



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 07:01 pm GMT

PDB ID : 5HM8  
Title : 2.85 Angstrom Crystal Structure of S-adenosylhomocysteinase from *Cryptosporidium parvum* in Complex with Adenosine and NAD.  
Authors : Minasov, G.; Shuvalova, L.; Halavaty, A.; Kiryukhina, O.; Dubrovskaya, I.; Bishop, B.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2016-01-15  
Resolution : 2.85 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ 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	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

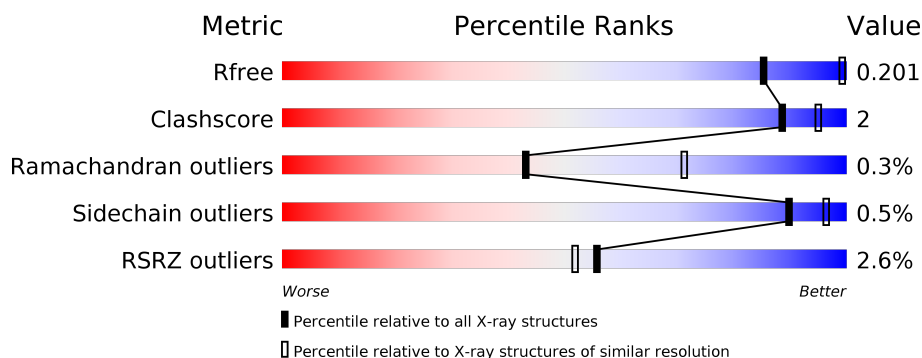
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	111664	2715 (2.90-2.82)
Clashscore	122126	2976 (2.90-2.82)
Ramachandran outliers	120053	2913 (2.90-2.82)
Sidechain outliers	120020	2916 (2.90-2.82)
RSRZ outliers	108989	2654 (2.90-2.82)

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	498	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> <div>•</div> </div>
1	B	498	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> <div>••</div> </div>
1	C	498	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> <div>••</div> </div>
1	D	498	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> <div>•</div> </div>
1	E	498	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> <div>•</div> </div>
1	F	498	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	498	<div><div></div><div>3%</div><div>90%</div><div>8% ..</div></div>
1	H	498	<div><div></div><div>2%</div><div>90%</div><div>7% ..</div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32193 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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	2	0
			3922	2493	657	744	28			
1	B	494	Total	C	N	O	S	0	0	0
			3902	2478	654	742	28			
1	C	488	Total	C	N	O	S	0	2	0
			3870	2459	647	735	29			
1	D	493	Total	C	N	O	S	0	0	0
			3893	2472	652	741	28			
1	E	489	Total	C	N	O	S	0	1	0
			3868	2459	647	733	29			
1	F	493	Total	C	N	O	S	0	2	0
			3909	2481	655	744	29			
1	G	494	Total	C	N	O	S	0	1	0
			3913	2487	655	743	28			
1	H	487	Total	C	N	O	S	0	0	0
			3845	2444	644	730	27			

There are 24 discrepancies between the modelled and reference sequences:

