



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 AM GMT

PDB ID : 2ZTM  
Title : T190S mutant of D-3-hydroxybutyrate dehydrogenase  
Authors : Nakashima, K.; Nakajima, Y.; Ito, K.; Yoshimoto, T.  
Deposited on : 2008-10-07  
Resolution : 2.30 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

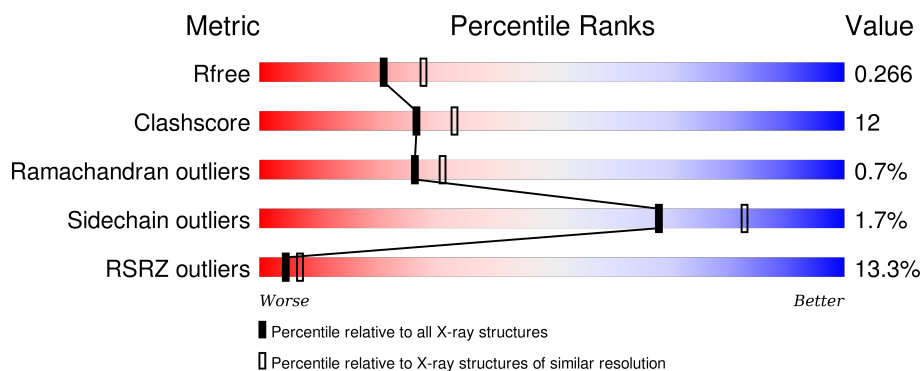
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	260	<div> <div>10%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	B	260	<div> <div>27%</div> <div>54%</div> <div>30%</div> <div>.</div> <div>14%</div> </div>
1	C	260	<div> <div>6%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
1	D	260	<div> <div>7%</div> <div>78%</div> <div>16%</div> <div>5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	406	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7551 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 D(-)-3-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1840	1155	327	355	3			
1	B	224	Total	C	N	O	S	0	0	0
			1598	1006	286	303	3			
1	C	250	Total	C	N	O	S	0	0	0
			1793	1131	317	341	4			
1	D	247	Total	C	N	O	S	0	0	0
			1771	1117	314	336	4			

There are 4 discrepancies between the modelled and reference sequences:

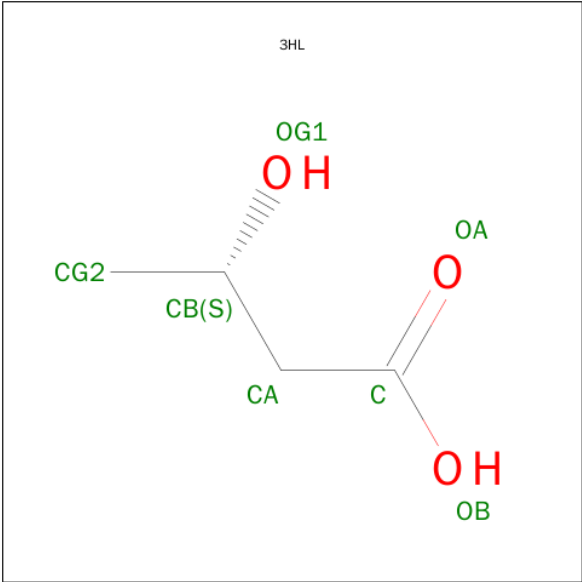
Chain	Residue	Modelled	Actual	Comment	Reference
A	190	SER	THR	ENGINEERED	UNP Q5KST5
B	190	SER	THR	ENGINEERED	UNP Q5KST5
C	190	SER	THR	ENGINEERED	UNP Q5KST5
D	190	SER	THR	ENGINEERED	UNP Q5KST5

- 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	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 (3S)-3-HYDROXYBUTANOIC ACID (three-letter code: 3HL) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

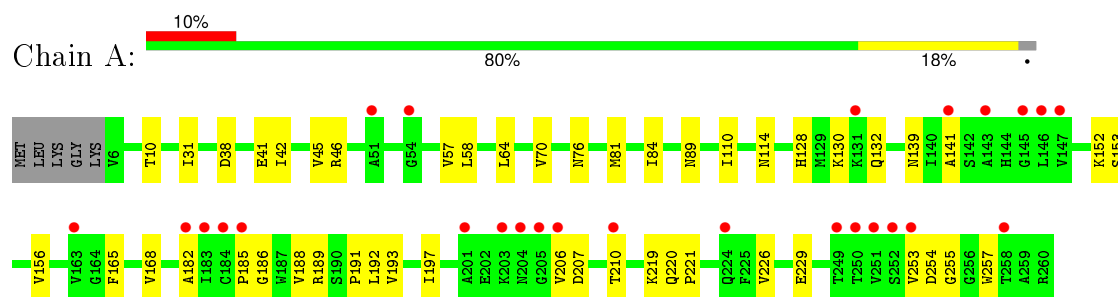
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	106	Total O 106 106	0	0
5	B	54	Total O 54 54	0	0
5	C	141	Total O 141 141	0	0
5	D	107	Total O 107 107	0	0

