



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:45 AM GMT

PDB ID : 3PVZ  
Title : UDP-N-acetylglucosamine 4,6-dehydratase from *Vibrio fischeri*  
Authors : Osipiuk, J.; Marshall, N.; Tesar, C.; Pearson, L.; Buck, K.; Joachimiak, A.;  
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Deposited on : 2010-12-07  
Resolution : 2.10 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

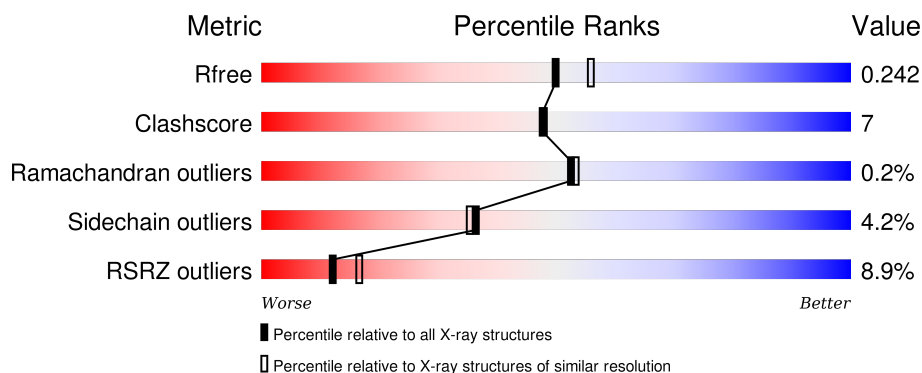
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	399	<div> <div>5%</div> <div>79%</div> <div>13%</div> <div>7%</div> </div>
1	B	399	<div> <div>12%</div> <div>61%</div> <div>13%</div> <div>25%</div> </div>
1	C	399	<div> <div>6%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>
1	D	399	<div> <div>7%</div> <div>75%</div> <div>17%</div> <div>7%</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
3	SCN	A	604	-	-	-	X
3	SCN	C	601	-	-	-	X
3	SCN	D	603	-	-	-	X
4	NA	A	607	-	-	-	X
4	NA	A	608	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12086 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.

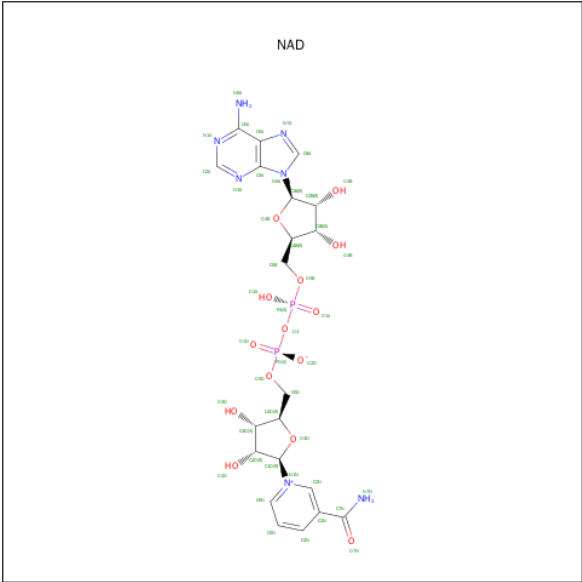
- Molecule 1 is a protein called UDP-N-acetylglucosamine 4,6-dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	Se	0	14	0
			3061	1959	511	574	5	12			
1	B	300	Total	C	N	O	S	Se	0	6	0
			2453	1561	417	460	3	12			
1	C	371	Total	C	N	O	S	Se	0	7	0
			3012	1925	502	567	5	13			
1	D	371	Total	C	N	O	S	Se	0	6	0
			3009	1921	501	570	5	12			

There are 12 discrepancies between the modelled and reference sequences:

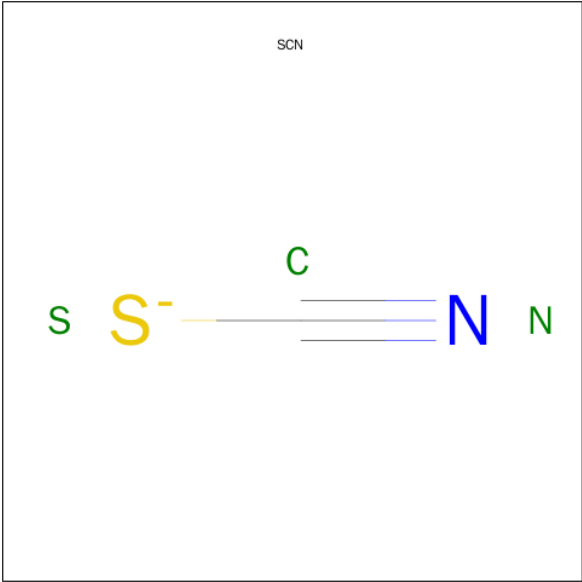
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q5E8L1
A	-1	ASN	-	EXPRESSION TAG	UNP Q5E8L1
A	0	ALA	-	EXPRESSION TAG	UNP Q5E8L1
B	-2	SER	-	EXPRESSION TAG	UNP Q5E8L1
B	-1	ASN	-	EXPRESSION TAG	UNP Q5E8L1
B	0	ALA	-	EXPRESSION TAG	UNP Q5E8L1
C	-2	SER	-	EXPRESSION TAG	UNP Q5E8L1
C	-1	ASN	-	EXPRESSION TAG	UNP Q5E8L1
C	0	ALA	-	EXPRESSION TAG	UNP Q5E8L1
D	-2	SER	-	EXPRESSION TAG	UNP Q5E8L1
D	-1	ASN	-	EXPRESSION TAG	UNP Q5E8L1
D	0	ALA	-	EXPRESSION TAG	UNP Q5E8L1

- 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		

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N S 3 1 1 1	0	0
3	A	1	Total C N S 3 1 1 1	0	0
3	C	1	Total C N S 3 1 1 1	0	0
3	D	1	Total C N S 3 1 1 1	0	0
3	D	1	Total C N S 3 1 1 1	0	0

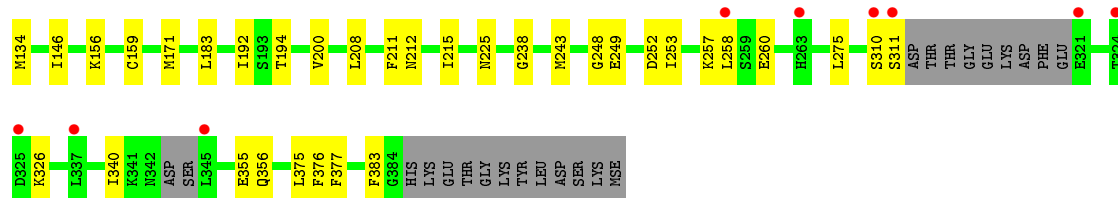
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Na 3 3	0	0

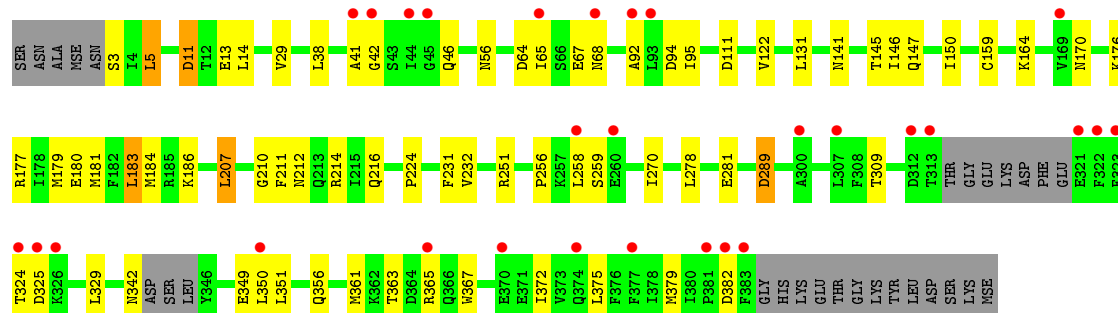
