



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 02:33 am GMT

PDB ID : 1NQO  
Title : Glyceraldehyde-3-Phosphate Dehydrogenase Mutant With Cys 149 Replaced By Ser Complexed With Nad<sup>+</sup> and D-Glyceraldehyde-3-Phosphate  
Authors : Didierjean, C.; Corbier, C.; Fatih, M.; Favier, F.; Boschi-Muller, S.; Branlant, G.; Aubry, A.  
Deposited on : 2003-01-22  
Resolution : 2.01 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

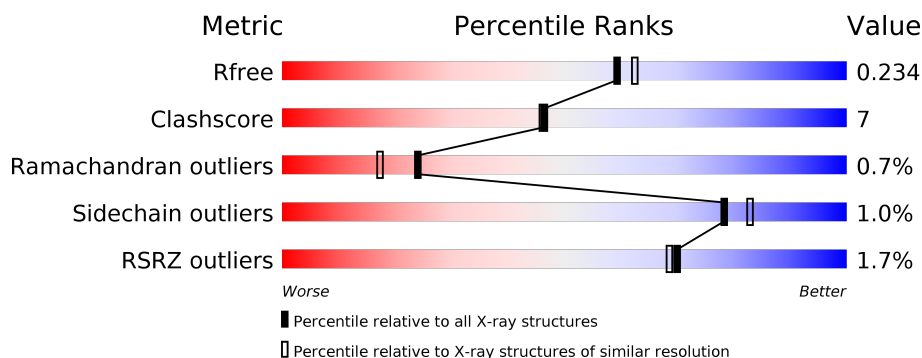
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>89%</span> <span>10%</span> </div> </div>
1	C	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>83%</span> <span>16%</span> </div> </div>
1	O	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>86%</span> <span>13%</span> </div> </div>
1	Q	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>83%</span> <span>17%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10991 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 Glyceraldehyde 3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	0	0
			2525	1582	445	490	8			
1	Q	334	Total	C	N	O	S	0	0	0
			2525	1582	445	490	8			
1	A	334	Total	C	N	O	S	0	0	0
			2525	1582	445	490	8			
1	C	334	Total	C	N	O	S	0	0	0
			2525	1582	445	490	8			

There are 4 discrepancies between the modelled and reference sequences:

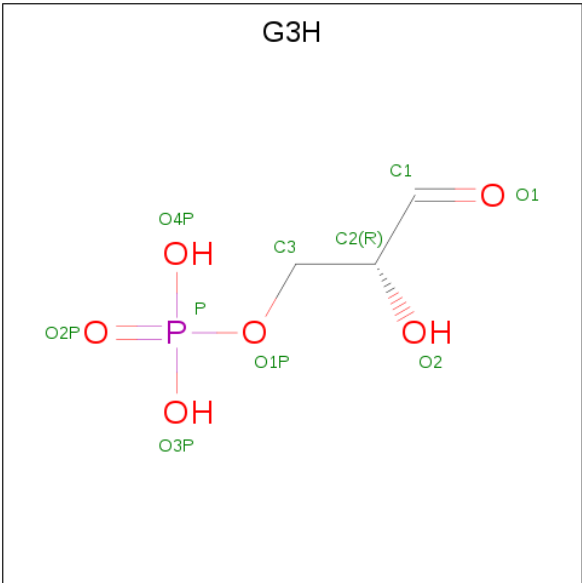
Chain	Residue	Modelled	Actual	Comment	Reference
O	149	SER	CYS	ENGINEERED	UNP P00362
Q	149	SER	CYS	ENGINEERED	UNP P00362
A	149	SER	CYS	ENGINEERED	UNP P00362
C	149	SER	CYS	ENGINEERED	UNP P00362

- 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	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
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		

- Molecule 3 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	1	Total	C	O	P	0	0
			10	3	6	1		
3	Q	1	Total	C	O	P	0	0
			10	3	6	1		
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		