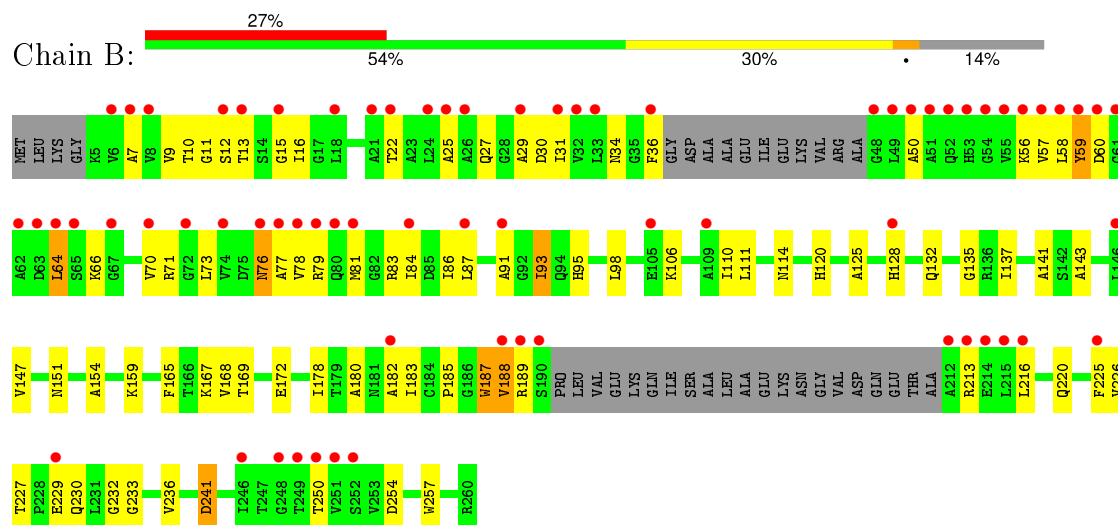
### 3 Residue-property plots [i](#)

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.

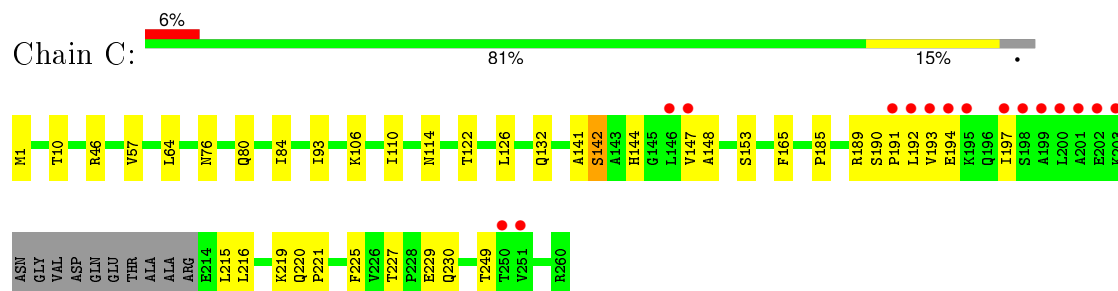
- Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase



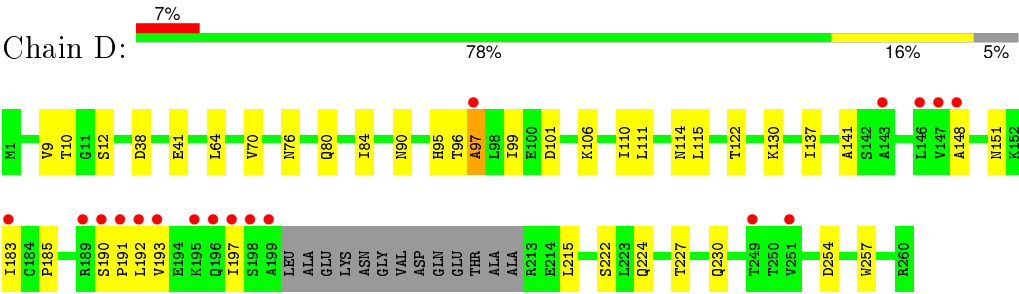
- Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase



- Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase



● Molecule 1: D(-)-3-hydroxybutyrate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.79Å 105.93Å 164.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 48.76 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.30) 99.5 (48.76-2.29)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.266 0.227 , 0.266	Depositor DCC
$R_{free}$ test set	2931 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58315 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7551	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3HL, 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	0.33	0/1866	0.59	0/2534
1	B	0.31	0/1621	0.55	0/2202
1	C	0.36	0/1818	0.60	0/2467
1	D	0.34	0/1796	0.59	0/2437
All	All	0.34	0/7101	0.59	0/9640

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	1840	0	1863	34	0
1	B	1598	0	1601	83	0
1	C	1793	0	1822	28	0
1	D	1771	0	1800	39	0
2	A	44	0	26	3	0
2	C	44	0	26	3	0
2	D	44	0	26	5	0
3	A	7	0	7	0	0
4	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	106	0	0	1	0
5	B	54	0	0	5	0
5	C	141	0	0	2	0
5	D	107	0	0	1	0
All	All	7551	0	7171	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 12.

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:B:188:VAL:HG12	1:B:189:ARG:H	1.34	0.90
1:B:34:ASN:HD21	1:B:64:LEU:HD11	1.35	0.89
1:C:84:ILE:H	1:C:132:GLN:HE22	1.24	0.85
1:B:216:LEU:HD11	1:B:225:PHE:CE1	2.14	0.83
1:B:59:TYR:HD2	1:B:60:ASP:N	1.76	0.83
1:A:206:VAL:HG12	1:A:207:ASP:H	1.45	0.81
1:B:76:ASN:HA	1:B:79:ARG:HE	1.46	0.81
1:B:64:LEU:H	1:B:64:LEU:HD12	1.45	0.80
1:B:83:ARG:HA	5:B:1395:HOH:O	1.86	0.75
1:B:128:HIS:O	1:B:132:GLN:HG3	1.87	0.74
1:B:98:LEU:HD23	1:B:151:ASN:ND2	2.07	0.70
1:C:194:GLU:HA	1:C:197:ILE:HD12	1.74	0.69
1:C:10:THR:HB	1:C:64:LEU:HD11	1.75	0.69
1:B:29:ALA:O	1:B:31:ILE:HD12	1.94	0.68
1:B:78:VAL:HG21	1:B:128:HIS:CD2	2.28	0.68
1:B:232:GLY:O	1:B:236:VAL:HG23	1.93	0.68
1:B:56:LYS:HG2	1:B:58:LEU:HD11	1.74	0.68
1:B:188:VAL:HG12	1:B:189:ARG:N	2.08	0.67
1:A:58:LEU:HD22	1:A:81:MET:HE3	1.77	0.66
1:B:9:VAL:HG12	1:B:12:SER:HB3	1.78	0.66
1:D:185:PRO:HG2	2:D:300:NAD:C5N	2.25	0.66
1:B:27:GLN:HG2	5:B:1360:HOH:O	1.96	0.65
1:A:152:LYS:O	1:A:156:VAL:HG23	1.98	0.64
1:B:93:ILE:HD13	1:B:93:ILE:H	1.62	0.64
1:A:206:VAL:HG12	1:A:207:ASP:N	2.13	0.64
1:D:197:ILE:HG12	1:D:215:LEU:HD13	1.80	0.63
1:D:64:LEU:HD22	1:D:70:VAL:HG22	1.81	0.63
1:A:206:VAL:HG11	1:A:210:THR:HG21	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HG13	1:C:110:ILE:HD13	1.81	0.62
1:C:192:LEU:O	1:C:192:LEU:HD23	2.00	0.62
1:B:95:HIS:CD2	1:B:106:LYS:HG3	2.35	0.62
1:B:76:ASN:HA	1:B:79:ARG:NE	2.15	0.61
1:B:30:ASP:HB3	1:B:81:MET:HE1	1.81	0.61
1:C:193:VAL:O	1:C:197:ILE:HG13	2.01	0.61
1:B:167:LYS:HE2	5:B:1405:HOH:O	1.99	0.61
1:B:16:ILE:HD11	1:B:188:VAL:HG21	1.82	0.60
1:B:110:ILE:O	1:B:114:ASN:HB2	2.02	0.60
1:A:165:PHE:CE1	1:C:153:SER:HB2	2.36	0.59
1:B:56:LYS:HG2	1:B:58:LEU:CD1	2.33	0.59
