



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:03 AM GMT

PDB ID : 1ML3  
Title : Evidences for a flip-flop catalytic mechanism of Trypanosoma cruzi glyceraldehyde-3-phosphatedehydrogenase, from its crystal structure in complex with reacted irreversible inhibitor 2-(2-phosphono-ethyl)-acrylicacid 4-nitro-phenyl ester  
Authors : Castilho, M.S.; Pavao, F.; Oliva, G.  
Deposited on : 2002-08-29  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

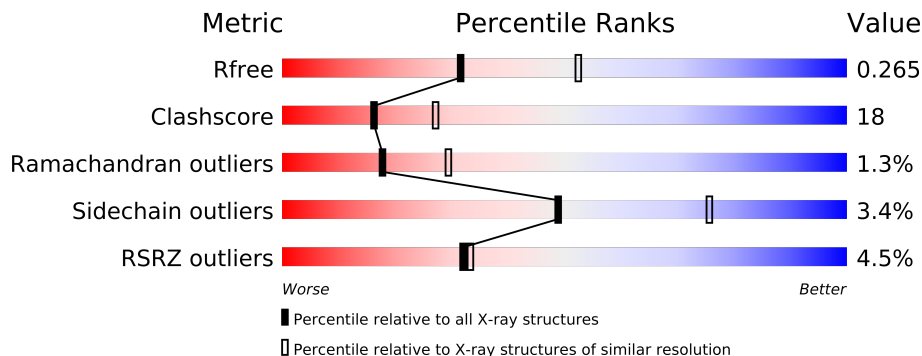
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	359	
1	B	359	
1	C	359	
1	D	359	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAD	B	1362	-	X
3	CYX	B	1166[A]	-	X
3	CYX	B	1166[B]	-	X
3	CYX	C	2166[A]	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
3	CYX	C	2166[B]	-	X
3	CYX	D	3166	-	X

## 2 Entry composition i

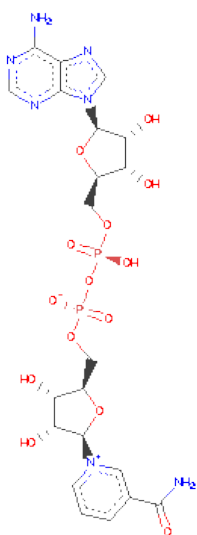
There are 4 unique types of molecules in this entry. The entry contains 11861 atoms, of which 0 are hydrogen and 0 are deuterium.

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, glycosomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	20	0	0
			2745	1725	486	520	14			
1	B	359	Total	C	N	O	S	52	1	0
			2747	1726	486	520	15			
1	C	359	Total	C	N	O	S	101	1	0
			2747	1726	486	520	15			
1	D	359	Total	C	N	O	S	12	0	0
			2745	1725	486	520	14			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



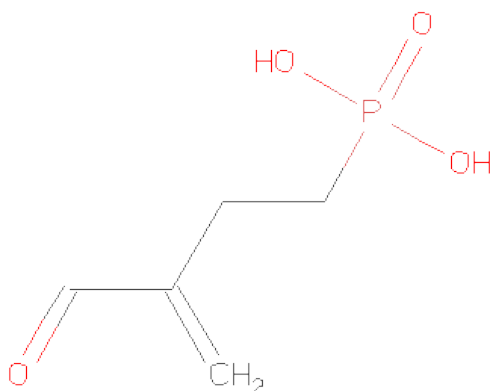
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is (3-FORMYL-BUT-3-ENYL)-PHOSPHONICACID (three-letter code: CYX) (formula:  $C_5H_9O_4P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	1
			20	10	8	2		
3	C	1	Total	C	O	P	0	1
			20	10	8	2		
3	D	1	Total	C	O	P	0	0
			10	5	4	1		

- Molecule 4 is water.

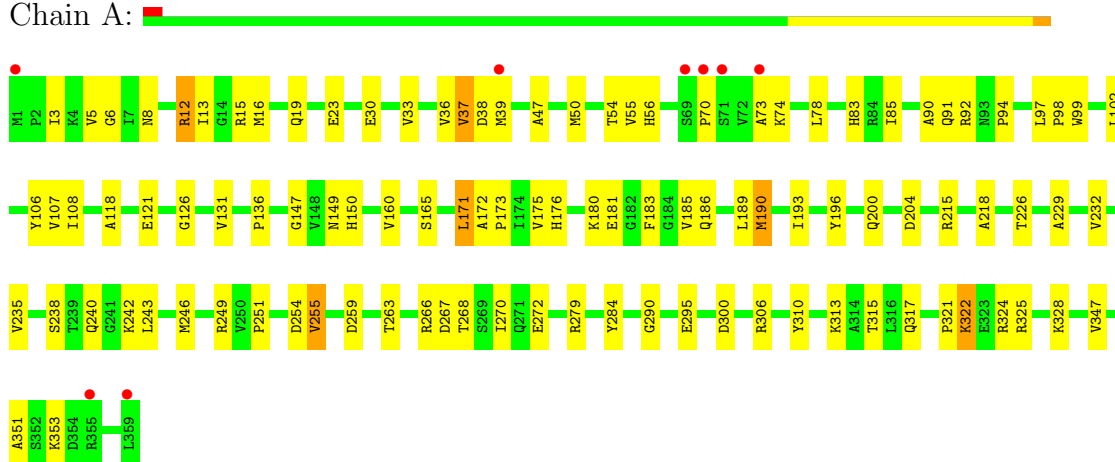
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	217	Total	O	0	0
			217	217		
4	B	161	Total	O	0	0
			161	161		
4	C	123	Total	O	0	0
			123	123		
4	D	194	Total	O	0	0
			194	194		

### 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 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.

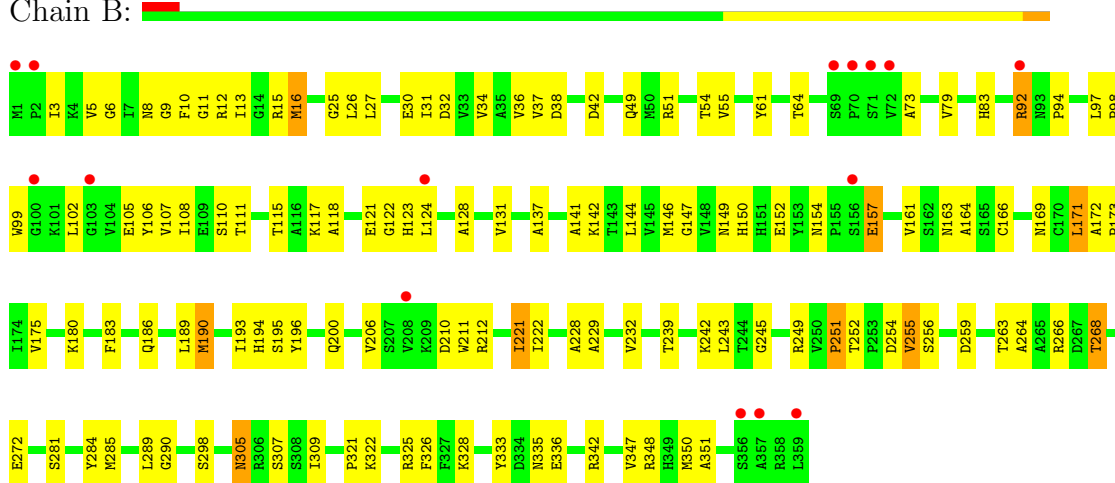
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase, glycosomal

