



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:01 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

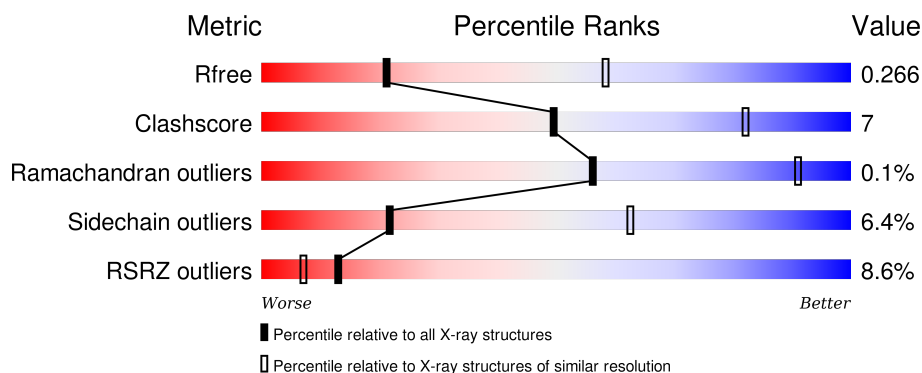
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	565	<div> <div>2%</div> <div>56%</div> <div>9%</div> <div>34%</div> </div>
1	B	565	<div> <div>15%</div> <div>74%</div> <div>21%</div> </div>
1	C	565	<div> <div>8%</div> <div>77%</div> <div>19%</div> </div>
1	D	565	<div> <div>3%</div> <div>55%</div> <div>11%</div> <div>33%</div> </div>

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
5	NAD	A	608	-	-	-	X

## 2 Entry composition

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

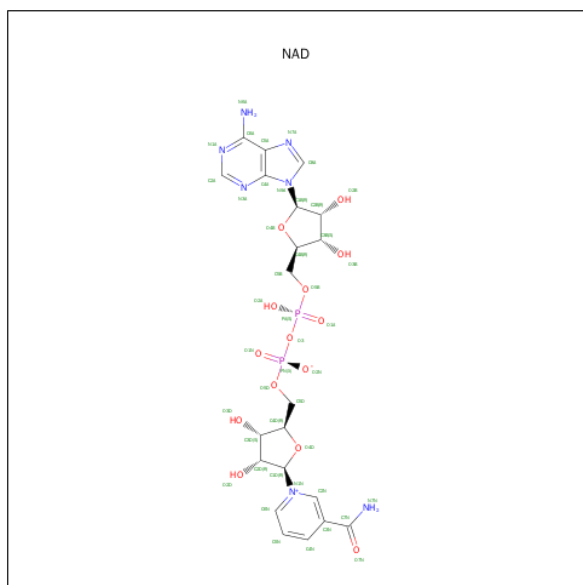
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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>).



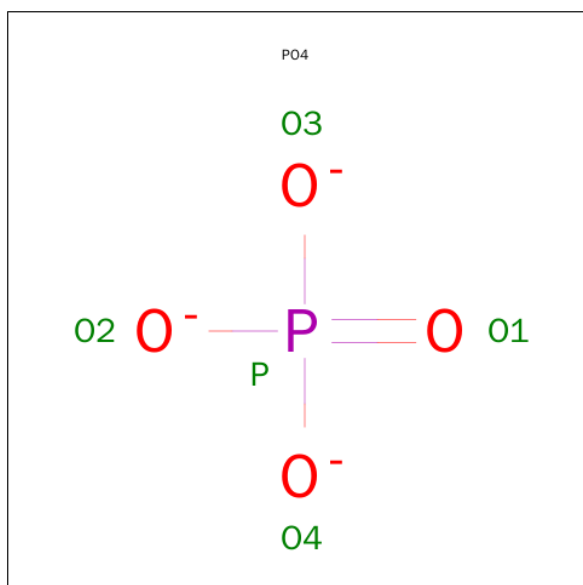
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
5	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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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).



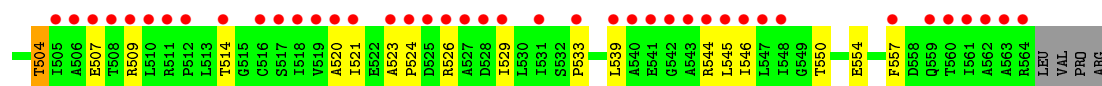
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

