



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:21 AM GMT

PDB ID : 3I3O  
Title : 2.06 Angstrom resolution crystal structure of a short chain dehydrogenase from Bacillus anthracis str. 'Ames Ancestor' in complex with NAD-acetone  
Authors : Halavaty, A.S.; Minasov, G.; Skarina, T.; Onopriyenko, O.; Peterson, S.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2009-06-30  
Resolution : 2.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

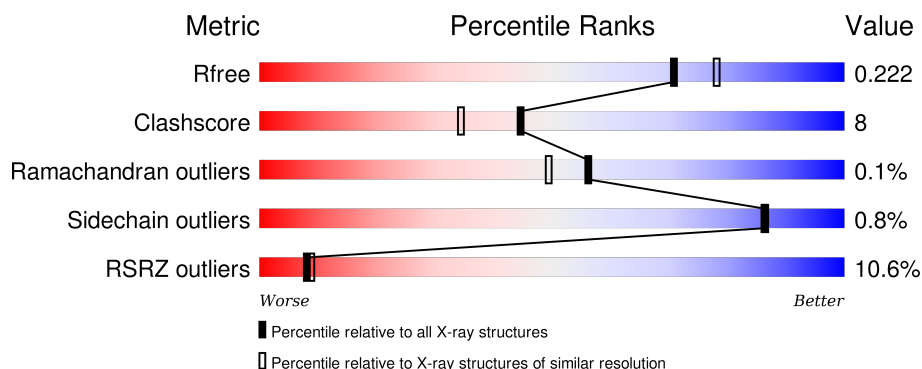
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	291	<div> <div>10%</div> <div>89%</div> <div>8%</div> </div>
1	B	291	<div> <div>9%</div> <div>89%</div> <div>8%</div> </div>
1	C	291	<div> <div>9%</div> <div>86%</div> <div>11%</div> </div>
1	D	291	<div> <div>7%</div> <div>87%</div> <div>11%</div> </div>
1	E	291	<div> <div>13%</div> <div>83%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	291	
1	G	291	
1	H	291	

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
4	CAC	A	327	-	-	-	X
4	CAC	B	321	-	-	-	X
4	CAC	B	328	-	-	-	X
4	CAC	C	322	-	-	-	X
4	CAC	D	324	-	-	-	X
4	CAC	E	325	-	-	-	X
4	CAC	F	329	-	-	-	X
4	CAC	H	323	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18804 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	3	0
			2181	1378	367	430	6			
1	B	283	Total	C	N	O	S	0	11	0
			2256	1421	380	449	6			
1	C	281	Total	C	N	O	S	0	5	0
			2190	1383	369	432	6			
1	D	283	Total	C	N	O	S	0	9	0
			2246	1417	381	442	6			
1	E	279	Total	C	N	O	S	0	9	0
			2208	1393	372	437	6			
1	F	270	Total	C	N	O	S	0	6	0
			2112	1337	354	416	5			
1	G	245	Total	C	N	O	S	0	4	0
			1893	1191	320	378	4			
1	H	270	Total	C	N	O	S	0	6	0
			2113	1335	357	416	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81UV8
A	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
A	0	ALA	-	EXPRESSION TAG	UNP Q81UV8
B	-2	SER	-	EXPRESSION TAG	UNP Q81UV8
B	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
B	0	ALA	-	EXPRESSION TAG	UNP Q81UV8
C	-2	SER	-	EXPRESSION TAG	UNP Q81UV8
C	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
C	0	ALA	-	EXPRESSION TAG	UNP Q81UV8
D	-2	SER	-	EXPRESSION TAG	UNP Q81UV8
D	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
D	0	ALA	-	EXPRESSION TAG	UNP Q81UV8
E	-2	SER	-	EXPRESSION TAG	UNP Q81UV8