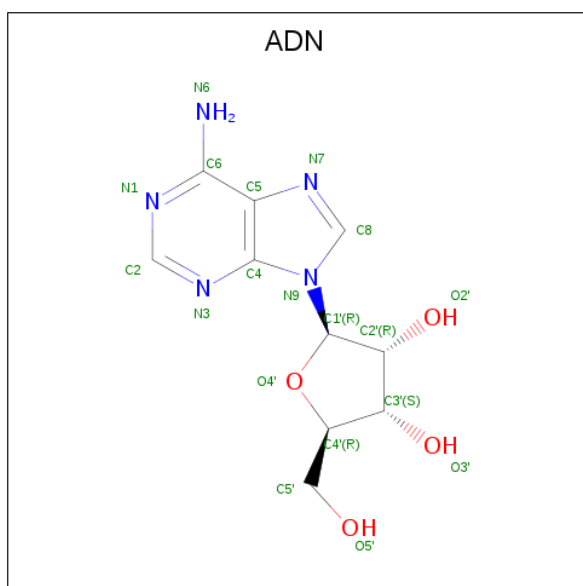
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5CPH1
A	-1	ASN	-	expression tag	UNP Q5CPH1
A	0	ALA	-	expression tag	UNP Q5CPH1
B	-2	SER	-	expression tag	UNP Q5CPH1
B	-1	ASN	-	expression tag	UNP Q5CPH1
B	0	ALA	-	expression tag	UNP Q5CPH1
C	-2	SER	-	expression tag	UNP Q5CPH1
C	-1	ASN	-	expression tag	UNP Q5CPH1
C	0	ALA	-	expression tag	UNP Q5CPH1
D	-2	SER	-	expression tag	UNP Q5CPH1
D	-1	ASN	-	expression tag	UNP Q5CPH1
D	0	ALA	-	expression tag	UNP Q5CPH1
E	-2	SER	-	expression tag	UNP Q5CPH1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q5CPH1
E	0	ALA	-	expression tag	UNP Q5CPH1
F	-2	SER	-	expression tag	UNP Q5CPH1
F	-1	ASN	-	expression tag	UNP Q5CPH1
F	0	ALA	-	expression tag	UNP Q5CPH1
G	-2	SER	-	expression tag	UNP Q5CPH1
G	-1	ASN	-	expression tag	UNP Q5CPH1
G	0	ALA	-	expression tag	UNP Q5CPH1
H	-2	SER	-	expression tag	UNP Q5CPH1
H	-1	ASN	-	expression tag	UNP Q5CPH1
H	0	ALA	-	expression tag	UNP Q5CPH1

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ).



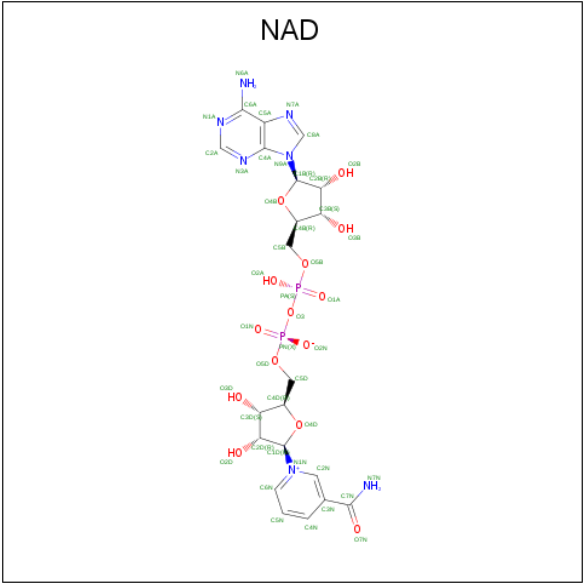
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		
2	C	1	Total	C	N	O	0	0
			19	10	5	4		
2	D	1	Total	C	N	O	0	0
			19	10	5	4		
2	E	1	Total	C	N	O	0	0
			19	10	5	4		
2	F	1	Total	C	N	O	0	0
			19	10	5	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			19	10	5	4		
2	H	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).

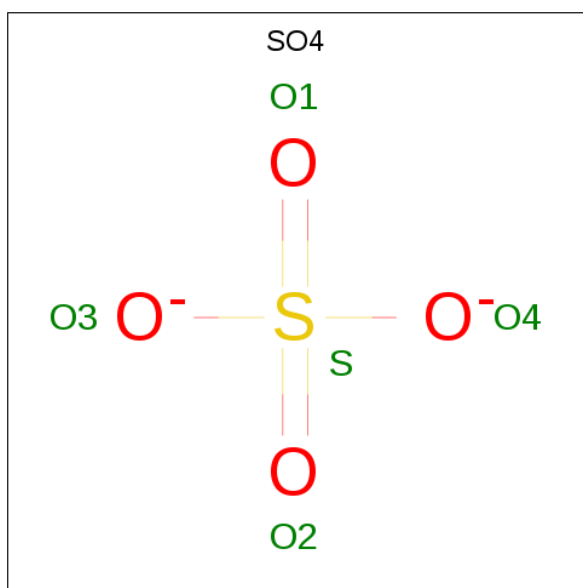


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	3	Total	Cl	0	0
			3	3		
4	D	4	Total	Cl	0	0
			4	4		
4	E	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		
4	B	3	Total	Cl	0	0
			3	3		
4	C	2	Total	Cl	0	0
			2	2		
4	A	3	Total	Cl	0	0
			3	3		
4	F	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