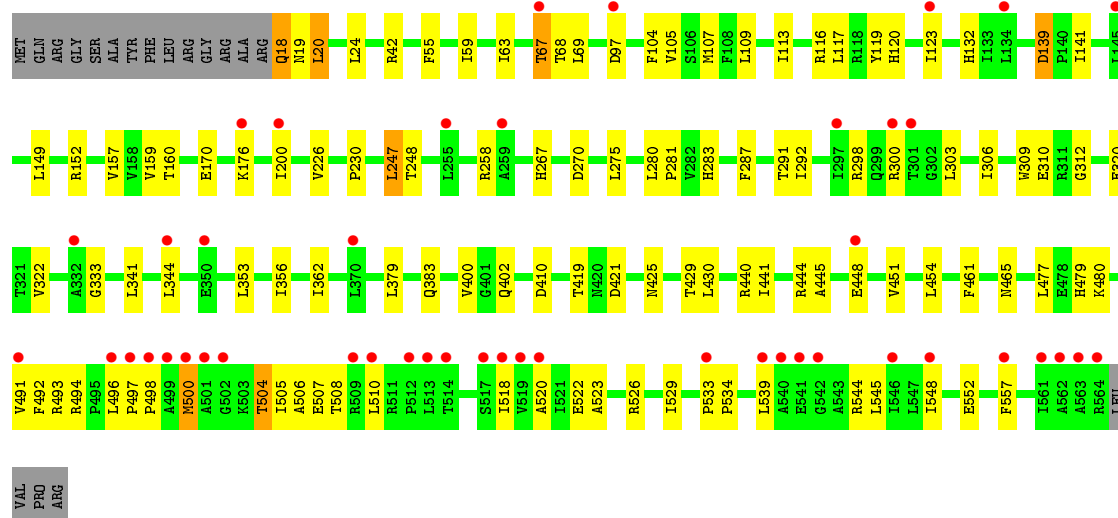
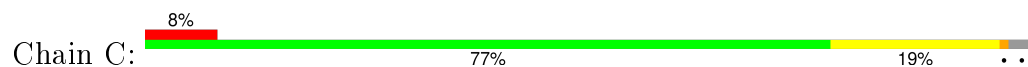
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	B	9	Total	O	0	0
			9	9		
7	C	18	Total	O	0	0
			18	18		
7	D	6	Total	O	0	0
			6	6		



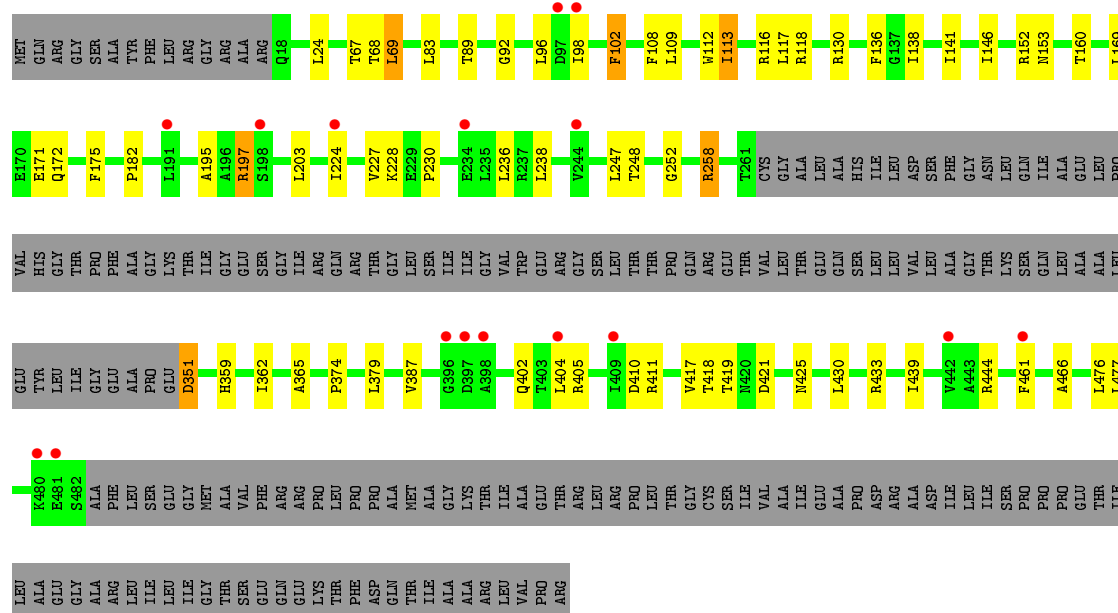




• Molecule 1: TrkA domain protein



• Molecule 1: TrkA domain protein



## 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 0.228 , 0.266	Depositor DCC
$R_{free}$ test set	2384 reflections (5.33%)	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> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.206 for h+2*l,k,-h-l 0.023 for h,-k,-h-l 0.028 for -h-2*l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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.

<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 [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2922	0	2957	33	0
1	B	4208	0	4282	77	0
1	C	4197	0	4269	64	0
1	D	2928	0	2962	40	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
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	26	6	0
5	B	44	0	26	4	0
5	C	44	0	26	6	0
5	D	44	0	26	6	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	14574	206	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 7.