1:D:185:PRO:HG2	2:D:300:NAD:H5N	1.84	0.58
1:B:172:GLU:OE1	1:D:99:ILE:HG13	2.04	0.58
1:B:71:ARG:HE	1:B:120:HIS:HD2	1.51	0.58
1:B:59:TYR:CD2	1:B:60:ASP:N	2.67	0.57
1:A:130:LYS:HD2	5:C:1273:HOH:O	2.04	0.57
1:C:1:MET:HG2	5:C:1359:HOH:O	2.03	0.57
1:B:183:ILE:O	1:B:185:PRO:HD3	2.04	0.57
1:D:193:VAL:O	1:D:197:ILE:HG13	2.06	0.56
1:C:227:THR:OG1	1:C:230:GLN:HG3	2.05	0.55
1:A:76:ASN:HB3	5:A:1406:HOH:O	2.07	0.55
1:C:10:THR:HB	1:C:64:LEU:CD1	2.37	0.54
1:B:25:ALA:HA	1:B:31:ILE:HD11	1.88	0.54
1:D:10:THR:HB	1:D:64:LEU:CD1	2.38	0.54
1:B:84:ILE:O	1:B:84:ILE:HG23	2.08	0.54
1:B:77:ALA:O	1:B:81:MET:HB2	2.08	0.54
1:B:9:VAL:CG1	1:B:12:SER:HB3	2.38	0.53
1:B:7:ALA:HA	1:B:86:ILE:O	2.09	0.53
1:B:71:ARG:HE	1:B:120:HIS:CD2	2.28	0.52
1:D:95:HIS:CD2	1:D:106:LYS:HG3	2.44	0.52
1:C:185:PRO:HB2	2:C:300:NAD:H5N	1.92	0.52
1:A:226:VAL:HG21	1:A:253:VAL:O	2.10	0.52
1:A:41:GLU:O	1:A:45:VAL:HG23	2.10	0.52
1:B:110:ILE:HD12	1:B:154:ALA:HB3	1.91	0.52
1:C:106:LYS:O	1:C:110:ILE:HG12	2.10	0.51
1:B:11:GLY:H	1:B:34:ASN:HD22	1.59	0.51
1:B:233:GLY:O	1:B:236:VAL:HB	2.10	0.51
1:D:122:THR:HG23	1:D:137:ILE:HD13	1.93	0.50
1:A:64:LEU:HD22	1:A:70:VAL:HG22	1.92	0.50
1:B:213:ARG:NH1	1:B:213:ARG:HB2	2.26	0.50
1:B:187:TRP:CE3	1:B:187:TRP:HA	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ASP:HB2	5:B:1163:HOH:O	2.10	0.50
1:D:96:THR:O	1:D:97:ALA:HB2	2.12	0.50
1:B:64:LEU:HB3	1:B:70:VAL:HG22	1.94	0.50
1:D:215:LEU:O	1:D:215:LEU:HD23	2.12	0.49
1:D:222:SER:O	1:D:224:GLN:HG3	2.12	0.49
1:B:91:ALA:HB3	5:B:1397:HOH:O	2.12	0.49
1:B:168:VAL:HG22	1:D:148:ALA:HB1	1.95	0.49
1:C:215:LEU:HD12	1:C:215:LEU:O	2.12	0.49
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.78	0.48
1:C:76:ASN:ND2	1:C:80:GLN:OE1	2.46	0.48
1:A:110:ILE:O	1:A:114:ASN:HB2	2.12	0.48
1:A:38:ASP:O	1:A:42:ILE:HG13	2.13	0.48
1:D:76:ASN:O	1:D:80:GLN:HG2	2.12	0.48
1:B:73:LEU:HD12	1:B:73:LEU:O	2.13	0.48
1:D:84:ILE:O	1:D:84:ILE:HG23	2.14	0.48
1:C:84:ILE:O	1:C:84:ILE:HG23	2.13	0.48
1:C:189:ARG:HE	1:C:194:GLU:HG2	1.79	0.48
1:D:110:ILE:O	1:D:114:ASN:HB2	2.14	0.48
1:D:64:LEU:CD2	1:D:70:VAL:HG22	2.43	0.47
1:B:31:ILE:N	1:B:31:ILE:HD12	2.29	0.47
1:B:60:ASP:HB3	1:B:73:LEU:HD13	1.96	0.47
1:B:22:THR:O	1:B:25:ALA:HB3	2.13	0.47
1:B:93:ILE:N	1:B:93:ILE:HD13	2.30	0.47
1:B:254:ASP:HB2	1:B:257:TRP:HB2	1.96	0.46
1:A:188:VAL:HG22	1:A:226:VAL:HB	1.96	0.46
1:A:84:ILE:HG23	1:A:84:ILE:O	2.15	0.46
1:A:206:VAL:HG11	1:A:210:THR:CG2	2.44	0.46
1:B:188:VAL:O	1:B:225:PHE:HD2	1.99	0.46
1:A:191:PRO:HD2	2:A:300:NAD:O2A	2.16	0.46
1:B:58:LEU:HD12	1:B:58:LEU:N	2.31	0.46
1:B:30:ASP:HB3	1:B:81:MET:CE	2.46	0.46
1:B:227:THR:OG1	1:B:230:GLN:HG3	2.16	0.46
1:B:187:TRP:HE3	1:B:187:TRP:HA	1.81	0.46
1:A:219:LYS:HB3	1:A:257:TRP:CE2	2.51	0.46
1:B:165:PHE:HE1	1:D:153:SER:HB2	1.81	0.46
1:B:98:LEU:HD23	1:B:151:ASN:HD21	1.80	0.45
1:B:168:VAL:CG2	1:D:148:ALA:HB1	2.46	0.45
1:D:38:ASP:HB3	1:D:41:GLU:HB2	1.97	0.45
1:B:87:LEU:HD22	1:B:125:ALA:HB2	1.99	0.45
1:D:10:THR:HB	1:D:64:LEU:HD11	1.98	0.45
