



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:10 PM GMT

PDB ID : 1NV8  
Title : N5-glutamine methyltransferase, HemK  
Authors : Schubert, H.L.; Phillips, J.D.; Hill, C.P.  
Deposited on : 2003-02-02  
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

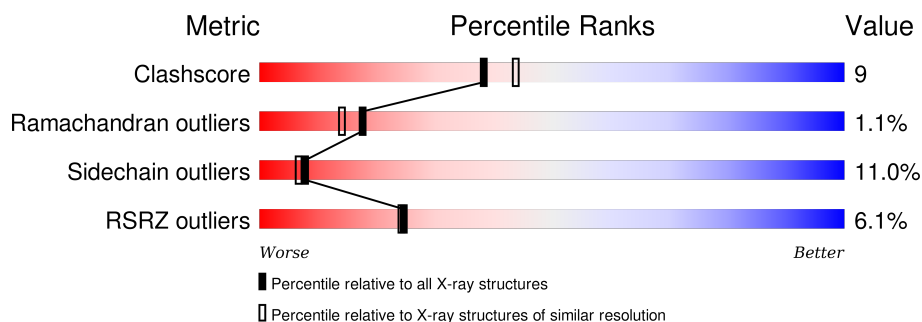
# 1 Overall quality at a glance

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))
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	284	
1	B	284	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAM	A	300	-	-	X	-
3	MEQ	A	400	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MEQ	B	401	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4603 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.

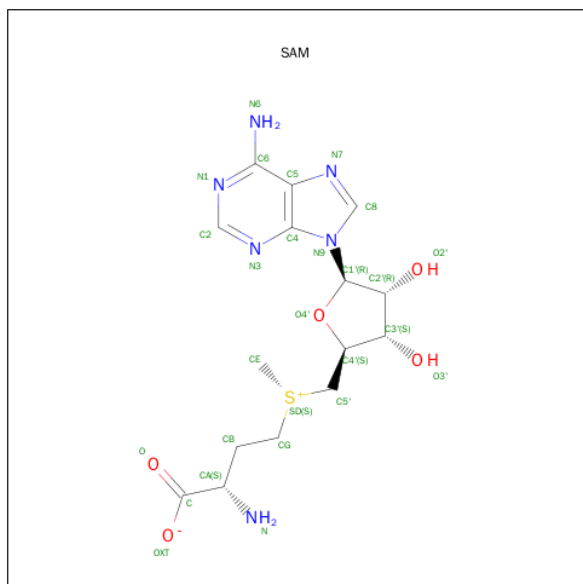
- Molecule 1 is a protein called hemK protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	4	0
			2168	1397	358	409	4			
1	B	267	Total	C	N	O	S	0	4	0
			2128	1373	349	402	4			

There are 4 discrepancies between the modelled and reference sequences:

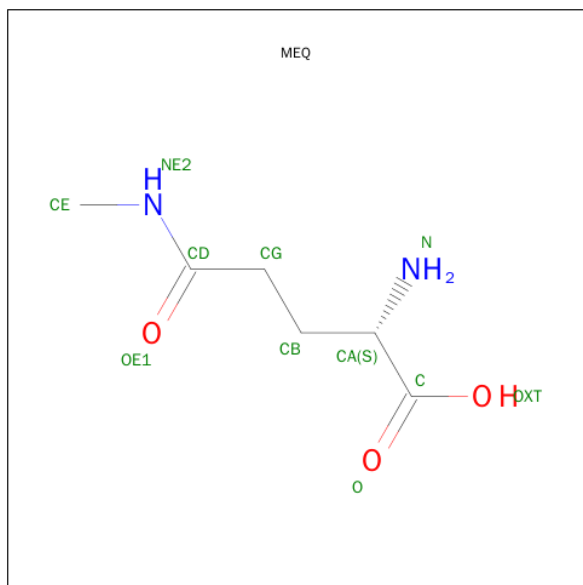
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9WYV8
A	-2	ALA	-	EXPRESSION TAG	UNP Q9WYV8
B	-1	GLY	-	EXPRESSION TAG	UNP Q9WYV8
B	-2	ALA	-	EXPRESSION TAG	UNP Q9WYV8