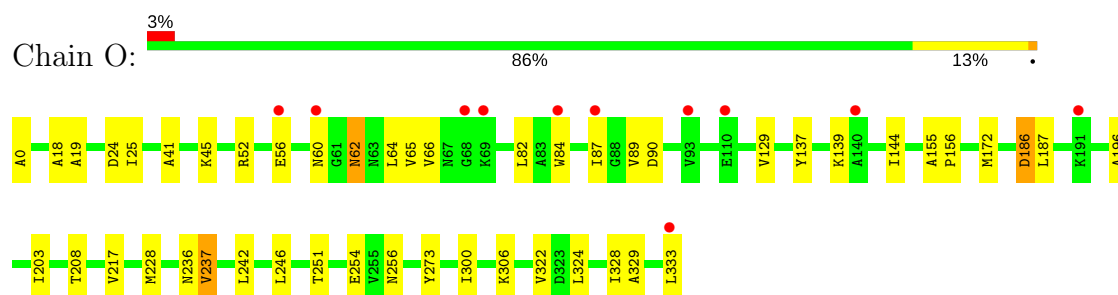
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	157	Total	O	0	0
			157	157		
4	Q	183	Total	O	0	0
			183	183		
4	A	170	Total	O	0	0
			170	170		
4	C	165	Total	O	0	0
			165	165		

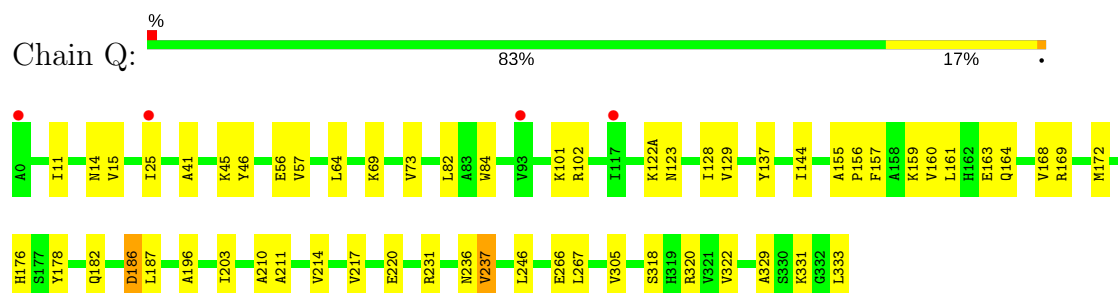
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

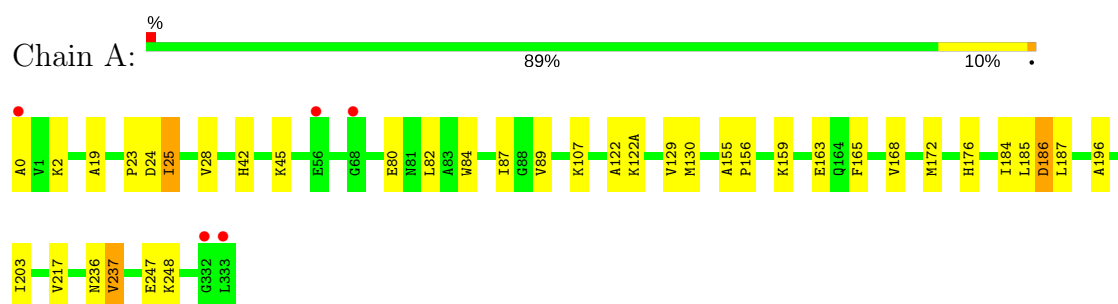
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase



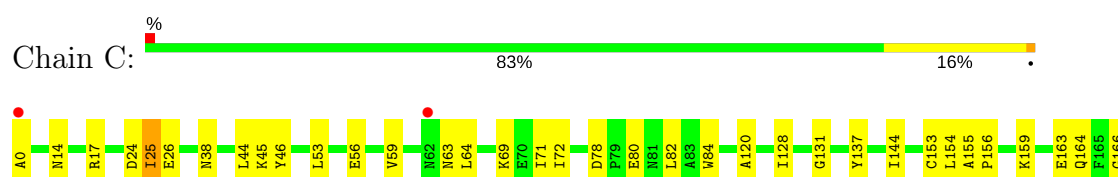
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase

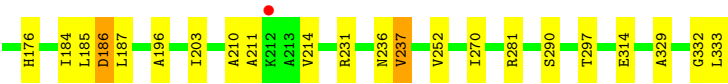


- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.31Å 87.84Å 119.41Å 90.00° 119.05° 90.00°	Depositor
Resolution (Å)	8.00 – 2.01 19.93 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.01) 93.0 (19.93-2.01)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.193 , 0.238 0.189 , 0.234	Depositor DCC
$R_{free}$ test set	7933 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 61.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: G3H, 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	0.30	0/2561	0.62	1/3474 (0.0%)
1	C	0.30	0/2561	0.62	1/3474 (0.0%)
1	O	0.29	0/2561	0.61	1/3474 (0.0%)
1	Q	0.30	0/2561	0.61	1/3474 (0.0%)
All	All	0.30	0/10244	0.62	4/13896 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	203	ILE	N-CA-C	-6.13	94.45	111.00
1	C	203	ILE	N-CA-C	-5.68	95.65	111.00
1	A	203	ILE	N-CA-C	-5.48	96.19	111.00
1	O	203	ILE	N-CA-C	-5.25	96.83	111.00