Chain A:



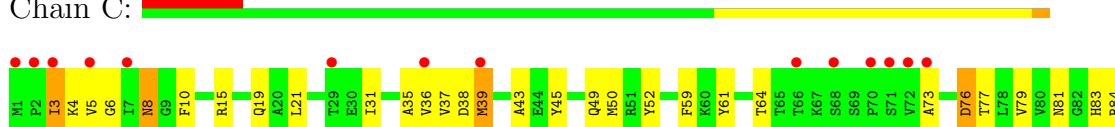
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase, glycosomal

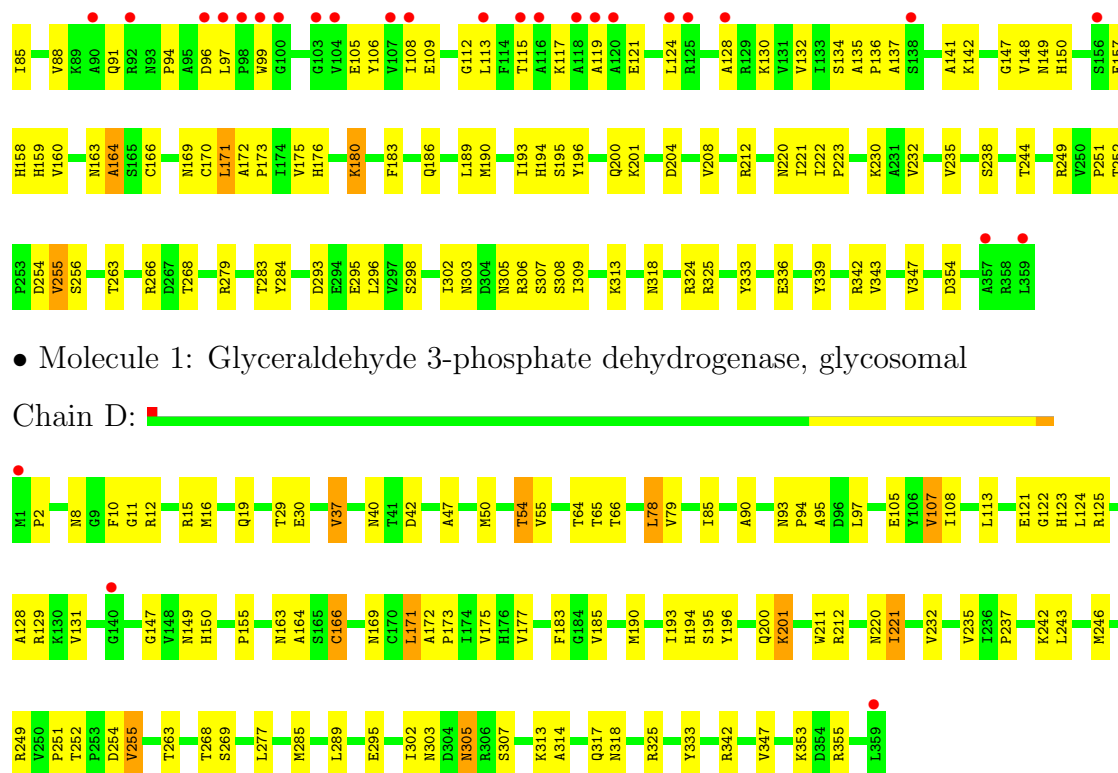
Chain B:



- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase, glycosomal

Chain C:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.46Å 85.26Å 105.15Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.50) 97.5 (19.88-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.265 0.199 , 0.265	Depositor DCC
$R_{free}$ test set	2455 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48450 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11861	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYX, 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	0.37	0/2798	0.61	0/3792
1	B	0.36	0/2804	0.60	1/3800 (0.0%)
1	C	0.34	0/2804	0.58	1/3800 (0.0%)
1	D	0.38	0/2798	0.62	1/3792 (0.0%)
All	All	0.36	0/11204	0.60	3/15184 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	ILE	N-CA-C	-6.01	94.77	111.00
1	B	221	ILE	N-CA-C	-5.67	95.70	111.00
1	C	221	ILE	N-CA-C	-5.28	96.75	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2745	0	2749	95	0
1	B	2747	0	2748	128	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2747	0	2748	110	0
1	D	2745	0	2748	87	0
2	B	44	0	26	3	0
2	C	44	0	26	0	0
2	D	44	0	26	2	0
3	B	20	0	12	2	0
3	C	20	0	12	1	0
3	D	10	0	6	0	0
4	A	217	0	0	13	0
4	B	161	0	0	13	0
4	C	123	0	0	14	0
4	D	194	0	0	4	0
All	All	11861	0	11101	396	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (396) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:183:PHE:HD1	1:D:268:THR:HG21	1.38	0.89
1:B:92:ARG:HA	1:B:92:ARG:HE	1.35	0.89
1:B:94:PRO:HA	1:B:97:LEU:HD23	1.56	0.87
1:B:305:ASN:HB3	4:B:1512:HOH:O	1.75	0.85
1:C:183:PHE:HD1	1:C:268:THR:HG21	1.42	0.85
1:D:47:ALA:HA	1:D:50:MET:HE3	1.59	0.85
1:D:107:VAL:HG13	1:D:131:VAL:HG22	1.59	0.84
1:A:8:ASN:HA	1:A:37:VAL:HG13	1.60	0.84
1:B:92:ARG:HA	1:B:92:ARG:NE	1.93	0.83
1:D:171:LEU:HD13	1:D:232:VAL:HG21	1.63	0.81
1:D:8:ASN:HA	1:D:37:VAL:HG13	1.63	0.80
1:D:30:GLU:HG3	4:D:3305:HOH:O	1.80	0.80
1:A:251:PRO:HB2	1:B:251:PRO:HB2	1.63	0.79
1:C:251:PRO:HB2	1:D:251:PRO:HB2	1.65	0.78
1:C:293:ASP:O	1:C:313:LYS:HE2	1.83	0.77
1:C:37:VAL:HB	1:C:88:VAL:HG23	1.68	0.76
1:C:21:LEU:HD11	1:C:31:ILE:HG21	1.66	0.75
1:A:215:ARG:HH21	1:D:54:THR:HG22	1.51	0.75
1:B:239:THR:HB	1:B:243:LEU:HD13	1.69	0.74
1:B:11:GLY:HA3	2:B:1362:NAD:H4B	1.69	0.74
1:B:200:GLN:NE2	1:B:249:ARG:HH11	1.84	0.74
1:D:147:GLY:H	1:D:150:HIS:CD2	2.06	0.73
1:D:313:LYS:O	1:D:317:GLN:HG3	1.89	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:GLY:H	1:A:150:HIS:CD2	2.06	0.73
1:B:8:ASN:HA	1:B:37:VAL:HG13	1.69	0.73
1:D:183:PHE:CD1	1:D:268:THR:HG21	2.22	0.73
1:A:94:PRO:HA	1:A:97:LEU:HD23	1.71	0.73
1:B:117:LYS:O	1:B:121:GLU:HG3	1.89	0.73
1:A:8:ASN:HD22	1:A:37:VAL:HG13	1.54	0.72
1:C:3:ILE:HG22	1:C:4:LYS:H	1.53	0.72
1:B:3:ILE:HB	1:B:31:ILE:HG12	1.71	0.72
1:C:124:LEU:HA	1:C:128:ALA:O	1.89	0.72
1:A:50:MET:HE1	1:A:78:LEU:HD22	1.72	0.71
1:D:64:THR:CG2	1:D:79:VAL:HB	2.20	0.71
1:C:117:LYS:O	1:C:121:GLU:HB2	1.90	0.71
1:C:108:ILE:HD11	1:C:347:VAL:HG21	1.72	0.71
1:C:196:TYR:HA	1:C:200:GLN:NE2	2.06	0.70
1:D:147:GLY:H	1:D:150:HIS:HD2	1.37	0.70
1:B:172:ALA:HB3	1:B:173:PRO:HD3	1.75	0.69
1:B:183:PHE:CD1	1:B:268:THR:HG21	2.28	0.69
1:C:183:PHE:CD1	1:C:268:THR:HG21	2.27	0.68
1:C:61:TYR:HD2	1:C:81:ASN:HB2	1.59	0.68
1:D:200:GLN:NE2	1:D:249:ARG:HH11	1.92	0.67
1:C:266:ARG:C	1:C:325:ARG:HE	1.98	0.67
1:D:196:TYR:HA	1:D:200:GLN:NE2	2.09	0.67
1:A:3:ILE:HG22	1:A:5:VAL:HG23	1.75	0.67
1:D:263:THR:HG21	4:D:3332:HOH:O	1.94	0.67
1:B:26:LEU:HD13	1:B:348:ARG:HD3	1.76	0.67
1:B:110:SER:HA	4:B:1466:HOH:O	1.94	0.67
1:A:321:PRO:HG2	4:A:449:HOH:O	1.94	0.66
1:C:64:THR:HG23	1:C:79:VAL:HB	1.77	0.66
1:D:37:VAL:HG22	2:D:1361:NAD:H2A	1.76	0.66
1:D:64:THR:HG22	1:D:79:VAL:HB	1.78	0.66
1:B:195:SER:HB2	1:B:252:THR:O	1.96	0.66
1:B:268:THR:HG22	1:B:272:GLU:OE2	1.96	0.66
1:B:107:VAL:CG1	1:B:131:VAL:HG22	2.26	0.66
1:C:105:GLU:HG3	1:C:106:TYR:H	1.60	0.65
1:D:107:VAL:CG1	1:D:131:VAL:HG22	2.26	0.65
1:B:194:HIS:NE2	3:B:1166[B]:CYX:H51	2.11	0.65
1:B:171:LEU:HD22	1:B:175:VAL:HG23	1.79	0.65
1:C:200:GLN:HE21	1:C:249:ARG:NH1	1.96	0.64
1:C:263:THR:HA	1:C:325:ARG:O	1.98	0.64
1:B:200:GLN:HE21	1:B:249:ARG:HH11	1.45	0.64
1:C:196:TYR:HA	1:C:200:GLN:HE22	1.62	0.64
1:A:16:MET:HG3	4:A:540:HOH:O	1.96	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:ILE:HD11	1:A:347:VAL:HG21	1.80	0.64
1:A:30:GLU:HG2	4:A:573:HOH:O	1.98	0.64
1:D:200:GLN:HE21	1:D:249:ARG:HH11	1.47	0.63
1:C:279:ARG:HG2	4:C:2238:HOH:O	1.99	0.63
1:B:83:HIS:HB2	4:B:1510:HOH:O	1.99	0.63
1:A:107:VAL:HG13	1:A:131:VAL:HG22	1.81	0.63
1:C:141:ALA:HA	4:C:2275:HOH:O	1.99	0.62
1:A:215:ARG:NH2	1:D:54:THR:HG22	2.14	0.62
1:A:15:ARG:O	1:A:19:GLN:HG3	2.00	0.62
1:A:94:PRO:O	1:A:97:LEU:HD23	2.00	0.62
1:B:36:VAL:HG23	1:B:36:VAL:O	2.00	0.62
1:C:8:ASN:HA	1:C:37:VAL:HG13	1.80	0.62
1:B:171:LEU:HD13	1:B:232:VAL:HG21	1.83	0.61
1:A:171:LEU:HD13	1:A:232:VAL:HG21	1.83	0.61
1:A:300:ASP:OD1	1:C:52:TYR:HB3	2.00	0.61
1:A:36:VAL:HG23	1:A:36:VAL:O	2.00	0.61
1:C:115:THR:HG23	1:C:137:ALA:HA	1.83	0.61
1:A:313:LYS:O	1:A:317:GLN:HG3	2.01	0.60
1:C:37:VAL:HB	1:C:88:VAL:CG2	2.30	0.60
1:B:106:TYR:OH	1:B:351:ALA:HA	2.01	0.60
1:B:183:PHE:CE1	1:B:268:THR:HG21	2.36	0.60
1:B:12:ARG:O	1:B:16:MET:HG2	2.01	0.60
1:A:254:ASP:O	1:A:255:VAL:HB	2.02	0.60
1:B:108:ILE:HD11	1:B:347:VAL:HG21	1.84	0.60