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

- Molecule 3 is N5-METHYLGLUTAMINE (three-letter code: MEQ) (formula:  $C_6H_{12}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	6	0
			10	6	2	2		

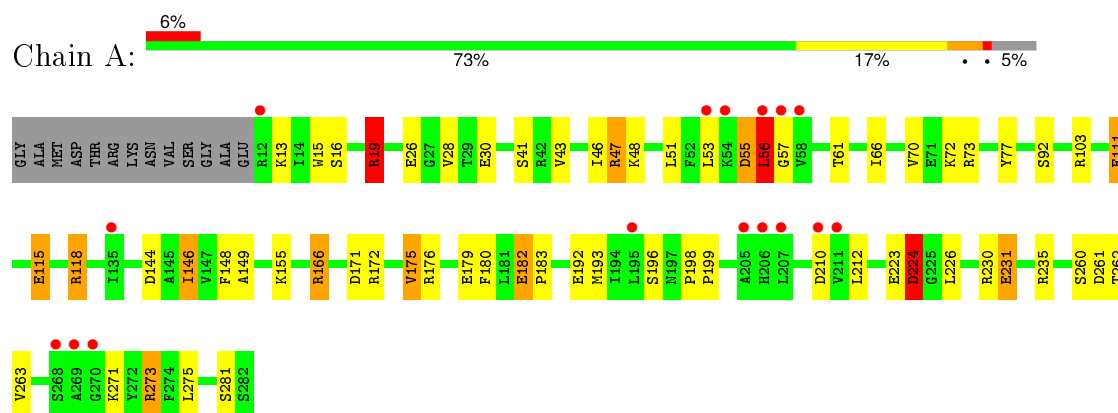
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		
4	B	96	Total	O	0	0
			96	96		

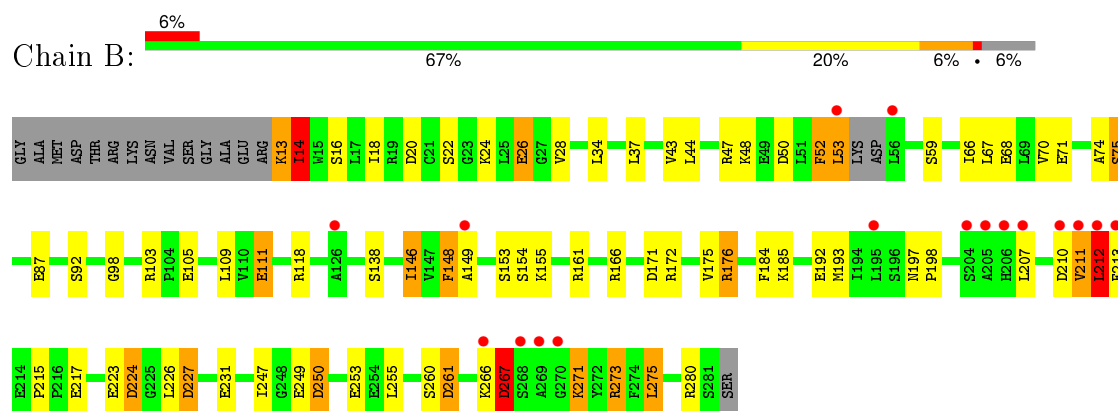
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: hemK protein



- Molecule 1: hemK protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.49 Å   59.06 Å   85.61 Å 90.00°   109.22°   90.00°	Depositor
Resolution (Å)	29.75 – 2.20 29.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.75-2.20) 94.7 (29.79-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.186   ,   0.253 0.196   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32326 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4603	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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, 0.375 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: MEQ, 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	1.35	9/2224 (0.4%)	1.26	19/2990 (0.6%)
1	B	1.42	8/2185 (0.4%)	1.30	19/2939 (0.6%)
All	All	1.39	17/4409 (0.4%)	1.28	38/5929 (0.6%)

