



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:37 AM GMT

PDB ID : 3SEQ  
Title : Crystal structure of C176A mutant of glutamine-dependent NAD<sup>+</sup> synthetase from *M. tuberculosis* in complex with AMPCPP and NaAD<sup>+</sup>  
Authors : Chuenchor, W.; Gerratana, B.  
Deposited on : 2011-06-10  
Resolution : 2.73 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

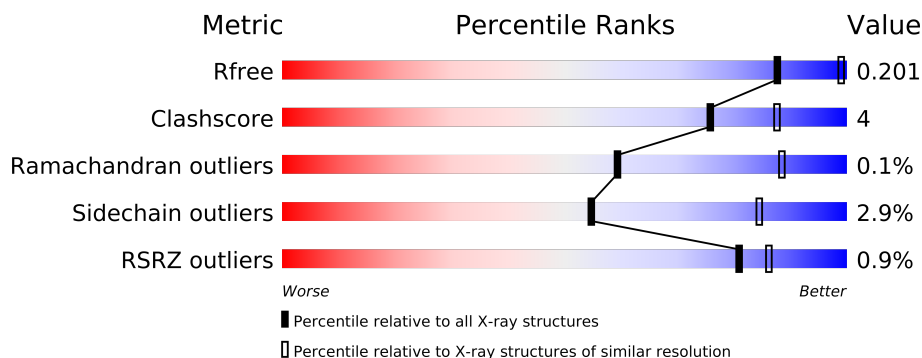
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.73 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))
$R_{free}$	66092	2164 (2.78-2.70)
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (2.78-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	680	
1	B	680	
1	C	680	
1	D	680	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	B	682	-	X
4	GOL	D	682	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20820 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

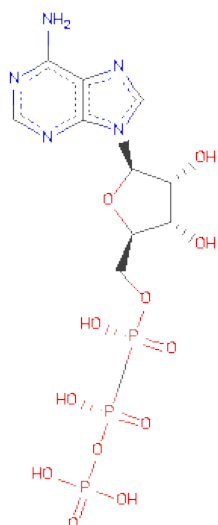
- Molecule 1 is a protein called Glutamine-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5102	3234	905	948	15			
1	B	658	Total	C	N	O	S	0	0	0
			5063	3215	894	939	15			
1	C	650	Total	C	N	O	S	0	0	0
			4992	3171	885	921	15			
1	D	650	Total	C	N	O	S	0	0	0
			5002	3174	887	926	15			

There are 8 discrepancies between the modelled and reference sequences:

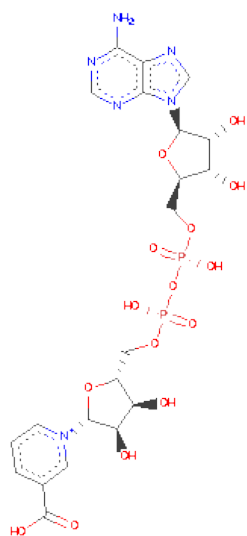
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P0A5L6
A	176	ALA	CYS	ENGINEERED MUTATION	UNP P0A5L6
B	0	SER	-	EXPRESSION TAG	UNP P0A5L6
B	176	ALA	CYS	ENGINEERED MUTATION	UNP P0A5L6
C	0	SER	-	EXPRESSION TAG	UNP P0A5L6
C	176	ALA	CYS	ENGINEERED MUTATION	UNP P0A5L6
D	0	SER	-	EXPRESSION TAG	UNP P0A5L6
D	176	ALA	CYS	ENGINEERED MUTATION	UNP P0A5L6

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONICACID ADENOSYL ESTER (three-letter code: APC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