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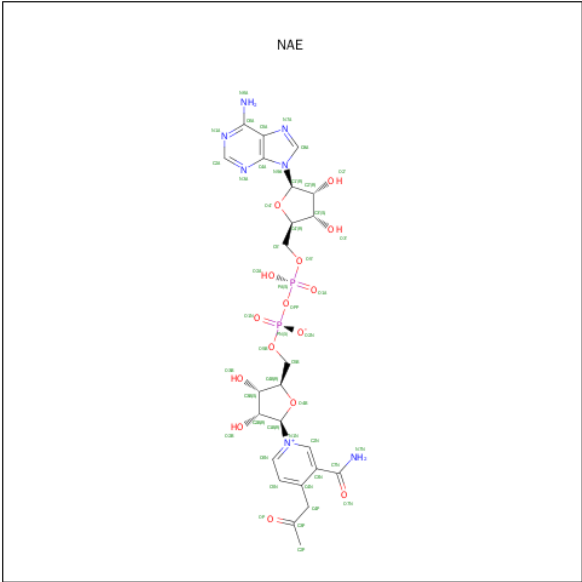
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
E	0	ALA	-	EXPRESSION TAG	UNP Q81UV8
F	-2	SER	-	EXPRESSION TAG	UNP Q81UV8
F	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
F	0	ALA	-	EXPRESSION TAG	UNP Q81UV8
G	-2	SER	-	EXPRESSION TAG	UNP Q81UV8
G	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
G	0	ALA	-	EXPRESSION TAG	UNP Q81UV8
H	-2	SER	-	EXPRESSION TAG	UNP Q81UV8
H	-1	ASN	-	EXPRESSION TAG	UNP Q81UV8
H	0	ALA	-	EXPRESSION TAG	UNP Q81UV8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

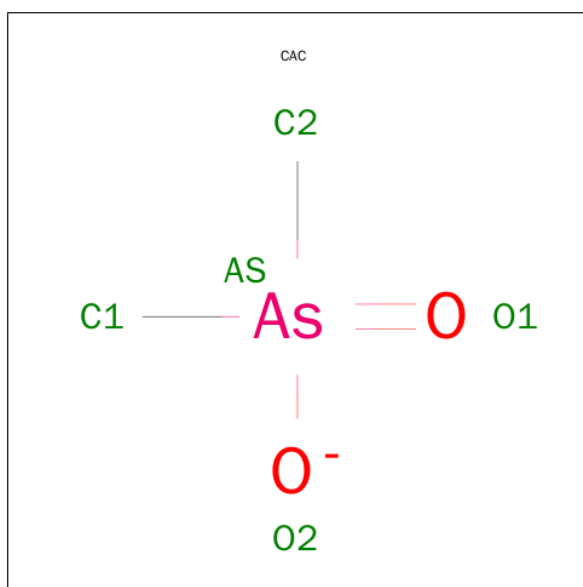
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is NICOTINAMIDE ADENINE DINUCLEOTIDE ACETONE ADDUCT (three-letter code: NAE) (formula: C<sub>24</sub>H<sub>31</sub>N<sub>7</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	24	7	15	2		
3	B	1	Total	C	N	O	P	0	0
			48	24	7	15	2		
3	C	1	Total	C	N	O	P	0	0
			48	24	7	15	2		
3	D	1	Total	C	N	O	P	0	0
			48	24	7	15	2		
3	E	1	Total	C	N	O	P	0	0
			48	24	7	15	2		
3	F	1	Total	C	N	O	P	0	0
			48	24	7	15	2		
3	H	1	Total	C	N	O	P	0	0
			48	24	7	15	2		

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	D	1	Total	As	C	O	0	0
			5	1	2	2		
4	E	1	Total	As	C	O	0	0
			5	1	2	2		
4	F	1	Total	As	C	O	0	0
			5	1	2	2		
4	G	1	Total	As	C	O	0	0
			5	1	2	2		
4	H	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