All (206) 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:69:LEU:HD23	1:D:68:THR:HA	1.59	0.84
1:A:247:LEU:H	5:A:608:NAD:H4N	1.45	0.82
1:C:226:VAL:HG12	5:C:610:NAD:H5N	1.62	0.80
1:A:69:LEU:HD22	1:B:70:GLY:HA3	1.62	0.80
1:A:69:LEU:CD2	1:B:70:GLY:HA3	2.13	0.79
1:C:419:THR:HG22	1:C:421:ASP:H	1.48	0.79
1:D:130:ARG:HG3	1:D:195:ALA:HB1	1.71	0.73
1:C:493:ARG:HD2	1:C:544:ARG:HD3	1.68	0.73
1:C:419:THR:HB	1:C:425:ASN:HD21	1.54	0.71
1:D:419:THR:HG22	1:D:421:ASP:H	1.56	0.68
1:A:247:LEU:N	5:A:608:NAD:H4N	2.09	0.67
1:D:227:VAL:HG22	1:D:236:LEU:HD22	1.75	0.67
1:C:444:ARG:HE	1:C:465:ASN:HD21	1.44	0.66
1:B:523:ALA:HB3	1:B:526:ARG:HB2	1.79	0.65
1:A:157:VAL:HG22	1:A:176:LYS:HB3	1.79	0.64
1:D:247:LEU:H	5:D:603:NAD:H4N	1.63	0.64
1:A:119:TYR:HB2	1:B:118:ARG:HH22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:THR:HB	1:C:362:ILE:HG12	1.81	0.63
1:A:419:THR:HG22	1:A:421:ASP:H	1.62	0.63
1:A:138:ILE:HG21	1:A:169:LEU:HD11	1.82	0.62
1:D:248:THR:HB	1:D:362:ILE:HG12	1.82	0.62
1:D:247:LEU:N	5:D:603:NAD:H4N	2.15	0.61
1:D:230:PRO:HD3	5:D:603:NAD:H72N	1.66	0.61
1:D:203:LEU:O	1:D:228:LYS:NZ	2.29	0.60
1:C:247:LEU:H	5:C:610:NAD:H4N	1.66	0.59
1:C:496:LEU:HD22	1:C:497:PRO:HD2	1.84	0.59
1:A:69:LEU:CD2	1:B:70:GLY:CA	2.80	0.59
1:C:504:THR:HG22	1:C:507:GLU:H	1.68	0.59
1:D:228:LYS:HD2	5:D:603:NAD:H1D	1.84	0.59
1:C:523:ALA:HB3	1:C:526:ARG:HB2	1.85	0.58
1:C:496:LEU:HD23	1:C:545:LEU:HD11	1.84	0.58
1:B:496:LEU:HD23	1:B:545:LEU:HD11	1.84	0.58
1:B:353:LEU:HB3	1:B:412:ALA:HA	1.86	0.58
1:D:113:ILE:HB	1:D:117:LEU:HD12	1.86	0.58
1:B:216:ARG:NH1	1:B:242:ASN:OD1	2.38	0.57
1:D:138:ILE:HG21	1:D:169:LEU:HD11	1.87	0.56
1:D:109:LEU:HA	1:D:112:TRP:HB3	1.86	0.56
1:C:500:MET:HG3	1:C:508:THR:HG21	1.88	0.56
1:B:493:ARG:HD3	1:B:544:ARG:HD2	1.86	0.56
1:C:505:ILE:HD13	1:C:518:ILE:HG21	1.87	0.56
1:C:230:PRO:HD3	5:C:610:NAD:H72N	1.71	0.56
1:B:270:ASP:HA	1:B:276:GLN:HG3	1.87	0.56
1:C:419:THR:HB	1:C:425:ASN:ND2	2.21	0.55
1:B:258:ARG:O	1:B:440:ARG:HD3	2.07	0.55
1:B:291:THR:HG22	1:B:322:VAL:HG22	1.89	0.55
1:B:169:LEU:HB3	1:B:175:PHE:HE1	1.71	0.55
1:B:496:LEU:HD22	1:B:497:PRO:HD2	1.88	0.55
1:A:203:LEU:O	1:A:228:LYS:NZ	2.35	0.55
1:B:356:ILE:HB	1:B:379:LEU:HD23	1.89	0.54
1:C:63:ILE:O	1:C:67:THR:HB	2.08	0.54
1:C:491:VAL:HG22	1:C:548:ILE:HG12	1.89	0.54
1:D:112:TRP:CE3	1:D:113:ILE:HG22	2.43	0.54
1:C:67:THR:O	1:C:68:THR:OG1	2.22	0.53
1:A:108:PHE:HA	1:A:111:PRO:HD2	1.91	0.53
1:B:353:LEU:HD12	1:B:411:ARG:HG2	1.90	0.53
1:C:258:ARG:HG2	1:C:461:PHE:CD1	2.45	0.52
1:B:520:ALA:HB3	1:B:546:ILE:HB	1.92	0.52
1:A:178:VAL:HG11	1:A:191:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:GLN:HB3	1:D:405:ARG:CZ	2.39	0.52
1:C:287:PHE:HE1	1:C:341:LEU:HD21	1.75	0.51
1:A:419:THR:HB	1:A:425:ASN:OD1	2.10	0.51
1:C:303:LEU:HD23	1:C:333:GLY:HA3	1.92	0.51
1:A:228:LYS:HD2	5:A:608:NAD:H1D	1.93	0.50
1:B:113:ILE:HG23	1:B:117:LEU:HD13	1.93	0.50
1:B:489:MET:HG2	1:B:550:THR:HA	1.93	0.50
1:A:105:VAL:HG23	1:A:109:LEU:HD23	1.93	0.50
1:B:419:THR:HG22	1:B:421:ASP:H	1.77	0.50
1:D:136:PHE:CD1	1:D:182:PRO:HB3	2.47	0.50
1:C:504:THR:HG23	1:C:506:ALA:H	1.77	0.50