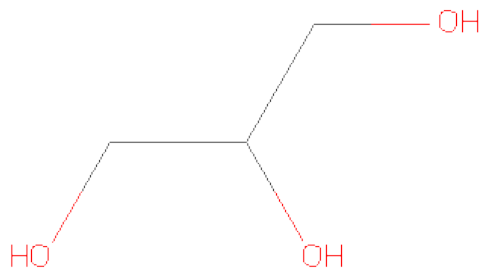
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is 1-[(2R,3R,4S,5R)-5-({[(R)-{[(R)-{(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]OXY}METHYL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]-3-CARBOXYPYRIDINIUM (three-letter code: NXX) (formula:  $C_{21}H_{27}N_6O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

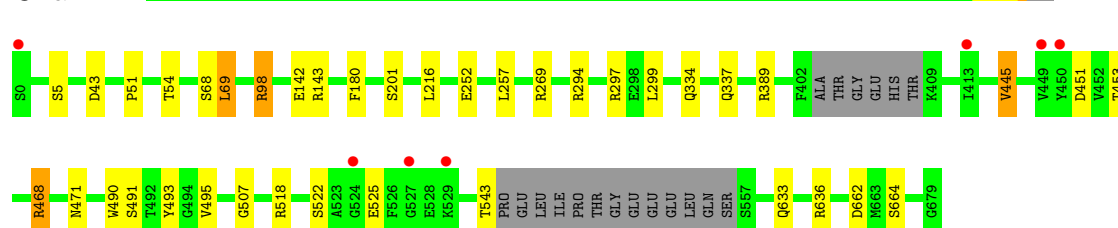
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	96	Total	O	0	0
			96	96		
5	B	92	Total	O	0	0
			92	92		
5	C	73	Total	O	0	0
			73	73		
5	D	88	Total	O	0	0
			88	88		

### 3 Residue-property plots

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

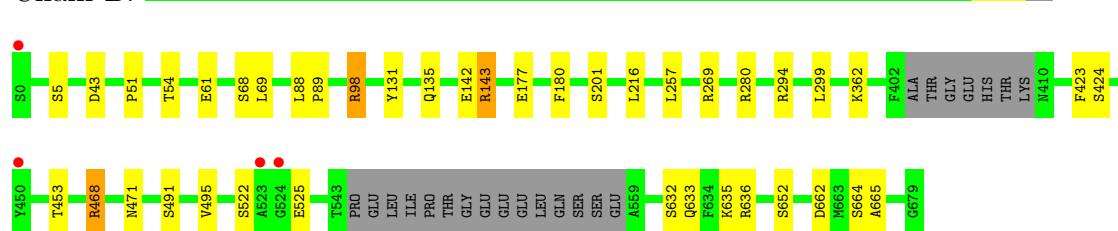
- Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain A:



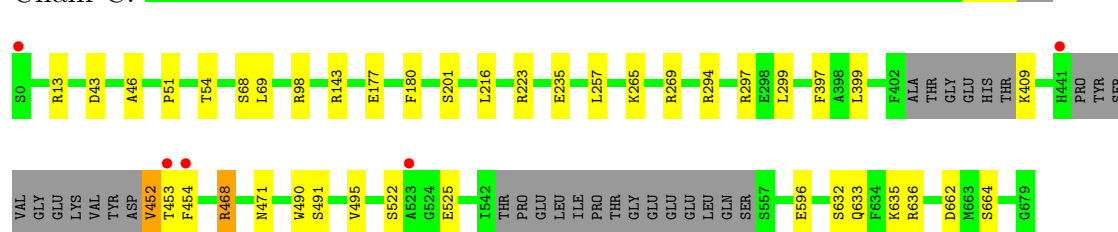
- Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain B:



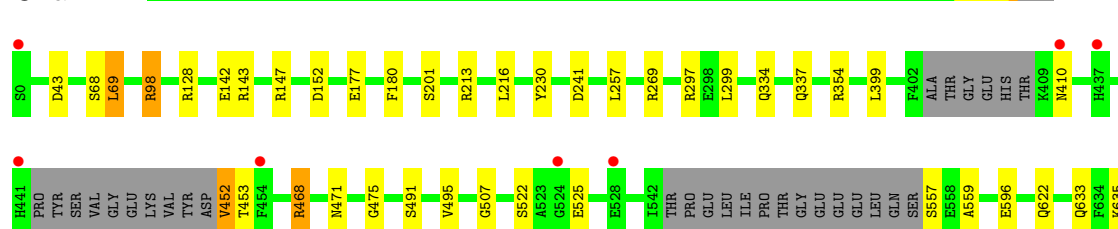
- Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain C:



- Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain D:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.17Å 178.17Å 214.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.09 – 2.73 40.09 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.09-2.73) 91.5 (40.09-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.21 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.163 , 0.212 0.152 , 0.201	Depositor DCC
$R_{free}$ test set	4188 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	1.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 11.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 88210 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.61	0/5222	0.73	2/7099 (0.0%)
1	B	0.62	0/5183	0.72	2/7049 (0.0%)
1	C	0.61	0/5108	0.71	2/6941 (0.0%)
1	D	0.62	0/5118	0.73	2/6955 (0.0%)
All	All	0.61	0/20631	0.72	8/28044 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	294	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	294	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	213	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	A	69	LEU	CA-CB-CG	-5.69	102.22	115.30
1	D	69	LEU	CA-CB-CG	-5.62	102.37	115.30
1	C	223	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	69	LEU	CA-CB-CG	-5.15	103.46	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	452	VAL	Peptide
1	D	452	VAL	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5102	0	0	17	1
1	B	5063	0	7	23	0
1	C	4992	0	0	19	0
1	D	5002	0	0	22	1
2	A	31	0	14	2	0
2	B	31	0	14	2	0
2	C	31	0	14	3	0
2	D	31	0	14	2	0
3	A	44	0	24	4	0
3	B	44	0	24	1	0
3	C	44	0	24	2	0
3	D	44	0	24	1	0
4	B	6	0	8	3	0
4	D	6	0	8	0	0
5	A	96	0	0	3	0
5	B	92	0	0	3	0
5	C	73	0	0	0	0
5	D	88	0	0	4	0
All	All	20820	0	175	80	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (80) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:633:GLN:OE1	1:D:636:ARG:NH1	2.04	0.90
1:A:633:GLN:OE1	1:A:636:ARG:NH1	2.06	0.88
1:A:468:ARG:NH2	1:D:495:VAL:O	2.08	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:633:GLN:OE1	1:C:636:ARG:NH1	2.07	0.86
1:B:633:GLN:OE1	1:B:636:ARG:NH1	2.10	0.84
1:B:468:ARG:NH2	1:C:495:VAL:O	2.11	0.83
1:B:495:VAL:O	1:C:468:ARG:NH2	2.13	0.82
2:D:680:APC:H3A1	2:D:680:APC:H3'	1.68	0.76
1:B:135:GLN:OE1	4:B:682:GOL:O2	2.03	0.75
1:A:495:VAL:O	1:D:468:ARG:NH2	2.21	0.73
1:A:468:ARG:NH1	1:A:471:ASN:OD1	2.24	0.71
1:A:252:GLU:OE2	5:A:725:HOH:O	2.08	0.71
1:A:297:ARG:NH2	1:B:142:GLU:OE2	2.23	0.70
1:B:468:ARG:NH1	1:B:471:ASN:OD1	2.25	0.69
1:C:468:ARG:NH1	1:C:471:ASN:OD1	2.26	0.67
1:D:468:ARG:NH1	1:D:471:ASN:OD1	2.27	0.67
1:B:131:TYR:N	4:B:682:GOL:HO1	1.93	0.65
1:D:128:ARG:NE	5:D:730:HOH:O	2.30	0.64
1:C:297:ARG:NH2	1:D:142:GLU:OE2	2.34	0.60
1:C:632:SER:OG	1:C:636:ARG:NH2	2.37	0.58
2:C:680:APC:H3A1	2:C:680:APC:H3'	1.85	0.57
1:B:43:ASP:OD2	1:B:269:ARG:NH2	2.38	0.56
1:A:493:TYR:N	3:A:681:NXX:O2A	2.39	0.56