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	2525	0	2572	25	0
1	C	2525	0	2572	41	0
1	O	2525	0	2572	37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	2525	0	2572	41	0
2	A	44	0	26	0	0
2	C	44	0	26	1	0
2	O	44	0	26	0	0
2	Q	44	0	26	0	0
3	A	10	0	5	2	0
3	C	10	0	5	0	0
3	O	10	0	5	0	0
3	Q	10	0	5	1	0
4	A	170	0	0	3	0
4	C	165	0	0	3	0
4	O	157	0	0	1	0
4	Q	183	0	0	3	0
All	All	10991	0	10412	141	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 (141) 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:O:45:LYS:HE3	1:O:52:ARG:HH21	1.20	1.03
1:A:2:LYS:HD3	1:A:28:VAL:HG11	1.55	0.88
1:O:45:LYS:HE3	1:O:52:ARG:NH2	1.88	0.87
1:A:19:ALA:HB1	1:A:25:ILE:HD11	1.58	0.85
1:Q:329:ALA:HA	1:Q:333:LEU:HD21	1.64	0.80
1:C:45:LYS:HE2	4:C:7355:HOH:O	1.81	0.80
1:C:329:ALA:HA	1:C:333:LEU:HD11	1.65	0.78
1:O:329:ALA:HA	1:O:333:LEU:HD11	1.68	0.76
1:C:210:ALA:O	1:C:214:VAL:HG23	1.90	0.71
1:O:90:ASP:HB3	1:O:333:LEU:HD23	1.75	0.69
1:C:329:ALA:HA	1:C:333:LEU:CD1	2.26	0.65
1:Q:101:LYS:HG2	1:Q:122(A):LYS:HD3	1.81	0.63
1:Q:25:ILE:HD13	1:Q:322:VAL:HG13	1.81	0.62
1:C:78:ASP:OD1	1:C:80:GLU:HG2	1.98	0.62
1:O:56:GLU:O	1:O:66:VAL:HA	1.99	0.62
1:C:45:LYS:HD3	1:C:45:LYS:O	1.99	0.61
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.82	0.61
1:C:187:LEU:O	1:C:196:ALA:HB1	2.01	0.61
1:A:159:LYS:O	1:A:163:GLU:HG3	2.01	0.60
1:C:38:ASN:HD22	1:C:59:VAL:HG21	1.64	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:ALA:HB3	1:A:24:ASP:O	2.01	0.59
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.84	0.59
1:Q:129:VAL:HG23	1:Q:217:VAL:HG11	1.84	0.59
1:Q:56:GLU:HG2	1:C:69:LYS:HE3	1.84	0.59
1:Q:331:LYS:HE2	1:A:23:PRO:HG2	1.85	0.58
1:A:187:LEU:O	1:A:196:ALA:HB1	2.04	0.58
1:Q:144:ILE:HD12	1:Q:144:ILE:N	2.19	0.58
1:Q:45:LYS:HE3	1:Q:57:VAL:HB	1.85	0.58
1:A:45:LYS:HB2	1:A:45:LYS:HZ2	1.69	0.57
1:C:176:HIS:HB3	1:C:231:ARG:HD3	1.86	0.56
1:O:87:ILE:HG13	1:O:89:VAL:HG23	1.87	0.56
1:O:0:ALA:HB3	1:O:24:ASP:O	2.06	0.56
1:O:60:ASN:HB2	1:O:65:VAL:HG23	1.87	0.56
1:O:18:ALA:HB3	1:O:322:VAL:HG21	1.88	0.56
1:Q:45:LYS:HD2	1:Q:46:TYR:CE2	2.41	0.55
1:A:236:ASN:O	1:A:237:VAL:HB	2.07	0.55
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.87	0.55
1:C:25:ILE:HD12	1:C:26:GLU:N	2.22	0.55
1:C:44:LEU:HG	1:C:53:LEU:HD22	1.89	0.54
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.42	0.54
1:A:45:LYS:HB2	1:A:45:LYS:NZ	2.23	0.54
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.89	0.54
3:Q:3337:G3H:H11	4:Q:3421:HOH:O	2.08	0.53
1:C:144:ILE:HD12	1:C:144:ILE:N	2.23	0.53
1:Q:246:LEU:HD12	1:Q:246:LEU:N	2.24	0.53
1:C:63:ASN:ND2	1:C:72:ILE:HA	2.24	0.53
1:O:144:ILE:N	1:O:144:ILE:HD12	2.24	0.52
1:Q:331:LYS:HE2	1:A:23:PRO:CG	2.40	0.52
1:C:131:GLY:HA3	1:C:270:ILE:CD1	2.40	0.52
