



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:52 AM GMT

PDB ID : 3N7U  
Title : NAD-dependent formate dehydrogenase from higher-plant *Arabidopsis thaliana* in complex with NAD and azide  
Authors : Shabalin, I.G.; Polyakov, K.M.; Serov, A.E.; Skirgello, O.E.; Sadykhov, E.G.; Dorovatovskiy, P.V.; Tishkov, V.I.; Popov, V.O.  
Deposited on : 2010-05-27  
Resolution : 2.00 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.

---

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

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

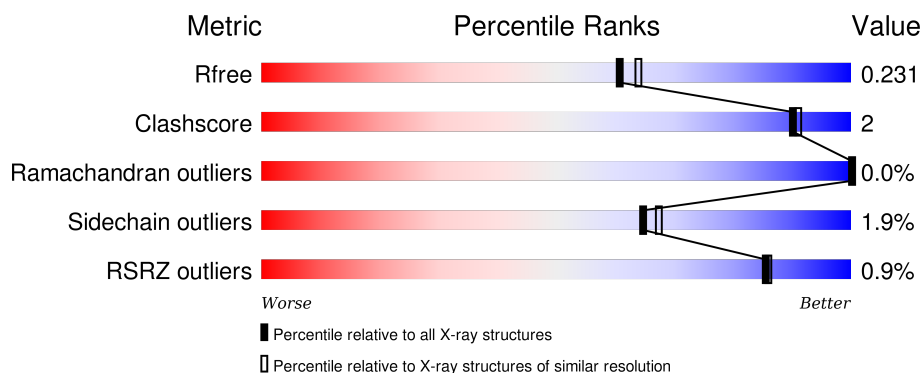
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	351	<div> <div>95%</div> <div>5%</div> </div>
1	B	351	<div> <div>95%</div> <div>5%</div> </div>
1	C	351	<div> <div>95%</div> <div>5%</div> </div>
1	D	351	<div> <div>95%</div> <div>5%</div> </div>
1	E	351	<div> <div>94%</div> <div>5%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	351	
1	G	351	
1	H	351	
1	I	351	
1	J	351	
1	K	351	
1	L	351	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	H	6	-	-	-	X
4	SO4	I	7	-	-	-	X
4	SO4	K	8	-	-	-	X
5	GOL	D	25	-	-	-	X
5	GOL	E	379	-	-	-	X
5	GOL	F	26	-	-	-	X
5	GOL	H	27	-	-	-	X
5	GOL	I	13	-	-	-	X
5	GOL	I	19	-	-	-	X
5	GOL	K	24	-	-	-	X
5	GOL	L	21	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37338 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 Formate dehydrogenase.

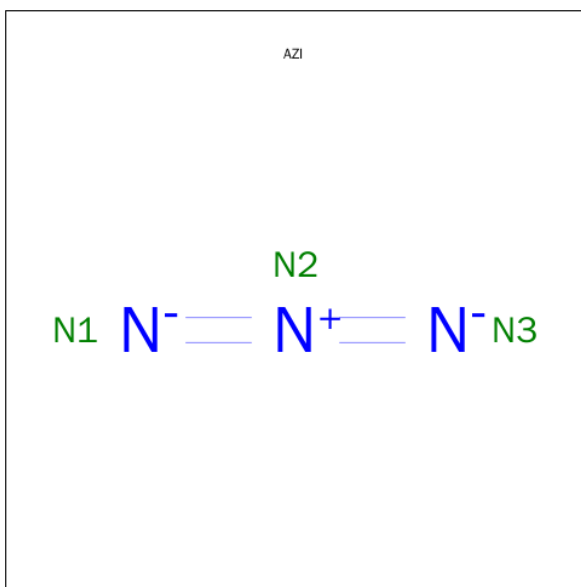
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	1	0
			2740	1741	472	513	14			
1	B	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	C	351	Total	C	N	O	S	0	1	0
			2740	1741	472	513	14			
1	D	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	E	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	F	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	G	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	H	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	I	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	J	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	K	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			
1	L	351	Total	C	N	O	S	0	0	0
			2739	1740	472	513	14			

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	B	1	Total N 3 3	0	0
3	C	1	Total N 3 3	0	0
3	D	1	Total N 3 3	0	0
3	E	1	Total N 3 3	0	0
3	F	1	Total N 3 3	0	0
3	G	1	Total N 3 3	0	0
3	H	1	Total N 3 3	0	0
3	I	1	Total N 3 3	0	0
3	J	1	Total N 3 3	0	0
3	K	1	Total N 3 3	0	0
3	L	1	Total N 3 3	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

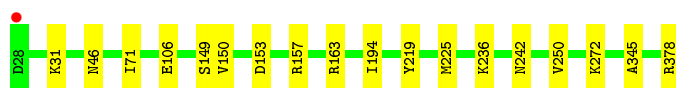
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	355	Total	O	0	0
			355	355		
6	B	353	Total	O	0	0
			353	353		
6	C	332	Total	O	0	0
			332	332		
6	D	344	Total	O	0	0
			344	344		
6	E	353	Total	O	0	0
			353	353		
6	F	275	Total	O	0	0
			275	275		
6	G	311	Total	O	0	0
			311	311		
6	H	293	Total	O	0	0
			293	293		
6	I	276	Total	O	0	0
			276	276		
6	J	233	Total	O	0	0
			233	233		
6	K	315	Total	O	0	0
			315	315		
6	L	305	Total	O	0	0
			305	305		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Formate dehydrogenase

Chain A: 



- Molecule 1: Formate dehydrogenase

Chain B: 



- Molecule 1: Formate dehydrogenase

Chain C: 



- Molecule 1: Formate dehydrogenase

Chain D: 

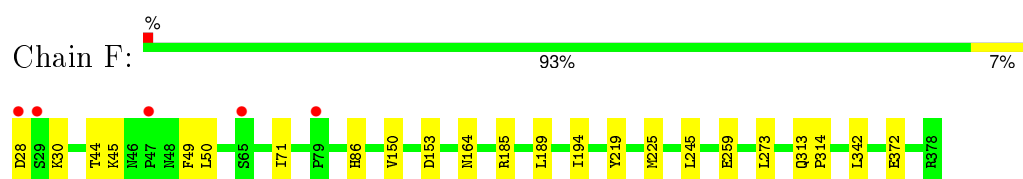


- Molecule 1: Formate dehydrogenase

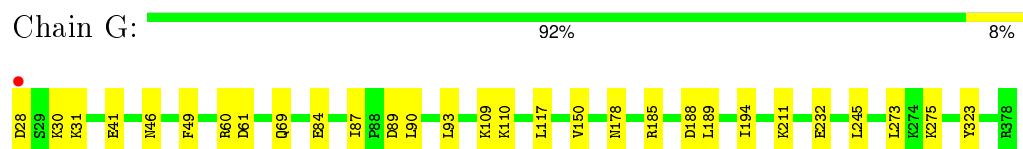
Chain E: 