1:B:7:ALA:HB2	1:B:86:ILE:HB	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HD2	1:A:255:GLY:O	2.17	0.45
1:D:190:SER:HB2	1:D:191:PRO:HD2	1.99	0.45
1:C:46:ARG:HG3	1:C:57:VAL:HG12	1.98	0.45
1:D:141:ALA:O	2:D:300:NAD:H6N	2.17	0.45
1:B:64:LEU:H	1:B:64:LEU:CD1	2.22	0.45
1:C:122:THR:O	1:C:126:LEU:HG	2.17	0.45
1:B:50:ALA:HB2	1:B:57:VAL:HB	1.99	0.45
1:B:59:TYR:C	1:B:59:TYR:CD2	2.89	0.44
1:B:169:THR:HA	1:D:99:ILE:HD11	1.98	0.44
1:A:31:ILE:O	1:A:57:VAL:HA	2.16	0.44
1:A:128:HIS:O	1:A:132:GLN:HG2	2.17	0.44
1:C:141:ALA:O	2:C:300:NAD:H6N	2.18	0.44
1:B:229:GLU:N	1:B:229:GLU:OE1	2.51	0.44
1:A:186:GLY:O	2:A:300:NAD:H4N	2.17	0.44
1:D:130:LYS:HE2	1:D:173:THR:HG22	1.99	0.44
1:D:111:LEU:HD23	1:D:111:LEU:O	2.18	0.44
1:B:59:TYR:HD2	1:B:60:ASP:H	1.61	0.44
1:B:64:LEU:C	1:B:66:LYS:H	2.21	0.43
1:B:135:GLY:HA3	1:B:178:ILE:HG23	2.00	0.43
1:B:25:ALA:CA	1:B:31:ILE:HD11	2.49	0.43
1:B:165:PHE:CE1	1:D:153:SER:HB2	2.53	0.43
1:C:216:LEU:HD21	1:C:225:PHE:CE2	2.53	0.43
1:B:137:ILE:O	1:B:180:ALA:HA	2.19	0.43
1:A:192:LEU:HD23	1:A:192:LEU:O	2.19	0.43
1:B:188:VAL:O	1:B:225:PHE:CD2	2.71	0.43
1:D:254:ASP:HB2	1:D:257:TRP:HB3	2.01	0.43
1:A:219:LYS:O	1:A:221:PRO:HD3	2.18	0.43
1:B:159:LYS:HA	1:B:159:LYS:HD3	1.83	0.43
1:D:9:VAL:HG12	1:D:12:SER:HB3	2.01	0.42
1:A:46:ARG:HG2	1:A:46:ARG:NH1	2.34	0.42
1:B:31:ILE:H	1:B:31:ILE:HD12	1.83	0.42
1:C:229:GLU:H	1:C:229:GLU:CD	2.22	0.42
1:A:168:VAL:HG22	1:C:148:ALA:HB1	2.02	0.42
1:B:188:VAL:HG13	1:B:226:VAL:O	2.20	0.42
1:C:142:SER:HB2	2:C:300:NAD:H6N	2.00	0.42
1:A:254:ASP:HB2	1:A:257:TRP:CB	2.49	0.42
1:B:143:ALA:O	1:B:147:VAL:HG22	2.19	0.42
1:B:34:ASN:ND2	1:B:64:LEU:HD11	2.18	0.42
1:D:96:THR:HA	1:D:151:ASN:O	2.20	0.42
1:B:111:LEU:HD23	1:D:111:LEU:HD21	2.02	0.42
1:A:139:ASN:O	1:A:182:ALA:HA	2.20	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:HD23	1:D:192:LEU:O	2.19	0.42
1:B:84:ILE:H	1:B:132:GLN:HE22	1.68	0.41
1:A:193:VAL:O	1:A:197:ILE:HG13	2.20	0.41
1:D:130:LYS:NZ	5:D:1288:HOH:O	2.50	0.41
1:D:227:THR:OG1	1:D:230:GLN:HG3	2.20	0.41
1:D:111:LEU:HD21	1:D:115:LEU:HD23	2.02	0.41
1:C:219:LYS:O	1:C:221:PRO:HD3	2.21	0.41
1:D:183:ILE:HG22	1:D:185:PRO:HD3	2.03	0.41
1:C:110:ILE:O	1:C:114:ASN:HB2	2.20	0.41
1:A:89:ASN:HB2	1:A:139:ASN:HD22	1.86	0.41
1:C:144:HIS:HA	1:C:147:VAL:O	2.21	0.41
1:B:182:ALA:HB3	1:B:250:THR:HG22	2.03	0.41
1:B:7:ALA:CB	1:B:86:ILE:HB	2.51	0.41
1:B:13:THR:HG21	1:B:36:PHE:O	2.21	0.41
1:B:172:GLU:CD	1:D:99:ILE:HG13	2.41	0.40
1:A:10:THR:HB	1:A:64:LEU:CD1	2.50	0.40
1:D:90:ASN:OD1	2:D:300:NAD:H4D	2.22	0.40
1:C:190:SER:HB2	1:C:191:PRO:CD	2.51	0.40
1:A:153:SER:HB2	1:C:165:PHE:CE1	2.56	0.40
1:B:10:THR:HA	1:B:34:ASN:HB3	2.02	0.40
1:D:185:PRO:O	2:D:300:NAD:H5N	2.21	0.40
1:A:185:PRO:HB2	2:A:300:NAD:C5N	2.52	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	253/260 (97%)	237 (94%)	14 (6%)	2 (1%)	24	27
1	B	218/260 (84%)	198 (91%)	17 (8%)	3 (1%)	14	13
1	C	246/260 (95%)	236 (96%)	9 (4%)	1 (0%)	39	48