1:C:131:GLY:HA3	1:C:270:ILE:HD13	1.91	0.52
1:Q:41:ALA:HB2	1:Q:64:LEU:CD2	2.40	0.52
1:O:52:ARG:HG2	1:O:52:ARG:HH11	1.75	0.52
1:O:187:LEU:O	1:O:196:ALA:HB1	2.09	0.52
1:O:333:LEU:N	1:O:333:LEU:HD12	2.25	0.52
1:C:0:ALA:HB3	1:C:24:ASP:O	2.10	0.51
1:Q:25:ILE:CD1	1:Q:322:VAL:HG13	2.40	0.51
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.46	0.51
1:C:281:ARG:NH1	4:C:7456:HOH:O	2.43	0.50
1:O:60:ASN:HB2	1:O:65:VAL:CG2	2.40	0.50
1:Q:187:LEU:O	1:Q:196:ALA:HB1	2.12	0.50
1:O:41:ALA:HB2	1:O:64:LEU:CD2	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:ASN:O	1:O:62:ASN:ND2	2.45	0.49
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.94	0.49
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.48	0.49
1:O:129:VAL:CG2	1:O:217:VAL:HG11	2.41	0.49
1:O:137:TYR:OH	1:O:328:ILE:HG23	2.13	0.49
1:O:236:ASN:O	1:O:237:VAL:HB	2.12	0.49
1:Q:266:GLU:HG3	1:Q:267:LEU:HG	1.95	0.49
1:C:332:GLY:C	1:C:333:LEU:HD12	2.33	0.49
1:C:45:LYS:HD2	1:C:46:TYR:CE1	2.48	0.49
1:Q:11:ILE:O	1:Q:15:VAL:HG23	2.13	0.49
1:C:236:ASN:O	1:C:237:VAL:HB	2.13	0.49
1:Q:160:VAL:O	1:Q:164:GLN:HB2	2.14	0.48
1:C:25:ILE:HD12	1:C:25:ILE:C	2.33	0.48
1:O:25:ILE:HD13	1:O:322:VAL:HG13	1.95	0.48
1:A:186:ASP:HA	1:A:196:ALA:O	2.14	0.48
1:Q:102:ARG:HD2	1:Q:123:ASN:O	2.13	0.48
1:Q:176:HIS:HB3	1:Q:231:ARG:HD3	1.94	0.47
1:O:300:ILE:HG13	4:O:1465:HOH:O	2.13	0.47
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.15	0.47
1:Q:41:ALA:HB2	1:Q:64:LEU:HD22	1.97	0.47
1:Q:64:LEU:HG	1:Q:73:VAL:CG2	2.44	0.47
1:O:324:LEU:O	1:O:328:ILE:HG13	2.15	0.47
1:A:176:HIS:NE2	3:A:5337:G3H:O1	2.48	0.46
1:A:80:GLU:HG2	4:A:5384:HOH:O	2.15	0.46
1:Q:246:LEU:HD11	1:Q:305:VAL:HG12	1.97	0.46
1:C:64:LEU:HB2	1:C:71:ILE:HB	1.97	0.46
1:A:122:ALA:C	1:A:122(A):LYS:HD3	2.36	0.45
1:O:137:TYR:CZ	1:O:328:ILE:HG23	2.51	0.45
1:Q:168:VAL:HG12	1:Q:169:ARG:HG2	1.98	0.45
1:Q:246:LEU:CD1	1:Q:246:LEU:N	2.80	0.45
1:C:184:ILE:HG22	1:C:185:LEU:HG	1.99	0.45
1:Q:159:LYS:O	1:Q:163:GLU:HG3	2.17	0.45
1:Q:69:LYS:HE3	1:C:56:GLU:OE2	2.17	0.44
1:C:128:ILE:HD11	1:C:137:TYR:HB2	1.98	0.44
1:O:84:TRP:HB3	1:O:89:VAL:HB	2.00	0.44
1:O:19:ALA:CB	1:O:25:ILE:HD11	2.48	0.44
1:Q:56:GLU:CG	1:C:69:LYS:HE3	2.48	0.44
1:O:208:THR:HG22	1:O:228:MET:HA	2.00	0.43
1:C:155:ALA:HB3	1:C:156:PRO:HD3	2.00	0.43
1:C:159:LYS:O	1:C:163:GLU:HG3	2.19	0.43
1:Q:182:GLN:HB3	4:Q:3443:HOH:O	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PHE:HA	1:A:248:LYS:HD3	1.99	0.43
3:A:5337:G3H:H11	4:A:5405:HOH:O	2.19	0.43
1:Q:157:PHE:O	1:Q:161:LEU:HG	2.18	0.43
1:C:154:LEU:CD2	1:C:214:VAL:HG21	2.49	0.43
1:O:251:THR:OG1	1:O:254:GLU:HG3	2.19	0.43
1:A:168:VAL:HG22	1:A:247:GLU:HG2	2.00	0.43
1:C:25:ILE:O	1:C:25:ILE:HG13	2.18	0.43