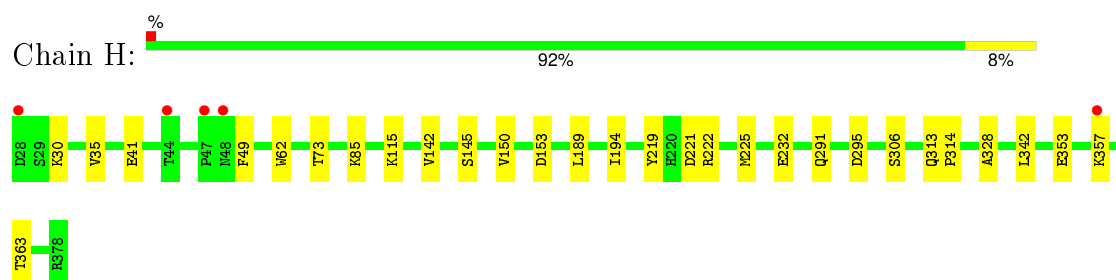
- Molecule 1: Formate dehydrogenase



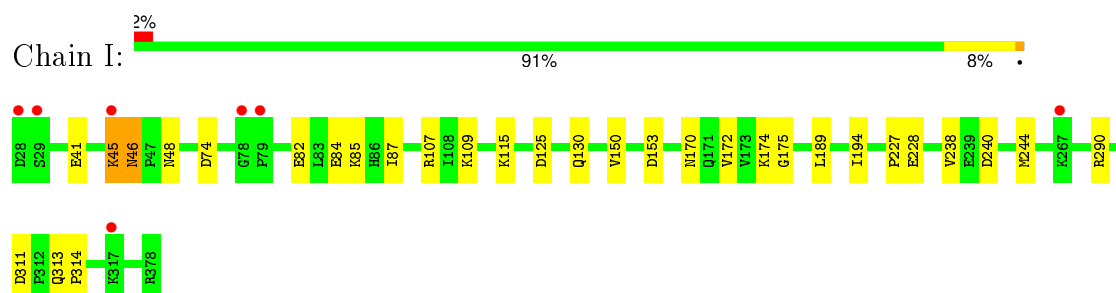
- Molecule 1: Formate dehydrogenase



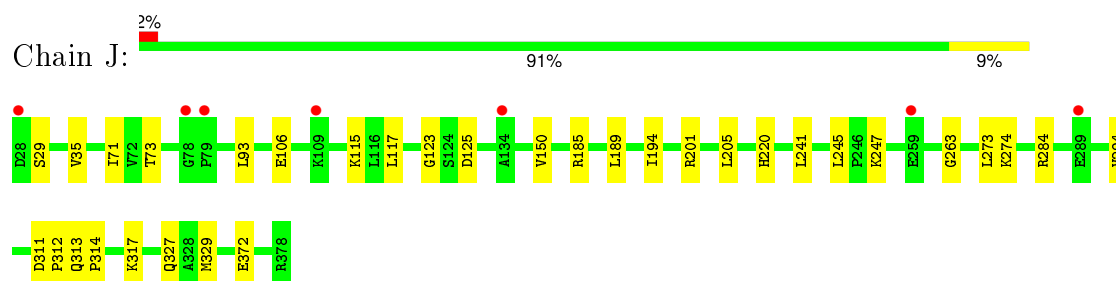
- Molecule 1: Formate dehydrogenase



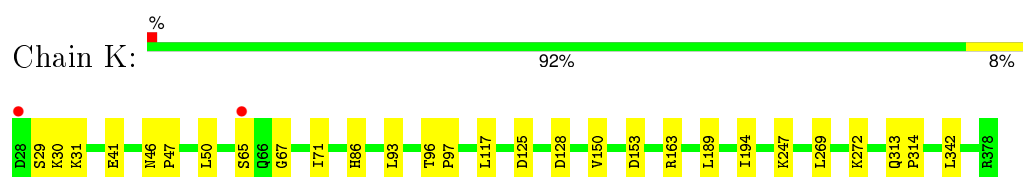
- Molecule 1: Formate dehydrogenase



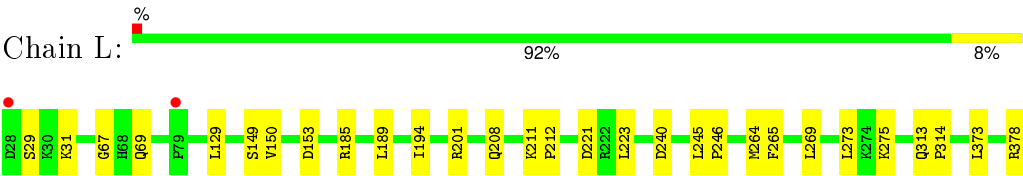
- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase



● Molecule 1: Formate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	229.62Å 217.68Å 139.11Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	19.99 – 2.00 19.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.00) 96.9 (19.88-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.189 , 0.231 0.191 , 0.231	Depositor DCC
$R_{free}$ test set	22264 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 63.2	EDS
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 443315 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	37338	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 55.10 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.3212e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, SO4, NAD, GOL

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	0.91	1/2804 (0.0%)	0.77	2/3796 (0.1%)
1	B	0.91	0/2796	0.77	0/3785
1	C	0.87	0/2804	0.74	0/3796
1	D	0.90	0/2796	0.76	1/3785 (0.0%)
1	E	0.98	0/2796	0.78	0/3785
1	F	0.87	0/2796	0.72	0/3785
1	G	0.95	0/2796	0.75	2/3785 (0.1%)
1	H	0.90	0/2796	0.75	1/3785 (0.0%)
1	I	0.87	0/2796	0.75	1/3785 (0.0%)
1	J	0.87	0/2796	0.77	0/3785
1	K	0.87	0/2796	0.74	1/3785 (0.0%)
1	L	0.92	0/2796	0.76	1/3785 (0.0%)
All	All	0.90	1/33568 (0.0%)	0.76	9/45442 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	ALA	CA-CB	5.08	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	373	LEU	CA-CB-CG	5.86	128.78	115.30
1	I	240	ASP	CB-CG-OD2	5.67	123.41	118.30
1	G	188	ASP	CB-CG-OD1	5.54	123.29	118.30
1	K	163	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	163	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	L	240	ASP	CB-CG-OD1	5.09	122.88	118.30
1	G	185	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	157	ARG	NE-CZ-NH2	-5.03	117.79	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	H	342	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2740	0	2743	8	0
1	B	2739	0	2744	10	0
1	C	2740	0	2743	11	0
1	D	2739	0	2744	8	0
1	E	2739	0	2744	14	0
1	F	2739	0	2744	11	0
1	G	2739	0	2744	19	0
1	H	2739	0	2744	15	0
1	I	2739	0	2744	16	0
1	J	2739	0	2744	15	0
1	K	2739	0	2744	12	0
1	L	2739	0	2744	15	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
2	E	44	0	26	1	0
2	F	44	0	26	1	0
2	G	44	0	26	1	0
2	H	44	0	26	1	0
2	I	44	0	26	1	0
2	J	44	0	26	1	0
2	K	44	0	26	1	0
2	L	44	0	26	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	K	5	0	0	0	0
5	B	6	0	8	1	0
5	C	12	0	16	1	0
5	D	24	0	32	2	0
5	E	6	0	8	0	0
5	F	6	0	8	0	0
5	G	6	0	8	3	0
5	H	12	0	16	0	0
5	I	18	0	24	0	0
5	K	18	0	24	1	0
5	L	6	0	8	0	0
6	A	355	0	0	2	0
6	B	353	0	0	3	0
6	C	332	0	0	3	0
6	D	344	0	0	1	0
6	E	353	0	0	4	0
6	F	275	0	0	0	0
6	G	311	0	0	0	0
6	H	293	0	0	2	0
6	I	276	0	0	1	0
6	J	233	0	0	2	0
6	K	315	0	0	0	0
6	L	305	0	0	1	0
All	All	37338	0	33390	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.