1:B:146:ILE:HG21	1:B:175:PHE:HD2	1.77	0.49
1:D:197:ARG:NH1	1:D:477:LEU:O	2.37	0.49
1:B:188:LEU:HA	1:B:191:LEU:HD12	1.94	0.49
1:D:112:TRP:CD1	1:D:116:ARG:HD2	2.48	0.49
1:C:67:THR:HG21	1:D:89:THR:HG23	1.95	0.49
1:C:247:LEU:N	5:C:610:NAD:H4N	2.27	0.49
1:D:258:ARG:HG2	1:D:461:PHE:CD1	2.47	0.49
1:C:105:VAL:HG13	1:C:109:LEU:HD23	1.95	0.49
1:B:520:ALA:HB1	1:B:529:ILE:HD11	1.94	0.48
1:D:351:ASP:OD1	1:D:351:ASP:N	2.44	0.48
1:C:18:GLN:HB2	1:C:19:ASN:H	1.44	0.48
1:B:482:SER:HA	1:B:485:LEU:HB2	1.96	0.48
1:A:107:MET:HG2	1:A:108:PHE:HD2	1.78	0.48
1:B:67:THR:HG23	1:B:69:LEU:H	1.78	0.48
1:D:433:ARG:NH1	1:D:439:ILE:O	2.47	0.48
1:B:272:PHE:CE2	1:B:274:ASN:HB3	2.49	0.48
1:B:227:VAL:HG22	1:B:229:GLU:H	1.79	0.48
1:C:298:ARG:NH1	1:C:523:ALA:O	2.46	0.48
1:C:157:VAL:HG22	1:C:176:LYS:HB3	1.96	0.48
1:A:359:HIS:CD2	1:A:379:LEU:HD13	2.49	0.48
1:D:109:LEU:O	1:D:113:ILE:HG23	2.14	0.47
1:A:356:ILE:HB	1:A:379:LEU:HD23	1.95	0.47
1:C:258:ARG:O	1:C:440:ARG:HD3	2.14	0.47
1:C:42:ARG:HD2	1:C:55:PHE:HA	1.95	0.47
1:B:141:ILE:HD13	1:B:466:ALA:HA	1.96	0.47
1:A:119:TYR:HE2	1:A:170:GLU:HG2	1.80	0.47
1:D:113:ILE:O	1:D:117:LEU:HB2	2.14	0.47
1:C:400:VAL:HG11	1:D:387:VAL:HA	1.97	0.47
1:C:510:LEU:HD11	1:C:557:PHE:HE1	1.79	0.47
1:C:492:PHE:HD1	1:C:494:ARG:HD3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:NH2	1:B:172:GLN:HE22	2.13	0.47
1:C:496:LEU:HD21	1:C:539:LEU:HD23	1.96	0.46
1:D:228:LYS:O	5:D:603:NAD:N7N	2.34	0.46
1:A:103:GLY:O	1:A:107:MET:HB3	2.15	0.46
1:A:480:LYS:H	1:A:480:LYS:HD3	1.78	0.46
1:D:67:THR:HG23	1:D:69:LEU:H	1.80	0.46
1:B:362:ILE:HD12	1:B:444:ARG:NE	2.31	0.46
1:D:402:GLN:HB2	1:D:405:ARG:HB2	1.96	0.46
1:C:119:TYR:CE2	1:C:170:GLU:HG3	2.51	0.46
1:B:146:ILE:HG21	1:B:175:PHE:CD2	2.50	0.46
1:C:105:VAL:O	1:C:109:LEU:HB3	2.15	0.46
1:B:281:PRO:HB2	1:B:283:HIS:CD2	2.51	0.46
1:D:252:GLY:HA3	1:D:365:ALA:HB3	1.98	0.46
1:B:124:GLU:HG2	1:B:125:LEU:H	1.80	0.46
1:A:161:ASP:HB3	1:A:182:PRO:HD3	1.97	0.46
1:B:173:GLU:HA	1:B:174:GLY:HA3	1.63	0.46
1:C:303:LEU:HD12	1:C:341:LEU:HD12	1.98	0.45
1:B:292:ILE:HD11	1:B:308:VAL:HG21	1.98	0.45
1:A:92:GLY:O	1:A:96:LEU:HB2	2.16	0.45
1:D:359:HIS:CD2	1:D:379:LEU:HD13	2.51	0.45
1:B:63:ILE:O	1:B:67:THR:HG22	2.17	0.45
1:D:418:THR:HG22	1:D:444:ARG:HH11	1.81	0.45
1:B:269:LEU:HG	1:B:271:SER:H	1.82	0.45
1:C:362:ILE:HD12	1:C:444:ARG:NE	2.32	0.45
1:C:19:ASN:HB3	1:C:107:MET:HG3	1.99	0.45
1:B:19:ASN:HB3	1:B:107:MET:SD	2.57	0.45
1:B:496:LEU:HA	1:B:497:PRO:HD2	1.90	0.44
1:C:200:ILE:HD11	1:C:477:LEU:HD11	2.00	0.44
1:B:504:THR:HG22	1:B:507:GLU:H	1.82	0.44
1:D:419:THR:HB	1:D:425:ASN:OD1	2.17	0.44
1:C:429:THR:HG23	1:C:441:ILE:HG21	1.98	0.44
1:D:418:THR:HG23	1:D:444:ARG:HD3	1.99	0.44
1:B:247:LEU:H	5:B:605:NAD:H4N	1.82	0.44
1:D:146:ILE:HG21	1:D:175:PHE:HD2	1.83	0.44
1:B:352:GLU:O	1:B:376:PRO:HG2	2.17	0.44
1:D:247:LEU:HB2	5:D:603:NAD:C5N	2.48	0.44
1:B:111:PRO:HB3	1:B:115:ARG:CZ	2.47	0.44
1:B:149:LEU:HB2	1:B:156:PHE:HE1	1.82	0.44
1:C:448:GLU:HA	1:C:451:VAL:HG23	1.99	0.43
1:C:291:THR:HG22	1:C:322:VAL:HG22	2.00	0.43
1:B:200:ILE:HD13	1:B:224:ILE:HB	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ARG:HH21	1:C:344:LEU:HD22	1.83	0.43