1:O:186:ASP:HA	1:O:196:ALA:O	2.18	0.43
1:A:80:GLU:HG3	1:A:107:LYS:HD3	2.00	0.42
1:O:41:ALA:HB2	1:O:64:LEU:HD22	2.01	0.42
1:A:184:ILE:HG22	1:A:185:LEU:HG	2.01	0.42
1:A:80:GLU:HA	4:A:5384:HOH:O	2.20	0.42
1:Q:211:ALA:HB3	4:Q:3447:HOH:O	2.19	0.42
1:C:17:ARG:HE	1:C:53:LEU:HD13	1.84	0.42
1:O:56:GLU:HA	1:O:56:GLU:OE1	2.20	0.42
1:Q:178:TYR:HA	1:Q:182:GLN:OE1	2.19	0.42
1:A:42:HIS:HA	1:A:45:LYS:HZ2	1.85	0.42
1:A:87:ILE:HG13	1:A:89:VAL:HG23	2.01	0.42
1:C:186:ASP:HA	1:C:196:ALA:O	2.18	0.42
1:O:256:ASN:HB3	1:O:273:TYR:OH	2.20	0.42
1:Q:333:LEU:HD22	1:Q:333:LEU:N	2.35	0.42
1:Q:186:ASP:HA	1:Q:196:ALA:O	2.20	0.42
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.54	0.42
1:C:252:VAL:HG13	1:C:297:THR:HG22	2.02	0.42
1:O:139:LYS:HD2	1:O:139:LYS:N	2.35	0.42
1:Q:210:ALA:O	1:Q:214:VAL:HG23	2.20	0.42
1:A:236:ASN:O	1:A:237:VAL:CB	2.66	0.41
1:C:120:ALA:HB2	2:C:7336:NAD:H1D	2.01	0.41
1:O:52:ARG:NH1	1:O:52:ARG:HG2	2.36	0.41
1:Q:128:ILE:HD11	1:Q:137:TYR:HB2	2.01	0.41
1:Q:25:ILE:O	1:Q:25:ILE:HG13	2.20	0.41
1:C:185:LEU:O	1:C:186:ASP:C	2.58	0.41
1:C:211:ALA:HB3	4:C:7426:HOH:O	2.19	0.41
1:Q:14:ASN:HB3	1:Q:318:SER:OG	2.21	0.41
1:Q:320:ARG:NE	1:Q:320:ARG:HA	2.34	0.41
1:C:153:CYS:HA	1:C:290:SER:HB2	2.03	0.41
1:O:242:LEU:O	1:O:306:LYS:HA	2.21	0.40
1:C:236:ASN:OD1	1:C:314:GLU:HG3	2.22	0.40
1:C:154:LEU:HD23	1:C:214:VAL:HG21	2.02	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	332/334 (99%)	314 (95%)	16 (5%)	2 (1%)	27	21
1	C	332/334 (99%)	316 (95%)	13 (4%)	3 (1%)	19	12
1	O	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	27	21
1	Q	332/334 (99%)	315 (95%)	15 (4%)	2 (1%)	27	21
All	All	1328/1336 (99%)	1260 (95%)	59 (4%)	9 (1%)	24	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	186	ASP
1	O	186	ASP
1	O	237	VAL
1	Q	186	ASP
1	Q	237	VAL
1	A	186	ASP
1	A	237	VAL
1	C	237	VAL
1	C	166	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	272/272 (100%)	269 (99%)	3 (1%)	76	80
1	C	272/272 (100%)	269 (99%)	3 (1%)	76	80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	272/272 (100%)	269 (99%)	3 (1%)	76	80
1	Q	272/272 (100%)	270 (99%)	2 (1%)	85	89
All	All	1088/1088 (100%)	1077 (99%)	11 (1%)	78	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	62	ASN
1	O	172	MET
1	O	246	LEU
1	Q	172	MET
1	Q	220	GLU
1	A	25	ILE
1	A	130	MET
1	A	172	MET
1	C	14	ASN
1	C	25	ILE
1	C	164	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	42	HIS
1	O	62	ASN
1	O	63	ASN
1	O	81	ASN
1	Q	38	ASN
1	Q	42	HIS
1	Q	62	ASN
1	Q	63	ASN
1	Q	81	ASN
1	Q	146	ASN
1	Q	319	HIS
1	A	38	ASN
1	A	60	ASN
1	A	63	ASN
1	A	146	ASN
1	A	164	GLN
1	C	14	ASN
1	C	38	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	63	ASN
1	C	81	ASN
1	C	146	ASN
1	C	164	GLN
1	C	319	HIS