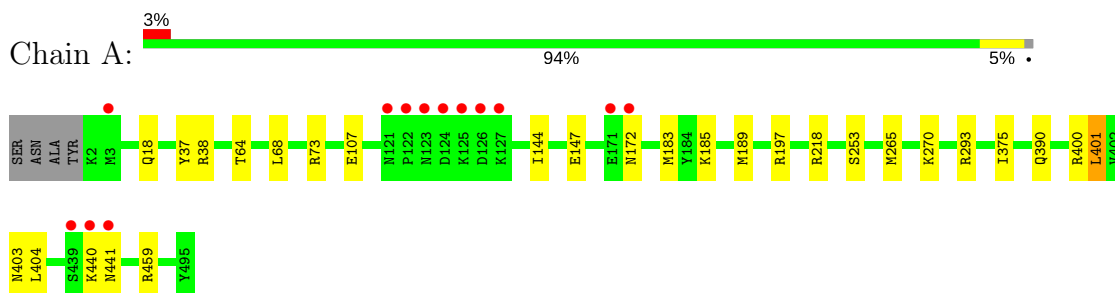
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	0
			80	80		
6	B	50	Total	O	0	0
			50	50		
6	C	72	Total	O	0	0
			72	72		
6	D	73	Total	O	0	0
			73	73		
6	E	74	Total	O	0	0
			74	74		
6	F	54	Total	O	0	1
			55	55		
6	G	68	Total	O	0	0
			68	68		
6	H	51	Total	O	0	0
			51	51		



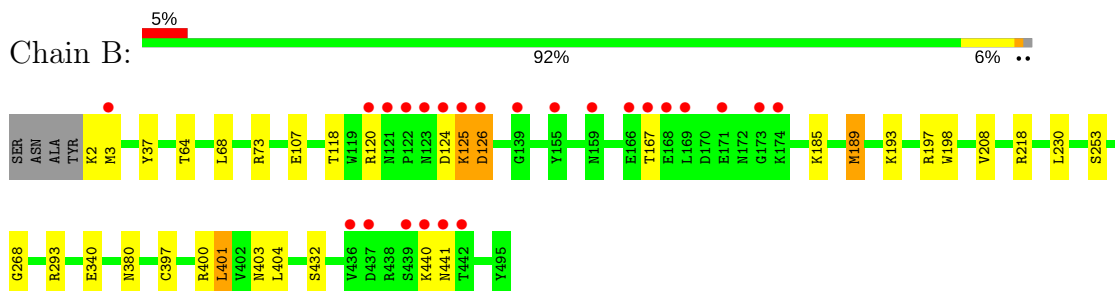
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

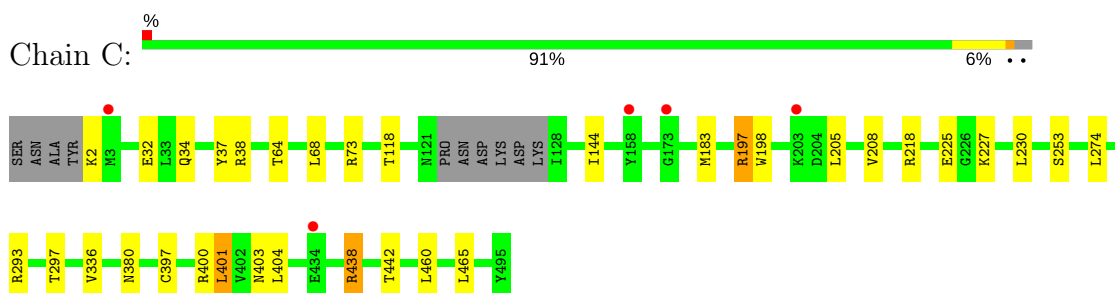
#### • Molecule 1: Adenosylhomocysteinase