All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ASP:HB2	5:G:9:GOL:H11	1.64	0.77
1:I:41:GLU:HG3	6:I:447:HOH:O	1.84	0.77
1:D:378:ARG:HH22	5:D:11:GOL:H32	1.52	0.75
1:L:211:LYS:HG2	1:L:212:PRO:HD3	1.71	0.72
1:H:291:GLN:NE2	1:H:295:ASP:OD2	2.24	0.69
1:I:175:GLY:O	1:J:317:LYS:HG2	1.93	0.67
1:E:28:ASP:N	6:E:1:HOH:O	2.29	0.66
1:G:61:ASP:HB2	5:G:9:GOL:C1	2.25	0.66
1:H:219:TYR:CZ	1:H:225:MET:HG3	2.30	0.66
1:G:211:LYS:HD3	1:G:232:GLU:O	1.96	0.65
1:I:87:ILE:HD13	1:I:107:ARG:HG2	1.78	0.65
1:E:245:LEU:HD23	1:E:251:ILE:HD11	1.79	0.65
1:C:184:TYR:CE1	1:C:185:ARG:HG3	2.35	0.62
1:G:31:LYS:HD3	1:G:69:GLN:OE1	1.99	0.62
1:H:150:VAL:HG21	2:H:401:NAD:C4N	2.30	0.62
1:H:62:TRP:HZ2	1:H:353:GLU:HG2	1.65	0.61
1:J:327:GLN:N	6:J:411:HOH:O	2.33	0.61
1:I:84:GLU:HA	1:I:87:ILE:HD12	1.82	0.61
1:J:189:LEU:HD11	1:J:194:ILE:HD11	1.82	0.61
1:F:164:ASN:HD21	1:F:185:ARG:NE	1.98	0.61
1:C:150:VAL:HG21	2:C:401:NAD:C4N	2.33	0.59
1:B:189:LEU:HD11	1:B:194:ILE:HD11	1.86	0.58
5:C:10:GOL:H31	6:C:688:HOH:O	2.04	0.57
1:K:128:ASP:HB2	5:K:24:GOL:H2	1.85	0.57
1:L:189:LEU:HD11	1:L:194:ILE:HD11	1.86	0.56
1:A:46:ASN:ND2	1:B:187:TYR:OH	2.37	0.56
5:B:16:GOL:H11	6:B:611:HOH:O	2.06	0.55
1:D:150:VAL:HG21	2:D:401:NAD:C4N	2.38	0.54
1:I:45:LYS:HD3	1:I:45:LYS:O	2.08	0.54
1:C:62:TRP:HE1	1:H:41:GLU:HB2	1.72	0.54
1:J:150:VAL:HG21	2:J:401:NAD:C4N	2.38	0.54
1:A:194[B]:ILE:HD12	1:A:250:VAL:HB	1.90	0.54
1:E:31:LYS:HG3	1:E:90:LEU:HA	1.89	0.53
1:G:31:LYS:CG	1:G:90:LEU:HA	2.38	0.53
1:L:245:LEU:HB2	1:L:246:PRO:HD3	1.92	0.52
1:G:150:VAL:HG21	2:G:401:NAD:C4N	2.39	0.52
1:C:38:LYS:HE3	1:C:40:ASN:HD21	1.74	0.52
1:H:85:LYS:HD2	6:H:507:HOH:O	2.09	0.52
1:E:274:LYS:HD3	6:E:464:HOH:O	2.08	0.52
1:G:93:LEU:HB3	1:G:117:LEU:HD23	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:LYS:HE3	1:K:71:ILE:HD12	1.91	0.52
1:K:93:LEU:HB3	1:K:117:LEU:HD23	1.92	0.52
1:I:227:PRO:HD2	1:I:228:GLU:OE2	2.10	0.51
1:H:62:TRP:CZ2	1:H:353:GLU:HG2	2.45	0.51
1:E:150:VAL:HG21	2:E:401:NAD:C4N	2.40	0.51
1:I:172:VAL:HG11	1:J:329:MET:HB2	1.92	0.51
1:F:189:LEU:HD11	1:F:194:ILE:HD11	1.93	0.51
1:B:130:GLN:HG3	6:B:513:HOH:O	2.09	0.51
1:H:189:LEU:HD11	1:H:194:ILE:HD11	1.93	0.50
1:I:238:VAL:HG11	1:I:244:MET:HB2	1.93	0.50
1:B:62:TRP:CZ2	1:B:353:GLU:HG2	2.45	0.50
1:J:201:ARG:O	1:J:205:LEU:HG	2.11	0.50
1:G:189:LEU:HD11	1:G:194:ILE:HD11	1.94	0.50
1:K:150:VAL:HG21	2:K:401:NAD:C4N	2.42	0.49
1:E:31:LYS:HD3	1:E:69:GLN:OE1	2.12	0.49
1:F:313:GLN:HA	1:F:314:PRO:C	2.32	0.49
1:G:245:LEU:HB3	1:G:273:LEU:HD23	1.94	0.49
1:L:373:LEU:O	1:L:378:ARG:NH2	2.46	0.49
1:G:31:LYS:HG2	1:G:90:LEU:HA	1.95	0.48
1:L:313:GLN:HA	1:L:314:PRO:C	2.34	0.48
1:I:313:GLN:HA	1:I:314:PRO:C	2.33	0.48
1:J:93:LEU:HB3	1:J:117:LEU:HD23	1.96	0.48
1:B:62:TRP:HZ2	1:B:353:GLU:HG2	1.79	0.48
1:B:150:VAL:HG21	2:B:401:NAD:C4N	2.44	0.48
1:J:245:LEU:HB3	1:J:273:LEU:HD23	1.97	0.47
1:L:150:VAL:HG21	2:L:401:NAD:C4N	2.45	0.47
1:F:28:ASP:O	1:F:30:LYS:HD3	2.14	0.47
1:F:150:VAL:HG21	2:F:401:NAD:C4N	2.43	0.47
1:D:30:LYS:NZ	6:D:673:HOH:O	2.48	0.47
1:K:269:LEU:HD12	1:K:272:LYS:HD2	1.96	0.47
1:I:46:ASN:ND2	1:I:48:ASN:H	2.13	0.47
1:G:28:ASP:OD1	1:G:28:ASP:N	2.48	0.47
1:A:378:ARG:NH2	6:A:508:HOH:O	2.47	0.47
1:H:232:GLU:HG2	6:H:602:HOH:O	2.14	0.47
1:J:123:GLY:HA3	1:J:284:ARG:NH2	2.30	0.47
1:K:189:LEU:HD11	1:K:194:ILE:HD11	1.96	0.47
1:I:170:ASN:O	1:I:174:LYS:HG3	2.16	0.46
1:K:313:GLN:HA	1:K:314:PRO:C	2.36	0.46
1:C:122:ILE:HD12	1:C:146:ASN:OD1	2.16	0.46
1:D:142:VAL:HG12	1:D:145:SER:HB3	1.97	0.46
1:L:269:LEU:O	1:L:269:LEU:HD23	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:VAL:HG12	1:H:145:SER:HB3	1.98	0.46
1:I:189:LEU:HD11	1:I:194:ILE:HD11	1.97	0.46