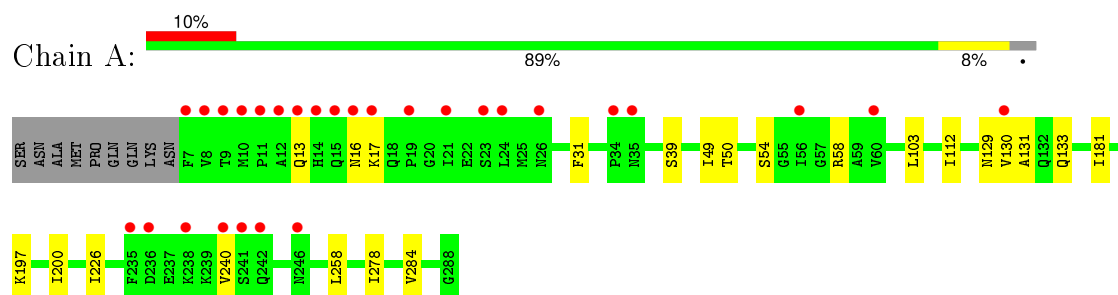
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	178	Total 179	O 179	0	3
6	B	221	Total 221	O 221	0	5
6	C	190	Total 191	O 191	0	5
6	D	169	Total 169	O 169	0	5
6	E	171	Total 174	O 174	0	6
6	F	100	Total 100	O 100	0	0
6	G	66	Total 66	O 66	0	1
6	H	115	Total 116	O 116	0	3



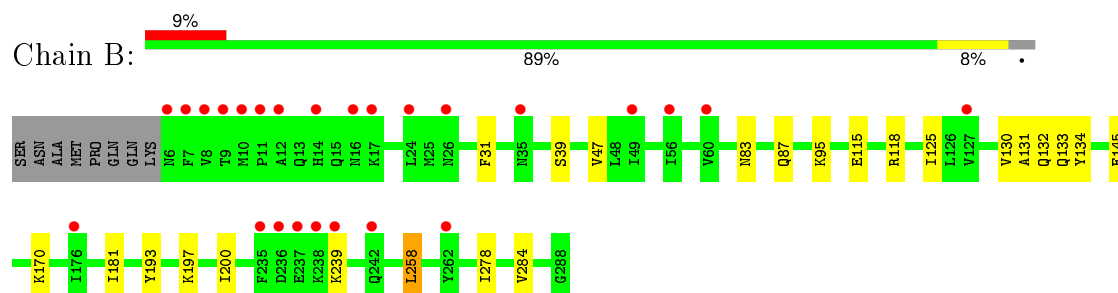
### 3 Residue-property plots [i](#)

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.

