



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:26 PM GMT

PDB ID : 4GX2  
Title : GsuK channel bound to NAD  
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.;  
Jiang, Y.  
Deposited on : 2012-09-03  
Resolution : 3.20 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>

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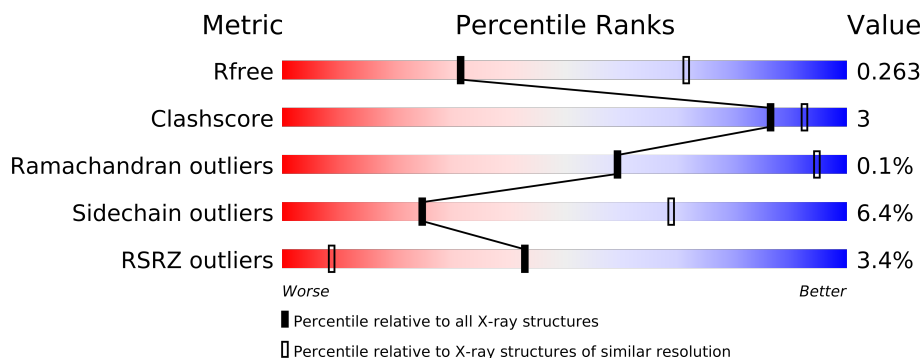
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	565	
1	B	565	
1	C	565	
1	D	565	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14511 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2922	1880	506	525	11			
1	B	548	Total	C	N	O	S	0	0	0
			4208	2693	729	771	15			
1	C	547	Total	C	N	O	S	0	0	0
			4197	2687	725	770	15			
1	D	376	Total	C	N	O	S	0	0	0
			2928	1883	507	527	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q74FS9
A	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
A	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
A	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
A	8	SER	-	EXPRESSION TAG	UNP Q74FS9
A	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
A	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
A	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
A	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
A	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
A	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
A	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	4	MET	-	EXPRESSION TAG	UNP Q74FS9
B	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
B	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
B	8	SER	-	EXPRESSION TAG	UNP Q74FS9
B	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
B	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
B	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
B	565	LEU	-	EXPRESSION TAG	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
B	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
B	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	4	MET	-	EXPRESSION TAG	UNP Q74FS9
C	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
C	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
C	8	SER	-	EXPRESSION TAG	UNP Q74FS9
C	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
C	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
C	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
C	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
C	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
C	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
C	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	4	MET	-	EXPRESSION TAG	UNP Q74FS9
D	5	GLN	-	EXPRESSION TAG	UNP Q74FS9
D	6	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	7	GLY	-	EXPRESSION TAG	UNP Q74FS9
D	8	SER	-	EXPRESSION TAG	UNP Q74FS9
D	52	ALA	GLU	ENGINEERED MUTATION	UNP Q74FS9
D	77	GLU	GLN	ENGINEERED MUTATION	UNP Q74FS9
D	97	ASP	LEU	ENGINEERED MUTATION	UNP Q74FS9
D	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
D	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
D	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
D	568	ARG	-	EXPRESSION TAG	UNP Q74FS9

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	5	Total K 5 5	0	0
2	D	1	Total K 1 1	0	0
2	C	5	Total K 5 5	0	0

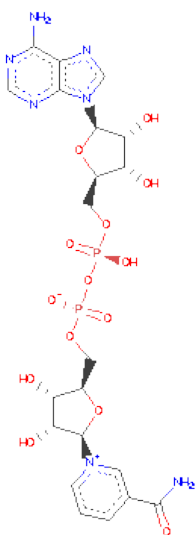
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		

- Molecule 5 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>).