1:C:96:ASP:HA	4:C:2210:HOH:O	2.01	0.60
1:C:19:GLN:HG3	1:C:59:PHE:HE1	1.67	0.60
1:C:148:VAL:HG13	1:C:176:HIS:CD2	2.36	0.60
1:A:107:VAL:CG1	1:A:131:VAL:HG22	2.31	0.60
1:A:147:GLY:H	1:A:150:HIS:HD2	1.51	0.59
1:C:19:GLN:HG3	1:C:59:PHE:CE1	2.37	0.59
1:A:94:PRO:HA	1:A:97:LEU:CD2	2.32	0.59
1:A:186:GLN:O	1:A:242:LYS:HD2	2.01	0.59
1:D:263:THR:HA	1:D:325:ARG:O	2.02	0.59
1:B:194:HIS:HB3	1:B:249:ARG:HD3	1.85	0.59
1:C:309:ILE:HD12	1:C:309:ILE:N	2.18	0.58
1:C:85:ILE:HD12	1:C:85:ILE:N	2.18	0.58
1:D:171:LEU:HD22	1:D:175:VAL:HG23	1.84	0.58
1:C:194:HIS:NE2	3:C:2166[A]:CYX:H51	2.18	0.58
1:B:54:THR:HG21	1:C:220:ASN:HD21	1.68	0.58
1:A:121:GLU:HG3	1:A:160:VAL:HG21	1.85	0.58
1:B:268:THR:HG22	1:B:272:GLU:CD	2.23	0.58
1:C:339:TYR:O	1:C:343:VAL:HG23	2.04	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:8:ASN:HA	1:B:37:VAL:CG1	2.34	0.57
1:A:6:GLY:O	1:A:107:VAL:HA	2.04	0.57
1:B:124:LEU:HA	1:B:128:ALA:O	2.04	0.57
1:A:99:TRP:HB2	1:A:126:GLY:O	2.04	0.57
1:A:176:HIS:HE1	4:A:545:HOH:O	1.88	0.57
1:C:5:VAL:HA	1:C:106:TYR:O	2.04	0.57
1:B:142:LYS:HB3	1:B:161:VAL:HG12	1.87	0.57
1:A:171:LEU:HD22	1:A:175:VAL:HG23	1.87	0.57
1:C:130:LYS:HE3	4:C:2289:HOH:O	2.04	0.57
1:B:254:ASP:O	1:B:255:VAL:HB	2.05	0.56
1:B:206:VAL:HG21	4:C:2230:HOH:O	2.04	0.56
1:B:147:GLY:H	1:B:150:HIS:CD2	2.23	0.56
1:D:121:GLU:HA	1:D:124:LEU:HD13	1.87	0.56
1:A:8:ASN:HA	1:A:37:VAL:CG1	2.34	0.56
1:B:144:LEU:HD22	1:B:150:HIS:HA	1.86	0.56
1:C:132:VAL:HG21	4:C:2231:HOH:O	2.05	0.56
1:B:64:THR:HG22	1:B:79:VAL:HB	1.87	0.56
1:B:149:ASN:O	1:B:152:GLU:HB2	2.06	0.56
1:B:124:LEU:HD23	1:B:128:ALA:O	2.05	0.56
1:C:35:ALA:HA	1:C:85:ILE:HG23	1.86	0.56
1:B:196:TYR:HA	1:B:200:GLN:NE2	2.21	0.56
1:D:50:MET:HE1	1:D:78:LEU:HG	1.86	0.55
1:D:85:ILE:HD12	1:D:85:ILE:N	2.21	0.55
1:B:200:GLN:HE21	1:B:249:ARG:NH1	2.03	0.55
1:D:8:ASN:HD22	1:D:37:VAL:CG1	2.20	0.55
1:D:185:VAL:HG11	1:D:243:LEU:HD11	1.89	0.55
1:D:108:ILE:HD11	1:D:347:VAL:HG21	1.89	0.55
1:B:239:THR:HA	1:B:242:LYS:HD2	1.89	0.55
1:D:94:PRO:HA	1:D:97:LEU:HD23	1.89	0.55
1:C:21:LEU:HD11	1:C:31:ILE:CG2	2.35	0.55
1:A:310:TYR:HE1	1:A:315:THR:HG1	1.55	0.55
1:A:13:ILE:HG21	4:A:566:HOH:O	2.06	0.55
1:D:47:ALA:HA	1:D:50:MET:CE	2.33	0.54
1:C:254:ASP:OD1	1:C:336:GLU:HG3	2.08	0.54
1:A:189:LEU:HD13	1:B:328:LYS:HB2	1.89	0.54
1:D:8:ASN:HD22	1:D:37:VAL:HG13	1.72	0.54
1:C:108:ILE:CD1	1:C:347:VAL:HG21	2.36	0.54
1:D:254:ASP:O	1:D:255:VAL:HB	2.07	0.54
1:B:64:THR:CG2	1:B:79:VAL:HB	2.38	0.54
1:A:263:THR:HA	1:A:325:ARG:O	2.07	0.54
1:C:136:PRO:HG3	4:C:2201:HOH:O	2.07	0.54
1:D:65:THR:HG22	1:D:78:LEU:HD12	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:ALA:O	1:B:121:GLU:HB2	2.08	0.54
1:A:70:PRO:HD3	4:A:453:HOH:O	2.07	0.54
1:C:200:GLN:NE2	1:C:249:ARG:HH11	2.06	0.54
1:B:190:MET:HG3	1:B:245:GLY:HA3	1.88	0.54
1:C:91:GLN:HG3	1:C:96:ASP:O	2.08	0.54
1:C:149:ASN:CG	1:C:235:VAL:HG13	2.28	0.54
1:D:193:ILE:N	1:D:193:ILE:HD12	2.23	0.54
1:A:193:ILE:HG22	1:B:221:ILE:HD13	1.90	0.54
1:B:27:LEU:HD11	1:B:83:HIS:HD2	1.72	0.53
1:B:193:ILE:HD12	1:B:193:ILE:N	2.23	0.53
1:B:228:ALA:O	1:B:232:VAL:HG23	2.07	0.53
1:D:302:ILE:O	1:D:303:ASN:HB2	2.07	0.53
1:A:200:GLN:NE2	1:A:249:ARG:HD2	2.22	0.53
1:C:254:ASP:O	1:C:255:VAL:HB	2.09	0.53
1:D:155:PRO:HG3	1:D:353:LYS:HB3	1.91	0.53
1:D:94:PRO:HA	1:D:97:LEU:CD2	2.39	0.52
1:C:180:LYS:NZ	4:C:2190:HOH:O	2.32	0.52
1:C:200:GLN:NE2	1:C:249:ARG:NH1	2.57	0.52
1:C:105:GLU:HG3	1:C:106:TYR:N	2.24	0.52
1:C:189:LEU:CD2	1:C:244:THR:HG22	2.38	0.52
1:C:94:PRO:O	1:C:97:LEU:HD23	2.09	0.52
1:B:27:LEU:HD11	1:B:83:HIS:CD2	2.45	0.52
1:B:97:LEU:HD11	4:B:1495:HOH:O	2.10	0.52
1:C:64:THR:CG2	1:C:79:VAL:HB	2.38	0.52
1:B:190:MET:HG2	1:B:229:ALA:HB2	1.91	0.52
1:C:302:ILE:O	1:C:303:ASN:HB2	2.10	0.52
1:C:6:GLY:HA3	1:C:99:TRP:HZ3	1.74	0.52
1:A:290:GLY:HA3	1:A:306:ARG:NH1	2.25	0.52
1:B:5:VAL:HG12	1:B:6:GLY:N	2.25	0.52
1:B:263:THR:HA	1:B:325:ARG:O	2.10	0.52
1:D:124:LEU:HD12	1:D:124:LEU:N	2.25	0.52
1:C:212:ARG:HG2	1:D:295:GLU:HB3	1.92	0.52
1:A:172:ALA:HB3	1:A:173:PRO:HD3	1.91	0.51
1:B:98:PRO:O	1:B:102:LEU:HD13	2.09	0.51
1:B:321:PRO:O	1:B:322:LYS:HB2	2.10	0.51
1:D:64:THR:HG23	1:D:79:VAL:HB	1.92	0.51
1:A:54:THR:HG21	1:D:220:ASN:HD21	1.74	0.51
1:B:38:ASP:HA	2:B:1362:NAD:H2A	1.91	0.51
1:A:196:TYR:HA	1:A:200:GLN:NE2	2.26	0.51
1:C:83:HIS:ND1	1:C:84:ARG:N	2.58	0.51
1:B:37:VAL:HG21	4:B:1495:HOH:O	2.10	0.51
1:C:195:SER:HB3	1:C:252:THR:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:98:PRO:HB2	1:B:102:LEU:HD13	1.92	0.51
1:C:3:ILE:HG22	1:C:4:LYS:N	2.23	0.51
1:A:183:PHE:HE1	1:A:268:THR:HG1	1.59	0.51
1:C:200:GLN:C	1:C:201:LYS:HD2	2.32	0.50
1:A:16:MET:CG	4:A:540:HOH:O	2.56	0.50
1:B:254:ASP:OD1	1:B:336:GLU:HG3	2.12	0.50
1:D:194:HIS:HB3	1:D:249:ARG:HD3	1.93	0.50
1:B:79:VAL:HG12	4:B:1487:HOH:O	2.10	0.50
1:B:9:GLY:HA3	1:B:111:THR:HG22	1.93	0.50
1:A:218:ALA:HB1	4:A:404:HOH:O	2.11	0.50
1:B:8:ASN:HD22	1:B:37:VAL:HG13	1.75	0.50
1:D:307:SER:OG	1:D:342:ARG:HD2	2.11	0.50
1:B:115:THR:HG23	1:B:137:ALA:HA	1.93	0.50
1:C:61:TYR:HD2	1:C:81:ASN:CB	2.25	0.49
1:D:105:GLU:HG3	1:D:129:ARG:HD3	1.94	0.49
1:A:200:GLN:HE22	1:A:249:ARG:HD2	1.76	0.49
1:C:318:ASN:CG	1:D:246:MET:HB3	2.33	0.49
1:B:239:THR:HB	1:B:243:LEU:CD1	2.40	0.49
1:B:99:TRP:CE3	1:B:99:TRP:HA	2.47	0.49
1:B:249:ARG:HH21	3:B:1166[B]:CYX:P7	2.36	0.49
