:CE2	2.40	0.56
1:A:255:ILE:HB	1:A:286:MET:HE1	1.85	0.55
1:B:446:ARG:O	1:B:471:LYS:HE2	2.06	0.54
1:B:259:PRO:HD2	1:B:260:MET:SD	2.48	0.54
1:D:300:ASP:OD2	1:D:420:ARG:NH2	2.40	0.53
1:D:301:GLU:HG2	1:D:386:HIS:HE1	1.73	0.53
1:B:337:ARG:HD3	3:B:608:HOH:O	2.09	0.53
1:C:258:GLU:O	1:C:258:GLU:CG	2.58	0.52
1:C:288:PRO:HB2	1:C:394:VAL:CG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PRO:HD2	1:A:260:MET:SD	2.50	0.51
1:C:288:PRO:CB	1:C:394:VAL:CG2	2.89	0.51
1:C:188:ILE:HG13	1:C:250:GLU:OE2	2.10	0.50
1:D:420:ARG:CD	3:D:543:HOH:O	2.56	0.50
1:B:268:ARG:CZ	1:B:443:ALA:HB1	2.42	0.50
1:B:466:ASN:HB3	3:B:487:HOH:O	2.12	0.50
1:D:467:LEU:HB3	3:D:619:HOH:O	2.12	0.50
1:B:376:LYS:HG3	1:B:434:THR:HG23	1.95	0.49
1:D:271:GLU:HB2	1:D:365:GLU:HG2	1.94	0.49
1:A:266:ASN:O	1:A:267:GLU:HB2	2.11	0.49
1:B:259:PRO:HD2	1:B:260:MET:HE3	1.94	0.49
1:A:234:ASP:OD1	1:A:234:ASP:N	2.47	0.48
1:D:295:LEU:HA	1:D:389:ALA:O	2.13	0.48
1:D:259:PRO:HD2	1:D:260:MET:SD	2.53	0.48
1:B:188:ILE:HG22	1:B:252:VAL:HG12	1.97	0.47
1:D:255:ILE:HG13	1:D:280:LEU:HD13	1.96	0.47
1:A:255:ILE:HD12	1:A:286:MET:CE	2.45	0.47
1:C:295:LEU:HD13	1:C:390:PHE:CD2	2.49	0.47
1:D:378:HIS:HB3	3:D:594:HOH:O	2.13	0.47
1:D:265:PHE:HB3	1:D:449:TYR:CE1	2.50	0.46
1:B:290:ILE:HG12	1:B:395:ALA:HB3	1.98	0.46
1:A:259:PRO:HG2	1:A:270:LEU:HD13	1.97	0.46
1:D:442:ILE:HG12	1:D:450:ASP:HB2	1.98	0.46
1:A:420:ARG:HD2	3:A:538:HOH:O	2.12	0.46
1:D:263:MET:CE	1:D:419:VAL:CG1	2.91	0.46
1:D:377:PHE:O	1:D:434:THR:HA	2.15	0.46
1:B:268:ARG:HD3	1:B:271:GLU:OE2	2.16	0.45
1:B:420:ARG:CD	3:B:538:HOH:O	2.60	0.45
1:C:190:LEU:HD13	1:C:248:LEU:HD21	1.98	0.45
1:A:337:ARG:NH2	1:A:469:ASP:HB2	2.32	0.45
1:A:371:ILE:HB	1:A:441:LEU:HB2	1.99	0.45
1:C:263:MET:HG3	1:C:419:VAL:HG21	1.98	0.45
1:D:345:ASP:OD2	1:D:347:ARG:NH2	2.48	0.45
1:C:223:ALA:O	1:C:227:VAL:HG23	2.16	0.44
1:C:295:LEU:CD1	1:C:390:PHE:CE2	3.00	0.44
1:A:365:GLU:OE1	3:A:615:HOH:O	2.20	0.44
1:C:288:PRO:HG3	1:C:394:VAL:HG21	1.99	0.44
1:A:263:MET:CE	1:A:419:VAL:HG11	2.47	0.44
1:C:394:VAL:HG12	1:C:405:LEU:HB3	1.99	0.44
1:D:437:GLY:HA3	1:D:454:VAL:O	2.17	0.43
1:D:285:ASN:CB	3:D:499:HOH:O	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HD12	1:A:286:MET:HE3	1.99	0.43
1:D:175:ARG:O	1:D:179:GLN:HB2	2.19	0.43
1:C:151:PHE:CE1	1:C:216:ALA:HB3	2.54	0.43
1:C:179:GLN:NE2	1:C:401:MET:SD	2.92	0.42
1:B:265:PHE:HB3	1:B:449:TYR:CE1	2.55	0.42
1:C:259:PRO:HD2	1:C:260:MET:SD	2.60	0.42
1:D:471:LYS:O	1:D:473:PRO:HD3	2.19	0.42
1:A:142:THR:HA	1:A:145:SER:HB3	2.00	0.42
1:B:344:PHE:CD2	1:B:420:ARG:HD2	2.55	0.41