1:B:429:THR:HG23	1:B:441:ILE:HG21	2.00	0.43
1:B:287:PHE:HD2	1:B:295:SER:HB2	1.83	0.43
1:B:149:LEU:HB2	1:B:156:PHE:CE1	2.53	0.43
1:B:492:PHE:HD1	1:B:494:ARG:HD3	1.83	0.43
1:B:448:GLU:HA	1:B:451:VAL:HG23	2.01	0.43
1:C:522:GLU:HB2	1:C:544:ARG:HB3	2.00	0.43
1:B:119:TYR:HE2	1:B:170:GLU:HG3	1.84	0.43
1:A:224:ILE:HD13	1:A:476:LEU:HB3	1.99	0.43
1:B:494:ARG:HG2	1:B:557:PHE:CE2	2.54	0.43
1:B:521:ILE:HG13	1:B:533:PRO:HG2	2.01	0.43
1:A:360:GLY:HA3	5:A:608:NAD:PA	2.58	0.43
1:A:69:LEU:HD21	1:B:70:GLY:CA	2.47	0.43
1:C:309:TRP:CZ2	1:C:312:GLY:HA2	2.54	0.43
1:B:476:LEU:O	1:B:480:LYS:HG2	2.19	0.43
1:B:494:ARG:NH2	1:B:554:GLU:OE2	2.52	0.43
1:A:247:LEU:HB2	5:A:608:NAD:C5N	2.49	0.42
1:C:267:HIS:CE1	1:C:270:ASP:HB2	2.54	0.42
1:C:281:PRO:HB2	1:C:283:HIS:ND1	2.34	0.42
1:B:226:VAL:HG12	5:B:605:NAD:H5N	2.01	0.42
1:C:117:LEU:HA	1:C:117:LEU:HD23	1.85	0.42
1:A:136:PHE:CD1	1:A:182:PRO:HB3	2.54	0.42
1:B:272:PHE:HB2	1:B:490:ALA:HB1	2.00	0.42
1:C:298:ARG:HG3	1:C:303:LEU:O	2.20	0.42
1:A:110:ALA:HB3	1:A:111:PRO:HD3	2.02	0.42
1:C:444:ARG:HE	1:C:465:ASN:ND2	2.11	0.42
1:C:275:LEU:HD23	1:C:491:VAL:HG12	2.02	0.42
1:C:356:ILE:HB	1:C:379:LEU:HD23	2.00	0.42
1:B:162:ASN:HB3	1:B:165:GLN:HB3	2.00	0.42
1:B:514:THR:HG21	1:B:557:PHE:HD1	1.84	0.42
1:C:520:ALA:HB1	1:C:529:ILE:HD11	2.01	0.42
1:A:474:GLY:O	1:A:478:GLU:HG2	2.20	0.42
1:B:257:ILE:HG22	1:B:369:PHE:CZ	2.54	0.42
1:A:67:THR:HG23	1:A:69:LEU:H	1.85	0.42
1:B:360:GLY:HA3	5:B:605:NAD:PA	2.60	0.42
1:B:275:LEU:HD23	1:B:491:VAL:HG13	2.02	0.42
1:C:445:ALA:HB2	1:C:454:LEU:HD12	2.02	0.41
1:A:228:LYS:C	5:A:608:NAD:H71N	2.23	0.41
1:B:335:LYS:HB2	1:B:335:LYS:HE3	1.95	0.41
1:B:309:TRP:CZ2	1:B:312:GLY:HA2	2.54	0.41
1:B:496:LEU:HD21	1:B:539:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ILE:O	1:D:102:PHE:HB3	2.21	0.41
1:B:359:HIS:CD2	1:B:379:LEU:HD13	2.55	0.41
1:C:139:ASP:OD1	1:C:141:ILE:HG12	2.21	0.41
1:B:248:THR:HG23	5:B:605:NAD:C2N	2.51	0.41
1:C:280:LEU:HA	1:C:281:PRO:HD2	1.94	0.41
1:C:230:PRO:HD3	5:C:610:NAD:N7N	2.36	0.41
1:D:224:ILE:HD13	1:D:476:LEU:HB3	2.02	0.41
1:C:533:PRO:HA	1:C:534:PRO:HD2	1.90	0.41
1:D:117:LEU:HA	1:D:117:LEU:HD23	1.65	0.41
1:B:307:GLY:HA2	1:B:317:PRO:HD3	2.01	0.41
1:B:181:SER:HA	1:B:182:PRO:HD3	1.90	0.41
1:D:141:ILE:HD13	1:D:466:ALA:HA	2.02	0.41
1:B:258:ARG:HG2	1:B:461:PHE:CG	2.56	0.40
1:B:110:ALA:HB3	1:B:111:PRO:HD3	2.03	0.40
1:C:20:LEU:H	1:C:20:LEU:HD22	1.86	0.40
1:B:136:PHE:CD1	1:B:182:PRO:HB3	2.56	0.40
1:D:92:GLY:O	1:D:96:LEU:HB2	2.20	0.40
1:C:419:THR:HG23	5:C:610:NAD:C8A	2.51	0.40
1:C:497:PRO:HA	1:C:498:PRO:HD3	1.90	0.40
1:B:271:SER:C	1:B:273:GLY:H	2.24	0.40
1:A:440:ARG:HA	1:A:460:ASP:OD2	2.21	0.40
1:B:188:LEU:HD23	1:B:191:LEU:HD12	2.04	0.40
1:C:55:PHE:O	1:C:59:ILE:HG12	2.22	0.40
1:B:426:ILE:O	1:B:430:LEU:HB2	2.22	0.40
1:B:345:ILE:N	1:B:346:GLY:HA2	2.36	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	546/565 (97%)	517 (95%)	28 (5%)	1 (0%)	52	88
1	C	545/565 (96%)	525 (96%)	20 (4%)	0	100	100
1	D	372/565 (66%)	358 (96%)	13 (4%)	1 (0%)	46	85
All	All	1834/2260 (81%)	1748 (95%)	84 (5%)	2 (0%)	56	91