### 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 ⓘ

8 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	$\# Z  > 2$
2	NAD	A	5336	-	40,48,48	1.10	3 (7%)	44,73,73	2.03	5 (11%)
3	G3H	A	5337	-	9,9,9	1.16	0	10,12,12	1.57	2 (20%)
2	NAD	C	7336	-	40,48,48	1.13	4 (10%)	44,73,73	2.05	5 (11%)
3	G3H	C	7337	-	9,9,9	1.10	0	10,12,12	1.68	3 (30%)
2	NAD	O	1336	-	40,48,48	1.07	3 (7%)	44,73,73	2.10	5 (11%)
3	G3H	O	1337	-	9,9,9	1.30	1 (11%)	10,12,12	1.56	3 (30%)
2	NAD	Q	3336	-	40,48,48	1.17	5 (12%)	44,73,73	2.05	6 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	G3H	Q	3337	-	9,9,9	1.14	0	10,12,12	1.65	2 (20%)

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	5336	-	-	0/22/62/62	0/5/5/5
3	G3H	A	5337	-	-	0/6/8/8	0/0/0/0
2	NAD	C	7336	-	-	0/22/62/62	0/5/5/5
3	G3H	C	7337	-	-	0/6/8/8	0/0/0/0
2	NAD	O	1336	-	-	0/22/62/62	0/5/5/5
3	G3H	O	1337	-	-	0/6/8/8	0/0/0/0
2	NAD	Q	3336	-	-	0/22/62/62	0/5/5/5
3	G3H	Q	3337	-	-	0/6/8/8	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7336	NAD	C5A-N7A	-2.21	1.31	1.39
2	Q	3336	NAD	C5A-N7A	-2.02	1.32	1.39
2	A	5336	NAD	C2A-N3A	2.02	1.35	1.32
2	O	1336	NAD	O4D-C1D	2.04	1.44	1.41
2	Q	3336	NAD	C4N-C3N	2.05	1.42	1.39
2	O	1336	NAD	O4B-C1B	2.08	1.44	1.41
2	C	7336	NAD	C2A-N3A	2.13	1.35	1.32
3	O	1337	G3H	C3-C2	2.15	1.54	1.51
2	Q	3336	NAD	C3N-C7N	2.56	1.54	1.50
2	A	5336	NAD	O4D-C1D	2.79	1.45	1.41
2	Q	3336	NAD	O4D-C1D	2.80	1.45	1.41
2	C	7336	NAD	C6N-N1N	2.84	1.42	1.35
2	A	5336	NAD	C6N-N1N	2.86	1.42	1.35
2	C	7336	NAD	O4D-C1D	2.89	1.45	1.41
2	Q	3336	NAD	C6N-N1N	3.05	1.43	1.35
2	O	1336	NAD	C6N-N1N	3.22	1.43	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1336	NAD	N3A-C2A-N1A	-11.59	118.94	128.86
2	Q	3336	NAD	N3A-C2A-N1A	-11.47	119.05	128.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5336	NAD	N3A-C2A-N1A	-11.34	119.15	128.86
2	C	7336	NAD	N3A-C2A-N1A	-11.07	119.39	128.86
2	O	1336	NAD	C1B-N9A-C4A	-3.18	121.14	126.64
3	O	1337	G3H	O2-C2-C1	-2.61	103.75	109.04
3	Q	3337	G3H	O2-C2-C1	-2.53	103.92	109.04
3	C	7337	G3H	O2-C2-C1	-2.48	104.01	109.04
2	Q	3336	NAD	C1B-N9A-C4A	-2.48	122.35	126.64
2	C	7336	NAD	C1B-N9A-C4A	-2.39	122.50	126.64
3	A	5337	G3H	O2-C2-C1	-2.38	104.22	109.04