1:D:242:LYS:HB3	1:D:242:LYS:HE2	1.72	0.41
1:D:271:GLU:HG2	1:D:271:GLU:H	1.74	0.41
1:D:259:PRO:HG2	1:D:270:LEU:HD23	2.01	0.41
1:D:251:GLN:HB3	1:D:281:LYS:HG3	2.03	0.41
1:B:370:ARG:HG3	1:B:442:ILE:CD1	2.51	0.41
1:C:456:GLN:HG3	1:C:463:LYS:HG3	2.02	0.41
1:C:274:LEU:O	1:C:277:LYS:HB2	2.21	0.41
1:A:379:MET:HG3	1:A:429:ALA:HB1	2.02	0.41
1:A:286:MET:HG3	1:A:361:LEU:HD23	2.01	0.41
1:C:377:PHE:O	1:C:434:THR:HA	2.21	0.40
1:B:339:PRO:HD2	1:B:473:PRO:HA	2.03	0.40
2:D:481:SAH:H4'	2:D:481:SAH:HG1	1.50	0.40
1:A:255:ILE:CB	1:A:286:MET:CE	2.92	0.40
1:A:263:MET:HE3	1:A:419:VAL:HG11	2.04	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	335/341 (98%)	319 (95%)	16 (5%)	0	100	100
1	B	335/341 (98%)	322 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	335/341 (98%)	326 (97%)	9 (3%)	0	100	100
1	D	335/341 (98%)	319 (95%)	15 (4%)	1 (0%)	46	50
All	All	1340/1364 (98%)	1286 (96%)	53 (4%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	477	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/296 (99%)	287 (98%)	6 (2%)	63	76
1	B	293/296 (99%)	287 (98%)	6 (2%)	63	76
1	C	293/296 (99%)	286 (98%)	7 (2%)	57	69
1	D	293/296 (99%)	284 (97%)	9 (3%)	47	59
All	All	1172/1184 (99%)	1144 (98%)	28 (2%)	57	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	A	283	SER
1	A	286	MET
1	A	382	SER
1	A	445	LYS
1	A	467	LEU
1	B	142	THR
1	B	210	LYS
1	B	221	GLN
1	B	258	GLU
1	B	346	ILE

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Mol	Chain	Res	Type
1	B	465	SER
1	C	143	GLU
1	C	169	ARG
1	C	187	LYS
1	C	221	GLN
1	C	237	VAL
1	C	258	GLU
1	C	287	PHE
1	D	143	GLU
1	D	146	SER
1	D	152	GLN
1	D	258	GLU
1	D	295	LEU
1	D	328	ARG
1	D	346	ILE
1	D	412	PRO
1	D	478	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	181	HIS
1	A	472	ASN
1	B	149	GLN
1	B	369	HIS
1	C	179	GLN
1	D	161	GLN
1	D	165	GLN
1	D	221	GLN
1	D	266	ASN
1	D	381	HIS
1	D	456	GLN
1	D	472	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	SAH	A	481	-	20,28,28	1.23	3 (15%)	19,40,40	2.88	2 (10%)
2	SAH	B	481	-	20,28,28	1.07	2 (10%)	19,40,40	3.21	2 (10%)
2	SAH	C	481	-	20,28,28	1.15	2 (10%)	19,40,40	2.84	2 (10%)
2	SAH	D	481	-	20,28,28	1.13	2 (10%)	19,40,40	3.35	6 (31%)

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	SAH	A	481	-	-	0/7/31/31	0/3/3/3
2	SAH	B	481	-	-	0/7/31/31	0/3/3/3
2	SAH	C	481	-	-	0/7/31/31	0/3/3/3
2	SAH	D	481	-	-	0/7/31/31	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	481	SAH	O4'-C4'	-2.06	1.40	1.45
2	B	481	SAH	C2-N1	2.17	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	481	SAH	C2-N1	2.50	1.38	1.33