1:I:150:VAL:HG21	2:I:401:NAD:C4N	2.46	0.46
1:F:71:ILE:HD13	1:F:86:HIS:CE1	2.51	0.46
1:F:219:TYR:CZ	1:F:225:MET:HG3	2.51	0.46
1:A:31:LYS:HE3	1:A:71:ILE:HD12	1.97	0.45
1:L:201:ARG:HD2	6:L:610:HOH:O	2.15	0.45
1:I:311:ASP:OD1	1:I:311:ASP:C	2.54	0.45
1:I:46:ASN:HD21	1:I:48:ASN:HB2	1.82	0.45
1:A:150:VAL:HG21	2:A:401:NAD:C4N	2.46	0.45
1:L:269:LEU:C	1:L:269:LEU:HD23	2.37	0.45
1:G:84:GLU:HA	1:G:87:ILE:HD12	1.98	0.45
1:J:35:VAL:HA	1:J:73:THR:O	2.17	0.45
1:B:313:GLN:HA	1:B:314:PRO:C	2.37	0.45
1:E:364:GLU:HB2	6:E:504:HOH:O	2.16	0.44
1:E:46:ASN:HA	1:E:47:PRO:HD2	1.90	0.44
1:L:31:LYS:HG3	1:L:69:GLN:OE1	2.18	0.44
1:K:71:ILE:HD13	1:K:86:HIS:CE1	2.53	0.44
1:E:31:LYS:HE3	1:E:71:ILE:HD12	2.00	0.44
1:I:82:GLU:HA	1:I:82:GLU:OE1	2.17	0.44
1:H:313:GLN:HA	1:H:314:PRO:C	2.37	0.44
6:C:654:HOH:O	1:G:275:LYS:HD2	2.16	0.44
1:E:201:ARG:NH2	6:E:515:HOH:O	2.36	0.43
1:L:245:LEU:HB3	1:L:273:LEU:HD23	2.00	0.43
1:G:31:LYS:HG3	1:G:90:LEU:HA	2.00	0.43
1:H:85:LYS:HB2	1:H:85:LYS:HE3	1.34	0.43
1:A:242:ASN:ND2	1:A:272:LYS:HE2	2.33	0.43
1:B:236:LYS:HD3	6:B:464:HOH:O	2.19	0.43
1:J:220:HIS:CD2	1:J:241:LEU:HD13	2.53	0.43
1:C:38:LYS:HE3	1:C:40:ASN:ND2	2.33	0.43
1:L:265:PHE:CD2	1:L:269:LEU:HD22	2.54	0.43
1:B:228:GLU:CD	1:B:228:GLU:H	2.20	0.43
1:H:35:VAL:HA	1:H:73:THR:O	2.19	0.43
1:H:221:ASP:OD1	1:H:222:ARG:N	2.52	0.43
1:E:201:ARG:O	1:E:205:LEU:HG	2.18	0.43
1:C:123:GLY:HA3	1:C:284:ARG:NH2	2.34	0.43
1:D:313:GLN:HA	1:D:314:PRO:C	2.39	0.43
1:D:189:LEU:HD11	1:D:194:ILE:HD11	2.01	0.43
1:K:50:LEU:HD12	1:K:342:LEU:HD23	2.01	0.43
1:E:245:LEU:HD23	1:E:251:ILE:CD1	2.48	0.42
1:G:110:LYS:HB3	1:G:110:LYS:HE2	1.80	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:129:LEU:HB3	1:L:373:LEU:HD21	2.00	0.42
1:G:31:LYS:CD	1:G:69:GLN:OE1	2.64	0.42
1:J:313:GLN:HA	1:J:314:PRO:C	2.39	0.42
1:F:245:LEU:HB3	1:F:273:LEU:HD23	2.00	0.42
1:C:317:LYS:HE3	6:C:425:HOH:O	2.20	0.42
1:E:313:GLN:HA	1:E:314:PRO:C	2.41	0.42
1:C:227:PRO:HD2	1:C:228:GLU:OE2	2.20	0.42
1:E:245:LEU:CD2	1:E:251:ILE:CD1	2.98	0.41
1:B:195:GLY:HA2	1:B:218:LEU:O	2.19	0.41
1:F:44:THR:HG22	1:F:45:LYS:HG2	2.02	0.41
1:K:29:SER:HB2	1:K:67:GLY:O	2.19	0.41
1:C:256:PRO:HD3	2:C:401:NAD:H52A	2.02	0.41
1:D:104:THR:HG22	5:D:25:GOL:H2	2.01	0.41
1:J:311:ASP:HA	1:J:312:PRO:HA	1.87	0.41
1:G:46:ASN:HB3	1:G:49:PHE:HB2	2.01	0.41
1:J:247:LYS:HG2	1:J:247:LYS:H	1.57	0.41
1:G:60:ARG:HD2	5:G:9:GOL:H31	2.01	0.41
1:J:294:VAL:HG13	6:J:434:HOH:O	2.19	0.41
1:L:29:SER:HB2	1:L:67:GLY:O	2.20	0.41
1:A:219:TYR:CZ	1:A:225:MET:HG3	2.56	0.41
1:L:221:ASP:HB3	1:L:223:LEU:O	2.21	0.41
1:A:106:GLU:HG3	6:A:448:HOH:O	2.20	0.40
1:C:41:GLU:HA	1:G:323:TYR:CZ	2.55	0.40
1:H:306:SER:HB2	1:H:328:ALA:HB3	2.02	0.40
1:K:46:ASN:HA	1:K:47:PRO:HD3	2.00	0.40
1:F:50:LEU:CD1	1:F:342:LEU:HD23	2.51	0.40
1:K:96:THR:HA	1:K:97:PRO:HD3	1.96	0.40
1:D:311:ASP:HA	1:D:312:PRO:HA	1.93	0.40
1:F:50:LEU:HD11	1:F:342:LEU:HD23	2.04	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	350/351 (100%)	340 (97%)	10 (3%)	0	100	100
1	B	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	C	350/351 (100%)	340 (97%)	10 (3%)	0	100	100
1	D	349/351 (99%)	338 (97%)	11 (3%)	0	100	100
1	E	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	F	349/351 (99%)	337 (97%)	12 (3%)	0	100	100
1	G	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	H	349/351 (99%)	340 (97%)	9 (3%)	0	100	100
1	I	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	J	349/351 (99%)	329 (94%)	19 (5%)	1 (0%)	46	41
1	K	349/351 (99%)	338 (97%)	11 (3%)	0	100	100
1	L	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
All	All	4190/4212 (100%)	4057 (97%)	132 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	263	GLY