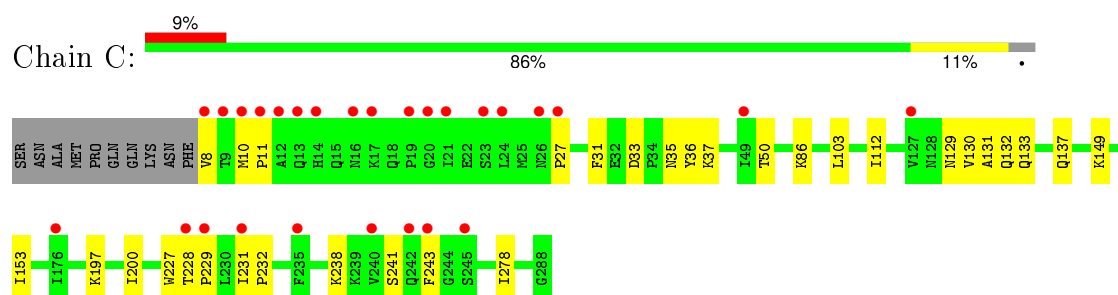
- Molecule 1: Short chain dehydrogenase



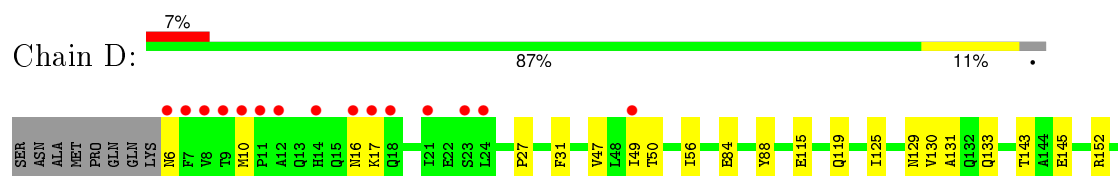
- Molecule 1: Short chain dehydrogenase

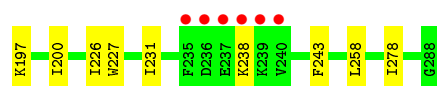


- Molecule 1: Short chain dehydrogenase

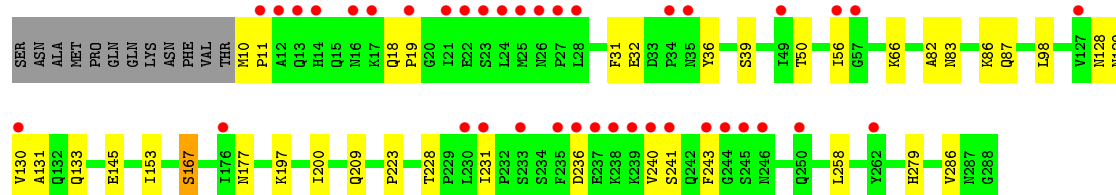
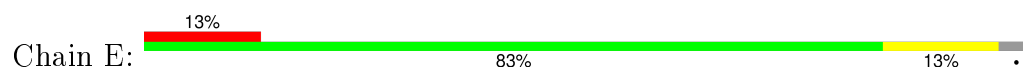


- Molecule 1: Short chain dehydrogenase

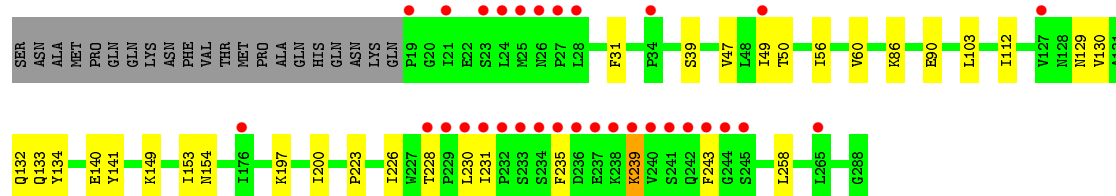
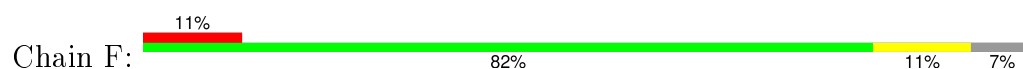




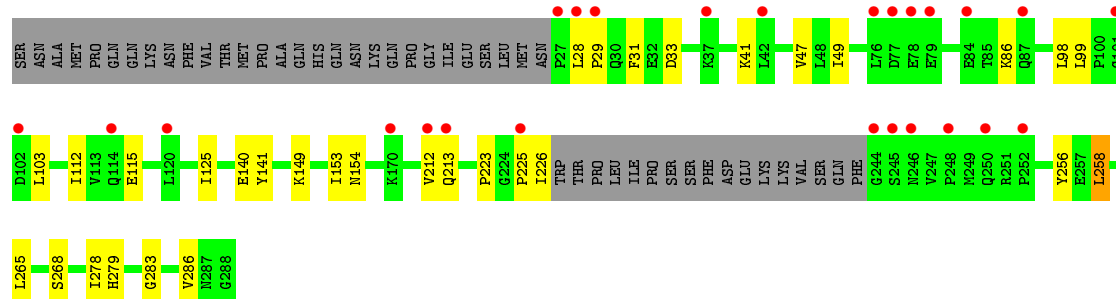
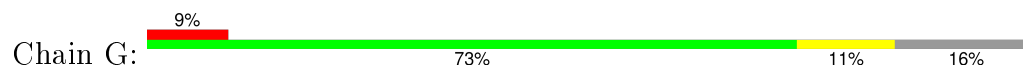
• Molecule 1: Short chain dehydrogenase