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	243/260 (94%)	233 (96%)	9 (4%)	1 (0%)	39	48
All	All	960/1040 (92%)	904 (94%)	49 (5%)	7 (1%)	26	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	ALA
1	D	97	ALA
1	A	141	ALA
1	B	15	GLY
1	C	142	SER
1	A	189	ARG
1	B	188	VAL

### 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	183/187 (98%)	181 (99%)	2 (1%)	80	90
1	B	156/187 (83%)	149 (96%)	7 (4%)	34	46
1	C	177/187 (95%)	175 (99%)	2 (1%)	80	90
1	D	175/187 (94%)	174 (99%)	1 (1%)	90	96
All	All	691/748 (92%)	679 (98%)	12 (2%)	68	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	229	GLU
1	B	59	TYR
1	B	64	LEU
1	B	76	ASN
1	B	93	ILE
1	B	187	TRP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	220	GLN
1	B	241	ASP
1	C	220	GLN
1	C	249	THR
1	D	101	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	89	ASN
1	A	139	ASN
1	A	204	ASN
1	B	34	ASN
1	B	89	ASN
1	B	95	HIS
1	B	120	HIS
1	B	132	GLN
1	B	139	ASN
1	B	151	ASN
1	C	89	ASN
1	C	132	GLN
1	C	139	ASN
1	D	89	ASN
1	D	95	HIS
1	D	132	GLN
1	D	139	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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	300	-	38,48,48	2.31	9 (23%)	47,73,73	2.16	9 (19%)
3	3HL	A	301	-	3,6,6	0.84	0	3,7,7	1.48	0
2	NAD	C	300	-	38,48,48	2.29	9 (23%)	47,73,73	2.19	7 (14%)
2	NAD	D	300	-	38,48,48	2.27	8 (21%)	47,73,73	2.15	6 (12%)