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%)	22	62
1	B	449/463 (97%)	423 (94%)	26 (6%)	25	66
1	C	448/463 (97%)	417 (93%)	31 (7%)	19	59
1	D	314/463 (68%)	293 (93%)	21 (7%)	20	60
All	All	1524/1852 (82%)	1426 (94%)	98 (6%)	22	62

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
1	B	172	GLN
1	C	276	GLN
1	C	425	ASN
1	C	465	ASN

### 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 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	-	38,48,48	1.65	6 (15%)	47,73,73	2.20	10 (21%)
6	PO4	B	604	-	4,4,4	0.47	0	6,6,6	0.27	0
5	NAD	B	605	-	38,48,48	1.64	5 (13%)	47,73,73	2.13	12 (25%)
6	PO4	C	609	-	4,4,4	0.47	0	6,6,6	0.28	0
5	NAD	C	610	-	38,48,48	1.64	5 (13%)	47,73,73	2.18	12 (25%)
5	NAD	D	603	-	38,48,48	1.65	6 (15%)	47,73,73	2.26	10 (21%)

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	-	-	0/22/62/62	0/5/5/5
6	PO4	B	604	-	-	0/0/0/0	0/0/0/0
5	NAD	B	605	-	-	0/22/62/62	0/5/5/5
6	PO4	C	609	-	-	0/0/0/0	0/0/0/0
5	NAD	C	610	-	-	0/22/62/62	0/5/5/5
5	NAD	D	603	-	-	0/22/62/62	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	NAD	C2D-C3D	-4.03	1.42	1.53
5	A	608	NAD	C2D-C3D	-4.03	1.42	1.53
5	C	610	NAD	C2D-C3D	-4.01	1.42	1.53
5	D	603	NAD	C2D-C3D	-4.01	1.42	1.53
5	C	610	NAD	C2B-C3B	-3.29	1.44	1.53
5	A	608	NAD	C2B-C3B	-3.29	1.44	1.53
5	B	605	NAD	C2B-C3B	-3.28	1.44	1.53
5	D	603	NAD	C2B-C3B	-3.24	1.44	1.53
5	D	603	NAD	O4D-C4D	-2.73	1.38	1.45
5	A	608	NAD	O4D-C4D	-2.67	1.38	1.45
5	C	610	NAD	O4D-C4D	-2.63	1.39	1.45
5	B	605	NAD	O4D-C4D	-2.54	1.39	1.45
5	D	603	NAD	O5D-C5D	-2.06	1.36	1.44
5	A	608	NAD	O5D-C5D	-2.03	1.36	1.44
5	A	608	NAD	C6A-N6A	2.60	1.43	1.34
5	B	605	NAD	C6A-N6A	2.62	1.43	1.34
5	C	610	NAD	C6A-N6A	2.64	1.43	1.34
5	D	603	NAD	C6A-N6A	2.65	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	608	NAD	C7N-N7N	4.99	1.43	1.33
5	D	603	NAD	C7N-N7N	5.00	1.43	1.33
5	B	605	NAD	C7N-N7N	5.08	1.43	1.33
5	C	610	NAD	C7N-N7N	5.09	1.43	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	610	NAD	N3A-C2A-N1A	-10.48	120.87	128.89
5	D	603	NAD	N3A-C2A-N1A	-10.39	120.94	128.89
5	B	605	NAD	N3A-C2A-N1A	-10.38	120.95	128.89
5	A	608	NAD	N3A-C2A-N1A	-10.24	121.05	128.89
5	D	603	NAD	PN-O3-PA	-4.66	119.66	132.73
5	D	603	NAD	C4D-O4D-C1D	-4.53	104.74	109.72
5	A	608	NAD	PN-O3-PA	-4.30	120.65	132.73
5	B	605	NAD	PN-O3-PA	-4.11	121.20	132.73
5	C	610	NAD	PN-O3-PA	-4.02	121.43	132.73
5	A	608	NAD	C4D-O4D-C1D	-3.99	105.33	109.72
5	C	610	NAD	C4D-O4D-C1D	-3.85	105.49	109.72
5	B	605	NAD	C4D-O4D-C1D	-2.92	106.51	109.72
5	D	603	NAD	O7N-C7N-N7N	-2.83	118.61	122.59
5	B	605	NAD	C1B-N9A-C4A	-2.82	122.69	126.94
5	A	608	NAD	C1B-N9A-C4A	-2.76	122.78	126.94
5	D	603	NAD	C1B-N9A-C4A	-2.75	122.79	126.94
5	A	608	NAD	C4A-C5A-N7A	-2.67	107.03	109.48
5	B	605	NAD	C4A-C5A-N7A	-2.66	107.03	109.48
5	C	610	NAD	C4A-C5A-N7A	-2.63	107.06	109.48
5	D	603	NAD	C4A-C5A-N7A	-2.61	107.08	109.48