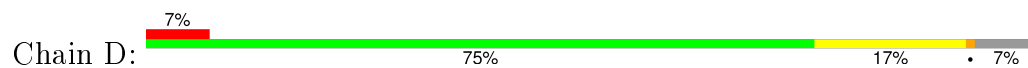
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	113	Total O 113 113	0	0
5	B	41	Total O 41 41	0	0
5	C	74	Total O 74 74	0	0
5	D	129	Total O 129 129	0	0





- Molecule 1: UDP-N-acetylglucosamine 4,6-dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.92Å 74.84Å 88.79Å 102.71° 95.15° 100.35°	Depositor
Resolution (Å)	38.00 – 2.10 38.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.00-2.10) 89.8 (38.74-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.187 , 0.233 0.197 , 0.242	Depositor DCC
$R_{free}$ test set	4852 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 97465 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: NA, SCN, 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	0.80	0/3145	0.79	1/4212 (0.0%)
1	B	0.74	0/2498	0.75	1/3327 (0.0%)
1	C	0.73	0/3076	0.75	2/4117 (0.0%)
1	D	0.78	2/3068 (0.1%)	0.76	1/4108 (0.0%)
All	All	0.76	2/11787 (0.0%)	0.76	5/15764 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	VAL	CB-CG2	5.54	1.64	1.52
1	D	67	GLU	CD-OE2	-5.12	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	111	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	94	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	252	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	C	133	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3061	0	3088	40	0
1	B	2453	0	2447	35	0
1	C	3012	0	3010	48	0
1	D	3009	0	3000	59	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	A	6	0	0	1	0
3	C	3	0	0	0	0
3	D	6	0	0	1	0
4	A	3	0	0	0	0
5	A	113	0	0	1	0
5	B	41	0	0	4	0
5	C	74	0	0	0	0
5	D	129	0	0	3	0
All	All	12086	0	11649	173	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 (173) 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:D:365[B]:ARG:HG3	1:D:365[B]:ARG:HH11	1.09	1.11
1:D:365[B]:ARG:HH11	1:D:365[B]:ARG:CG	1.67	1.05
1:D:184:MSE:HE1	1:D:251:ARG:HD3	1.40	1.02
1:C:243:MSE:HA	1:C:243:MSE:HE2	1.44	0.99
1:B:123:ARG:O	1:B:126:LYS:HG2	1.72	0.90
1:D:365[B]:ARG:HG3	1:D:365[B]:ARG:NH1	1.88	0.87
1:C:26:LEU:HD21	1:C:243:MSE:CE	2.11	0.80
1:C:65:ILE:HD13	1:D:65[B]:ILE:HD12	1.63	0.79
1:D:365[B]:ARG:NH1	1:D:365[B]:ARG:CG	2.40	0.76
1:A:134:MSE:HE1	1:A:172:MSE:HG2	1.67	0.75
1:B:216:GLN:NE2	5:B:427:HOH:O	2.20	0.74
1:D:65[B]:ILE:HD11	1:D:94:ASP:HB2	1.72	0.72
1:A:98[B]:ILE:HD13	1:B:362:LYS:HG2	1.73	0.70
1:A:10:ARG:NH1	1:A:14:LEU:CD1	2.57	0.68
1:C:46:GLN:HG2	1:C:73:LEU:HD13	1.78	0.66