### 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	291/290 (100%)	288 (99%)	3 (1%)	82	85
1	B	290/290 (100%)	287 (99%)	3 (1%)	82	85
1	C	291/290 (100%)	288 (99%)	3 (1%)	82	85
1	D	290/290 (100%)	286 (99%)	4 (1%)	74	77
1	E	290/290 (100%)	283 (98%)	7 (2%)	57	58
1	F	290/290 (100%)	286 (99%)	4 (1%)	74	77
1	G	290/290 (100%)	285 (98%)	5 (2%)	68	71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	290/290 (100%)	284 (98%)	6 (2%)	61	63
1	I	290/290 (100%)	280 (97%)	10 (3%)	44	41
1	J	290/290 (100%)	282 (97%)	8 (3%)	51	50
1	K	290/290 (100%)	284 (98%)	6 (2%)	61	63
1	L	290/290 (100%)	284 (98%)	6 (2%)	61	63
All	All	3482/3480 (100%)	3417 (98%)	65 (2%)	65	67

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	153	ASP
1	A	236	LYS
1	B	153	ASP
1	B	185	ARG
1	B	268	GLU
1	C	28	ASP
1	C	153	ASP
1	C	268	GLU
1	D	77	GLU
1	D	149	SER
1	D	153	ASP
1	D	268	GLU
1	E	30	LYS
1	E	38	LYS
1	E	69	GLN
1	E	87	ILE
1	E	153	ASP
1	E	185	ARG
1	E	251	ILE
1	F	49	PHE
1	F	153	ASP
1	F	259	GLU
1	F	372	GLU
1	G	30	LYS
1	G	41	GLU
1	G	89	ASP
1	G	109	LYS
1	G	178	ASN
1	H	30	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	49	PHE
1	H	115	LYS
1	H	153	ASP
1	H	357	LYS
1	H	363	THR
1	I	45	LYS
1	I	46	ASN
1	I	74	ASP
1	I	85	LYS
1	I	109	LYS
1	I	115	LYS
1	I	125	ASP
1	I	130	GLN
1	I	153	ASP
1	I	290	ARG
1	J	29	SER
1	J	71	ILE
1	J	106	GLU
1	J	115	LYS
1	J	125	ASP
1	J	185	ARG
1	J	274	LYS
1	J	372	GLU
1	K	30	LYS
1	K	41	GLU
1	K	65	SER
1	K	125	ASP
1	K	153	ASP
1	K	247	LYS
1	L	149	SER
1	L	153	ASP
1	L	185	ARG
1	L	208	GLN
1	L	264	MET
1	L	275	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	B	178	ASN
1	B	254	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	178	ASN
1	C	208	GLN
1	C	254	ASN
1	D	178	ASN
1	E	178	ASN
1	F	164	ASN
1	F	178	ASN
1	F	254	ASN
1	G	178	ASN
1	H	178	ASN
1	H	254	ASN
1	I	46	ASN
1	I	130	GLN
1	I	178	ASN
1	I	254	ASN
1	J	178	ASN
1	K	178	ASN
1	L	208	GLN
1	L	326	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