5	A	608	NAD	O7N-C7N-N7N	-2.61	118.93	122.59
5	C	610	NAD	C1B-N9A-C4A	-2.54	123.10	126.94
5	B	605	NAD	O7N-C7N-N7N	-2.49	119.08	122.59
5	C	610	NAD	O7N-C7N-N7N	-2.34	119.30	122.59
5	D	603	NAD	O3-PN-O5D	2.08	108.44	102.94
5	A	608	NAD	C2B-C3B-C4B	2.08	106.88	102.61
5	B	605	NAD	C2B-C3B-C4B	2.09	106.91	102.61
5	C	610	NAD	C2B-C3B-C4B	2.13	107.00	102.61
5	C	610	NAD	C3N-C7N-N7N	2.16	120.18	117.82
5	B	605	NAD	O5B-C5B-C4B	2.22	117.31	109.12
5	C	610	NAD	O3-PN-O5D	2.26	108.93	102.94
5	B	605	NAD	O3-PN-O5D	2.36	109.19	102.94
5	B	605	NAD	C3N-C7N-N7N	2.37	120.41	117.82
5	C	610	NAD	O5B-C5B-C4B	2.65	118.88	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	NAD	O4B-C1B-N9A	3.00	114.38	108.10
5	D	603	NAD	O3-PA-O5B	3.05	111.02	102.94
5	A	608	NAD	O3-PA-O5B	3.09	111.12	102.94
5	A	608	NAD	O4B-C1B-N9A	3.09	114.58	108.10
5	D	603	NAD	O4B-C1B-N9A	3.11	114.62	108.10
5	B	605	NAD	O3-PA-O5B	3.32	111.74	102.94
5	C	610	NAD	O4B-C1B-N9A	3.34	115.08	108.10
5	C	610	NAD	O3-PA-O5B	3.47	112.14	102.94
5	A	608	NAD	C3N-C7N-N7N	3.55	121.70	117.82
5	D	603	NAD	C3N-C7N-N7N	3.81	121.99	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	608	NAD	6	0
5	B	605	NAD	4	0
5	C	610	NAD	6	0
5	D	603	NAD	6	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	375/565 (66%)	0.32	12 (3%)	51	36	64, 90, 166, 214	0
1	B	548/565 (96%)	0.93	85 (15%)	3	2	67, 115, 249, 357	0
1	C	547/565 (96%)	0.62	46 (8%)	14	7	66, 111, 192, 261	0
1	D	376/565 (66%)	0.30	16 (4%)	39	25	60, 89, 168, 234	0
All	All	1846/2260 (81%)	0.59	159 (8%)	13	7	60, 100, 212, 357	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	LEU	12.1
1	B	543	ALA	12.1
1	B	516	CYS	9.9
1	B	542	GLY	9.6
1	C	561	ILE	8.9
1	B	563	ALA	8.5
1	B	518	ILE	8.4
1	B	510	LEU	8.2
1	C	562	ALA	8.1
1	B	561	ILE	8.0
1	B	541	GLU	7.9
1	B	497	PRO	7.8
1	B	517	SER	7.6
1	C	564	ARG	7.3
1	B	495	PRO	6.4
1	C	501	ALA	6.1
1	B	564	ARG	6.0
1	A	398	ALA	6.0
1	A	404	LEU	5.9
1	B	508	THR	5.8
1	B	519	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	297	ILE	5.7
1	C	500	MET	5.7
1	B	509	ARG	5.7
1	B	540	ALA	5.6
1	B	526	ARG	5.5
1	B	492	PHE	5.4
1	B	562	ALA	5.3
1	C	541	GLU	5.2
1	C	542	GLY	5.0
1	D	398	ALA	4.9
1	B	498	PRO	4.9
1	B	494	ARG	4.8
1	C	97	ASP	4.7
1	B	499	ALA	4.6
1	B	97	ASP	4.4
1	C	502	GLY	4.3
1	B	525	ASP	4.3
1	B	500	MET	4.2
1	B	507	GLU	4.2
1	D	481	GLU	4.1
1	B	529	ILE	4.1
1	B	545	LEU	4.1
1	B	438	HIS	4.1
1	B	521	ILE	4.0
1	D	397	ASP	3.9
1	C	519	VAL	3.9
1	B	528	ASP	3.8
1	B	546	ILE	3.8
1	B	557	PHE	3.8
1	B	524	PRO	3.8
1	B	506	ALA	3.8
1	A	441	ILE	3.7
1	B	292	ILE	3.7
1	D	409	ILE	3.7
1	B	317	PRO	3.7
1	D	480	LYS	3.5
1	C	539	LEU	3.5
1	C	301	THR	3.5
1	C	448	GLU	3.5
1	C	499	ALA	3.5
1	B	443	ALA	3.5
1	B	255	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	498	PRO	3.4
1	C	332	ALA	3.4
1	A	397	ASP	3.4
1	B	548	ILE	3.4
1	B	514	THR	3.4
1	B	512	PRO	3.4
1	D	97	ASP	3.4
1	D	198	SER	3.4
1	C	510	LEU	3.3