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	300	-	-	0/22/62/62	0/5/5/5
3	3HL	A	301	-	-	0/2/4/4	0/0/0/0
2	NAD	C	300	-	-	0/22/62/62	0/5/5/5
2	NAD	D	300	-	-	0/22/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NAD	C2N-C3N	-2.95	1.34	1.39
2	C	300	NAD	C2N-C3N	-2.70	1.34	1.39
2	D	300	NAD	C2N-C3N	-2.53	1.35	1.39
2	C	300	NAD	O2B-C2B	-2.22	1.37	1.43
2	A	300	NAD	C3D-C4D	2.01	1.58	1.53
2	D	300	NAD	O4D-C4D	2.10	1.49	1.45
2	A	300	NAD	O4D-C4D	2.18	1.50	1.45
2	C	300	NAD	C3D-C4D	2.23	1.59	1.53
2	A	300	NAD	O4D-C1D	2.46	1.44	1.41
2	D	300	NAD	O4D-C1D	2.52	1.44	1.41
2	C	300	NAD	O4D-C1D	2.69	1.44	1.41
2	C	300	NAD	C6N-N1N	2.79	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	NAD	C6N-N1N	2.84	1.43	1.35
2	A	300	NAD	C6N-N1N	2.85	1.43	1.35
2	C	300	NAD	C4A-N3A	3.49	1.40	1.35
2	A	300	NAD	C4A-N3A	3.61	1.40	1.35
2	D	300	NAD	C4A-N3A	3.71	1.41	1.35
2	C	300	NAD	C2A-N3A	4.53	1.40	1.32
2	D	300	NAD	C2A-N3A	4.63	1.40	1.32
2	A	300	NAD	C2A-N3A	4.65	1.40	1.32
2	C	300	NAD	C5N-C4N	6.11	1.51	1.38
2	D	300	NAD	C5N-C4N	6.15	1.51	1.38
2	A	300	NAD	C5N-C4N	6.45	1.52	1.38
2	A	300	NAD	C4N-C3N	8.08	1.53	1.39
2	D	300	NAD	C4N-C3N	8.14	1.53	1.39
2	C	300	NAD	C4N-C3N	8.28	1.53	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	NAD	N3A-C2A-N1A	-9.13	121.90	128.89
2	A	300	NAD	N3A-C2A-N1A	-9.08	121.94	128.89
2	D	300	NAD	N3A-C2A-N1A	-9.01	122.00	128.89
2	C	300	NAD	C5N-C4N-C3N	-7.90	110.41	120.33
2	D	300	NAD	C5N-C4N-C3N	-7.63	110.74	120.33
2	A	300	NAD	C5N-C4N-C3N	-6.77	111.83	120.33
2	A	300	NAD	C4B-O4B-C1B	-3.49	105.89	109.72
2	A	300	NAD	C2B-C1B-N9A	-3.47	109.00	114.29
2	C	300	NAD	C4B-O4B-C1B	-2.90	106.53	109.72
2	C	300	NAD	C2B-C1B-N9A	-2.74	110.10	114.29
2	D	300	NAD	C2B-C1B-N9A	-2.42	110.59	114.29
2	A	300	NAD	C1B-N9A-C4A	-2.20	123.63	126.94
2	C	300	NAD	O2B-C2B-C3B	2.04	118.47	111.83
2	D	300	NAD	C3N-C7N-N7N	2.16	120.19	117.82
2	A	300	NAD	O2B-C2B-C3B	2.27	119.21	111.83
2	A	300	NAD	C3N-C7N-N7N	2.40	120.45	117.82
2	D	300	NAD	C2N-C3N-C4N	2.42	120.98	118.29
2	A	300	NAD	C2N-C3N-C4N	2.42	120.98	118.29
2	C	300	NAD	C2N-C3N-C4N	2.42	120.99	118.29
2	A	300	NAD	C2A-N1A-C6A	3.79	125.54	118.77
2	D	300	NAD	C2A-N1A-C6A	3.86	125.66	118.77
2	C	300	NAD	C2A-N1A-C6A	3.86	125.67	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NAD	3	0
2	C	300	NAD	3	0
2	D	300	NAD	5	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	255/260 (98%)	0.62	26 (10%) 9 13	20, 40, 64, 78	0
1	B	224/260 (86%)	1.52	69 (30%) 1 1	32, 56, 79, 83	0
1	C	250/260 (96%)	0.25	16 (6%) 23 31	19, 28, 64, 79	0
1	D	247/260 (95%)	0.36	19 (7%) 16 23	21, 34, 65, 85	1 (0%)
All	All	976/1040 (93%)	0.67	130 (13%) 4 7	19, 39, 74, 85	1 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	ALA	7.8