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
1	B	0	3
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	GLU	CD-OE2	-8.71	1.16	1.25
1	B	193	MET	SD-CE	-7.39	1.36	1.77
1	A	111[A]	GLU	CD-OE1	6.64	1.32	1.25
1	A	111[B]	GLU	CD-OE1	6.64	1.32	1.25
1	A	182	GLU	CD-OE1	6.38	1.32	1.25
1	A	196	SER	CB-OG	5.93	1.50	1.42
1	A	175	VAL	CB-CG1	-5.92	1.40	1.52
1	B	211	VAL	CA-CB	5.92	1.67	1.54
1	B	231	GLU	CD-OE1	5.91	1.32	1.25
1	B	231	GLU	CD-OE2	5.88	1.32	1.25
1	A	193	MET	SD-CE	-5.79	1.45	1.77
1	B	192	GLU	CD-OE1	-5.73	1.19	1.25
1	A	179	GLU	CG-CD	5.63	1.60	1.51
1	A	166	ARG	CG-CD	5.55	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	SER	CB-OG	5.31	1.49	1.42
1	A	192	GLU	CD-OE2	-5.16	1.20	1.25
1	B	148	PHE	CD1-CE1	5.00	1.49	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	MET	CG-SD-CE	-12.26	80.58	100.20
1	A	166	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	B	250	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	56	LEU	CA-CB-CG	8.11	133.95	115.30
1	A	118	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	B	172	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	172	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	166	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	176	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	267	ASP	CB-CG-OD2	7.53	125.08	118.30
1	B	210	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	172	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	B	103	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	273	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	A	103	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	103	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	A	193	MET	CG-SD-CE	-6.74	89.41	100.20
1	A	144	ASP	CB-CG-OD2	6.66	124.29	118.30
1	B	176	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	B	118[A]	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	118[B]	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	176	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	B	176	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	280	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	227	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	212	LEU	N-CA-CB	5.47	121.34	110.40
1	A	103	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	19	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	224	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	171	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	230	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	47	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	171	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	118	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	111[A]	GLU	N-CA-CB	5.16	119.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[B]	GLU	N-CA-CB	5.16	119.89	110.60
1	A	210	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	212	LEU	CB-CG-CD2	5.09	119.66	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	SER	Peptide
1	A	55	ASP	Peptide
1	B	211	VAL	Peptide
1	B	212	LEU	Peptide
1	B	52	PHE	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2168	0	2209	27	0
1	B	2128	0	2154	34	0
2	A	27	0	22	11	0
2	B	27	0	22	7	0
3	A	10	0	11	11	0
3	B	10	0	11	8	0
4	A	137	0	0	3	1
4	B	96	0	0	3	0
All	All	4603	0	4429	79	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 9.