1:C:635:LYS:NZ	3:C:681:NXX:O1N	2.39	0.55
1:C:399:LEU:N	2:C:680:APC:N1	2.55	0.54
1:D:43:ASP:OD2	1:D:269:ARG:NH2	2.41	0.54
1:B:632:SER:OG	1:B:636:ARG:NH2	2.41	0.54
1:A:389:ARG:CD	5:A:753:HOH:O	2.56	0.54
1:C:43:ASP:OD2	1:C:269:ARG:NH2	2.41	0.53
2:A:680:APC:H3A2	2:A:680:APC:O2G	2.09	0.53
1:B:61:GLU:N	4:B:682:GOL:HO3	2.07	0.53
1:A:180:PHE:CD2	1:A:216:LEU:CD1	2.93	0.51
2:B:680:APC:O2G	2:B:680:APC:H3A2	2.11	0.51
1:B:662:ASP:N	1:B:662:ASP:OD1	2.43	0.51
1:C:662:ASP:N	1:C:662:ASP:OD1	2.44	0.51
1:A:43:ASP:OD2	1:A:269:ARG:NH2	2.44	0.51
1:D:507:GLY:N	5:D:733:HOH:O	2.46	0.49
1:B:180:PHE:CD2	1:B:216:LEU:CD1	2.96	0.49
1:D:147:ARG:NH1	1:D:152:ASP:OD2	2.45	0.49
1:D:635:LYS:NZ	3:D:681:NXX:O1N	2.47	0.48
1:D:399:LEU:N	2:D:680:APC:N1	2.62	0.48
1:C:180:PHE:CD2	1:C:216:LEU:CD1	2.98	0.47
1:A:507:GLY:N	5:A:722:HOH:O	2.47	0.47
1:B:635:LYS:NZ	3:B:681:NXX:O1N	2.48	0.46
1:D:180:PHE:CD2	1:D:216:LEU:CD1	2.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:525:GLU:OE1	1:B:525:GLU:CA	2.64	0.45
1:D:98:ARG:CG	1:D:98:ARG:NH1	2.76	0.45
1:A:525:GLU:OE1	1:A:525:GLU:CA	2.64	0.45
2:A:680:APC:O2A	3:A:681:NXX:C7N	2.65	0.45
1:D:68:SER:N	5:D:688:HOH:O	2.49	0.45
1:B:88:LEU:N	1:B:89:PRO:CD	2.81	0.44
1:A:98:ARG:CG	1:A:98:ARG:NH1	2.80	0.44
1:D:557:SER:C	1:D:559:ALA:N	2.71	0.44
1:C:490:TRP:NE1	3:C:681:NXX:H2N	2.33	0.44
1:D:622:GLN:NE2	5:D:766:HOH:O	2.50	0.44
1:A:662:ASP:N	1:A:662:ASP:OD1	2.50	0.44
1:D:354:ARG:NH2	1:D:641:ASN:OD1	2.52	0.43
1:C:98:ARG:NH1	1:C:98:ARG:CG	2.81	0.43
1:B:51:PRO:O	1:B:54:THR:OG1	2.36	0.42
1:A:490:TRP:NE1	3:A:681:NXX:H2N	2.34	0.42
1:B:652:SER:OG	1:D:241:ASP:OD1	2.38	0.42
1:B:280:ARG:NH1	5:B:749:HOH:O	2.52	0.42
1:B:362:LYS:NZ	5:B:759:HOH:O	2.53	0.42
3:A:681:NXX:O2P	1:D:475:GLY:O	2.37	0.41
1:D:525:GLU:OE1	1:D:525:GLU:CA	2.65	0.41
1:A:51:PRO:O	1:A:54:THR:OG1	2.39	0.41
1:B:665:ALA:N	5:B:733:HOH:O	2.53	0.41
1:C:235:GLU:OE2	1:C:265:LYS:NZ	2.54	0.41
1:C:452:VAL:C	1:C:454:PHE:N	2.72	0.41
1:D:662:ASP:OD1	1:D:662:ASP:N	2.54	0.41
1:A:445:VAL:CG1	1:A:445:VAL:O	2.68	0.41
1:C:397:PHE:O	2:C:680:APC:H2	2.21	0.41
2:B:680:APC:H5'2	2:B:680:APC:H3A2	1.73	0.41
1:B:98:ARG:NH1	1:B:98:ARG:CG	2.84	0.41
1:B:423:PHE:CG	1:B:424:SER:N	2.89	0.41
1:D:230:TYR:CD1	1:D:230:TYR:C	2.94	0.41
1:C:525:GLU:CA	1:C:525:GLU:OE1	2.67	0.40
1:B:143:ARG:NH1	1:B:143:ARG:CG	2.85	0.40
1:C:51:PRO:O	1:C:54:THR:OG1	2.39	0.40
1:C:13:ARG:O	1:C:46:ALA:N	2.55	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	Distance(Å)	Clash(Å)
1:A:142:GLU:OE2	1:D:297:ARG:NH2[8_555]	2.15	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	655/680 (96%)	631 (96%)	24 (4%)	0	100	100
1	B	652/680 (96%)	626 (96%)	25 (4%)	1 (0%)	56	85
1	C	642/680 (94%)	618 (96%)	23 (4%)	1 (0%)	56	85
1	D	642/680 (94%)	621 (97%)	20 (3%)	1 (0%)	56	85
All	All	2591/2720 (95%)	2496 (96%)	92 (4%)	3 (0%)	59	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	177	GLU
1	D	177	GLU
1	B	177	GLU