1:D:324:THR:HG22	1:D:325:ASP:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:MSE:HA	1:C:243:MSE:CE	2.25	0.65
1:B:390:LYS:NZ	5:B:411:HOH:O	2.30	0.65
1:B:46[A]:GLN:HG2	1:B:73:LEU:HD13	1.78	0.64
1:B:46[B]:GLN:HG2	1:B:47:ALA:N	2.12	0.64
1:C:65:ILE:CD1	1:D:65[B]:ILE:HD12	2.28	0.64
1:C:377:PHE:CE2	1:C:383:PHE:O	2.51	0.63
1:B:126:LYS:NZ	1:B:127:ASP:OD2	2.33	0.62
1:B:53:PHE:CE2	1:B:84:ILE:HD13	2.34	0.62
1:D:179:MSE:HE3	1:D:183:LEU:HD22	1.82	0.61
1:A:134:MSE:HE2	1:A:172:MSE:SE	2.51	0.61
1:C:26:LEU:HD21	1:C:243:MSE:HE1	1.82	0.60
1:D:122:VAL:HG13	1:D:170:ASN:ND2	2.17	0.59
1:C:156:LYS:NZ	1:C:248:GLY:O	2.36	0.58
1:A:3:SER:OG	1:A:277[B]:GLN:NE2	2.37	0.57
1:D:281[A]:GLU:OE2	5:D:523:HOH:O	2.18	0.57
1:C:48:VAL:HG12	1:C:238:GLY:HA2	1.86	0.57
1:D:146:ILE:O	1:D:150:ILE:HD12	2.05	0.56
1:D:41:ALA:HB3	1:D:64:ASP:CG	2.26	0.56
1:A:327:GLU:O	1:A:329:LEU:CD1	2.54	0.55
1:B:159:CYS:SG	1:B:183:LEU:HD21	2.47	0.54
1:D:232:VAL:HG11	3:D:603:SCN:C	2.38	0.54
1:A:7:LEU:HD21	1:A:274:TYR:HA	1.90	0.54
1:A:178[B]:ILE:HD11	1:A:379:MSE:HB3	1.89	0.53
1:D:65[B]:ILE:HD11	1:D:94:ASP:CB	2.37	0.53
1:A:165:ALA:CB	1:A:324:THR:HG23	2.39	0.53
1:B:64:ASP:O	1:B:92:ALA:HA	2.09	0.53
1:A:121:HIS:HB3	1:A:123[A]:ARG:NE	2.23	0.52
1:D:65[B]:ILE:CD1	1:D:94:ASP:HB2	2.38	0.52
1:D:375:LEU:O	1:D:379:MSE:HG2	2.09	0.52
1:C:133:ARG:HD2	5:D:442:HOH:O	2.10	0.52
1:D:147:GLN:HA	1:D:150:ILE:HD12	1.92	0.51
1:D:361:MSE:HB3	1:D:367:TRP:HB3	1.92	0.51
1:B:29:VAL:HG11	1:B:246:ILE:CG2	2.40	0.51
1:B:194:THR:OG1	1:B:253:ILE:HG23	2.11	0.51
1:A:307:LEU:HD23	1:A:309[B]:THR:CG2	2.40	0.51
1:A:165:ALA:HB1	1:A:324:THR:HG23	1.92	0.50
1:D:324:THR:CG2	1:D:325:ASP:N	2.75	0.50
1:A:327:GLU:O	1:A:329:LEU:HD12	2.10	0.50
1:D:159:CYS:SG	1:D:183:LEU:HD21	2.51	0.50
1:C:310:SER:O	1:C:311:SER:CB	2.59	0.50
1:D:212:ASN:OD1	1:D:216:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ARG:NH1	1:D:180:GLU:OE1	2.44	0.49
1:C:26:LEU:CD2	1:C:243:MSE:HE1	2.42	0.49
5:B:411:HOH:O	1:D:56:ASN:HB2	2.12	0.49
1:B:46[B]:GLN:CG	1:B:47:ALA:N	2.76	0.49
1:A:206:SER:HB2	3:A:604:SCN:C	2.43	0.49
1:A:10:ARG:NH1	1:A:14:LEU:HD13	2.27	0.49
1:A:10:ARG:NH1	1:A:14:LEU:HD12	2.28	0.49
1:D:64:ASP:O	1:D:92:ALA:HA	2.12	0.49
1:A:10:ARG:CZ	1:A:14:LEU:CD1	2.90	0.49
1:B:51:GLU:OE2	1:B:235:GLN:HG2	2.11	0.49
1:C:377:PHE:HE2	1:C:383:PHE:O	1.94	0.48
1:B:97:SER:HB2	1:B:99:GLU:OE1	2.13	0.48
1:A:329:LEU:HD12	1:A:329:LEU:N	2.29	0.48
1:C:98:ILE:HD12	1:D:365[B]:ARG:HH12	1.78	0.48