2	A	5336	NAD	C1B-N9A-C4A	-2.33	122.61	126.64
3	C	7337	G3H	O1-C1-C2	-2.12	119.95	125.00
3	O	1337	G3H	O1-C1-C2	-2.04	120.13	125.00
3	A	5337	G3H	P-O1P-C3	2.04	123.92	118.30
2	A	5336	NAD	C5N-C4N-C3N	2.10	122.81	120.35
2	Q	3336	NAD	O2D-C2D-C3D	2.17	118.77	111.83
2	Q	3336	NAD	C5N-C4N-C3N	2.23	122.96	120.35
2	O	1336	NAD	C5N-C4N-C3N	2.54	123.33	120.35
2	C	7336	NAD	C5N-C4N-C3N	2.58	123.37	120.35
3	O	1337	G3H	P-O1P-C3	2.60	125.45	118.30
2	A	5336	NAD	C4A-C5A-N7A	2.64	111.96	109.41
2	C	7336	NAD	C2A-N1A-C6A	2.67	123.29	118.75
3	Q	3337	G3H	P-O1P-C3	2.70	125.74	118.30
2	A	5336	NAD	C2A-N1A-C6A	2.71	123.35	118.75
3	C	7337	G3H	P-O1P-C3	2.73	125.80	118.30
2	Q	3336	NAD	C2A-N1A-C6A	2.75	123.43	118.75
2	C	7336	NAD	C4A-C5A-N7A	2.76	112.08	109.41
2	O	1336	NAD	C2A-N1A-C6A	2.86	123.61	118.75
2	Q	3336	NAD	C4A-C5A-N7A	3.09	112.40	109.41
2	O	1336	NAD	C4A-C5A-N7A	3.33	112.62	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5337	G3H	2	0
2	C	7336	NAD	1	0
3	Q	3337	G3H	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	-0.20	5 (1%) 73 72	8, 15, 28, 37	0
1	C	334/334 (100%)	-0.24	3 (0%) 84 83	8, 16, 28, 35	0
1	O	334/334 (100%)	-0.06	11 (3%) 46 46	6, 18, 35, 45	0
1	Q	334/334 (100%)	-0.18	4 (1%) 79 78	8, 15, 28, 33	0
All	All	1336/1336 (100%)	-0.17	23 (1%) 70 68	6, 16, 30, 45	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	GLY	3.0
1	C	0	ALA	3.0
1	A	333	LEU	2.7
1	O	60	ASN	2.6
1	O	333	LEU	2.6
1	A	0	ALA	2.6
1	O	69	LYS	2.5
1	O	93	VAL	2.5
1	A	56	GLU	2.5
1	Q	25	ILE	2.5
1	Q	0	ALA	2.4
1	A	68	GLY	2.4
1	O	191	LYS	2.3
1	Q	93	VAL	2.2
1	C	62	ASN	2.2
1	C	212	LYS	2.2
1	Q	117	ILE	2.2
1	O	110	GLU	2.2
1	O	87	ILE	2.1
1	O	140	ALA	2.1
1	O	68	GLY	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	84	TRP	2.1
1	O	56	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	G3H	Q	3337	10/10	0.60	0.32	43,49,54,54	0
3	G3H	A	5337	10/10	0.68	0.29	42,46,48,48	0
3	G3H	C	7337	10/10	0.70	0.32	42,47,49,51	0
3	G3H	O	1337	10/10	0.76	0.21	26,37,46,46	0
2	NAD	C	7336	44/44	0.97	0.08	8,11,13,14	0
2	NAD	A	5336	44/44	0.97	0.08	6,12,14,15	0
2	NAD	O	1336	44/44	0.97	0.07	7,13,16,18	0
2	NAD	Q	3336	44/44	0.98	0.07	5,10,12,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.