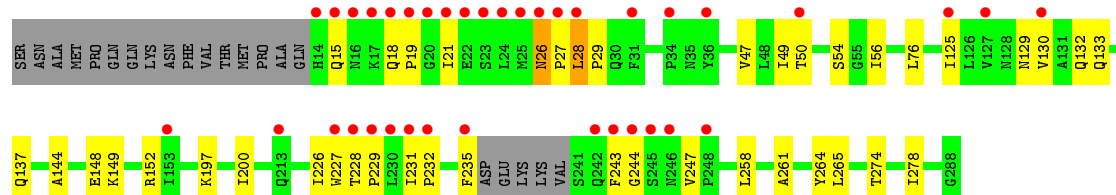
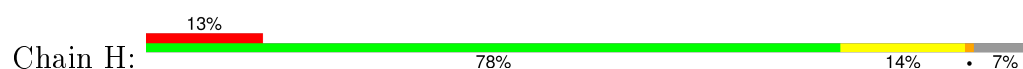
• Molecule 1: Short chain dehydrogenase



• Molecule 1: Short chain dehydrogenase



• Molecule 1: Short chain dehydrogenase



## 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, $\alpha$ , $\beta$ , $\gamma$	131.76 Å   168.16 Å   107.19 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.95 – 2.06 29.56 – 2.06	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.95-2.06) 100.0 (29.56-2.06)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.80 (at 2.06 Å)	Xtriage
Refinement program	REFMAC 5.5.0051	Depositor
R, $R_{free}$	0.161   ,   0.205 0.182   ,   0.222	Depositor DCC
$R_{free}$ test set	7384 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.947	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	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	0 of 147192 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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 24.65 % 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 3.6785e-03. 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: CAC, MG, NAE, 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	0.73	0/2223	0.74	1/3015 (0.0%)
1	B	0.75	0/2298	0.75	1/3117 (0.0%)
1	C	0.78	0/2231	0.74	0/3025
1	D	0.70	0/2288	0.74	0/3102
1	E	0.70	0/2249	0.74	1/3050 (0.0%)
1	F	0.62	0/2151	0.70	0/2916
1	G	0.66	0/1924	0.71	0/2606
1	H	0.63	0/2152	0.73	0/2918
All	All	0.70	0/17516	0.73	3/23749 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	CA-CB-CG	-7.23	98.67	115.30
1	E	167	SER	CB-CA-C	-5.14	100.33	110.10
1	A	58	ARG	NE-CZ-NH2	-5.08	117.76	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	2181	0	2157	22	0
1	B	2256	0	2214	24	0
1	C	2190	0	2172	30	0
1	D	2246	0	2218	37	0
1	E	2208	0	2178	46	0
1	F	2112	0	2099	42	0
1	G	1893	0	1871	22	0
1	H	2113	0	2087	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
3	A	48	0	30	13	0
3	B	48	0	29	14	0
3	C	48	0	30	7	0
3	D	48	0	29	8	0
3	E	48	0	29	15	0
3	F	48	0	29	9	0
3	H	48	0	30	7	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	D	1	0	0	0	0
6	A	179	0	0	1	0
6	B	221	0	0	3	0
6	C	191	0	0	4	0
6	D	169	0	0	4	0
6	E	174	0	0	1	0
6	F	100	0	0	2	0
6	G	66	0	0	2	0
6	H	116	0	0	2	0
All	All	18804	0	17202	274	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 8.

The worst 5 of 274 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:C:10:MET:HE3	1:C:27:PRO:HD2	1.48	0.94
1:C:132:GLN:HE22	1:C:149:LYS:HE2	1.34	0.91
1:A:130:VAL:HG23	3:A:311:NAE:C1'	2.01	0.91
1:D:56:ILE:HG12	1:D:258[B]:LEU:HD22	1.55	0.89
1:F:226:ILE:O	1:F:231:ILE:HD11	1.72	0.89