1:D:131[A]:LEU:HD11	1:D:372:ILE:HG21	1.95	0.48
1:A:42:GLY:O	1:A:46:GLN:HG3	2.13	0.48
1:C:208:LEU:HD23	1:C:211:PHE:CE2	2.49	0.48
1:B:239:GLU:O	1:B:243:MSE:HG2	2.13	0.48
1:C:114:LEU:HD12	1:C:114:LEU:N	2.29	0.48
1:B:7:LEU:O	1:B:7:LEU:HD23	2.14	0.48
1:B:19:ILE:HD12	1:B:20:ASN:N	2.29	0.48
1:C:44:ILE:O	1:C:48:VAL:HG13	2.14	0.47
1:C:159:CYS:O	1:C:194:THR:HA	2.14	0.47
1:D:184:MSE:CE	1:D:251:ARG:HD3	2.29	0.47
1:C:26:LEU:HD21	1:C:243:MSE:HE3	1.94	0.47
1:A:368:THR:OG1	1:A:371:GLU:HB2	2.15	0.47
1:D:289:ASP:N	1:D:289:ASP:OD1	2.46	0.47
1:A:90:THR:O	1:B:126:LYS:CE	2.63	0.47
1:A:15:PHE:CE1	1:A:337:LEU:HD23	2.50	0.47
1:C:26:LEU:CG	1:C:243:MSE:HE1	2.44	0.47
1:A:13:GLU:HB3	5:A:509:HOH:O	2.13	0.47
1:D:207:LEU:HD11	1:D:224:PRO:HD3	1.96	0.47
1:B:249:GLU:OE2	1:B:341:LYS:NZ	2.48	0.47
1:A:160[B]:VAL:HG12	1:A:161:SER:O	2.15	0.47
1:C:5:LEU:HD11	1:C:13:GLU:HG2	1.97	0.47
1:A:146:ILE:HG21	1:A:186:LYS:HB3	1.98	0.46
1:D:131[A]:LEU:CD1	1:D:372:ILE:HG21	2.45	0.46
1:B:56:ASN:ND2	5:B:410:HOH:O	2.48	0.46
1:C:212:ASN:ND2	1:D:216:GLN:OE1	2.48	0.46
1:C:146:ILE:HD11	1:C:183:LEU:HD23	1.97	0.46
1:A:134:MSE:CE	1:A:172:MSE:SE	3.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ILE:HG23	1:D:365[B]:ARG:NH1	2.32	0.45
1:C:26:LEU:HD11	1:C:243:MSE:HE3	1.99	0.45
1:A:64:ASP:O	1:A:92:ALA:HA	2.16	0.45
1:C:208:LEU:CD2	1:C:211:PHE:CE2	3.00	0.45
1:C:64:ASP:O	1:C:92:ALA:HA	2.16	0.45
1:C:215:ILE:HD11	1:C:275:LEU:HD21	1.99	0.45
1:D:122:VAL:CG1	1:D:170:ASN:ND2	2.80	0.45
1:B:7:LEU:HD13	1:B:202:PHE:CZ	2.52	0.45
1:A:147:GLN:HA	1:A:150:ILE:HD12	1.98	0.44
1:B:19:ILE:C	1:B:19:ILE:HD12	2.38	0.44
1:A:125:GLU:CG	1:A:171:MSE:HB2	2.47	0.44
1:D:210:GLY:O	1:D:214:ARG:HG2	2.18	0.44
1:D:363:THR:O	1:D:365[B]:ARG:HD2	2.18	0.44
1:D:365[B]:ARG:HH11	1:D:365[B]:ARG:HG2	1.71	0.44
1:B:51:GLU:OE2	1:B:235:GLN:CG	2.66	0.44
1:C:26:LEU:HG	1:C:243:MSE:HE1	2.00	0.44
1:A:71:VAL:O	1:A:75[B]:ARG:HG3	2.18	0.44
1:D:176:LYS:NZ	2:D:501:NAD:O2D	2.51	0.44
1:A:172:MSE:HB3	1:A:172:MSE:HE3	1.90	0.43
1:B:161:SER:C	1:B:162:THR:O	2.57	0.43
1:A:323:PHE:CD1	1:A:329:LEU:HD21	2.52	0.43
1:C:146:ILE:HD11	1:C:183:LEU:CD2	2.49	0.43
1:B:29:VAL:HG11	1:B:246:ILE:HG21	2.01	0.43
1:D:324:THR:HG22	1:D:325:ASP:H	1.83	0.43
1:B:240:LEU:HD11	1:B:254:PHE:HB3	2.01	0.43
1:C:94:ASP:O	1:C:97:SER:CB	2.67	0.43
1:D:181:MSE:HB3	1:D:351:LEU:HD21	2.01	0.43
1:C:310:SER:O	1:C:311:SER:HB3	2.19	0.43
1:C:171:MSE:HE3	1:C:376:PHE:CE2	2.54	0.42
1:B:156:LYS:HG2	1:B:245:CYS:O	2.19	0.42