1:C:180:LYS:HA	1:C:180:LYS:HE3	1.94	0.49
1:B:32:ASP:HB2	1:B:83:HIS:CE1	2.48	0.49
1:C:295:GLU:HG3	1:D:211:TRP:HB2	1.95	0.49
1:A:8:ASN:ND2	1:A:37:VAL:HG13	2.24	0.48
1:A:183:PHE:CZ	1:A:272:GLU:HG2	2.47	0.48
1:A:33:VAL:O	1:A:83:HIS:HE1	1.95	0.48
1:C:172:ALA:HB3	1:C:173:PRO:HD3	1.95	0.48
1:D:305:ASN:C	1:D:305:ASN:HD22	2.16	0.48
1:B:200:GLN:NE2	1:B:249:ARG:NH1	2.58	0.48
1:C:94:PRO:HA	1:C:97:LEU:HD23	1.95	0.48
1:A:204:ASP:OD1	1:D:54:THR:HG23	2.13	0.48
1:B:171:LEU:HD12	1:B:190:MET:HE2	1.95	0.48
1:A:118:ALA:O	1:A:121:GLU:HB2	2.14	0.48
1:C:193:ILE:N	1:C:193:ILE:HD12	2.28	0.48
1:C:296:LEU:O	1:D:212:ARG:HD3	2.13	0.48
1:A:118:ALA:HA	1:A:121:GLU:OE2	2.14	0.48
1:B:98:PRO:HB2	1:B:102:LEU:CD1	2.44	0.48
1:A:185:VAL:HG11	1:A:243:LEU:HD11	1.94	0.48
1:A:190:MET:HG2	1:A:229:ALA:HB2	1.95	0.48
1:B:285:MET:HB3	1:B:289:LEU:HB3	1.95	0.48
1:B:266:ARG:NH1	1:B:268:THR:HG23	2.29	0.47
1:D:200:GLN:C	1:D:201:LYS:HD2	2.34	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:5:VAL:HG22	1:A:106:TYR:HB2	1.95	0.47
1:A:149:ASN:CG	1:A:235:VAL:HG13	2.35	0.47
1:C:141:ALA:HB1	1:C:160:VAL:O	2.14	0.47
1:C:8:ASN:ND2	1:C:37:VAL:HG13	2.29	0.47
1:D:12:ARG:O	1:D:16:MET:HG2	2.14	0.47
1:A:54:THR:CG2	1:D:220:ASN:HD21	2.28	0.47
1:A:324:ARG:HD2	4:A:569:HOH:O	2.14	0.47
1:D:169:ASN:O	1:D:307:SER:HB3	2.14	0.47
1:D:195:SER:HB3	1:D:252:THR:O	2.14	0.47
1:A:322:LYS:NZ	1:A:322:LYS:HA	2.29	0.47
1:D:166:CYS:HB2	1:D:333:TYR:HE2	1.79	0.47
1:A:91:GLN:HG3	1:A:97:LEU:HD13	1.97	0.47
1:C:109:GLU:HA	1:C:109:GLU:OE2	2.14	0.47
1:A:259:ASP:OD1	1:A:328:LYS:NZ	2.48	0.47
1:B:99:TRP:HE3	1:B:99:TRP:HA	1.79	0.47
1:C:171:LEU:HD22	1:C:175:VAL:HG23	1.97	0.47
1:C:230:LYS:HD2	4:C:2234:HOH:O	2.15	0.47
1:B:61:TYR:CD1	1:B:61:TYR:N	2.83	0.47
1:D:19:GLN:HE21	1:D:19:GLN:HB3	1.60	0.47
1:C:147:GLY:H	1:C:150:HIS:CD2	2.33	0.46
1:B:194:HIS:O	1:B:249:ARG:HA	2.15	0.46
1:B:281:SER:HB2	1:B:289:LEU:O	2.15	0.46
1:A:295:GLU:HG3	1:B:211:TRP:HB2	1.98	0.46
1:B:298:SER:HB2	4:B:1412:HOH:O	2.14	0.46
1:A:226:THR:HG22	1:A:246:MET:HA	1.97	0.46
1:C:113:LEU:N	4:C:2232:HOH:O	2.48	0.46
1:C:36:VAL:HG13	1:C:85:ILE:HG21	1.98	0.46
1:C:21:LEU:C	1:C:21:LEU:HD23	2.36	0.46
1:D:242:LYS:O	1:D:243:LEU:HD12	2.15	0.46
1:B:49:GLN:HA	4:B:1364:HOH:O	2.15	0.46
1:C:222:ILE:HA	1:C:223:PRO:HD3	1.82	0.46
1:C:283:THR:OG1	1:C:284:TYR:N	2.44	0.46
1:C:266:ARG:HA	1:C:325:ARG:HH21	1.81	0.46
1:A:183:PHE:CE1	1:A:272:GLU:HG2	2.51	0.46
1:A:106:TYR:OH	1:A:351:ALA:HA	2.16	0.46
1:D:342:ARG:NE	1:D:342:ARG:HA	2.30	0.46
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.80	0.46
1:A:266:ARG:HD2	1:A:267:ASP:O	2.16	0.46
1:D:122:GLY:HA2	1:D:125:ARG:NH1	2.31	0.45
1:B:305:ASN:ND2	1:B:305:ASN:H	2.13	0.45
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.82	0.45
1:A:47:ALA:HA	1:A:50:MET:HE3	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:SER:O	1:A:242:LYS:HE2	2.17	0.45
1:C:163:ASN:O	1:C:164:ALA:HB3	2.16	0.45
1:C:268:THR:O	1:C:324:ARG:HG2	2.17	0.45
1:B:328:LYS:NZ	4:B:1386:HOH:O	2.49	0.45
1:B:239:THR:O	1:B:242:LYS:HB2	2.16	0.45
1:D:200:GLN:HE21	1:D:249:ARG:NH1	2.13	0.45
1:B:117:LYS:HB2	1:B:141:ALA:HB2	1.99	0.45
1:A:263:THR:HG23	1:B:326:PHE:CE1	2.52	0.45
1:A:38:ASP:OD1	1:A:39:MET:N	2.49	0.45
1:C:307:SER:OG	1:C:342:ARG:HD2	2.16	0.45
1:C:105:GLU:CG	1:C:106:TYR:H	2.29	0.44
1:A:99:TRP:CE3	1:A:99:TRP:HA	2.52	0.44
1:D:124:LEU:HA	1:D:128:ALA:O	2.16	0.44
1:B:115:THR:CG2	1:B:137:ALA:HA	2.47	0.44
1:D:200:GLN:HB3	4:D:3171:HOH:O	2.17	0.44
1:B:51:ARG:HG3	4:B:1409:HOH:O	2.16	0.44
1:C:50:MET:O	1:C:59:PHE:HB2	2.17	0.44
1:B:309:ILE:N	1:B:309:ILE:HD12	2.33	0.44
1:D:40:ASN:OD1	1:D:42:ASP:HB3	2.17	0.44
1:D:37:VAL:CG2	1:D:90:ALA:HA	2.48	0.44
1:B:13:ILE:HG12	2:B:1362:NAD:O2N	2.17	0.44
1:B:34:VAL:HG11	1:B:102:LEU:HB3	1.99	0.44
1:A:85:ILE:HD12	1:A:85:ILE:N	2.32	0.44
1:C:8:ASN:HD22	1:C:37:VAL:HG13	1.82	0.44
1:B:196:TYR:HA	1:B:200:GLN:HE22	1.80	0.44
1:B:12:ARG:HG3	1:B:12:ARG:HH11	1.82	0.44
1:B:25:GLY:HA2	4:B:1464:HOH:O	2.17	0.44
1:C:10:PHE:CE2	1:C:15:ARG:HG2	2.52	0.44
1:C:134:SER:O	1:C:135:ALA:HB2	2.18	0.44
1:D:149:ASN:CG	1:D:235:VAL:HG13	2.38	0.44
1:B:54:THR:CG2	1:C:220:ASN:HD21	2.30	0.44
1:A:246:MET:HG2	1:B:328:LYS:HE2	1.99	0.44
1:B:200:GLN:HB3	4:B:1375:HOH:O	2.18	0.43
1:A:180:LYS:HE3	1:A:284:TYR:CE2	2.53	0.43
1:D:2:PRO:HG3	1:D:29:THR:O	2.17	0.43
1:A:353:LYS:HE2	4:A:544:HOH:O	2.18	0.43
1:D:254:ASP:O	1:D:255:VAL:CB	2.67	0.43
1:C:119:ALA:C	1:C:121:GLU:H	2.21	0.43
1:D:107:VAL:HG11	1:D:123:HIS:HB3	2.01	0.43
1:D:95:ALA:HA	1:D:122:GLY:O	2.19	0.43
1:C:43:ALA:HB2	1:C:76:ASP:HA	2.01	0.43
1:A:36:VAL:CG2	1:A:36:VAL:O	2.66	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:259:ASP:OD1	1:B:328:LYS:HE3	2.18	0.43
1:B:290:GLY:O	1:B:309:ILE:HA	2.18	0.43
1:B:10:PHE:CE2	1:B:15:ARG:HG2	2.53	0.43
1:B:212:ARG:HB3	1:B:222:ILE:HG23	2.00	0.43
1:B:342:ARG:HA	1:B:342:ARG:NE	2.34	0.43
1:B:108:ILE:CD1	1:B:347:VAL:HG21	2.48	0.43
1:A:270:ILE:HD11	1:A:315:THR:CG2	2.49	0.43
1:D:268:THR:HB	1:D:269:SER:H	1.65	0.42
1:B:30:GLU:O	1:B:31:ILE:HG13	2.18	0.42
1:B:350:MET:O	1:B:351:ALA:C	2.56	0.42
1:A:254:ASP:O	1:A:255:VAL:CB	2.67	0.42
1:C:19:GLN:NE2	4:C:2240:HOH:O	2.51	0.42
1:D:50:MET:CE	1:D:78:LEU:HG	2.48	0.42
1:A:180:LYS:HE2	4:A:545:HOH:O	2.18	0.42
1:C:77:THR:HG23	1:C:85:ILE:O	2.19	0.42