52 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	$\# Z  > 2$
4	SO4	A	1	-	4,4,4	0.40	0	6,6,6	0.36	0
2	NAD	A	401	-	38,48,48	1.06	3 (7%)	47,73,73	1.83	5 (10%)
3	AZI	A	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	B	16	-	5,5,5	0.49	0	5,5,5	0.61	0
4	SO4	B	2	-	4,4,4	0.21	0	6,6,6	0.44	0
2	NAD	B	401	-	38,48,48	0.96	3 (7%)	47,73,73	1.81	6 (12%)
3	AZI	B	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	C	10	-	5,5,5	0.61	0	5,5,5	0.55	0
5	GOL	C	17	-	5,5,5	0.42	0	5,5,5	0.25	0
4	SO4	C	3	-	4,4,4	0.25	0	6,6,6	0.37	0
2	NAD	C	401	-	38,48,48	1.17	3 (7%)	47,73,73	2.05	5 (10%)
3	AZI	C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	D	11	-	5,5,5	0.63	0	5,5,5	1.28	1 (20%)
5	GOL	D	18	-	5,5,5	0.63	0	5,5,5	0.97	0
5	GOL	D	22	-	5,5,5	0.40	0	5,5,5	0.43	0
5	GOL	D	25	-	5,5,5	0.46	0	5,5,5	0.29	0
4	SO4	D	4	-	4,4,4	0.39	0	6,6,6	0.18	0
2	NAD	D	401	-	38,48,48	1.09	2 (5%)	47,73,73	1.85	5 (10%)
3	AZI	D	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	E	379	-	5,5,5	0.29	0	5,5,5	0.25	0
2	NAD	E	401	-	38,48,48	1.29	4 (10%)	47,73,73	1.81	5 (10%)
3	AZI	E	403	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	F	20	-	4,4,4	0.33	0	6,6,6	0.41	0
5	GOL	F	26	-	5,5,5	0.28	0	5,5,5	0.77	0
2	NAD	F	401	-	38,48,48	1.10	2 (5%)	47,73,73	1.87	8 (17%)
3	AZI	F	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAD	G	401	-	38,48,48	1.21	5 (13%)	47,73,73	1.89	7 (14%)
3	AZI	G	403	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	G	5	-	4,4,4	0.17	0	6,6,6	0.53	0
5	GOL	G	9	-	5,5,5	0.81	0	5,5,5	0.79	0
5	GOL	H	12	-	5,5,5	0.18	0	5,5,5	0.53	0
5	GOL	H	27	-	5,5,5	0.50	0	5,5,5	1.02	0
2	NAD	H	401	-	38,48,48	1.11	3 (7%)	47,73,73	1.81	7 (14%)
3	AZI	H	403	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	H	6	-	4,4,4	0.32	0	6,6,6	0.11	0
5	GOL	I	13	-	5,5,5	0.42	0	5,5,5	0.83	0
5	GOL	I	19	-	5,5,5	0.61	0	5,5,5	0.49	0
5	GOL	I	23	-	5,5,5	0.45	0	5,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	I	401	-	38,48,48	1.03	2 (5%)	47,73,73	1.80	4 (8%)
3	AZI	I	403	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	I	7	-	4,4,4	0.05	0	6,6,6	0.44	0
2	NAD	J	401	-	38,48,48	1.14	2 (5%)	47,73,73	1.99	9 (19%)
3	AZI	J	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	K	14	-	5,5,5	0.17	0	5,5,5	0.95	0
5	GOL	K	15	-	5,5,5	0.36	0	5,5,5	0.61	0
5	GOL	K	24	-	5,5,5	0.37	0	5,5,5	0.57	0
2	NAD	K	401	-	38,48,48	1.10	4 (10%)	47,73,73	1.88	9 (19%)
3	AZI	K	403	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	K	8	-	4,4,4	0.45	0	6,6,6	0.26	0
5	GOL	L	21	-	5,5,5	0.44	0	5,5,5	0.93	0
2	NAD	L	401	-	38,48,48	1.25	2 (5%)	47,73,73	1.88	9 (19%)
3	AZI	L	403	-	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	NAD	A	401	-	-	0/22/62/62	0/5/5/5
3	AZI	A	403	-	-	0/0/0/0	0/0/0/0
5	GOL	B	16	-	-	0/4/4/4	0/0/0/0
4	SO4	B	2	-	-	0/0/0/0	0/0/0/0
2	NAD	B	401	-	-	0/22/62/62	0/5/5/5
3	AZI	B	403	-	-	0/0/0/0	0/0/0/0
5	GOL	C	10	-	-	0/4/4/4	0/0/0/0
5	GOL	C	17	-	-	0/4/4/4	0/0/0/0
4	SO4	C	3	-	-	0/0/0/0	0/0/0/0
2	NAD	C	401	-	-	0/22/62/62	0/5/5/5
3	AZI	C	403	-	-	0/0/0/0	0/0/0/0
5	GOL	D	11	-	-	0/4/4/4	0/0/0/0
5	GOL	D	18	-	-	0/4/4/4	0/0/0/0
5	GOL	D	22	-	-	0/4/4/4	0/0/0/0
5	GOL	D	25	-	-	0/4/4/4	0/0/0/0
4	SO4	D	4	-	-	0/0/0/0	0/0/0/0
2	NAD	D	401	-	-	0/22/62/62	0/5/5/5
3	AZI	D	403	-	-	0/0/0/0	0/0/0/0
5	GOL	E	379	-	-	0/4/4/4	0/0/0/0
2	NAD	E	401	-	-	0/22/62/62	0/5/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AZI	E	403	-	-	0/0/0/0	0/0/0/0
4	SO4	F	20	-	-	0/0/0/0	0/0/0/0
5	GOL	F	26	-	-	0/4/4/4	0/0/0/0
2	NAD	F	401	-	-	0/22/62/62	0/5/5/5
3	AZI	F	403	-	-	0/0/0/0	0/0/0/0
2	NAD	G	401	-	-	0/22/62/62	0/5/5/5
3	AZI	G	403	-	-	0/0/0/0	0/0/0/0
4	SO4	G	5	-	-	0/0/0/0	0/0/0/0
5	GOL	G	9	-	-	0/4/4/4	0/0/0/0
5	GOL	H	12	-	-	0/4/4/4	0/0/0/0
5	GOL	H	27	-	-	0/4/4/4	0/0/0/0
2	NAD	H	401	-	-	0/22/62/62	0/5/5/5
3	AZI	H	403	-	-	0/0/0/0	0/0/0/0
4	SO4	H	6	-	-	0/0/0/0	0/0/0/0
5	GOL	I	13	-	-	0/4/4/4	0/0/0/0
5	GOL	I	19	-	-	0/4/4/4	0/0/0/0
5	GOL	I	23	-	-	0/4/4/4	0/0/0/0
2	NAD	I	401	-	-	0/22/62/62	0/5/5/5
3	AZI	I	403	-	-	0/0/0/0	0/0/0/0
4	SO4	I	7	-	-	0/0/0/0	0/0/0/0
2	NAD	J	401	-	-	0/22/62/62	0/5/5/5
3	AZI	J	403	-	-	0/0/0/0	0/0/0/0
5	GOL	K	14	-	-	0/4/4/4	0/0/0/0
5	GOL	K	15	-	-	0/4/4/4	0/0/0/0
5	GOL	K	24	-	-	0/4/4/4	0/0/0/0
2	NAD	K	401	-	-	0/22/62/62	0/5/5/5
3	AZI	K	403	-	-	0/0/0/0	0/0/0/0
4	SO4	K	8	-	-	0/0/0/0	0/0/0/0
5	GOL	L	21	-	-	0/4/4/4	0/0/0/0
2	NAD	L	401	-	-	0/22/62/62	0/5/5/5
3	AZI	L	403	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	NAD	PA-O2A	-2.31	1.45	1.54
2	G	401	NAD	C8A-N7A	-2.16	1.30	1.34
2	B	401	NAD	PA-O2A	-2.14	1.45	1.54
2	K	401	NAD	PA-O2A	-2.03	1.46	1.54
2	C	401	NAD	C2N-C3N	2.00	1.42	1.39
2	E	401	NAD	C2A-N3A	2.05	1.35	1.32
2	H	401	NAD	C7N-N7N	2.05	1.37	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	NAD	C7N-N7N	2.06	1.37	1.33
2	K	401	NAD	C7N-N7N	2.11	1.37	1.33
2	H	401	NAD	O4B-C1B	2.20	1.44	1.41
2	D	401	NAD	O4D-C1D	2.28	1.44	1.41
2	B	401	NAD	O4D-C1D	2.29	1.44	1.41
2	K	401	NAD	O4D-C1D	2.50	1.44	1.41
2	F	401	NAD	O4B-C1B	2.50	1.44	1.41
2	I	401	NAD	O4B-C1B	2.64	1.44	1.41
2	A	401	NAD	O4D-C1D	2.69	1.44	1.41
2	I	401	NAD	O4D-C1D	2.69	1.44	1.41
2	C	401	NAD	O4B-C1B	2.72	1.44	1.41
2	A	401	NAD	O4B-C1B	2.80	1.44	1.41
2	G	401	NAD	O4B-C1B	2.81	1.44	1.41
2	L	401	NAD	O4B-C1B	2.88	1.44	1.41
2	G	401	NAD	C2N-C3N	2.90	1.43	1.39
2	G	401	NAD	O4D-C1D	2.90	1.44	1.41
2	B	401	NAD	O4B-C1B	2.97	1.45	1.41
2	J	401	NAD	O4D-C1D	3.09	1.45	1.41
2	E	401	NAD	O4D-C1D	3.20	1.45	1.41
2	H	401	NAD	O4D-C1D	3.22	1.45	1.41
2	A	401	NAD	C2N-C3N	3.25	1.43	1.39
2	F	401	NAD	O4D-C1D	3.42	1.45	1.41
2	K	401	NAD	O4B-C1B	3.62	1.45	1.41
2	J	401	NAD	O4B-C1B	3.63	1.45	1.41
2	E	401	NAD	O4B-C1B	3.66	1.45	1.41
2	C	401	NAD	O4D-C1D	3.98	1.46	1.41
2	D	401	NAD	O4B-C1B	4.05	1.46	1.41
2	L	401	NAD	O4D-C1D	4.30	1.46	1.41