1:C:44:ILE:HD11	1:C:200:VAL:HG21	2.01	0.42
1:D:231:PHE:CE1	1:D:270:ILE:HD11	2.54	0.42
1:C:34:ARG:HB3	1:C:59:LYS:HD2	2.00	0.42
1:D:141:ASN:O	1:D:145:THR:HG23	2.19	0.42
1:D:146:ILE:HG22	1:D:150:ILE:HD11	2.02	0.42
1:C:121[A]:HIS:NE2	1:D:68:ASN:OD1	2.52	0.42
1:A:15:PHE:CE1	1:A:337:LEU:CD2	3.03	0.42
1:C:253:ILE:HB	1:C:340:ILE:HB	2.01	0.42
1:B:159:CYS:O	1:B:194:THR:HA	2.20	0.42
1:C:97:SER:OG	1:C:99:GLU:OE1	2.38	0.42
1:C:119:LEU:O	1:C:134:MSE:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HD21	1:D:256:PRO:HB2	2.01	0.42
1:B:29:VAL:HG11	1:B:246:ILE:HG23	2.02	0.41
1:D:179:MSE:HE3	1:D:183:LEU:CD2	2.50	0.41
1:A:178[B]:ILE:CD1	1:A:379:MSE:HB3	2.49	0.41
1:A:307:LEU:HD23	1:A:309[B]:THR:HG22	2.02	0.41
1:C:215:ILE:HD11	1:C:275:LEU:CD2	2.50	0.41
1:D:207:LEU:HD22	1:D:211:PHE:CE1	2.55	0.41
1:D:42:GLY:O	1:D:46:GLN:HG3	2.20	0.41
1:A:272:VAL:HG13	1:A:282:PRO:HG2	2.02	0.41
1:C:249:GLU:O	1:C:252:ASP:HB2	2.20	0.41
1:D:5:LEU:HD12	1:D:5:LEU:HA	1.95	0.41
1:C:26:LEU:HD11	1:C:243:MSE:CE	2.51	0.41
1:D:65[B]:ILE:HD11	1:D:94:ASP:OD2	2.21	0.41
1:B:229[B]:ARG:HD3	1:B:231:PHE:CZ	2.56	0.41
1:D:179:MSE:CE	1:D:183:LEU:HD22	2.49	0.41
1:A:74:VAL:O	1:A:78:ARG:HG2	2.21	0.41
1:A:136:ASP:OD2	1:B:99:GLU:OE2	2.38	0.41
1:A:38:LEU:HB3	1:A:95:ILE:HD11	2.03	0.41
1:B:5:LEU:HG	1:B:233:THR:HG21	2.03	0.41
1:D:147:GLN:NE2	1:D:186:LYS:HE3	2.36	0.41
1:B:172:MSE:HE3	1:B:172:MSE:HB3	2.02	0.40
1:D:365[B]:ARG:NH1	5:D:433:HOH:O	2.54	0.40
1:C:94:ASP:O	1:C:97:SER:HB2	2.21	0.40
1:B:156:LYS:NZ	1:B:248:GLY:O	2.33	0.40
1:C:171:MSE:CE	1:C:376:PHE:CD2	3.05	0.40
1:D:38:LEU:HB3	1:D:95:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/399 (96%)	375 (98%)	7 (2%)	0	100	100
1	B	295/399 (74%)	284 (96%)	9 (3%)	2 (1%)	26	21
1	C	372/399 (93%)	368 (99%)	4 (1%)	0	100	100
1	D	371/399 (93%)	362 (98%)	8 (2%)	1 (0%)	46	45
All	All	1420/1596 (89%)	1389 (98%)	28 (2%)	3 (0%)	52	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	THR
1	B	166	ALA
1	D	13	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/338 (102%)	329 (96%)	14 (4%)	37	36
1	B	271/338 (80%)	256 (94%)	15 (6%)	27	23
1	C	334/338 (99%)	325 (97%)	9 (3%)	52	56
1	D	334/338 (99%)	316 (95%)	18 (5%)	27	24
All	All	1282/1352 (95%)	1226 (96%)	56 (4%)	36	33

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	58	GLN
1	A	123[A]	ARG
1	A	123[B]	ARG
1	A	161	SER
1	A	164	LYS
1	A	278	LEU
1	A	284[A]	LEU

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Mol	Chain	Res	Type
1	A	284[B]	LEU