1:A:99:TRP:HE3	1:A:99:TRP:HA	1.84	0.42
1:C:170:CYS:HA	1:C:308:SER:HB2	2.02	0.42
1:B:180:LYS:HD3	1:B:284:TYR:CE2	2.54	0.42
1:B:183:PHE:HD1	1:B:268:THR:HG21	1.76	0.42
1:D:193:ILE:H	1:D:193:ILE:HD12	1.82	0.42
1:A:136:PRO:CG	1:A:165:SER:HB3	2.49	0.42
1:C:61:TYR:CD2	1:C:81:ASN:HB2	2.45	0.42
1:C:171:LEU:HD13	1:C:232:VAL:HG21	2.01	0.42
1:D:149:ASN:HA	4:D:3197:HOH:O	2.19	0.42
1:A:181:GLU:OE2	1:A:279:ARG:NH2	2.52	0.42
1:B:256:SER:HB2	1:B:333:TYR:CZ	2.54	0.42
1:B:54:THR:HG23	1:C:204:ASP:OD2	2.20	0.42
1:B:305:ASN:N	1:B:305:ASN:HD22	2.18	0.42
1:C:45:TYR:O	1:C:49:GLN:HG3	2.19	0.42
1:B:186:GLN:HG3	1:B:264:ALA:O	2.19	0.42
1:A:55:VAL:HG13	1:A:56:HIS:CD2	2.55	0.42
1:D:93:ASN:HA	1:D:94:PRO:HD3	1.93	0.42
1:D:314:ALA:O	1:D:318:ASN:ND2	2.52	0.42
1:C:298:SER:HB3	1:D:221:ILE:HB	2.02	0.42
1:B:242:LYS:C	1:B:243:LEU:HD12	2.40	0.42
1:B:9:GLY:CA	1:B:111:THR:HG22	2.48	0.42
1:D:172:ALA:HB3	1:D:173:PRO:HD3	2.01	0.42
1:B:94:PRO:HB3	1:B:123:HIS:CG	2.55	0.41
1:C:50:MET:HB3	4:C:2276:HOH:O	2.19	0.41
1:B:169:ASN:O	1:B:307:SER:HB3	2.20	0.41
1:D:285:MET:HB3	1:D:289:LEU:HB3	2.02	0.41
1:C:208:VAL:HG13	4:C:2283:HOH:O	2.18	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:305:ASN:N	1:B:305:ASN:ND2	2.68	0.41
1:C:194:HIS:O	1:C:249:ARG:HA	2.20	0.41
1:B:348:ARG:HD2	4:B:1461:HOH:O	2.19	0.41
1:B:171:LEU:HD22	1:B:175:VAL:CG2	2.49	0.41
1:A:196:TYR:HA	1:A:200:GLN:HE22	1.85	0.41
1:B:94:PRO:HB2	1:B:122:GLY:C	2.41	0.41
1:A:94:PRO:C	1:A:97:LEU:HD23	2.41	0.41
1:C:343:VAL:O	1:C:347:VAL:HG23	2.20	0.41
1:C:113:LEU:O	1:C:113:LEU:HG	2.20	0.41
1:A:204:ASP:OD1	1:D:54:THR:CG2	2.69	0.41
1:A:200:GLN:HB3	4:A:366:HOH:O	2.20	0.41
1:D:177:VAL:HG11	1:D:277:LEU:HD23	2.03	0.41
1:A:74:LYS:HE2	4:A:489:HOH:O	2.20	0.41
1:B:154:ASN:HB3	1:B:157:GLU:HB3	2.02	0.41
1:A:94:PRO:CA	1:A:97:LEU:HD23	2.45	0.41
1:C:295:GLU:HB3	1:D:212:ARG:HG2	2.02	0.41
1:A:136:PRO:HG3	1:A:165:SER:HB3	2.03	0.41
1:C:112:GLY:N	4:C:2232:HOH:O	2.54	0.41
1:B:146:MET:HB2	1:B:342:ARG:HD3	2.02	0.41
1:C:256:SER:HB2	1:C:333:TYR:CZ	2.55	0.41
1:A:97:LEU:N	1:A:97:LEU:HD22	2.36	0.41
1:C:169:ASN:O	1:C:307:SER:HB3	2.21	0.41
1:D:163:ASN:O	1:D:164:ALA:HB3	2.21	0.41
1:C:186:GLN:HB2	1:C:263:THR:OG1	2.21	0.40
1:A:204:ASP:OD2	1:D:54:THR:HG23	2.21	0.40
1:B:190:MET:O	1:B:190:MET:HG3	2.21	0.40
1:D:124:LEU:HD12	1:D:124:LEU:H	1.84	0.40
1:B:163:ASN:O	1:B:164:ALA:HB3	2.20	0.40
1:C:38:ASP:CG	1:C:39:MET:H	2.24	0.40
1:A:37:VAL:CG2	1:A:90:ALA:HA	2.51	0.40
1:C:142:LYS:HG2	1:C:158:HIS:CE1	2.56	0.40
1:D:10:PHE:CZ	1:D:15:ARG:HG3	2.56	0.40
1:D:11:GLY:HA3	2:D:1361:NAD:O5B	2.22	0.40
1:A:121:GLU:CG	1:A:160:VAL:HG21	2.48	0.40
1:C:130:LYS:HZ3	1:C:159:HIS:CD2	2.39	0.40
1:B:94:PRO:CA	1:B:97:LEU:HD23	2.39	0.40
1:B:118:ALA:HA	1:B:121:GLU:CD	2.42	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	357/359 (99%)	331 (93%)	23 (6%)	3 (1%)	27	46
1	B	358/359 (100%)	323 (90%)	28 (8%)	7 (2%)	11	17
1	C	358/359 (100%)	306 (86%)	45 (13%)	7 (2%)	11	17
1	D	357/359 (99%)	331 (93%)	24 (7%)	2 (1%)	33	55
All	All	1430/1436 (100%)	1291 (90%)	120 (8%)	19 (1%)	18	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	ALA
1	C	73	ALA
1	A	73	ALA
1	A	255	VAL
1	B	42	ASP
1	B	157	GLU
1	B	255	VAL
1	C	3	ILE
1	C	39	MET
1	C	157	GLU
1	D	255	VAL
1	B	335	ASN
1	C	255	VAL
1	B	210	ASP
1	C	164	ALA
1	C	76	ASP
1	D	237	PRO
1	A	98	PRO
1	B	251	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/296 (100%)	287 (97%)	9 (3%)	53	80
1	B	297/296 (100%)	287 (97%)	10 (3%)	49	75
1	C	297/296 (100%)	287 (97%)	10 (3%)	49	75
1	D	296/296 (100%)	283 (96%)	13 (4%)	39	64
All	All	1186/1184 (100%)	1144 (96%)	42 (4%)	49	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	23	GLU
1	A	37	VAL
1	A	92	ARG
1	A	102	LEU
1	A	171	LEU
1	A	190	MET
1	A	240	GLN
1	A	322	LYS
1	B	16	MET
1	B	55	VAL
1	B	92	ARG
1	B	105	GLU
1	B	166[A]	CYS
1	B	166[B]	CYS
1	B	171	LEU
1	B	190	MET
1	B	268	THR
1	B	305	ASN
1	C	8	ASN
1	C	166[A]	CYS
1	C	166[B]	CYS
1	C	171	LEU
1	C	180	LYS
1	C	190	MET
1	C	238	SER
1	C	305	ASN
1	C	306	ARG
1	C	354	ASP
1	D	37	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	54	THR
1	D	55	VAL
1	D	66	THR
1	D	78	LEU
1	D	107	VAL
1	D	113	LEU
1	D	166	CYS
1	D	171	LEU
1	D	190	MET
1	D	201	LYS
1	D	305	ASN
1	D	355	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	19	GLN
1	A	150	HIS
1	A	159	HIS
1	A	176	HIS
1	A	200	GLN
1	B	8	ASN
1	B	19	GLN
1	B	83	HIS
1	B	150	HIS
1	B	176	HIS
1	B	200	GLN
1	B	305	ASN
1	C	8	ASN
1	C	19	GLN
1	C	49	GLN
1	C	150	HIS
1	C	151	HIS
1	C	159	HIS
1	C	176	HIS
1	C	200	GLN
1	C	305	ASN
1	D	8	ASN
1	D	19	GLN
1	D	81	ASN
1	D	150	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	151	HIS
1	D	159	HIS
1	D	176	HIS
1	D	200	GLN
1	D	305	ASN
1	D	341	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
3	CYX	B	1166[A]	1	9,9,9	3.02	6 (66%)	12,12,12	1.29	1 (8%)
3	CYX	B	1166[B]	1	9,9,9	2.98	6 (66%)	12,12,12	1.20	1 (8%)
2	NAD	B	1362	-	48,48,48	1.48	7 (14%)	73,73,73	1.61	13 (17%)
2	NAD	C	1360	-	48,48,48	1.37	7 (14%)	73,73,73	1.67	12 (16%)
3	CYX	C	2166[A]	1	9,9,9	2.94	6 (66%)	12,12,12	1.23	1 (8%)
3	CYX	C	2166[B]	1	9,9,9	2.92	6 (66%)	12,12,12	1.24	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	D	1361	-	48,48,48	1.45	8 (16%)	73,73,73	1.65	12 (16%)
3	CYX	D	3166	1	9,9,9	3.05	7 (77%)	12,12,12	1.24	1 (8%)