2	C	481	SAH	C2-N1	2.59	1.38	1.33
2	D	481	SAH	C2-N1	2.66	1.39	1.33
2	B	481	SAH	C2-N3	3.43	1.38	1.32
2	D	481	SAH	C2-N3	3.60	1.38	1.32
2	C	481	SAH	C2-N3	3.61	1.38	1.32
2	A	481	SAH	C2-N3	3.87	1.39	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	481	SAH	N3-C2-N1	-13.21	118.78	128.89
2	D	481	SAH	N3-C2-N1	-13.01	118.93	128.89
2	C	481	SAH	N3-C2-N1	-11.55	120.05	128.89
2	A	481	SAH	N3-C2-N1	-11.42	120.15	128.89
2	D	481	SAH	CB-CG-SD	-2.74	108.29	113.57
2	A	481	SAH	C5'-SD-CG	-2.73	94.22	102.41
2	B	481	SAH	C1'-N9-C4	-2.43	123.27	126.94
2	D	481	SAH	C5'-SD-CG	-2.37	95.29	102.41
2	D	481	SAH	C4-C5-N7	-2.30	107.36	109.48
2	D	481	SAH	C1'-N9-C4	-2.12	123.73	126.94
2	D	481	SAH	O3'-C3'-C4'	-2.12	104.69	111.05
2	C	481	SAH	C2'-C1'-N9	2.37	117.91	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	481	SAH	1	0
2	C	481	SAH	2	0
2	D	481	SAH	1	0

## 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<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	337/341 (98%)	-0.08	11 (3%) 50 49	20, 30, 43, 75	0
1	B	337/341 (98%)	-0.14	7 (2%) 67 65	15, 30, 43, 68	0
1	C	337/341 (98%)	0.02	21 (6%) 24 23	19, 31, 45, 73	0
1	D	337/341 (98%)	-0.26	9 (2%) 58 57	23, 30, 42, 73	0
All	All	1348/1364 (98%)	-0.12	48 (3%) 46 45	15, 30, 43, 75	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	THR	7.8
1	D	142	THR	6.7
1	D	478	THR	5.8
1	D	144	GLU	5.8
1	B	478	THR	5.6
1	A	144	GLU	4.9
1	C	144	GLU	4.6
1	B	144	GLU	4.6
1	C	478	THR	4.5
1	A	142	THR	4.3
1	D	477	TYR	4.3
1	C	477	TYR	3.9
1	B	145	SER	3.9
1	C	148	VAL	3.7
1	C	199	LEU	3.6
1	B	148	VAL	3.4
1	C	142	THR	3.4
1	B	477	TYR	3.3
1	A	148	VAL	3.1
1	C	145	SER	2.9
1	A	478	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	378	HIS	2.8
1	A	145	SER	2.8
1	C	284	GLY	2.8
1	A	199	LEU	2.7
1	C	149	GLN	2.6
1	A	257	SER	2.6
1	A	259	PRO	2.6
1	C	181	HIS	2.5
1	C	147	ALA	2.5
1	C	257	SER	2.5
1	B	170	THR	2.5
1	D	347	ARG	2.4
1	C	260	MET	2.4
1	C	401	MET	2.4
1	C	283	SER	2.4
1	C	228	LYS	2.4
1	A	477	TYR	2.3
1	C	192	VAL	2.3
1	C	182	THR	2.2
1	A	192	VAL	2.2
1	C	398	GLY	2.1
1	C	143	GLU	2.1
1	D	173	TYR	2.1
1	A	264	LEU	2.1
1	D	475	PHE	2.1
1	C	221	GLN	2.0
1	D	145	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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
2	SAH	C	481	26/26	0.93	0.13	-0.26	27,29,31,32	0
2	SAH	A	481	26/26	0.96	0.13	-0.29	23,26,28,31	0
2	SAH	B	481	26/26	0.96	0.10	-0.58	27,29,32,32	0
2	SAH	D	481	26/26	0.96	0.09	-0.60	24,27,31,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.