1	C	199	ALA	7.8
1	C	193	VAL	7.2
1	D	198	SER	6.7
1	C	200	LEU	6.5
1	D	193	VAL	6.4
1	B	31	ILE	6.0
1	D	199	ALA	5.8
1	C	191	PRO	5.7
1	B	58	LEU	5.7
1	C	197	ILE	5.4
1	B	51	ALA	5.3
1	D	197	ILE	5.3
1	B	55	VAL	5.2
1	A	201	ALA	5.2
1	A	204	ASN	5.1
1	B	33	LEU	5.1
1	B	189	ARG	4.9
1	C	198	SER	4.9
1	B	13	THR	4.7
1	B	62	ALA	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	196	GLN	4.5
1	B	212	ALA	4.5
1	D	146	LEU	4.4
1	B	63	ASP	4.4
1	B	91	ALA	4.3
1	B	32	VAL	4.3
1	B	214	GLU	4.3
1	B	7	ALA	4.1
1	B	216	LEU	4.0
1	B	67	GLY	3.9
1	B	49	LEU	3.9
1	B	64	LEU	3.9
1	C	146	LEU	3.9
1	A	163	VAL	3.9
1	C	195	LYS	3.8
1	B	15	GLY	3.8
1	B	52	GLN	3.7
1	B	56	LYS	3.7
1	A	184	CYS	3.7
1	B	57	VAL	3.6
1	A	146	LEU	3.6
1	B	53	HIS	3.6
1	D	192	LEU	3.6
1	B	18	LEU	3.5
1	B	188	VAL	3.4
1	D	191	PRO	3.4
1	A	131	LYS	3.3
1	D	249	THR	3.3
1	B	128	HIS	3.3
1	A	251	VAL	3.3
1	B	25	ALA	3.3
1	B	59	TYR	3.2
1	B	6	VAL	3.2
1	A	51	ALA	3.2
1	D	97	ALA	3.1
1	B	76	ASN	3.1
1	B	225	PHE	3.1
1	A	54	GLY	3.1
1	B	22	THR	3.1
1	B	36	PHE	3.1
1	B	21	ALA	3.1
1	D	190	SER	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	183	ILE	3.0
1	A	250	THR	3.0
1	A	249	THR	3.0
1	B	215	LEU	3.0
1	B	250	THR	3.0
1	B	213	ARG	3.0
1	C	202	GLU	3.0
1	A	182	ALA	2.9
1	B	50	ALA	2.9
1	B	8	VAL	2.9
1	B	229	GLU	2.9
1	B	78	VAL	2.8
1	B	80	GLN	2.8
1	A	205	GLY	2.8
1	B	182	ALA	2.8
1	B	105	GLU	2.8
1	B	12	SER	2.7
1	B	84	ILE	2.7
1	B	54	GLY	2.7
1	B	70	VAL	2.7
1	B	81	MET	2.7
1	B	72	GLY	2.7
1	B	249	THR	2.7
1	A	253	VAL	2.6
1	B	190	SER	2.6
1	B	29	ALA	2.6
1	D	251	VAL	2.6
1	A	210	THR	2.6
1	B	77	ALA	2.6
1	C	147	VAL	2.6
1	C	192	LEU	2.5
1	B	79	ARG	2.5
1	B	248	GLY	2.5
1	A	206	VAL	2.5
1	B	74	VAL	2.5
1	B	24	LEU	2.4
1	B	61	GLY	2.4
1	C	203	LYS	2.4
1	D	189	ARG	2.4
1	B	48	GLY	2.3
1	C	251	VAL	2.3
1	B	252	SER	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	109	ALA	2.3
1	B	246	ILE	2.3
1	D	147	VAL	2.3
1	D	195	LYS	2.3
1	A	203	LYS	2.2
1	A	185	PRO	2.2
1	A	258	THR	2.2
1	B	251	VAL	2.2
1	B	26	ALA	2.2
1	A	145	GLY	2.2
1	A	224	GLN	2.1
1	A	252	SER	2.1
1	B	87	LEU	2.1
1	C	250	THR	2.1
1	D	143	ALA	2.1
1	A	147	VAL	2.1
1	B	65	SER	2.1
1	A	141	ALA	2.1
1	D	148	ALA	2.1
1	A	143	ALA	2.0
1	C	194	GLU	2.0
1	D	183	ILE	2.0
1	B	146	LEU	2.0
1	D	182	ALA	2.0
1	B	60	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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



of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	406	1/1	0.79	0.38	4.79	42,42,42,42	0
4	MG	B	401	1/1	0.93	0.28	1.99	42,42,42,42	0
2	NAD	A	300	44/44	0.93	0.15	-0.04	34,40,43,44	0
3	3HL	A	301	7/7	0.96	0.17	-0.18	45,47,48,48	0
2	NAD	C	300	44/44	0.96	0.12	-0.33	31,38,44,47	0
2	NAD	D	300	44/44	0.93	0.12	-0.57	39,46,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.