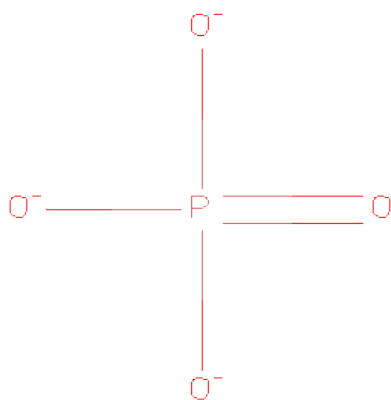
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
5	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

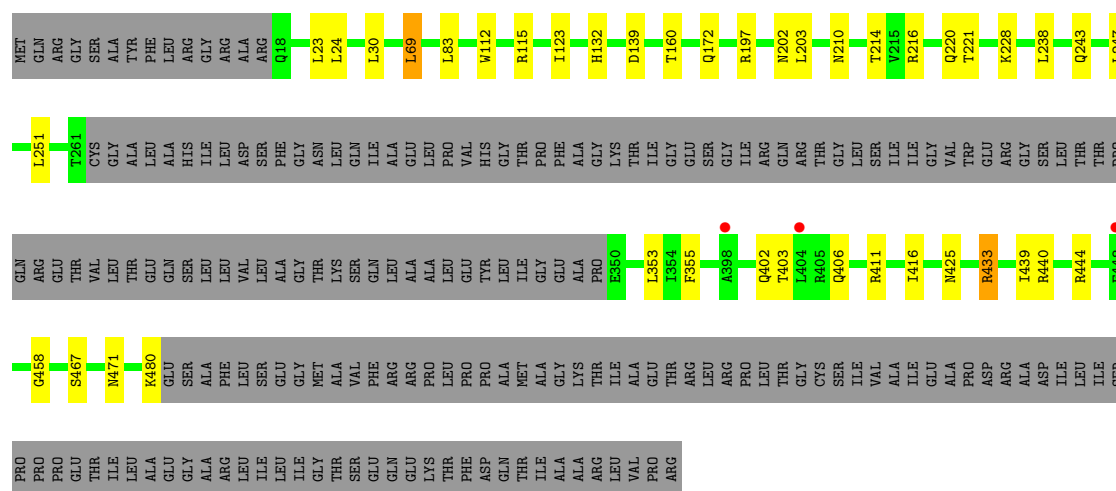
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	B	9	Total	O	0	0
			9	9		
7	C	18	Total	O	0	0
			18	18		
7	D	6	Total	O	0	0
			6	6		

### 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.

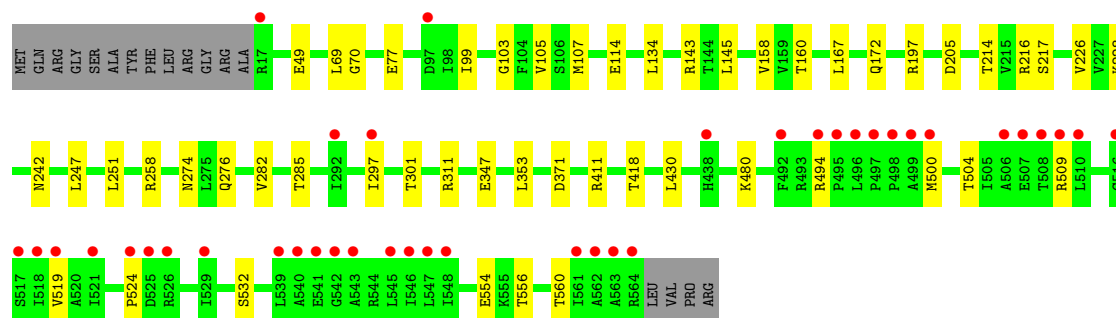
- Molecule 1: TrkA domain protein

Chain A: 



- Molecule 1: TrkA domain protein

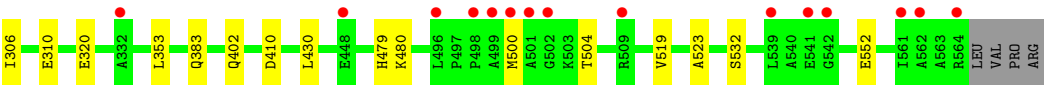
Chain B: 