### 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	525/548 (96%)	506 (96%)	19 (4%)	47	78
1	B	517/548 (94%)	505 (98%)	12 (2%)	63	90
1	C	509/548 (93%)	496 (97%)	13 (3%)	59	87
1	D	512/548 (93%)	496 (97%)	16 (3%)	52	83
All	All	2063/2192 (94%)	2003 (97%)	60 (3%)	55	84

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	68	SER
1	A	69	LEU
1	A	98	ARG
1	A	143	ARG
1	A	201	SER
1	A	257	LEU
1	A	299	LEU
1	A	334	GLN
1	A	337	GLN
1	A	445	VAL
1	A	451	ASP
1	A	453	THR
1	A	468	ARG
1	A	491	SER
1	A	518	ARG
1	A	522	SER
1	A	543	THR
1	A	664	SER
1	B	5	SER
1	B	68	SER
1	B	98	ARG
1	B	143	ARG
1	B	201	SER
1	B	257	LEU
1	B	299	LEU
1	B	453	THR
1	B	468	ARG
1	B	491	SER
1	B	522	SER
1	B	664	SER
1	C	68	SER
1	C	69	LEU
1	C	143	ARG
1	C	201	SER
1	C	257	LEU
1	C	299	LEU
1	C	409	LYS
1	C	453	THR
1	C	468	ARG
1	C	491	SER
1	C	522	SER
1	C	596	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	664	SER
1	D	69	LEU
1	D	98	ARG
1	D	143	ARG
1	D	201	SER
1	D	257	LEU
1	D	299	LEU
1	D	334	GLN
1	D	337	GLN
1	D	410	ASN
1	D	452	VAL
1	D	453	THR
1	D	468	ARG
1	D	491	SER
1	D	522	SER
1	D	596	GLU
1	D	664	SER