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
3	CYX	B	1166[A]	1	-	0/6/8/8	0/0/0/0
3	CYX	B	1166[B]	1	-	0/6/8/8	0/0/0/0
2	NAD	B	1362	-	-	0/30/62/62	0/3/5/5
2	NAD	C	1360	-	-	0/30/62/62	0/3/5/5
3	CYX	C	2166[A]	1	-	0/6/8/8	0/0/0/0
3	CYX	C	2166[B]	1	-	0/6/8/8	0/0/0/0
2	NAD	D	1361	-	-	0/30/62/62	0/3/5/5
3	CYX	D	3166	1	-	0/6/8/8	0/0/0/0

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3166	CYX	P7-O10	5.04	1.61	1.50
3	C	2166[A]	CYX	P7-O10	4.89	1.61	1.50
3	B	1166[A]	CYX	P7-O10	4.84	1.61	1.50
2	D	1361	NAD	C3N-C7N	4.72	1.58	1.50
3	C	2166[B]	CYX	P7-O10	4.71	1.61	1.50
3	B	1166[B]	CYX	P7-O10	4.62	1.60	1.50
2	B	1362	NAD	C3N-C7N	4.29	1.57	1.50
2	C	1360	NAD	C3N-C7N	4.23	1.57	1.50
3	B	1166[B]	CYX	P7-C6	-4.03	1.75	1.79
2	D	1361	NAD	C2N-N1N	3.94	1.40	1.35
3	C	2166[B]	CYX	P7-C6	-3.86	1.75	1.79
3	B	1166[A]	CYX	P7-C6	-3.82	1.75	1.79
2	C	1360	NAD	C2N-N1N	3.79	1.40	1.35
3	C	2166[A]	CYX	P7-C6	-3.54	1.75	1.79
3	D	3166	CYX	P7-O8	3.51	1.61	1.54
3	B	1166[B]	CYX	P7-O9	3.49	1.61	1.54
2	B	1362	NAD	O4B-C1B	3.48	1.46	1.41
3	C	2166[A]	CYX	P7-O9	3.46	1.61	1.54
2	B	1362	NAD	C6N-N1N	3.45	1.45	1.35
2	B	1362	NAD	C2N-N1N	3.44	1.39	1.35
3	B	1166[B]	CYX	P7-O8	3.42	1.61	1.54