- Molecule 1: TrkA domain protein

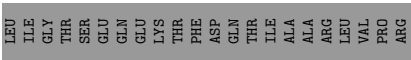
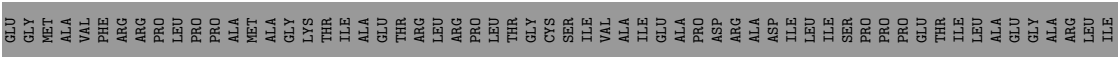
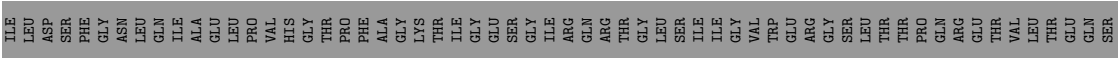
Chain C: 





• Molecule 1: TrkA domain protein

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.55Å 111.10Å 164.56Å 90.00° 134.78° 90.00°	Depositor
Resolution (Å)	41.14 – 3.20 49.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.14-3.20) 94.1 (49.31-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.230 , 0.270 0.222 , 0.263	Depositor DCC
$R_{free}$ test set	2381 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 62.1	EDS
Estimated twinning fraction	0.206 for h+2*k,-h-l 0.023 for h,-k,-h-l 0.028 for -h-2*k,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 47121 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	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 37.45 % 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 4.2821e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: K, ZN, CA, PO4, NAD

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	0.22	0/2982	0.42	0/4060
1	B	0.22	0/4291	0.41	0/5843
1	C	0.23	0/4280	0.42	0/5829
1	D	0.23	0/2988	0.43	0/4068
All	All	0.22	0/14541	0.42	0/19800

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2922	0	0	13	0
1	B	4208	0	0	13	0
1	C	4197	0	0	5	0
1	D	2928	0	0	9	0
2	A	5	0	0	0	0
2	B	1	0	0	0	0
2	C	5	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	44	0	0	0	0
5	B	44	0	0	0	0
5	C	44	0	0	1	0
5	D	44	0	0	1	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
7	A	17	0	0	0	0
7	B	9	0	0	0	0
7	C	18	0	0	0	0
7	D	6	0	0	0	0
All	All	14511	0	0	38	0