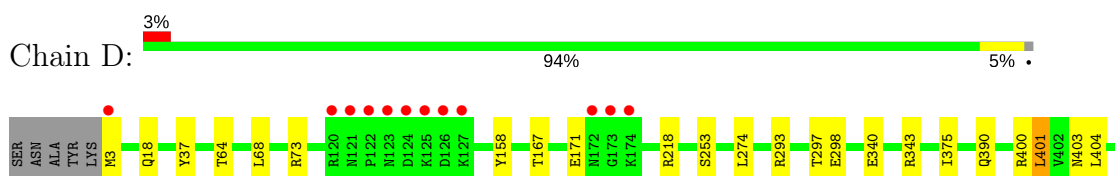
#### • Molecule 1: Adenosylhomocysteinase

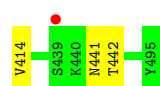


#### • Molecule 1: Adenosylhomocysteinase

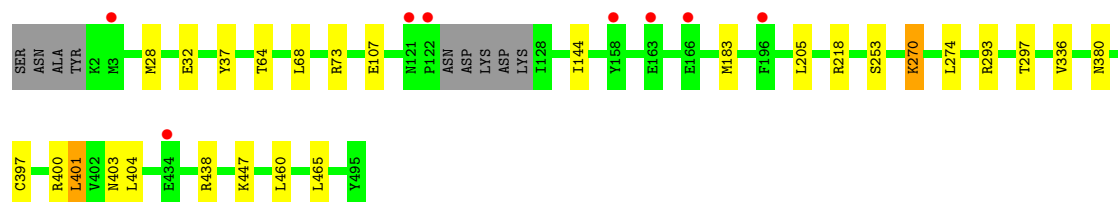
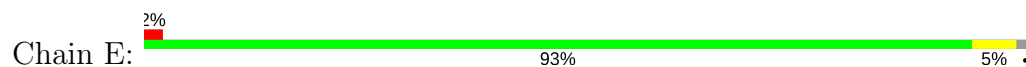


#### • Molecule 1: Adenosylhomocysteinase

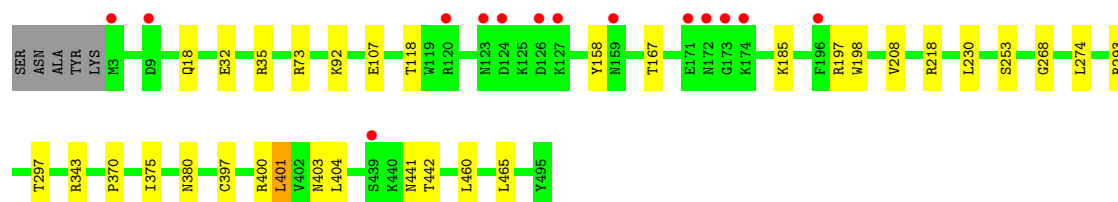
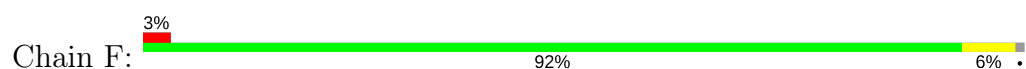




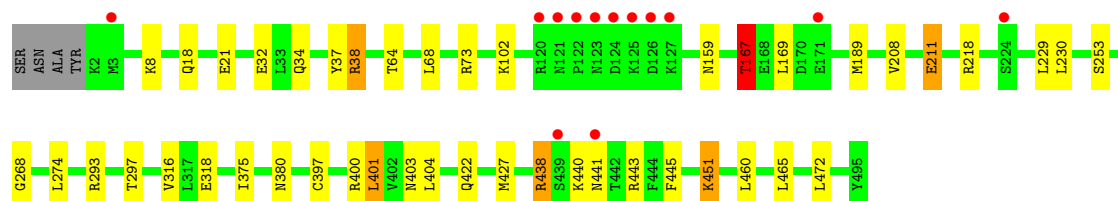
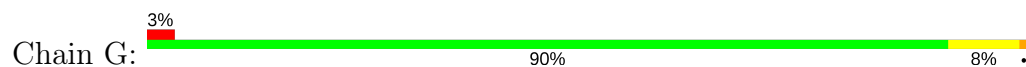
● Molecule 1: Adenosylhomocysteinase