1	A	288	GLU
1	A	309[A]	THR
1	A	309[B]	THR
1	A	321	GLU
1	A	327	GLU
1	B	5	LEU
1	B	14	LEU
1	B	17	GLN
1	B	18	ASP
1	B	26	LEU
1	B	29	VAL
1	B	43	SER
1	B	84	ILE
1	B	98	ILE
1	B	125	GLU
1	B	127	ASP
1	B	169	VAL
1	B	183	LEU
1	B	203	SER
1	B	356	GLN
1	C	24	LYS
1	C	192	ILE
1	C	225	ASN
1	C	257	LYS
1	C	258	LEU
1	C	260	GLU
1	C	355	GLU
1	C	356	GLN
1	C	375	LEU
1	D	3	SER
1	D	5	LEU
1	D	11[A]	ASP
1	D	11[B]	ASP
1	D	164	LYS
1	D	183	LEU
1	D	207	LEU
1	D	258	LEU
1	D	259	SER
1	D	278	LEU
1	D	289	ASP
1	D	309	THR

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Mol	Chain	Res	Type
1	D	329	LEU
1	D	342	ASN
1	D	349	GLU
1	D	350	LEU
1	D	356	GLN
1	D	382	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	ASN
1	C	212	ASN
1	C	225	ASN
1	C	263	HIS
1	C	301	GLN
1	D	170	ASN
1	D	342	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z  > 2$
2	NAD	A	501	-	38,48,48	1.13	2 (5%)	47,73,73	2.34	11 (23%)
3	SCN	A	604	-	2,2,2	1.82	1 (50%)	1,1,1	0.44	0
3	SCN	A	605	-	2,2,2	1.56	1 (50%)	1,1,1	0.42	0
2	NAD	B	501	-	38,48,48	1.29	4 (10%)	47,73,73	2.22	11 (23%)
2	NAD	C	501	-	38,48,48	1.01	2 (5%)	47,73,73	1.94	10 (21%)
3	SCN	C	601	-	2,2,2	1.58	1 (50%)	1,1,1	0.06	0
2	NAD	D	501	-	38,48,48	1.03	2 (5%)	47,73,73	2.26	10 (21%)
3	SCN	D	602	-	2,2,2	1.37	0	1,1,1	0.25	0
3	SCN	D	603	-	2,2,2	1.29	0	1,1,1	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	SCN	A	604	-	-	0/0/0/0	0/0/0/0
3	SCN	A	605	-	-	0/0/0/0	0/0/0/0
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
3	SCN	C	601	-	-	0/0/0/0	0/0/0/0
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5
3	SCN	D	602	-	-	0/0/0/0	0/0/0/0
3	SCN	D	603	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C4A-N3A	-3.38	1.30	1.35
2	C	501	NAD	C4A-N3A	-2.76	1.31	1.35
2	A	501	NAD	C8A-N7A	-2.54	1.29	1.34
2	D	501	NAD	C8A-N7A	-2.37	1.30	1.34
2	C	501	NAD	O4B-C1B	2.04	1.43	1.41
3	A	605	SCN	C-S	2.11	1.77	1.63
3	C	601	SCN	C-S	2.17	1.77	1.63
2	B	501	NAD	C2N-C3N	2.24	1.42	1.39
3	A	604	SCN	C-S	2.50	1.79	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	C7N-N7N	2.64	1.38	1.33
2	B	501	NAD	O4B-C1B	3.17	1.45	1.41
2	B	501	NAD	O4D-C1D	3.64	1.45	1.41
2	A	501	NAD	O4D-C1D	3.75	1.45	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	N3A-C2A-N1A	-10.51	120.84	128.89
2	B	501	NAD	N3A-C2A-N1A	-9.47	121.64	128.89
2	D	501	NAD	N3A-C2A-N1A	-8.93	122.06	128.89
2	C	501	NAD	PN-O3-PA	-6.32	114.97	132.73
2	C	501	NAD	N3A-C2A-N1A	-6.13	124.20	128.89
2	D	501	NAD	PN-O3-PA	-5.16	118.22	132.73