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	283/291 (97%)	274 (97%)	9 (3%)	0	100	100
1	B	292/291 (100%)	280 (96%)	12 (4%)	0	100	100
1	C	284/291 (98%)	272 (96%)	12 (4%)	0	100	100
1	D	290/291 (100%)	281 (97%)	9 (3%)	0	100	100
1	E	286/291 (98%)	273 (96%)	13 (4%)	0	100	100
1	F	274/291 (94%)	263 (96%)	11 (4%)	0	100	100
1	G	245/291 (84%)	235 (96%)	10 (4%)	0	100	100
1	H	272/291 (94%)	260 (96%)	10 (4%)	2 (1%)	26	14
All	All	2226/2328 (96%)	2138 (96%)	86 (4%)	2 (0%)	56	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	26	ASN
1	H	28	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	239/244 (98%)	238 (100%)	1 (0%)	93	94
1	B	248/244 (102%)	245 (99%)	3 (1%)	78	76
1	C	240/244 (98%)	239 (100%)	1 (0%)	93	94
1	D	246/244 (101%)	242 (98%)	4 (2%)	70	67
1	E	242/244 (99%)	241 (100%)	1 (0%)	93	94
1	F	231/244 (95%)	230 (100%)	1 (0%)	93	94
1	G	205/244 (84%)	203 (99%)	2 (1%)	82	81
1	H	231/244 (95%)	229 (99%)	2 (1%)	84	84
All	All	1882/1952 (96%)	1867 (99%)	15 (1%)	86	86

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	16	ASN
1	D	17	LYS
1	G	268	SER
1	D	6	ASN
1	G	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	128	ASN
1	E	129	ASN
1	H	18	GLN
1	D	119	GLN
1	F	132	GLN

### 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 ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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$
3	NAE	A	311	2	42,52,52	2.09	7 (16%)	52,79,79	3.08	13 (25%)
4	CAC	A	327	-	0,4,4	0.00	-	0,6,6	0.00	-
3	NAE	B	311	2	42,52,52	2.00	6 (14%)	52,79,79	2.86	13 (25%)
4	CAC	B	321	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	328	-	0,4,4	0.00	-	0,6,6	0.00	-
3	NAE	C	311	2	42,52,52	2.10	5 (11%)	52,79,79	2.68	13 (25%)
4	CAC	C	322	-	0,4,4	0.00	-	0,6,6	0.00	-
3	NAE	D	311	2	42,52,52	2.01	8 (19%)	52,79,79	2.70	16 (30%)
4	CAC	D	324	-	0,4,4	0.00	-	0,6,6	0.00	-
3	NAE	E	311	2	42,52,52	1.91	6 (14%)	52,79,79	3.04	14 (26%)
4	CAC	E	325	-	0,4,4	0.00	-	0,6,6	0.00	-
3	NAE	F	311	2	42,52,52	1.98	6 (14%)	52,79,79	2.81	11 (21%)
4	CAC	F	329	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	G	326	-	0,4,4	0.00	-	0,6,6	0.00	-
3	NAE	H	311	2	42,52,52	2.03	6 (14%)	52,79,79	2.74	11 (21%)
4	CAC	H	323	-	0,4,4	0.00	-	0,6,6	0.00	-

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	NAE	A	311	2	-	0/26/66/66	0/5/5/5
4	CAC	A	327	-	-	0/0/0/0	0/0/0/0
3	NAE	B	311	2	-	0/26/66/66	0/5/5/5
4	CAC	B	321	-	-	0/0/0/0	0/0/0/0
4	CAC	B	328	-	-	0/0/0/0	0/0/0/0
3	NAE	C	311	2	-	0/26/66/66	0/5/5/5
4	CAC	C	322	-	-	0/0/0/0	0/0/0/0
3	NAE	D	311	2	-	0/26/66/66	0/5/5/5
4	CAC	D	324	-	-	0/0/0/0	0/0/0/0
3	NAE	E	311	2	-	0/26/66/66	0/5/5/5
4	CAC	E	325	-	-	0/0/0/0	0/0/0/0
3	NAE	F	311	2	-	0/26/66/66	0/5/5/5
4	CAC	F	329	-	-	0/0/0/0	0/0/0/0
4	CAC	G	326	-	-	0/0/0/0	0/0/0/0
3	NAE	H	311	2	-	0/26/66/66	0/5/5/5
4	CAC	H	323	-	-	0/0/0/0	0/0/0/0

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	311	NAE	C3N-C7N	-3.92	1.45	1.50
3	B	311	NAE	C2N-C3N	-2.56	1.35	1.38
3	F	311	NAE	C2N-C3N	-2.52	1.35	1.38
3	D	311	NAE	C6N-C5N	-2.43	1.32	1.38
3	H	311	NAE	C2N-C3N	-2.38	1.35	1.38