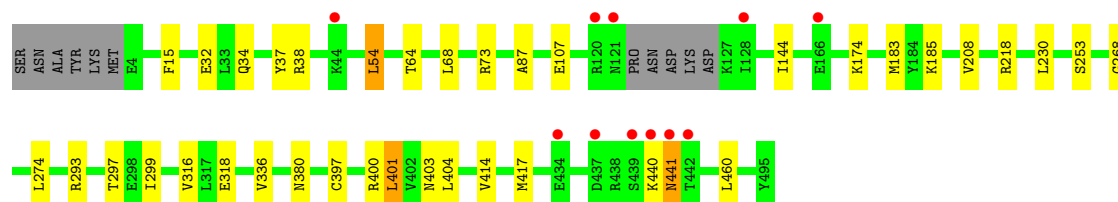
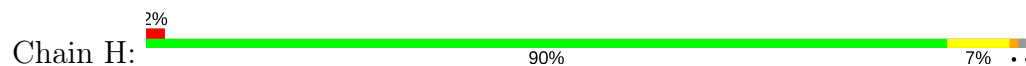
● Molecule 1: Adenosylhomocysteinase



● Molecule 1: Adenosylhomocysteinase



● Molecule 1: Adenosylhomocysteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.84Å 185.31Å 122.44Å 90.00° 97.85° 90.00°	Depositor
Resolution (Å)	29.93 – 2.85 29.93 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.93-2.85) 98.5 (29.93-2.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.173 , 0.200 0.174 , 0.201	Depositor DCC
$R_{free}$ test set	5493 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: ADN, SO4, NAD, CL

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	0.54	1/3987 (0.0%)	1.20	17/5375 (0.3%)
1	B	0.52	1/3966 (0.0%)	0.87	12/5348 (0.2%)
1	C	0.52	0/3932	0.89	10/5300 (0.2%)
1	D	0.54	0/3957	0.90	10/5337 (0.2%)
1	E	0.52	1/3931 (0.0%)	0.86	9/5300 (0.2%)
1	F	0.55	1/3973 (0.0%)	1.20	14/5358 (0.3%)
1	G	0.56	3/3978 (0.1%)	1.10	23/5364 (0.4%)
1	H	0.51	0/3907	0.91	9/5268 (0.2%)
All	All	0.53	7/31631 (0.0%)	1.00	104/42650 (0.2%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	73	ARG	CZ-NH2	-7.46	1.23	1.33
1	A	73	ARG	CZ-NH2	-7.36	1.23	1.33
1	B	432	SER	CA-CB	7.35	1.64	1.52
1	G	211	GLU	CD-OE2	-6.12	1.19	1.25
1	G	21	GLU	CD-OE2	5.68	1.31	1.25

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	ARG	NE-CZ-NH2	-45.36	97.62	120.30
1	A	73	ARG	NE-CZ-NH2	-45.06	97.77	120.30
1	F	73	ARG	NE-CZ-NH1	42.71	141.66	120.30
1	A	73	ARG	NE-CZ-NH1	42.58	141.59	120.30
1	G	293	ARG	NE-CZ-NH1	21.35	130.97	120.30

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	3922	0	3981	15	0
1	B	3902	0	3961	15	0
1	C	3870	0	3926	20	0
1	D	3893	0	3948	12	0
1	E	3868	0	3928	14	0
1	F	3909	0	3961	16	0
1	G	3913	0	3969	26	0
1	H	3845	0	3904	22	0
2	A	19	0	13	1	0
2	B	19	0	13	1	0
2	C	19	0	13	1	0
2	D	19	0	13	1	0
2	E	19	0	13	1	0
2	F	19	0	13	1	0
2	G	19	0	13	1	0
2	H	19	0	13	1	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	3	0
3	E	44	0	26	2	0
3	F	44	0	26	2	0
3	G	44	0	26	2	0
3	H	44	0	26	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	E	5	0	0	0	0
5	G	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	80	0	0	1	0
6	B	50	0	0	1	0
6	C	72	0	0	0	0
6	D	73	0	0	1	0
6	E	74	0	0	0	0
6	F	55	0	0	0	0
6	G	68	0	0	0	0
6	H	51	0	0	0	0
All	All	32193	0	31890	135	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 2.