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 3.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:203:LEU:O	1:D:228:LYS:NZ	2.29	0.65
1:A:112:TRP:NE1	1:B:114:GLU:OE2	2.30	0.64
1:A:203:LEU:O	1:A:228:LYS:NZ	2.35	0.60
1:A:247:LEU:O	1:A:251:LEU:N	2.36	0.59
1:D:228:LYS:O	5:D:603:NAD:N7N	2.34	0.59
1:A:69:LEU:CD2	1:B:70:GLY:CA	2.80	0.59
1:B:216:ARG:NH1	1:B:242:ASN:OD1	2.38	0.57
1:C:67:THR:O	1:C:68:THR:OG1	2.22	0.57
1:D:197:ARG:NH1	1:D:477:LEU:O	2.37	0.56
1:D:467:SER:O	1:D:471:ASN:ND2	2.39	0.55
1:A:467:SER:O	1:A:471:ASN:ND2	2.43	0.51
1:A:402:GLN:O	1:A:406:GLN:N	2.44	0.51
1:C:228:LYS:O	5:C:610:NAD:N7N	2.44	0.50
1:B:99:ILE:O	1:B:103:GLY:N	2.44	0.49
1:D:351:ASP:N	1:D:351:ASP:OD1	2.44	0.48
1:D:402:GLN:O	1:D:406:GLN:N	2.47	0.48
1:D:247:LEU:O	1:D:251:LEU:N	2.46	0.48
1:D:433:ARG:NH1	1:D:439:ILE:O	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:298:ARG:NH1	1:C:523:ALA:O	2.46	0.48
1:B:247:LEU:O	1:B:251:LEU:N	2.47	0.46
1:D:109:LEU:O	1:D:113:ILE:N	2.49	0.45
1:B:556:THR:O	1:B:560:THR:OG1	2.34	0.45
1:A:433:ARG:NH2	1:A:458:GLY:O	2.50	0.45
1:A:433:ARG:NH1	1:A:439:ILE:O	2.50	0.45
1:A:210:ASN:O	1:A:214:THR:OG1	2.36	0.43
1:A:425:ASN:ND2	1:A:444:ARG:O	2.52	0.43
1:A:355:PHE:O	1:A:416:ILE:N	2.51	0.43
1:B:282:VAL:O	1:B:285:THR:OG1	2.36	0.43
1:B:494:ARG:NH2	1:B:554:GLU:OE2	2.52	0.43
1:A:216:ARG:NH1	1:A:221:THR:O	2.53	0.42
1:B:297:ILE:O	1:B:301:THR:OG1	2.39	0.41
1:C:519:VAL:O	1:C:532:SER:N	2.53	0.41
1:B:205:ASP:OD2	1:B:228:LYS:N	2.54	0.41
1:B:519:VAL:O	1:B:532:SER:N	2.54	0.41
1:B:214:THR:O	1:B:217:SER:OG	2.39	0.41
1:B:49:GLU:OE1	1:B:77:GLU:N	2.54	0.41
1:C:282:VAL:O	1:C:285:THR:OG1	2.40	0.40
1:A:139:ASP:OD2	1:A:202:ASN:ND2	2.55	0.40

There are no symmetry-related clashes.

## 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	371/565 (66%)	348 (94%)	23 (6%)	0	100	100
1	B	546/565 (97%)	517 (95%)	28 (5%)	1 (0%)	56	93
1	C	545/565 (96%)	525 (96%)	20 (4%)	0	100	100
1	D	372/565 (66%)	358 (96%)	13 (4%)	1 (0%)	50	91
All	All	1834/2260 (81%)	1748 (95%)	84 (5%)	2 (0%)	59	95

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	374	PRO
1	B	524	PRO

### 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	313/463 (68%)	293 (94%)	20 (6%)	25	69
1	B	449/463 (97%)	423 (94%)	26 (6%)	28	73
1	C	448/463 (97%)	417 (93%)	31 (7%)	22	65
1	D	314/463 (68%)	293 (93%)	21 (7%)	23	66
All	All	1524/1852 (82%)	1426 (94%)	98 (6%)	25	69

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	24	LEU
1	A	30	LEU
1	A	69	LEU
1	A	83	LEU
1	A	115	ARG
1	A	123	ILE
1	A	132	HIS
1	A	160	THR
1	A	172	GLN
1	A	197	ARG
1	A	220	GLN
1	A	238	LEU
1	A	243	GLN
1	A	353	LEU
1	A	403	THR
1	A	411	ARG
1	A	433	ARG
1	A	440	ARG
1	A	480	LYS
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	105	VAL
1	B	107	MET
1	B	134	LEU
1	B	143	ARG
1	B	145	LEU
1	B	158	VAL
1	B	160	THR
1	B	167	LEU
1	B	172	GLN
1	B	197	ARG
1	B	226	VAL
1	B	258	ARG
1	B	274	ASN
1	B	276	GLN
1	B	311	ARG
1	B	347	GLU
1	B	353	LEU
1	B	371	ASP
1	B	411	ARG
1	B	418	THR
1	B	430	LEU
1	B	480	LYS
1	B	500	MET
1	B	504	THR
1	B	509	ARG
1	C	18	GLN
1	C	20	LEU
1	C	24	LEU
1	C	67	THR
1	C	97	ASP
1	C	104	PHE
1	C	113	ILE
1	C	116	ARG
1	C	120	HIS
1	C	123	ILE
1	C	132	HIS
1	C	139	ASP
1	C	149	LEU
1	C	152	ARG
1	C	159	VAL
1	C	160	THR
1	C	247	LEU