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAD	N3A-C2A-N1A	-10.56	120.81	128.89
2	I	401	NAD	N3A-C2A-N1A	-10.07	121.18	128.89
2	H	401	NAD	N3A-C2A-N1A	-9.94	121.28	128.89
2	D	401	NAD	N3A-C2A-N1A	-9.90	121.31	128.89
2	A	401	NAD	N3A-C2A-N1A	-9.84	121.36	128.89
2	B	401	NAD	N3A-C2A-N1A	-9.82	121.37	128.89
2	J	401	NAD	N3A-C2A-N1A	-9.75	121.43	128.89
2	G	401	NAD	N3A-C2A-N1A	-9.28	121.78	128.89
2	K	401	NAD	N3A-C2A-N1A	-9.17	121.88	128.89
2	E	401	NAD	N3A-C2A-N1A	-8.73	122.21	128.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	401	NAD	N3A-C2A-N1A	-8.51	122.38	128.89
2	F	401	NAD	N3A-C2A-N1A	-8.13	122.67	128.89
2	G	401	NAD	O7N-C7N-N7N	-3.99	116.99	122.59
2	K	401	NAD	C4A-C5A-N7A	-3.76	106.02	109.48
2	J	401	NAD	O7N-C7N-N7N	-3.65	117.46	122.59
2	D	401	NAD	O3-PN-O5D	-3.50	93.64	102.94
2	A	401	NAD	O7N-C7N-N7N	-3.16	118.15	122.59
2	F	401	NAD	O4D-C4D-C3D	-3.04	99.02	105.15
2	B	401	NAD	C1B-N9A-C4A	-2.98	122.44	126.94
2	L	401	NAD	C4A-C5A-N7A	-2.83	106.87	109.48
2	F	401	NAD	O7N-C7N-N7N	-2.79	118.67	122.59
2	G	401	NAD	C1B-N9A-C4A	-2.70	122.87	126.94
2	B	401	NAD	O3-PN-O5D	-2.68	95.83	102.94
5	D	11	GOL	O1-C1-C2	-2.57	97.74	110.18
2	K	401	NAD	C4B-O4B-C1B	-2.55	106.91	109.72
2	J	401	NAD	C4A-C5A-N7A	-2.50	107.18	109.48
2	H	401	NAD	C4B-O4B-C1B	-2.49	106.98	109.72
2	A	401	NAD	O3-PN-O5D	-2.49	96.34	102.94
2	L	401	NAD	O7N-C7N-N7N	-2.45	119.14	122.59
2	C	401	NAD	C1B-N9A-C4A	-2.43	123.27	126.94
2	G	401	NAD	C4A-C5A-N7A	-2.41	107.26	109.48
2	A	401	NAD	C1B-N9A-C4A	-2.40	123.32	126.94
2	H	401	NAD	C4A-C5A-N7A	-2.39	107.28	109.48
2	J	401	NAD	PN-O3-PA	-2.39	126.03	132.73
2	C	401	NAD	O3-PN-O5D	-2.38	96.63	102.94
2	F	401	NAD	C4A-C5A-N7A	-2.33	107.34	109.48
2	I	401	NAD	C4B-O4B-C1B	-2.28	107.21	109.72
2	D	401	NAD	PN-O3-PA	-2.28	126.34	132.73
2	B	401	NAD	PN-O3-PA	-2.22	126.48	132.73
2	J	401	NAD	C1B-N9A-C4A	-2.20	123.62	126.94
2	G	401	NAD	O3-PN-O5D	-2.20	97.10	102.94
2	E	401	NAD	C1B-N9A-C4A	-2.15	123.70	126.94
2	K	401	NAD	PN-O3-PA	-2.14	126.71	132.73
2	F	401	NAD	O3-PN-O5D	-2.14	97.25	102.94
2	L	401	NAD	C1B-N9A-C4A	-2.14	123.72	126.94
2	H	401	NAD	O7N-C7N-N7N	-2.13	119.59	122.59
2	H	401	NAD	O5D-PN-O1N	-2.13	101.34	109.62
2	H	401	NAD	O3-PN-O5D	-2.09	97.38	102.94
2	L	401	NAD	PN-O3-PA	-2.07	126.91	132.73
2	I	401	NAD	C5N-C4N-C3N	-2.06	117.74	120.33
2	E	401	NAD	PN-O3-PA	-2.06	126.94	132.73
2	K	401	NAD	C1B-N9A-C4A	-2.03	123.88	126.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAD	C4A-C5A-N7A	-2.02	107.62	109.48
2	J	401	NAD	O3-PA-O5B	2.04	108.35	102.94
2	K	401	NAD	C3N-C2N-N1N	2.08	122.76	120.36
2	I	401	NAD	O2N-PN-O1N	2.11	123.95	112.53
2	L	401	NAD	O2A-PA-O3	2.11	114.67	105.09
2	K	401	NAD	O4B-C4B-C3B	2.14	109.45	105.15
2	J	401	NAD	C4D-O4D-C1D	2.26	112.20	109.72
2	B	401	NAD	C2B-C1B-N9A	2.31	117.82	114.29
2	J	401	NAD	O2A-PA-O3	2.33	115.68	105.09
2	E	401	NAD	C3N-C7N-N7N	2.41	120.45	117.82
2	L	401	NAD	C3N-C7N-N7N	2.45	120.50	117.82
2	B	401	NAD	O2A-PA-O3	2.48	116.37	105.09
2	H	401	NAD	C3N-C7N-N7N	2.56	120.62	117.82
2	K	401	NAD	O3-PA-O5B	2.56	109.73	102.94
2	K	401	NAD	C3N-C7N-N7N	2.62	120.69	117.82
2	G	401	NAD	O2A-PA-O3	2.70	117.36	105.09
2	L	401	NAD	C4D-O4D-C1D	2.73	112.72	109.72
2	D	401	NAD	C3N-C7N-N7N	2.92	121.01	117.82
2	A	401	NAD	C3N-C7N-N7N	3.31	121.44	117.82
2	F	401	NAD	C3N-C7N-N7N	3.31	121.44	117.82
2	G	401	NAD	O7N-C7N-C3N	3.49	123.40	119.59
2	C	401	NAD	C3N-C7N-N7N	3.72	121.89	117.82
2	F	401	NAD	C4D-O4D-C1D	3.73	113.82	109.72
2	J	401	NAD	C3N-C7N-N7N	4.03	122.23	117.82
2	C	401	NAD	O4D-C1D-N1N	4.13	112.67	108.13
2	E	401	NAD	O4D-C1D-N1N	4.44	113.01	108.13
2	L	401	NAD	O4D-C1D-N1N	4.55	113.14	108.13
2	F	401	NAD	O4D-C1D-N1N	5.22	113.87	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	1	0
5	B	16	GOL	1	0
2	B	401	NAD	1	0
5	C	10	GOL	1	0
2	C	401	NAD	2	0
5	D	11	GOL	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	25	GOL	1	0
2	D	401	NAD	1	0
2	E	401	NAD	1	0
2	F	401	NAD	1	0
2	G	401	NAD	1	0
5	G	9	GOL	3	0
2	H	401	NAD	1	0
2	I	401	NAD	1	0
2	J	401	NAD	1	0
5	K	24	GOL	1	0
2	K	401	NAD	1	0