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

10 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	APC	A	680	-	33,33,33	1.24	4 (12%)	52,52,52	1.87	11 (21%)
3	NXX	A	681	-	48,48,48	0.92	4 (8%)	73,73,73	1.75	8 (10%)
2	APC	B	680	-	33,33,33	1.52	2 (6%)	52,52,52	1.91	11 (21%)
3	NXX	B	681	-	48,48,48	0.94	3 (6%)	73,73,73	1.74	8 (10%)
4	GOL	B	682	-	5,5,5	0.36	0	5,5,5	0.21	0
2	APC	C	680	-	33,33,33	1.54	3 (9%)	52,52,52	1.99	14 (26%)
3	NXX	C	681	-	48,48,48	1.04	3 (6%)	73,73,73	1.64	10 (13%)
2	APC	D	680	-	33,33,33	1.34	4 (12%)	52,52,52	1.94	11 (21%)
3	NXX	D	681	-	48,48,48	1.05	2 (4%)	73,73,73	1.81	9 (12%)
4	GOL	D	682	-	5,5,5	0.69	0	5,5,5	0.53	0

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	APC	A	680	-	-	0/20/38/38	0/1/3/3
3	NXX	A	681	-	-	0/30/62/62	0/3/5/5
2	APC	B	680	-	-	0/20/38/38	0/1/3/3
3	NXX	B	681	-	-	0/30/62/62	0/3/5/5
4	GOL	B	682	-	-	0/4/4/4	0/0/0/0
2	APC	C	680	-	-	0/20/38/38	0/1/3/3
3	NXX	C	681	-	-	0/30/62/62	0/3/5/5
2	APC	D	680	-	-	0/20/38/38	0/1/3/3
3	NXX	D	681	-	-	0/30/62/62	0/3/5/5
4	GOL	D	682	-	-	0/4/4/4	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	680	APC	PA-C3A	5.50	1.84	1.79
2	B	680	APC	PA-C3A	4.84	1.84	1.79
2	B	680	APC	PB-C3A	4.51	1.83	1.79
3	D	681	NXX	PN-O3A	3.87	1.66	1.59
2	C	680	APC	PB-C3A	3.63	1.82	1.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	680	APC	PB-C3A	3.52	1.82	1.79
2	D	680	APC	PA-C3A	3.36	1.82	1.79
3	D	681	NXX	PA-O3A	3.34	1.65	1.59
2	A	680	APC	PA-C3A	3.15	1.82	1.79
2	A	680	APC	PB-C3A	3.15	1.82	1.79
3	C	681	NXX	PA-O3A	3.12	1.65	1.59
3	C	681	NXX	PN-O3A	3.02	1.65	1.59
3	C	681	NXX	C4A-N9A	-2.92	1.33	1.37
2	A	680	APC	C4-N9	-2.91	1.33	1.37
3	B	681	NXX	PN-O3A	2.72	1.64	1.59
2	C	680	APC	C4-N9	-2.62	1.33	1.37
3	A	681	NXX	PN-O3A	2.23	1.63	1.59
3	A	681	NXX	O4B-C1B	2.23	1.44	1.41
2	D	680	APC	C4-N9	-2.18	1.34	1.37
2	A	680	APC	PA-O2A	-2.11	1.51	1.56
2	D	680	APC	O4'-C1'	2.09	1.44	1.41
3	B	681	NXX	PA-O3A	2.08	1.63	1.59
3	A	681	NXX	O4M-C1M	2.05	1.44	1.41
3	A	681	NXX	PA-O3A	2.05	1.63	1.59
3	B	681	NXX	O4B-C1B	2.02	1.44	1.41