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Mol	Chain	Res	Type
1	C	292	ILE
1	C	306	ILE
1	C	310	GLU
1	C	320	GLU
1	C	353	LEU
1	C	383	GLN
1	C	402	GLN
1	C	410	ASP
1	C	430	LEU
1	C	479	HIS
1	C	480	LYS
1	C	500	MET
1	C	504	THR
1	C	552	GLU
1	D	24	LEU
1	D	69	LEU
1	D	83	LEU
1	D	102	PHE
1	D	108	PHE
1	D	113	ILE
1	D	118	ARG
1	D	152	ARG
1	D	153	ASN
1	D	160	THR
1	D	171	GLU
1	D	172	GLN
1	D	197	ARG
1	D	238	LEU
1	D	258	ARG
1	D	351	ASP
1	D	404	LEU
1	D	410	ASP
1	D	411	ARG
1	D	417	VAL
1	D	430	LEU

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 ⓘ

Of 26 ligands modelled in this entry, 20 are monoatomic - leaving 6 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	$\# Z  > 2$
5	NAD	A	608	-	48,48,48	1.55	8 (16%)	73,73,73	2.03	17 (23%)
6	PO4	B	604	-	4,4,4	0.29	0	6,6,6	0.31	0
5	NAD	B	605	-	48,48,48	1.53	7 (14%)	73,73,73	1.96	18 (24%)
6	PO4	C	609	-	4,4,4	0.29	0	6,6,6	0.31	0
5	NAD	C	610	-	48,48,48	1.53	7 (14%)	73,73,73	2.03	18 (24%)
5	NAD	D	603	-	48,48,48	1.54	8 (16%)	73,73,73	2.07	17 (23%)

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
5	NAD	A	608	-	-	1/30/62/62	0/3/5/5
6	PO4	B	604	-	-	0/0/0/0	0/0/0/0
5	NAD	B	605	-	-	0/30/62/62	0/3/5/5
6	PO4	C	609	-	-	0/0/0/0	0/0/0/0
5	NAD	C	610	-	-	0/30/62/62	0/3/5/5
5	NAD	D	603	-	-	1/30/62/62	0/3/5/5

All (30) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	610	NAD	C7N-N7N	4.58	1.43	1.33
5	B	605	NAD	C7N-N7N	4.58	1.43	1.33
5	D	603	NAD	C7N-N7N	4.51	1.43	1.33
5	A	608	NAD	C7N-N7N	4.50	1.43	1.33
5	A	608	NAD	C2D-C3D	-3.94	1.42	1.53
5	B	605	NAD	C2D-C3D	-3.95	1.42	1.53
5	C	610	NAD	C2D-C3D	-3.92	1.42	1.53
5	D	603	NAD	C2D-C3D	-3.92	1.42	1.53
5	C	610	NAD	C2B-C3B	-3.22	1.44	1.53
5	A	608	NAD	C2B-C3B	-3.21	1.44	1.53
5	B	605	NAD	C2B-C3B	-3.21	1.44	1.53
5	D	603	NAD	C2B-C3B	-3.17	1.44	1.53
5	A	608	NAD	C2D-C1D	-2.87	1.49	1.53
5	D	603	NAD	C2D-C1D	-2.76	1.49	1.53
5	D	603	NAD	O4D-C4D	-2.70	1.38	1.45
5	B	605	NAD	C2D-C1D	-2.69	1.49	1.53
5	C	610	NAD	C2D-C1D	-2.68	1.49	1.53
5	A	608	NAD	O4D-C4D	-2.63	1.38	1.45
5	C	610	NAD	O4D-C4D	-2.60	1.39	1.45
5	B	605	NAD	O4D-C4D	-2.51	1.39	1.45
5	D	603	NAD	C6A-N6A	2.51	1.43	1.35
5	C	610	NAD	C6A-N6A	2.50	1.43	1.35
5	B	605	NAD	C6A-N6A	2.48	1.43	1.35
5	A	608	NAD	C6A-N6A	2.46	1.43	1.35
5	D	603	NAD	PN-O5D	-2.26	1.52	1.60
5	A	608	NAD	PN-O5D	-2.22	1.52	1.60
5	B	605	NAD	PN-O5D	-2.16	1.53	1.60
5	C	610	NAD	PN-O5D	-2.11	1.53	1.60
5	D	603	NAD	O5D-C5D	-2.04	1.36	1.44
5	A	608	NAD	O5D-C5D	-2.01	1.36	1.44