The worst 5 of 135 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:G:68:LEU:HD13	1:G:427:MET:HE2	1.59	0.82
1:G:68:LEU:HD13	1:G:427:MET:CE	2.13	0.78
1:G:68:LEU:CD1	1:G:427:MET:HE2	2.22	0.69
1:G:229:LEU:O	1:G:438:ARG:NH1	2.24	0.69
1:G:68:LEU:CD1	1:G:427:MET:CE	2.75	0.65

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	494/498 (99%)	475 (96%)	17 (3%)	2 (0%)	36	66
1	B	492/498 (99%)	472 (96%)	17 (4%)	3 (1%)	27	57
1	C	486/498 (98%)	468 (96%)	17 (4%)	1 (0%)	49	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	491/498 (99%)	471 (96%)	18 (4%)	2 (0%)	36	66
1	E	486/498 (98%)	468 (96%)	17 (4%)	1 (0%)	49	78
1	F	493/498 (99%)	474 (96%)	18 (4%)	1 (0%)	49	78
1	G	493/498 (99%)	475 (96%)	17 (3%)	1 (0%)	49	78
1	H	483/498 (97%)	464 (96%)	18 (4%)	1 (0%)	49	78
All	All	3918/3984 (98%)	3767 (96%)	139 (4%)	12 (0%)	43	71

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	ASP
1	A	401	LEU
1	B	401	LEU
1	C	401	LEU
1	D	401	LEU

### 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	434/435 (100%)	434 (100%)	0	100	100
1	B	432/435 (99%)	430 (100%)	2 (0%)	90	96
1	C	428/435 (98%)	427 (100%)	1 (0%)	94	98
1	D	431/435 (99%)	427 (99%)	4 (1%)	81	93
1	E	428/435 (98%)	428 (100%)	0	100	100
1	F	433/435 (100%)	430 (99%)	3 (1%)	85	95
1	G	433/435 (100%)	428 (99%)	5 (1%)	74	90
1	H	425/435 (98%)	423 (100%)	2 (0%)	90	96
All	All	3444/3480 (99%)	3427 (100%)	17 (0%)	90	96

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	167	THR
1	F	441	ASN
1	G	441	ASN
1	D	442	THR
1	G	451	LYS

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](#)

Of 40 ligands modelled in this entry, 19 are monoatomic - leaving 21 for Mogul analysis.

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	ADN	A	501	-	18,21,21	1.02	1 (5%)	16,31,31	2.26	4 (25%)
3	NAD	A	502	-	40,48,48	0.84	1 (2%)	44,73,73	1.61	4 (9%)
5	SO4	A	506	-	4,4,4	0.41	0	6,6,6	0.09	0
2	ADN	B	501	-	18,21,21	1.01	1 (5%)	16,31,31	2.10	3 (18%)
3	NAD	B	502	-	40,48,48	0.83	1 (2%)	44,73,73	1.48	3 (6%)
5	SO4	B	506	-	4,4,4	0.44	0	6,6,6	0.10	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADN	C	501	-	18,21,21	1.02	1 (5%)	16,31,31	2.20	4 (25%)
3	NAD	C	502	-	40,48,48	0.87	3 (7%)	44,73,73	1.53	5 (11%)
5	SO4	C	505	-	4,4,4	0.44	0	6,6,6	0.17	0
2	ADN	D	501	-	18,21,21	1.02	1 (5%)	16,31,31	2.36	4 (25%)
3	NAD	D	502	-	40,48,48	0.81	1 (2%)	44,73,73	1.47	4 (9%)
2	ADN	E	501	-	18,21,21	0.94	1 (5%)	16,31,31	2.28	3 (18%)
3	NAD	E	502	-	40,48,48	0.89	1 (2%)	44,73,73	1.50	4 (9%)
5	SO4	E	504	-	4,4,4	0.45	0	6,6,6	0.15	0
2	ADN	F	501	-	18,21,21	0.99	1 (5%)	16,31,31	2.37	4 (25%)
3	NAD	F	502	-	40,48,48	0.86	1 (2%)	44,73,73	1.64	5 (11%)
2	ADN	G	501	-	18,21,21	1.03	1 (5%)	16,31,31	2.17	3 (18%)
3	NAD	G	502	-	40,48,48	0.81	1 (2%)	44,73,73	1.56	5 (11%)
5	SO4	G	506	-	4,4,4	0.44	0	6,6,6	0.10	0
2	ADN	H	501	-	18,21,21	1.09	1 (5%)	16,31,31	2.15	4 (25%)
3	NAD	H	502	-	40,48,48	0.93	2 (5%)	44,73,73	1.48	5 (11%)