2	A	501	NAD	PN-O3-PA	-4.83	119.16	132.73
2	B	501	NAD	PN-O3-PA	-4.42	120.30	132.73
2	C	501	NAD	C4B-O4B-C1B	-4.26	105.04	109.72
2	D	501	NAD	C4B-O4B-C1B	-4.21	105.09	109.72
2	D	501	NAD	O7N-C7N-C3N	-3.80	115.44	119.59
2	C	501	NAD	C2B-C1B-N9A	-3.19	109.41	114.29
2	A	501	NAD	O7N-C7N-C3N	-2.90	116.42	119.59
2	B	501	NAD	C4B-O4B-C1B	-2.82	106.62	109.72
2	A	501	NAD	C4B-O4B-C1B	-2.64	106.82	109.72
2	B	501	NAD	C1B-N9A-C4A	-2.48	123.20	126.94
2	D	501	NAD	O5B-C5B-C4B	-2.33	100.54	109.12
2	D	501	NAD	O5D-PN-O1N	-2.32	100.59	109.62
2	C	501	NAD	C5N-C4N-C3N	-2.29	117.46	120.33
2	B	501	NAD	O5D-PN-O1N	-2.24	100.92	109.62
2	C	501	NAD	O5D-PN-O1N	-2.23	100.95	109.62
2	A	501	NAD	C2B-C1B-N9A	-2.22	110.90	114.29
2	B	501	NAD	O7N-C7N-N7N	-2.22	119.47	122.59
2	B	501	NAD	C4A-C5A-N7A	-2.13	107.52	109.48
2	A	501	NAD	O5D-PN-O1N	-2.07	101.57	109.62
2	B	501	NAD	O2N-PN-O3	2.03	114.30	105.09
2	A	501	NAD	O2A-PA-O3	2.08	114.51	105.09
2	C	501	NAD	O2N-PN-O3	2.12	114.73	105.09
2	C	501	NAD	O3-PA-O5B	2.40	109.29	102.94
2	B	501	NAD	C3N-C7N-N7N	2.61	120.67	117.82
2	C	501	NAD	O2A-PA-O3	2.62	116.96	105.09
2	B	501	NAD	O3-PA-O5B	2.92	110.69	102.94
2	A	501	NAD	O2N-PN-O3	3.15	119.37	105.09
2	D	501	NAD	O2N-PN-O3	3.28	119.98	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	501	NAD	O3-PA-O5B	3.56	112.39	102.94
2	A	501	NAD	O4D-C1D-N1N	3.70	112.20	108.13
2	D	501	NAD	O4D-C1D-N1N	3.77	112.28	108.13
2	D	501	NAD	C3N-C7N-N7N	3.99	122.19	117.82
2	D	501	NAD	O3-PA-O5B	4.11	113.84	102.94
2	C	501	NAD	O4D-C1D-N1N	4.18	112.72	108.13
2	A	501	NAD	C3N-C7N-N7N	4.75	123.01	117.82
2	B	501	NAD	O4D-C1D-N1N	5.67	114.36	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	SCN	1	0
2	D	501	NAD	1	0
3	D	603	SCN	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	360/399 (90%)	0.24	21 (5%) 26 34	23, 43, 77, 92	0
1	B	288/399 (72%)	0.72	49 (17%) 2 3	26, 53, 102, 124	0
1	C	359/399 (89%)	0.18	23 (6%) 23 30	30, 48, 67, 81	0
1	D	359/399 (89%)	0.37	29 (8%) 15 20	22, 47, 80, 94	0
All	All	1366/1596 (85%)	0.36	122 (8%) 12 16	22, 47, 83, 124	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	ILE	8.7
1	B	230	TYR	7.7
1	B	215	ILE	6.6
1	B	337	LEU	6.4
1	B	7	LEU	6.0
1	B	16	HIS	6.0
1	B	220	PRO	5.6
1	C	345	LEU	5.3
1	B	229[A]	ARG	5.3
1	B	19	ILE	5.0
1	B	338	GLY	5.0
1	B	11	ASP	4.8
1	B	332	ALA	4.7
1	B	231	PHE	4.4
1	B	12	THR	4.3
1	C	311	SER	4.1
1	D	300	ALA	4.1
1	D	313	THR	3.9
1	B	219	GLN	3.9
1	B	5	LEU	3.9
1	D	323	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	255	PHE	3.7