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	610	NAD	N3A-C2A-N1A	-9.37	120.87	128.71
5	D	603	NAD	N3A-C2A-N1A	-9.29	120.94	128.71
5	B	605	NAD	N3A-C2A-N1A	-9.28	120.95	128.71
5	A	608	NAD	N3A-C2A-N1A	-9.16	121.05	128.71
5	C	610	NAD	O4B-C1B-N9A	7.14	115.08	108.44
5	D	603	NAD	O4B-C1B-N9A	6.64	114.62	108.44
5	A	608	NAD	O4B-C1B-N9A	6.60	114.58	108.44
5	B	605	NAD	O4B-C1B-N9A	6.38	114.38	108.44
5	D	603	NAD	C4D-O4D-C1D	-4.61	104.74	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	608	NAD	C4D-O4D-C1D	-4.06	105.33	109.75
5	C	610	NAD	N3A-C4A-N9A	4.02	132.70	125.43
5	D	603	NAD	N3A-C4A-N9A	4.02	132.69	125.43
5	A	608	NAD	N3A-C4A-N9A	3.98	132.62	125.43
5	B	605	NAD	N3A-C4A-N9A	3.95	132.57	125.43
5	C	610	NAD	C4D-O4D-C1D	-3.92	105.49	109.75
5	D	603	NAD	C3B-C2B-C1B	3.77	106.81	100.91
5	D	603	NAD	C3N-C7N-N7N	3.71	121.99	117.77
5	C	610	NAD	C3B-C2B-C1B	3.67	106.66	100.91
5	A	608	NAD	C3B-C2B-C1B	3.57	106.49	100.91
5	A	608	NAD	C3N-C7N-N7N	3.45	121.70	117.77
5	B	605	NAD	C3B-C2B-C1B	3.16	105.85	100.91
5	B	605	NAD	C3D-C2D-C1D	3.10	105.76	100.91
5	D	603	NAD	PN-O3-PA	-3.09	119.66	132.95
5	C	610	NAD	O2N-PN-O1N	-3.06	109.49	118.72
5	B	605	NAD	O2N-PN-O1N	-3.03	109.58	118.72
5	B	605	NAD	C4D-O4D-C1D	-2.98	106.51	109.75
5	A	608	NAD	C4A-C5A-N7A	-2.91	107.03	109.52
5	B	605	NAD	C4A-C5A-N7A	-2.91	107.03	109.52
5	C	610	NAD	C3D-C2D-C1D	2.89	105.44	100.91
5	C	610	NAD	C4A-C5A-N7A	-2.88	107.06	109.52
5	A	608	NAD	PN-O3-PA	-2.86	120.65	132.95
5	A	608	NAD	C3D-C2D-C1D	2.86	105.38	100.91
5	D	603	NAD	C4A-C5A-N7A	-2.85	107.08	109.52
5	D	603	NAD	O2N-PN-O1N	-2.81	110.23	118.72
5	A	608	NAD	O2N-PN-O1N	-2.81	110.26	118.72
5	D	603	NAD	O7N-C7N-N7N	-2.75	118.61	122.59