All (79) 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)
2:A:300:SAM:HE2	3:A:400:MEQ:CE	1.53	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:300:SAM:HE2	3:A:400:MEQ:HE1	1.25	1.18
2:A:300:SAM:HE3	3:A:400:MEQ:CE	1.74	1.13
2:A:300:SAM:CE	3:A:400:MEQ:HE1	1.73	1.12
2:A:300:SAM:CE	3:A:400:MEQ:HE2	1.68	1.09
2:B:301:SAM:CE	3:B:401:MEQ:CE	2.37	1.02
2:A:300:SAM:HE2	3:A:400:MEQ:HE2	1.29	1.01
1:B:260:SER:O	1:B:261:ASP:HB2	1.58	1.00
2:A:300:SAM:HE3	3:A:400:MEQ:HE3	1.47	0.94
2:A:300:SAM:CE	3:A:400:MEQ:HE3	1.94	0.94
2:B:301:SAM:CE	3:B:401:MEQ:HE2	2.04	0.87
1:A:260:SER:O	1:A:261:ASP:HB2	1.73	0.85
2:B:301:SAM:HE3	3:B:401:MEQ:CE	2.05	0.84
2:A:300:SAM:HE1	3:A:400:MEQ:CE	2.10	0.81
1:B:260:SER:O	1:B:261:ASP:CB	2.25	0.79
2:B:301:SAM:HE3	3:B:401:MEQ:HE3	1.64	0.79
2:A:300:SAM:HE1	3:A:400:MEQ:HE2	1.61	0.77
2:B:301:SAM:HE2	3:B:401:MEQ:CE	2.13	0.77
1:B:227:ASP:OD2	4:B:447:HOH:O	2.03	0.76
2:B:301:SAM:HE2	3:B:401:MEQ:HE2	1.68	0.76
1:B:213:PHE:O	4:B:423:HOH:O	2.06	0.72
1:A:231:GLU:CD	1:A:235[B]:ARG:HE	1.99	0.65
1:B:13:LYS:N	1:B:16:SER:HG	1.92	0.65
1:B:50:ASP:OD2	1:B:53:LEU:HD22	1.96	0.64
1:A:180:PHE:CE2	1:A:231:GLU:HG2	2.34	0.61
1:A:19:ARG:HH11	1:A:19:ARG:HG2	1.65	0.61
1:A:146:ILE:HD11	1:A:148:PHE:CZ	2.39	0.57
1:A:231:GLU:O	1:A:235[B]:ARG:HG3	2.04	0.57
1:B:13:LYS:HD2	1:B:14:ILE:HG22	1.87	0.57
1:A:260:SER:O	1:A:261:ASP:CB	2.47	0.57
1:B:275:LEU:C	1:B:275:LEU:HD12	2.26	0.56
1:A:275:LEU:HD12	1:A:275:LEU:C	2.25	0.56
1:A:13:LYS:HE3	1:A:56:LEU:HD13	1.89	0.55
2:A:300:SAM:HE3	3:A:400:MEQ:HE1	1.58	0.52
1:A:26:GLU:HA	1:A:26:GLU:OE1	2.11	0.51
1:B:223:GLU:HG2	4:B:465:HOH:O	2.09	0.51
1:B:105[B]:GLU:OE2	1:B:267:ASP:OD1	2.29	0.50
1:A:66:ILE:O	1:A:70:VAL:HG23	2.12	0.50
1:A:180:PHE:CZ	1:A:231:GLU:HG2	2.47	0.49
1:B:247:ILE:HG21	1:B:255:LEU:HD13	1.94	0.49
1:B:28:VAL:O	1:B:28:VAL:HG12	2.12	0.49
1:B:198:PRO:O	3:B:401:MEQ:CE	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HD23	1:B:212:LEU:O	2.13	0.47
1:A:115:GLU:HB2	1:A:118:ARG:NH2	2.30	0.47
1:B:28:VAL:HG21	1:B:74:ALA:HA	1.98	0.46
1:A:92:SER:O	1:A:166:ARG:HD3	2.15	0.46
1:A:224:ASP:HB3	1:A:226:LEU:H	1.80	0.46
1:B:146:ILE:HD11	1:B:148:PHE:CZ	2.52	0.45
1:A:149:ALA:O	1:A:175:VAL:HA	2.16	0.45
1:B:26:GLU:HA	1:B:26:GLU:OE1	2.17	0.44
1:B:247:ILE:HG21	1:B:255:LEU:CD1	2.46	0.44
1:A:15:TRP:HZ2	1:A:51:LEU:O	2.01	0.44
1:B:250:ASP:OD1	1:B:250:ASP:N	2.41	0.44
1:B:275:LEU:HD12	1:B:275:LEU:O	2.17	0.44
1:A:73:ARG:HD2	1:A:77:TYR:O	2.18	0.44
1:A:262:THR:HG22	1:A:263:VAL:N	2.33	0.44
1:A:223:GLU:HG3	4:A:477:HOH:O	2.18	0.44
1:B:176:ARG:HD2	1:B:184:PHE:CZ	2.53	0.43
1:B:109:LEU:C	1:B:109:LEU:HD23	2.39	0.43
1:B:98:GLY:HA2	1:B:215:PRO:HG3	2.01	0.43
1:B:67:LEU:O	1:B:71:GLU:HG2	2.19	0.43
1:B:249:GLU:OE1	1:B:271:LYS:NZ	2.48	0.42
1:B:66:ILE:O	1:B:70:VAL:HG23	2.19	0.42
1:B:273:ARG:HD2	1:B:273:ARG:HA	1.89	0.42
1:A:231:GLU:CD	1:A:235[B]:ARG:NE	2.71	0.42
1:B:18:ILE:HD13	1:B:37:LEU:CD2	2.50	0.42
1:B:161:ARG:HG2	1:B:175:VAL:CG1	2.49	0.42
1:B:75:SER:O	1:B:213:PHE:CZ	2.73	0.41
1:B:224:ASP:HB3	1:B:226:LEU:H	1.85	0.41
1:A:115:GLU:HG2	4:A:460:HOH:O	2.20	0.41
1:A:198:PRO:HB2	1:A:199:PRO:HD2	2.02	0.41
1:B:197:ASN:OD1	3:B:401:MEQ:HE1	2.21	0.41
1:A:262:THR:HG22	1:A:263:VAL:O	2.20	0.41
1:A:46:ILE:HG23	1:A:47:ARG:N	2.36	0.41
1:A:182:GLU:N	1:A:183:PRO:CD	2.84	0.41
1:B:149:ALA:O	1:B:175:VAL:HA	2.21	0.41
1:A:111[A]:GLU:OE2	4:A:535:HOH:O	2.22	0.41
1:B:44:LEU:HA	1:B:44:LEU:HD23	1.86	0.41
2:B:301:SAM:H4'	2:B:301:SAM:HG1	1.92	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)
4:A:449:HOH:O	4:A:526:HOH:O[4_555]	2.17	0.03