1	A	325	ASP	3.7
1	B	8	ILE	3.7
1	B	20	ASN	3.7
1	B	198	ALA	3.6
1	D	325	ASP	3.6
1	B	342	ASN	3.6
1	C	63	VAL	3.6
1	B	17	GLN	3.5
1	C	263	HIS	3.4
1	C	65	ILE	3.4
1	A	297[A]	THR	3.4
1	A	284[A]	LEU	3.3
1	D	326	LYS	3.3
1	D	377	PHE	3.3
1	A	95	ILE	3.2
1	B	15	PHE	3.2
1	B	233	THR	3.2
1	B	392	LEU	3.2
1	B	199	ASN	3.2
1	D	65[A]	ILE	3.2
1	C	66	SER	3.1
1	A	300	ALA	3.1
1	B	13	GLU	3.1
1	D	312	ASP	3.1
1	B	256	PRO	3.0
1	D	41	ALA	3.0
1	B	384	GLY	3.0
1	C	16	HIS	3.0
1	B	164	LYS	3.0
1	D	382	ASP	3.0
1	B	257	LYS	3.0
1	C	119	LEU	2.9
1	B	6	SER	2.9
1	B	9	GLY	2.9
1	D	381	PRO	2.9
1	D	365[A]	ARG	2.9
1	D	370	GLU	2.9
1	C	20	ASN	2.8
1	A	321	GLU	2.8
1	A	324	THR	2.7
1	A	116	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	340	ILE	2.7
1	B	387	GLU	2.7
1	B	165	ALA	2.7
1	A	38	LEU	2.6
1	B	388	THR	2.6
1	A	44	ILE	2.6
1	C	324	THR	2.6
1	D	169	VAL	2.6
1	D	322	PHE	2.6
1	C	258	LEU	2.6
1	B	389	GLY	2.5
1	D	93	LEU	2.5
1	D	307	LEU	2.5
1	A	63	VAL	2.5
1	D	321	GLU	2.5
1	D	258	LEU	2.5
1	A	260[A]	GLU	2.5
1	A	118	ALA	2.5
1	A	117	SER	2.5
1	A	65	ILE	2.5
1	B	14	LEU	2.4
1	C	325	ASP	2.4
1	C	310	SER	2.4
1	B	163	ASP	2.4
1	D	68	ASN	2.4
1	C	73	LEU	2.4
1	B	232	VAL	2.3
1	A	309[A]	THR	2.3
1	C	12	THR	2.3
1	B	336	ASN	2.3
1	C	38	LEU	2.3
1	B	346	TYR	2.3
1	B	335	ASP	2.3
1	D	42	GLY	2.3
1	C	117	SER	2.2
1	C	321	GLU	2.2
1	B	10	ARG	2.2
1	C	337	LEU	2.2
1	A	160[A]	VAL	2.2
1	A	382	ASP	2.2
1	A	323	PHE	2.2
1	B	334	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	92	ALA	2.2
1	D	260	GLU	2.2
1	C	116	LEU	2.2
1	D	350	LEU	2.2
1	D	383	PHE	2.2
1	B	218	ASN	2.2
1	A	93	LEU	2.1
1	C	39	GLY	2.1
1	C	92	ALA	2.1
1	D	44	ILE	2.1
1	D	374	GLN	2.1
1	B	339	ILE	2.1
1	C	45	GLY	2.1
1	B	393	ASP	2.0
1	A	370	GLU	2.0
1	D	324	THR	2.0
1	D	45	GLY	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
3	SCN	C	601	3/3	0.96	0.25	6.29	71,71,72,72	0
3	SCN	A	604	3/3	0.95	0.22	5.29	61,61,64,66	0
4	NA	A	607	1/1	0.92	0.17	4.57	40,40,40,40	0
3	SCN	D	603	3/3	0.97	0.22	3.14	52,52,54,55	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	A	608	1/1	0.83	0.14	2.76	43,43,43,43	0
3	SCN	A	605	3/3	0.98	0.19	1.21	51,51,52,53	0
3	SCN	D	602	3/3	0.97	0.16	0.91	61,61,63,64	0
2	NAD	A	501	44/44	0.98	0.18	-0.30	24,29,36,39	0
2	NAD	D	501	44/44	0.97	0.17	-0.33	25,31,40,41	0
4	NA	A	606	1/1	0.91	0.10	-0.39	42,42,42,42	0
2	NAD	C	501	44/44	0.98	0.16	-0.45	28,32,37,39	0
2	NAD	B	501	44/44	0.96	0.13	-0.72	26,34,48,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.