1	A	448	GLU	3.3
1	B	505	ILE	3.3
1	D	191	LEU	3.3
1	C	509	ARG	3.2
1	B	439	ILE	3.2
1	B	547	LEU	3.2
1	B	17	ARG	3.2
1	B	416	ILE	3.2
1	B	527	ALA	3.1
1	C	297	ILE	3.1
1	C	563	ALA	3.1
1	B	306	ILE	3.1
1	A	97	ASP	3.1
1	A	409	ILE	3.1
1	C	557	PHE	3.0
1	C	300	ARG	3.0
1	B	539	LEU	3.0
1	B	531	ILE	2.9
1	C	496	LEU	2.9
1	B	448	GLU	2.9
1	B	523	ALA	2.8
1	B	484	PHE	2.8
1	C	370	LEU	2.8
1	B	198	SER	2.7
1	B	287	PHE	2.7
1	C	517	SER	2.7
1	B	157	VAL	2.7
1	A	67	THR	2.7
1	A	399	THR	2.6
1	C	540	ALA	2.6
1	B	559	GLN	2.6
1	B	560	THR	2.6
1	C	518	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	497	PRO	2.6
1	B	398	ALA	2.5
1	B	176	LYS	2.5
1	D	396	GLY	2.5
1	B	184	ASP	2.5
1	A	117	LEU	2.5
1	B	341	LEU	2.5
1	C	533	PRO	2.4
1	D	234	GLU	2.4
1	C	67	THR	2.4
1	A	118	ARG	2.4
1	B	134	LEU	2.4
1	C	145	LEU	2.4
1	C	259	ALA	2.4
1	B	102	PHE	2.4
1	B	174	GLY	2.4
1	A	102	PHE	2.4
1	B	335	LYS	2.4
1	B	234	GLU	2.3
1	C	134	LEU	2.3
1	C	255	LEU	2.3
1	B	473	LEU	2.3
1	C	512	PRO	2.2
1	C	344	LEU	2.2
1	B	224	ILE	2.2
1	B	511	ARG	2.2
1	C	491	VAL	2.2
1	C	546	ILE	2.2
1	C	548	ILE	2.2
1	C	513	LEU	2.2
1	C	200	ILE	2.2
1	D	98	ILE	2.2
1	B	520	ALA	2.2
1	B	301	THR	2.2
1	D	461	PHE	2.1
1	B	354	ILE	2.1
1	D	224	ILE	2.1
1	D	404	LEU	2.1
1	C	176	LYS	2.1
1	C	514	THR	2.1
1	C	520	ALA	2.1
1	B	442	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	463	VAL	2.1
1	B	236	LEU	2.1
1	C	350	GLU	2.1
1	C	123	ILE	2.1
1	D	244	VAL	2.0
1	B	113	ILE	2.0
1	B	305	ILE	2.0
1	B	544	ARG	2.0
1	D	442	VAL	2.0
1	B	175	PHE	2.0
1	B	300	ARG	2.0
1	B	533	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAD	A	608	44/44	0.76	0.41	0.79	67,221,245,282	0
4	CA	C	608	1/1	0.90	0.23	0.18	90,90,90,90	0
5	NAD	C	610	44/44	0.82	0.27	-0.04	78,179,210,212	0
4	CA	B	603	1/1	0.99	0.23	-0.07	89,89,89,89	0
5	NAD	D	603	44/44	0.81	0.27	-0.19	83,197,221,223	0
6	PO4	B	604	5/5	0.83	0.27	-0.38	131,134,136,137	0
4	CA	C	607	1/1	0.95	0.23	-0.52	87,87,87,87	0
6	PO4	C	609	5/5	0.93	0.22	-0.78	139,139,142,142	0
5	NAD	B	605	44/44	0.88	0.19	-1.01	57,151,214,216	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	C	603	1/1	0.99	0.15	-1.29	68,68,68,68	1
2	K	A	602	1/1	0.91	0.24	-1.29	87,87,87,87	1
2	K	A	601	1/1	0.99	0.16	-1.50	88,88,88,88	1
2	K	C	602	1/1	0.96	0.21	-1.52	64,64,64,64	1
4	CA	A	607	1/1	0.97	0.16	-1.74	89,89,89,89	0
2	K	A	603	1/1	0.87	0.16	-1.81	71,71,71,71	1
2	K	C	601	1/1	0.91	0.14	-2.04	73,73,73,73	1
2	K	A	605	1/1	0.64	0.26	-	136,136,136,136	1
3	ZN	A	606	1/1	0.98	0.31	-	91,91,91,91	0
2	K	C	604	1/1	0.94	0.28	-	100,100,100,100	1
3	ZN	C	606	1/1	0.97	0.29	-	87,87,87,87	0
2	K	A	604	1/1	0.98	0.31	-	109,109,109,109	1
2	K	B	601	1/1	0.54	0.62	-	222,222,222,222	1
3	ZN	B	602	1/1	0.98	0.29	-	92,92,92,92	0
2	K	D	601	1/1	0.96	0.22	-	136,136,136,136	1
2	K	C	605	1/1	0.78	0.50	-	207,207,207,207	1
3	ZN	D	602	1/1	0.99	0.28	-	81,81,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.