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	ADN	A	501	-	-	0/2/22/22	0/3/3/3
3	NAD	A	502	-	-	0/22/62/62	0/5/5/5
5	SO4	A	506	-	-	0/0/0/0	0/0/0/0
2	ADN	B	501	-	-	0/2/22/22	0/3/3/3
3	NAD	B	502	-	-	0/22/62/62	0/5/5/5
5	SO4	B	506	-	-	0/0/0/0	0/0/0/0
2	ADN	C	501	-	-	0/2/22/22	0/3/3/3
3	NAD	C	502	-	-	0/22/62/62	0/5/5/5
5	SO4	C	505	-	-	0/0/0/0	0/0/0/0
2	ADN	D	501	-	-	0/2/22/22	0/3/3/3
3	NAD	D	502	-	-	0/22/62/62	0/5/5/5
2	ADN	E	501	-	-	0/2/22/22	0/3/3/3
3	NAD	E	502	-	-	0/22/62/62	0/5/5/5
5	SO4	E	504	-	-	0/0/0/0	0/0/0/0
2	ADN	F	501	-	-	0/2/22/22	0/3/3/3
3	NAD	F	502	-	-	0/22/62/62	0/5/5/5
2	ADN	G	501	-	-	0/2/22/22	0/3/3/3
3	NAD	G	502	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	G	506	-	-	0/0/0/0	0/0/0/0
2	ADN	H	501	-	-	0/2/22/22	0/3/3/3
3	NAD	H	502	-	-	0/22/62/62	0/5/5/5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	NAD	C8A-N9A	-2.02	1.34	1.36
3	H	502	NAD	O4D-C1D	2.12	1.44	1.41
3	C	502	NAD	O4D-C1D	2.36	1.44	1.41
2	E	501	ADN	C5-C4	2.39	1.45	1.40
2	A	501	ADN	C5-C4	2.41	1.45	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	ADN	N3-C2-N1	-7.37	122.55	128.86
3	A	502	NAD	N3A-C2A-N1A	-7.34	122.58	128.86
2	D	501	ADN	N3-C2-N1	-7.23	122.67	128.86
2	E	501	ADN	N3-C2-N1	-7.14	122.75	128.86
3	F	502	NAD	N3A-C2A-N1A	-7.00	122.88	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADN	1	0
3	A	502	NAD	1	0
2	B	501	ADN	1	0
3	B	502	NAD	1	0
2	C	501	ADN	1	0
3	C	502	NAD	2	0
2	D	501	ADN	1	0
3	D	502	NAD	3	0
2	E	501	ADN	1	0
3	E	502	NAD	2	0
2	F	501	ADN	1	0
3	F	502	NAD	2	0
2	G	501	ADN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	502	NAD	2	0
2	H	501	ADN	1	0
3	H	502	NAD	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	494/498 (99%)	-0.41	13 (2%) 56 52	33, 50, 85, 151	0
1	B	494/498 (99%)	-0.17	24 (4%) 29 25	34, 67, 136, 176	0
1	C	488/498 (97%)	-0.44	5 (1%) 82 81	34, 53, 88, 122	0
1	D	493/498 (98%)	-0.40	13 (2%) 56 52	32, 52, 95, 148	0
1	E	489/498 (98%)	-0.37	8 (1%) 72 70	38, 56, 90, 134	0
1	F	493/498 (98%)	-0.30	14 (2%) 53 48	33, 56, 97, 136	0
1	G	494/498 (99%)	-0.39	13 (2%) 56 52	37, 53, 88, 154	0
1	H	487/498 (97%)	-0.31	11 (2%) 60 57	36, 67, 107, 147	0
All	All	3932/3984 (98%)	-0.35	101 (2%) 56 52	32, 56, 102, 176	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	123	ASN	5.7
1	H	441	ASN	5.6
1	B	441	ASN	5.5
1	D	122	PRO	5.4
1	F	126	ASP	5.3