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	311	NAE	N3A-C2A-N1A	-12.07	119.65	128.89
3	E	311	NAE	N3A-C2A-N1A	-11.52	120.08	128.89
3	C	311	NAE	N3A-C2A-N1A	-11.34	120.21	128.89
3	F	311	NAE	N3A-C2A-N1A	-11.25	120.28	128.89
3	A	311	NAE	N3A-C2A-N1A	-10.81	120.61	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	311	NAE	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	311	NAE	14	0
3	C	311	NAE	7	0
4	C	322	CAC	1	0
3	D	311	NAE	8	0
3	E	311	NAE	15	0
3	F	311	NAE	9	0
3	H	311	NAE	7	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	282/291 (96%)	0.31	28 (9%) 9 10	7, 16, 26, 38	0
1	B	283/291 (97%)	0.25	25 (8%) 12 13	7, 13, 23, 32	0
1	C	281/291 (96%)	0.35	27 (9%) 10 11	8, 14, 24, 31	0
1	D	283/291 (97%)	0.23	21 (7%) 17 19	11, 16, 27, 33	0
1	E	279/291 (95%)	0.44	39 (13%) 4 4	2, 15, 25, 36	0
1	F	270/291 (92%)	0.50	31 (11%) 6 7	12, 18, 27, 31	0
1	G	245/291 (84%)	0.70	25 (10%) 9 9	10, 20, 28, 37	0
1	H	270/291 (92%)	0.55	37 (13%) 4 4	10, 18, 31, 40	0
All	All	2193/2328 (94%)	0.41	233 (10%) 8 9	2, 16, 27, 40	0

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ASN	9.9
1	A	7	PHE	9.7
1	D	7	PHE	8.9
1	H	26	ASN	8.9
1	B	7	PHE	8.0

### 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
4	CAC	A	327	5/5	0.89	0.40	23.16	51,53,54,56	5
4	CAC	B	328	5/5	0.69	0.41	13.70	61,61,62,62	5
4	CAC	B	321	5/5	0.93	0.35	7.55	54,58,59,61	5
4	CAC	E	325	5/5	0.93	0.25	6.84	46,50,52,53	5
4	CAC	C	322	5/5	0.89	0.27	6.16	37,41,46,54	5
4	CAC	F	329	5/5	0.91	0.28	4.81	52,53,54,56	5
4	CAC	D	324	5/5	0.92	0.30	3.81	44,46,48,53	5
4	CAC	H	323	5/5	0.89	0.26	3.32	48,51,51,58	5
4	CAC	G	326	5/5	0.94	0.19	1.51	46,47,49,50	5
3	NAE	H	311	48/48	0.80	0.23	0.75	30,40,46,49	48
3	NAE	A	311	48/48	0.90	0.17	0.41	23,31,38,44	0
3	NAE	C	311	48/48	0.86	0.17	0.23	22,32,39,42	48
3	NAE	F	311	48/48	0.88	0.17	0.19	25,36,40,43	48
5	CL	D	308	1/1	0.89	0.10	0.02	51,51,51,51	0
3	NAE	B	311	48/48	0.92	0.13	-0.10	18,26,35,44	0
3	NAE	D	311	48/48	0.92	0.13	-0.11	25,30,37,45	48
3	NAE	E	311	48/48	0.92	0.14	-0.32	21,33,37,42	48
2	MG	E	305	1/1	0.61	0.13	-0.44	45,45,45,45	0
2	MG	F	303	1/1	0.74	0.10	-0.87	40,40,40,40	0
2	MG	C	304	1/1	0.81	0.11	-0.94	38,38,38,38	0
2	MG	H	307	1/1	0.70	0.09	-1.10	40,40,40,40	0
2	MG	D	302	1/1	0.84	0.07	-1.41	39,39,39,39	0
2	MG	A	306	1/1	0.95	0.04	-1.79	35,35,35,35	0
2	MG	B	301	1/1	0.87	0.08	-2.14	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.