2	L	401	NAD	1	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	351/351 (100%)	-0.53	1 (0%) 94 94	12, 19, 32, 45	0
1	B	351/351 (100%)	-0.51	2 (0%) 90 90	12, 20, 33, 50	0
1	C	351/351 (100%)	-0.44	1 (0%) 94 94	15, 22, 35, 51	0
1	D	351/351 (100%)	-0.57	3 (0%) 85 86	14, 20, 32, 49	0
1	E	351/351 (100%)	-0.54	2 (0%) 90 90	10, 18, 31, 44	0
1	F	351/351 (100%)	-0.23	5 (1%) 78 78	13, 25, 42, 58	0
1	G	351/351 (100%)	-0.43	1 (0%) 94 94	10, 22, 33, 48	0
1	H	351/351 (100%)	-0.35	5 (1%) 78 78	11, 22, 38, 57	0
1	I	351/351 (100%)	-0.12	7 (1%) 68 69	13, 25, 42, 55	0
1	J	351/351 (100%)	-0.04	7 (1%) 68 69	12, 26, 43, 50	0
1	K	351/351 (100%)	-0.42	2 (0%) 90 90	15, 23, 36, 56	0
1	L	351/351 (100%)	-0.50	2 (0%) 90 90	13, 21, 33, 49	0
All	All	4212/4212 (100%)	-0.39	38 (0%) 85 86	10, 22, 37, 58	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	28	ASP	5.6
1	K	28	ASP	5.0
1	I	28	ASP	4.6
1	G	28	ASP	4.2
1	J	28	ASP	4.1
1	I	78	GLY	3.7
1	C	28	ASP	3.6
1	F	28	ASP	3.6
1	I	79	PRO	3.6
1	L	28	ASP	3.3
1	F	29	SER	3.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	134	ALA	3.0
1	J	79	PRO	2.9
1	F	79	PRO	2.9
1	B	28	ASP	2.8
1	H	47	PRO	2.7
1	D	28	ASP	2.7
1	J	78	GLY	2.7
1	L	79	PRO	2.7
1	I	317	LYS	2.6
1	B	29	SER	2.6
1	K	65	SER	2.6
1	F	65	SER	2.5
1	H	44	THR	2.5
1	A	28	ASP	2.3
1	I	29	SER	2.3
1	E	47	PRO	2.3
1	I	45	LYS	2.2
1	E	28	ASP	2.2
1	J	109	LYS	2.2
1	J	289	GLU	2.1
1	D	29	SER	2.1
1	I	267	LYS	2.1
1	F	47	PRO	2.1
1	H	48	ASN	2.1
1	H	357	LYS	2.1
1	D	231	LYS	2.0
1	J	259	GLU	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	GOL	D	25	6/6	0.82	0.26	9.89	51,54,55,55	0
5	GOL	L	21	6/6	0.78	0.21	8.66	44,47,47,49	0
5	GOL	E	379	6/6	0.91	0.19	8.18	35,39,40,43	0
5	GOL	H	27	6/6	0.85	0.17	5.09	35,39,40,45	0
5	GOL	F	26	6/6	0.89	0.14	4.32	44,48,49,50	0
4	SO4	K	8	5/5	0.98	0.14	3.43	32,32,33,34	0
5	GOL	I	13	6/6	0.90	0.16	3.09	26,33,35,36	0
4	SO4	H	6	5/5	0.98	0.15	2.97	32,33,34,36	0
5	GOL	I	19	6/6	0.87	0.20	2.95	36,41,41,43	0
5	GOL	K	24	6/6	0.83	0.14	2.62	44,44,45,46	0
4	SO4	I	7	5/5	0.93	0.16	2.51	53,53,56,56	0
4	SO4	B	2	5/5	0.96	0.15	1.51	45,46,48,48	0
4	SO4	D	4	5/5	0.98	0.14	1.41	43,44,45,48	0
4	SO4	C	3	5/5	0.97	0.18	1.39	46,46,49,49	0
5	GOL	I	23	6/6	0.82	0.15	1.33	41,42,43,45	0
5	GOL	K	15	6/6	0.92	0.11	0.78	36,38,39,40	0
3	AZI	D	403	3/3	0.99	0.09	0.45	16,16,18,18	0
3	AZI	E	403	3/3	0.98	0.08	0.12	12,12,13,15	0
3	AZI	J	403	3/3	0.98	0.08	0.03	19,19,20,22	0
4	SO4	F	20	5/5	0.94	0.13	-0.05	26,28,29,29	5
2	NAD	H	401	44/44	0.97	0.07	-0.51	12,16,21,23	0
2	NAD	F	401	44/44	0.97	0.08	-0.52	14,20,26,27	0
2	NAD	K	401	44/44	0.98	0.07	-0.67	14,17,23,24	0
2	NAD	G	401	44/44	0.98	0.07	-0.67	14,19,24,25	0
3	AZI	L	403	3/3	0.99	0.07	-0.67	17,17,18,22	0
3	AZI	I	403	3/3	0.99	0.07	-0.80	18,18,19,19	0
2	NAD	C	401	44/44	0.97	0.08	-0.82	13,21,23,25	0
3	AZI	G	403	3/3	0.98	0.06	-0.86	17,17,18,19	0
3	AZI	H	403	3/3	0.99	0.07	-0.94	15,15,15,17	0
5	GOL	H	12	6/6	0.97	0.08	-0.94	24,26,26,29	0
3	AZI	B	403	3/3	0.99	0.07	-0.98	12,12,13,15	0
2	NAD	J	401	44/44	0.98	0.07	-1.03	13,19,33,35	0
2	NAD	E	401	44/44	0.99	0.06	-1.07	9,14,17,17	0
2	NAD	I	401	44/44	0.98	0.07	-1.19	12,17,24,26	0
2	NAD	A	401	44/44	0.98	0.06	-1.20	11,17,21,23	0
2	NAD	B	401	44/44	0.98	0.07	-1.22	13,17,22,23	0
2	NAD	L	401	44/44	0.99	0.05	-1.22	11,17,23,25	0
3	AZI	C	403	3/3	0.99	0.07	-1.24	15,15,16,17	0
5	GOL	K	14	6/6	0.97	0.06	-1.36	23,24,25,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	D	401	44/44	0.98	0.06	-1.45	14,18,23,25	0
3	AZI	A	403	3/3	0.99	0.06	-1.70	14,14,14,15	0
3	AZI	K	403	3/3	0.99	0.05	-2.08	13,13,17,18	0
3	AZI	F	403	3/3	0.99	0.04	-2.26	13,13,17,20	0
5	GOL	B	16	6/6	0.90	0.16	-	42,43,45,49	0
5	GOL	C	10	6/6	0.92	0.12	-	39,42,45,47	0
4	SO4	G	5	5/5	0.93	0.21	-	28,28,31,32	5
5	GOL	C	17	6/6	0.87	0.19	-	49,50,51,53	0
4	SO4	A	1	5/5	0.98	0.12	-	47,48,49,50	0
5	GOL	D	22	6/6	0.85	0.19	-	50,53,54,54	0
5	GOL	D	11	6/6	0.74	0.20	-	53,55,56,56	0
5	GOL	G	9	6/6	0.93	0.09	-	31,36,38,38	0
5	GOL	D	18	6/6	0.92	0.19	-	43,45,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.