### 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 ⓘ

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<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	B	505	1/1	0.60	0.20	75,75,75,75	0
4	CL	D	505	1/1	0.78	0.31	72,72,72,72	0
4	CL	G	503	1/1	0.79	0.21	72,72,72,72	0
4	CL	D	506	1/1	0.85	0.14	75,75,75,75	0
4	CL	F	503	1/1	0.86	0.11	69,69,69,69	0
5	SO4	B	506	5/5	0.86	0.31	131,136,138,155	0
4	CL	A	505	1/1	0.87	0.14	64,64,64,64	0
4	CL	F	504	1/1	0.87	0.12	72,72,72,72	0
4	CL	A	503	1/1	0.88	0.12	64,64,64,64	0
4	CL	E	503	1/1	0.88	0.19	71,71,71,71	0
4	CL	C	504	1/1	0.88	0.15	61,61,61,61	0
4	CL	C	503	1/1	0.90	0.11	73,73,73,73	0
4	CL	G	504	1/1	0.91	0.09	60,60,60,60	0
5	SO4	G	506	5/5	0.91	0.30	96,107,110,111	0
4	CL	G	505	1/1	0.92	0.08	62,62,62,62	0
5	SO4	A	506	5/5	0.93	0.38	101,101,109,113	0
4	CL	B	504	1/1	0.93	0.13	72,72,72,72	0
5	SO4	E	504	5/5	0.94	0.28	101,102,108,113	0
4	CL	A	504	1/1	0.94	0.16	72,72,72,72	0
4	CL	D	504	1/1	0.95	0.08	72,72,72,72	0
4	CL	D	503	1/1	0.95	0.04	75,75,75,75	0
5	SO4	C	505	5/5	0.95	0.31	99,100,108,109	0
2	ADN	E	501	19/19	0.97	0.13	42,50,65,66	0
2	ADN	G	501	19/19	0.97	0.16	40,44,62,64	0
2	ADN	H	501	19/19	0.97	0.14	50,59,62,63	0
3	NAD	G	502	44/44	0.97	0.14	34,40,48,55	0
3	NAD	A	502	44/44	0.97	0.13	30,35,43,47	0
2	ADN	C	501	19/19	0.97	0.15	41,46,63,63	0
2	ADN	A	501	19/19	0.98	0.15	35,39,51,52	0
3	NAD	E	502	44/44	0.98	0.12	32,42,48,53	0
2	ADN	B	501	19/19	0.98	0.13	45,56,62,65	0
3	NAD	B	502	44/44	0.98	0.11	35,41,49,57	0
4	CL	B	503	1/1	0.98	0.09	71,71,71,71	0
2	ADN	F	501	19/19	0.98	0.19	40,43,49,49	0
3	NAD	C	502	44/44	0.98	0.12	30,41,47,51	0
3	NAD	D	502	44/44	0.98	0.12	26,30,34,36	0
2	ADN	D	501	19/19	0.98	0.16	37,42,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	H	503	1/1	0.98	0.05	71,71,71,71	0
3	NAD	H	502	44/44	0.98	0.11	40,43,51,54	0
3	NAD	F	502	44/44	0.98	0.11	30,33,38,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.