5	B	605	NAD	PN-O3-PA	-2.74	121.20	132.95
5	C	610	NAD	O5B-C5B-C4B	2.71	118.88	108.94
5	C	610	NAD	PN-O3-PA	-2.68	121.43	132.95
5	C	610	NAD	C5A-C4A-N3A	-2.64	119.95	125.70
5	D	603	NAD	C3D-C2D-C1D	2.62	105.00	100.91
5	D	603	NAD	C5A-C4A-N3A	-2.61	120.01	125.70
5	A	608	NAD	C5A-C4A-N3A	-2.59	120.06	125.70
5	B	605	NAD	C5A-C4A-N3A	-2.57	120.10	125.70
5	A	608	NAD	O7N-C7N-N7N	-2.54	118.93	122.59
5	B	605	NAD	O7N-C7N-N7N	-2.43	119.08	122.59
5	A	608	NAD	C8A-N9A-C4A	2.39	108.72	106.90
5	D	603	NAD	C8A-N9A-C4A	2.35	108.69	106.90
5	B	605	NAD	C8A-N9A-C4A	2.34	108.68	106.90
5	B	605	NAD	C3N-C7N-N7N	2.32	120.41	117.77
5	C	610	NAD	C2A-N3A-C4A	2.30	120.55	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	NAD	C1B-N9A-C4A	-2.29	122.69	126.64
5	B	605	NAD	O5B-C5B-C4B	2.28	117.31	108.94
5	C	610	NAD	O7N-C7N-N7N	-2.28	119.30	122.59
5	D	603	NAD	C2A-N3A-C4A	2.27	120.47	114.01
5	B	605	NAD	C2A-N3A-C4A	2.25	120.42	114.01
5	A	608	NAD	C1B-N9A-C4A	-2.23	122.78	126.64
5	D	603	NAD	C1B-N9A-C4A	-2.22	122.79	126.64
5	A	608	NAD	C2A-N3A-C4A	2.22	120.33	114.01
5	C	610	NAD	C2B-C3B-C4B	2.18	107.00	102.65
5	A	608	NAD	N7A-C8A-N9A	-2.17	108.23	114.36
5	B	605	NAD	N7A-C8A-N9A	-2.15	108.28	114.36
5	D	603	NAD	N7A-C8A-N9A	-2.15	108.29	114.36
5	B	605	NAD	C2B-C3B-C4B	2.14	106.91	102.65
5	C	610	NAD	C8A-N9A-C4A	2.14	108.53	106.90
5	A	608	NAD	C2B-C3B-C4B	2.12	106.88	102.65
5	C	610	NAD	C3N-C7N-N7N	2.12	120.18	117.77
5	C	610	NAD	N7A-C8A-N9A	-2.07	108.49	114.36
5	C	610	NAD	C1B-N9A-C4A	-2.04	123.10	126.64
5	D	603	NAD	C2B-C3B-C4B	2.01	106.67	102.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	603	NAD	C2D-C1D-N1N-C6N
5	A	608	NAD	C2D-C1D-N1N-C6N