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	681	NXX	N3A-C2A-N1A	-10.61	119.84	128.71
3	A	681	NXX	N3A-C2A-N1A	-9.35	120.89	128.71
3	C	681	NXX	N3A-C2A-N1A	-9.18	121.03	128.71
3	B	681	NXX	N3A-C2A-N1A	-8.96	121.22	128.71
2	A	680	APC	N3-C2-N1	-7.74	122.24	128.71
2	D	680	APC	N3-C2-N1	-7.44	122.49	128.71
2	B	680	APC	N3-C2-N1	-7.15	122.73	128.71
2	C	680	APC	N3-C2-N1	-7.02	122.84	128.71
3	B	681	NXX	N3A-C4A-N9A	4.96	134.38	125.43
3	D	681	NXX	N3A-C4A-N9A	4.92	134.32	125.43
2	B	680	APC	N3-C4-N9	4.77	134.04	125.43
3	B	681	NXX	O4M-C1M-N1N	-4.67	103.17	107.95
3	A	681	NXX	N3A-C4A-N9A	4.56	133.66	125.43
3	A	681	NXX	C2M-C1M-N1N	-4.36	106.48	113.86
2	B	680	APC	O5'-PA-O1A	-4.33	103.40	114.21
2	D	680	APC	N3-C4-N9	4.26	133.12	125.43
2	C	680	APC	N3-C4-N9	4.15	132.92	125.43
2	A	680	APC	N3-C4-N9	3.98	132.62	125.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	680	APC	O5'-PA-O1A	-3.95	104.36	114.21
2	C	680	APC	O4'-C1'-N9	-3.92	104.80	108.44
2	C	680	APC	O3B-PB-O1B	-3.90	103.25	111.51
3	C	681	NXX	N3A-C4A-N9A	3.85	132.38	125.43
2	C	680	APC	O5'-PA-O1A	-3.65	105.09	114.21
3	D	681	NXX	C2A-N3A-C4A	3.61	124.30	114.01
2	D	680	APC	O2B-PB-C3A	3.50	114.67	106.61
3	B	681	NXX	C5A-C4A-N3A	-3.47	118.14	125.70
3	B	681	NXX	C3M-C2M-C1M	3.43	106.28	100.91
3	B	681	NXX	C2A-N3A-C4A	3.37	123.59	114.01
3	D	681	NXX	C5A-C4A-N3A	-3.36	118.39	125.70
2	A	680	APC	C2'-C1'-N9	-3.29	104.81	113.27
2	A	680	APC	O5'-PA-O1A	-3.28	106.02	114.21
2	C	680	APC	PA-C3A-PB	3.28	122.33	117.62
3	A	681	NXX	O4M-C1M-N1N	3.26	111.28	107.95
2	D	680	APC	PA-C3A-PB	3.25	122.30	117.62
3	A	681	NXX	C3M-C2M-C1M	3.22	105.94	100.91
2	A	680	APC	O2B-PB-O1B	3.21	120.93	110.93
2	B	680	APC	C5-C4-N3	-3.17	118.79	125.70
2	C	680	APC	O5'-C5'-C4'	3.15	120.49	108.94
3	C	681	NXX	C8A-N9A-C4A	3.12	109.28	106.90
3	A	681	NXX	C2A-N3A-C4A	3.11	122.87	114.01
3	A	681	NXX	C5A-C4A-N3A	-3.01	119.14	125.70
2	C	680	APC	O1A-PA-C3A	2.95	116.91	109.49
2	A	680	APC	O3B-PB-O1B	-2.84	105.49	111.51
3	C	681	NXX	C2A-N3A-C4A	2.84	122.10	114.01
3	D	681	NXX	O3A-PN-O5M	-2.78	90.96	103.41
2	B	680	APC	O2B-PB-O1B	2.78	119.57	110.93
2	D	680	APC	O1B-PB-C3A	-2.68	102.76	109.49
2	D	680	APC	C5-C4-N3	-2.67	119.90	125.70
3	D	681	NXX	O2N-PN-O3A	2.64	117.68	105.14
3	C	681	NXX	O2N-PN-O3A	2.61	117.53	105.14
2	B	680	APC	O3B-PB-C3A	2.60	114.80	106.62
2	A	680	APC	C3'-C2'-C1'	2.56	104.92	100.91
2	B	680	APC	C2-N3-C4	2.52	121.18	114.01
2	C	680	APC	O2B-PB-O1B	2.48	118.65	110.93
2	A	680	APC	C5-C4-N3	-2.39	120.49	125.70
3	B	681	NXX	O1A-PA-O3A	2.39	116.45	105.14