## 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	273/284 (96%)	259 (95%)	12 (4%)	2 (1%)	26	25
1	B	267/284 (94%)	251 (94%)	12 (4%)	4 (2%)	13	9
All	All	540/568 (95%)	510 (94%)	24 (4%)	6 (1%)	17	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	ILE
1	B	267	ASP
1	B	26	GLU
1	A	48	LYS
1	A	57	GLY
1	B	52	PHE

### 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	239/244 (98%)	219 (92%)	20 (8%)	14	13
1	B	234/244 (96%)	202 (86%)	32 (14%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	473/488 (97%)	421 (89%)	52 (11%)	<b>8</b> <b>7</b>

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	19	ARG
1	A	28	VAL
1	A	30	GLU
1	A	41	SER
1	A	43	VAL
1	A	47	ARG
1	A	53	LEU
1	A	55	ASP
1	A	56	LEU
1	A	61	THR
1	A	72	LYS
1	A	115	GLU
1	A	146	ILE
1	A	155	LYS
1	A	212	LEU
1	A	224	ASP
1	A	231	GLU
1	A	271	LYS
1	A	273	ARG
1	B	13	LYS
1	B	14	ILE
1	B	20	ASP
1	B	22	SER
1	B	24	LYS
1	B	34	LEU
1	B	43	VAL
1	B	48	LYS
1	B	53	LEU
1	B	59	SER
1	B	68	GLU
1	B	75	SER
1	B	87	GLU
1	B	92	SER
1	B	111[A]	GLU
1	B	111[B]	GLU
1	B	146	ILE

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Mol	Chain	Res	Type
1	B	153	SER
1	B	154	SER
1	B	155	LYS
1	B	166	ARG
1	B	185	LYS
1	B	207	LEU
1	B	212	LEU
1	B	217	GLU
1	B	224	ASP
1	B	253	GLU
1	B	261	ASP
1	B	266	LYS
1	B	271	LYS
1	B	273	ARG
1	B	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS

### 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](#)

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	SAM	A	300	3	21,29,29	1.22	3 (14%)	17,42,42	3.50	4 (23%)
3	MEQ	A	400	2	8,9,10	1.39	1 (12%)	7,10,12	2.33	4 (57%)
2	SAM	B	301	-	21,29,29	2.22	4 (19%)	17,42,42	4.86	6 (35%)
3	MEQ	B	401	-	8,9,10	10.87	3 (37%)	7,10,12	8.46	3 (42%)