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	375/565 (66%)	0.12	3 (0%) 83 35	64, 90, 166, 214	0
1	B	548/565 (96%)	0.49	40 (7%) 15 3	67, 115, 249, 357	0
1	C	547/565 (96%)	0.31	17 (3%) 47 10	66, 111, 192, 261	0
1	D	376/565 (66%)	0.12	4 (1%) 77 27	60, 89, 168, 234	0
All	All	1846/2260 (81%)	0.29	64 (3%) 43 8	60, 100, 212, 357	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	LEU	7.9
1	B	543	ALA	7.3
1	B	516	CYS	6.4
1	B	541	GLU	5.7
1	B	542	GLY	5.5
1	C	564	ARG	5.1
1	C	561	ILE	5.1
1	C	562	ALA	4.9
1	B	518	ILE	4.9
1	B	510	LEU	4.7
1	B	561	ILE	4.7
1	B	563	ALA	4.7
1	B	497	PRO	4.5
1	B	495	PRO	4.2
1	C	500	MET	4.2
1	B	526	ARG	4.1
1	B	509	ARG	4.1
1	B	564	ARG	4.1
1	C	501	ALA	3.9
1	C	541	GLU	3.7
1	B	494	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	398	ALA	3.5
1	B	540	ALA	3.4
1	B	519	VAL	3.3
1	B	297	ILE	3.3
1	B	508	THR	3.3
1	A	404	LEU	3.3
1	B	507	GLU	3.1
1	B	517	SER	3.1
1	B	562	ALA	3.0
1	B	492	PHE	3.0
1	C	502	GLY	2.9
1	D	481	GLU	2.8
1	B	500	MET	2.7
1	D	480	LYS	2.6
1	C	542	GLY	2.6
1	D	398	ALA	2.5
1	C	539	LEU	2.5
1	B	545	LEU	2.5
1	B	498	PRO	2.4
1	B	17	ARG	2.4
1	C	448	GLU	2.4
1	B	438	HIS	2.4
1	B	525	ASP	2.4
1	C	499	ALA	2.3
1	B	506	ALA	2.3
1	C	498	PRO	2.3
1	B	499	ALA	2.3
1	C	97	ASP	2.2
1	B	548	ILE	2.2
1	B	521	ILE	2.2
1	B	97	ASP	2.2
1	B	524	PRO	2.2
1	C	300	ARG	2.2
1	B	546	ILE	2.2
1	B	547	LEU	2.2
1	D	409	ILE	2.1
1	A	448	GLU	2.1
1	B	529	ILE	2.1
1	C	496	LEU	2.1
1	B	292	ILE	2.1
1	B	539	LEU	2.1
1	C	509	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	332	ALA	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
3	ZN	A	606	1/1	0.30	1.56	91,91,91,91	0
3	ZN	D	602	1/1	0.28	1.56	81,81,81,81	0
3	ZN	C	606	1/1	0.29	1.24	87,87,87,87	0
3	ZN	B	602	1/1	0.29	0.90	92,92,92,92	0
5	NAD	A	608	44/44	0.42	0.90	67,221,245,282	0
4	CA	B	603	1/1	0.24	0.17	89,89,89,89	0
4	CA	C	608	1/1	0.23	0.08	90,90,90,90	0
2	K	A	604	1/1	0.34	0.02	109,109,109,109	1
5	NAD	C	610	44/44	0.27	-0.00	78,179,210,212	0
4	CA	C	607	1/1	0.24	-0.21	87,87,87,87	0
5	NAD	D	603	44/44	0.27	-0.21	83,197,221,223	0
6	PO4	B	604	5/5	0.27	-0.38	131,134,136,137	0
2	K	C	604	1/1	0.28	-0.40	100,100,100,100	1
2	K	A	605	1/1	0.23	-0.68	136,136,136,136	1
6	PO4	C	609	5/5	0.23	-0.72	139,139,142,142	0
5	NAD	B	605	44/44	0.19	-1.01	57,151,214,216	0
2	K	A	602	1/1	0.25	-1.13	87,87,87,87	1
2	K	C	603	1/1	0.15	-1.31	68,68,68,68	1
2	K	A	601	1/1	0.16	-1.44	88,88,88,88	1
2	K	D	601	1/1	0.21	-1.55	136,136,136,136	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	C	602	1/1	0.21	-1.58	64,64,64,64	1
4	CA	A	607	1/1	0.17	-1.74	89,89,89,89	0
2	K	A	603	1/1	0.17	-1.78	71,71,71,71	1
2	K	C	601	1/1	0.14	-2.07	73,73,73,73	1
2	K	C	605	1/1	0.49	-	207,207,207,207	1
2	K	B	601	1/1	0.63	-	222,222,222,222	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.