3	B	681	NXX	C4M-O4M-C1M	2.37	112.32	109.75
2	D	680	APC	C2-N3-C4	2.36	120.74	114.01
2	A	680	APC	C2-N3-C4	2.36	120.73	114.01
3	A	681	NXX	O3A-PN-O5M	-2.35	92.90	103.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	681	NXX	C3M-C2M-C1M	2.33	104.56	100.91
2	B	680	APC	O4'-C1'-N9	-2.33	106.28	108.44
2	B	680	APC	O5'-C5'-C4'	2.31	117.43	108.94
3	C	681	NXX	O2M-C2M-C3M	-2.30	104.36	111.83
2	C	680	APC	C5-C4-N3	-2.29	120.71	125.70
3	D	681	NXX	C3M-C2M-C1M	2.28	104.47	100.91
3	C	681	NXX	C5A-C4A-N3A	-2.28	120.74	125.70
2	B	680	APC	O5'-PA-C3A	2.26	109.57	103.97
2	D	680	APC	O2A-PA-O1A	2.24	117.89	110.93
3	D	681	NXX	C4A-C5A-N7A	-2.24	107.61	109.52
2	B	680	APC	O2B-PB-O3B	-2.21	101.71	107.18
2	D	680	APC	O3G-PG-O2G	2.20	116.16	107.61
2	C	680	APC	O4'-C4'-C5'	2.17	117.12	109.36
2	C	680	APC	C2-N3-C4	2.13	120.07	114.01
3	D	681	NXX	N7A-C8A-N9A	-2.13	108.35	114.36
3	C	681	NXX	O1A-PA-O3A	2.12	115.21	105.14
2	A	680	APC	O3B-PB-C3A	2.11	113.27	106.62
3	C	681	NXX	C6N-N1N-C2N	-2.10	119.67	122.04
2	D	680	APC	O4'-C1'-N9	2.08	110.38	108.44
2	A	680	APC	C8-N9-C4	2.08	108.49	106.90
2	C	680	APC	O2A-PA-O1A	2.05	117.32	110.93
2	C	680	APC	C8-N9-C4	2.01	108.43	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	661/680 (97%)	-0.50	7 (1%) 77 83	13, 30, 56, 87	0
1	B	658/680 (96%)	-0.52	4 (0%) 86 91	14, 30, 55, 87	0
1	C	650/680 (95%)	-0.49	5 (0%) 83 88	17, 32, 56, 89	0
1	D	650/680 (95%)	-0.50	8 (1%) 75 82	14, 30, 55, 90	0
All	All	2619/2720 (96%)	-0.50	24 (0%) 81 86	13, 31, 56, 90	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	SER	4.6
1	C	0	SER	4.3
1	B	0	SER	3.6
1	D	441	HIS	3.5
1	C	454	PHE	3.4
1	D	410	ASN	3.0
1	C	441	HIS	3.0
1	D	0	SER	2.8
1	A	524	GLY	2.8
1	C	523	ALA	2.7
1	B	523	ALA	2.6
1	D	437	HIS	2.5
1	A	450	TYR	2.5
1	D	454	PHE	2.5
1	A	529	LYS	2.4
1	D	678	LYS	2.3
1	D	528	GLU	2.3
1	A	527	GLY	2.3
1	B	524	GLY	2.2
1	A	413	ILE	2.2
1	B	450	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	449	VAL	2.1
1	C	453	THR	2.0
1	D	524	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	D	682	6/6	0.36	10.76	36,68,74,81	0
4	GOL	B	682	6/6	0.17	5.32	38,48,57,60	0
3	NXX	D	681	44/44	0.19	1.96	27,65,132,135	0
3	NXX	C	681	44/44	0.20	1.83	39,73,144,154	0
2	APC	D	680	31/31	0.16	1.76	41,63,114,119	0
3	NXX	B	681	44/44	0.18	1.26	27,79,151,156	0
3	NXX	A	681	44/44	0.17	0.61	31,59,121,140	0
2	APC	B	680	31/31	0.13	0.51	38,59,112,160	0
2	APC	A	680	31/31	0.13	0.06	32,59,102,161	0
2	APC	C	680	31/31	0.12	-0.21	37,61,103,140	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.