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	300	3	-	0/8/33/33	0/3/3/3
3	MEQ	A	400	2	-	1/7/9/11	0/0/0/0
2	SAM	B	301	-	-	0/8/33/33	0/3/3/3
3	MEQ	B	401	-	-	1/7/9/11	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MEQ	CB-CG	-27.25	0.61	1.52
2	B	301	SAM	CG-CB	-8.66	1.41	1.52
2	A	300	SAM	C4-N3	-2.62	1.31	1.35
2	B	301	SAM	C4-N3	-2.00	1.32	1.35
2	A	300	SAM	C2-N3	2.11	1.35	1.32
2	B	301	SAM	C2-N1	2.33	1.38	1.33
2	A	300	SAM	O4'-C1'	2.45	1.44	1.41
3	A	400	MEQ	OE1-CD	2.83	1.29	1.23
2	B	301	SAM	C2-N3	2.91	1.37	1.32
3	B	401	MEQ	O-C	5.16	1.43	1.19
3	B	401	MEQ	CG-CD	13.10	1.76	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	SAM	N3-C2-N1	-17.26	115.68	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SAM	N3-C2-N1	-11.05	120.43	128.89
3	B	401	MEQ	O-C-CA	-6.19	109.36	125.49
2	B	301	SAM	O4'-C1'-N9	-5.55	96.47	108.10
2	A	300	SAM	O4'-C1'-N9	-5.53	96.51	108.10
3	A	400	MEQ	O-C-CA	-3.72	115.80	125.49
3	A	400	MEQ	CB-CG-CD	-3.25	105.53	113.27
2	A	300	SAM	C1'-N9-C4	-2.87	122.61	126.94
2	B	301	SAM	C1'-N9-C4	-2.73	122.82	126.94
3	B	401	MEQ	CE-NE2-CD	-2.03	103.83	121.86
3	A	400	MEQ	CE-NE2-CD	-2.02	103.95	121.86
2	B	301	SAM	C2-N1-C6	2.23	122.74	118.77
3	A	400	MEQ	CB-CA-N	2.76	118.37	110.52
2	B	301	SAM	CE-SD-CG	2.78	125.39	99.84
2	A	300	SAM	C2'-C1'-N9	5.73	123.05	114.29
2	B	301	SAM	C2'-C1'-N9	6.39	124.05	114.29
3	B	401	MEQ	CB-CG-CD	21.36	164.03	113.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	MEQ	CG-CD-NE2-CE
3	A	400	MEQ	CG-CD-NE2-CE

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	SAM	11	0
3	A	400	MEQ	11	0
2	B	301	SAM	7	0
3	B	401	MEQ	8	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	271/284 (95%)	0.04	16 (5%) 26 25	22, 37, 66, 87	0
1	B	267/284 (94%)	0.15	17 (6%) 23 22	21, 41, 66, 81	0
All	All	538/568 (94%)	0.10	33 (6%) 25 24	21, 38, 66, 87	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	LEU	5.6
1	B	211	VAL	4.6
1	B	212	LEU	3.9
1	B	207	LEU	3.7
1	A	58	VAL	3.3
1	B	210	ASP	3.2
1	A	53	LEU	3.2
1	B	269	ALA	3.0
1	B	205	ALA	2.8
1	A	12	ARG	2.8
1	B	270	GLY	2.6
1	B	268	SER	2.6
1	A	207	LEU	2.6
1	A	270	GLY	2.6
1	B	206	HIS	2.5
1	B	266	LYS	2.5
1	A	269	ALA	2.5
1	A	210	ASP	2.5
1	A	268	SER	2.5
1	B	126	ALA	2.4
1	B	53	LEU	2.4
1	A	57	GLY	2.3
1	B	149	ALA	2.3
1	A	211	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	2.3
1	B	213	PHE	2.2
1	A	135	ILE	2.2
1	A	195	LEU	2.1
1	A	54	LYS	2.1
1	B	56	LEU	2.0
1	A	205	ALA	2.0
1	A	206	HIS	2.0
1	B	204	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
3	MEQ	A	400	10/11	0.61	0.28	6.08	38,59,65,65	1
3	MEQ	B	401	10/11	0.65	0.30	1.68	44,57,67,67	6
2	SAM	B	301	27/27	0.97	0.13	-0.21	22,28,31,33	1
2	SAM	A	300	27/27	0.97	0.13	-0.39	20,26,28,30	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.