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2166[B]	CYX	P7-O9	3.37	1.61	1.54
3	C	2166[A]	CYX	P7-O8	3.36	1.61	1.54
3	D	3166	CYX	P7-O9	3.35	1.61	1.54
2	D	1361	NAD	C4N-C3N	3.33	1.45	1.39
3	D	3166	CYX	P7-C6	-3.25	1.75	1.79
3	B	1166[A]	CYX	P7-O9	3.23	1.61	1.54
3	B	1166[A]	CYX	P7-O8	3.14	1.60	1.54
2	C	1360	NAD	C6N-N1N	3.12	1.44	1.35
2	D	1361	NAD	C6N-N1N	3.09	1.44	1.35
3	C	2166[B]	CYX	P7-O8	3.06	1.60	1.54
3	B	1166[A]	CYX	C6-C5	2.96	1.56	1.52
2	C	1360	NAD	O4B-C1B	2.94	1.45	1.41
3	B	1166[A]	CYX	C1-C2	2.92	1.55	1.45
2	C	1360	NAD	C4N-C3N	2.92	1.44	1.39
2	B	1362	NAD	C4N-C3N	2.80	1.44	1.39
2	D	1361	NAD	O4B-C1B	2.74	1.45	1.41
3	D	3166	CYX	C6-C5	2.70	1.56	1.52
3	D	3166	CYX	C1-C2	2.70	1.54	1.45
3	B	1166[B]	CYX	C1-C2	2.65	1.54	1.45
3	C	2166[B]	CYX	C6-C5	2.62	1.56	1.52
3	C	2166[A]	CYX	C1-C2	2.56	1.54	1.45
3	C	2166[B]	CYX	C1-C2	2.50	1.54	1.45
3	C	2166[A]	CYX	C6-C5	2.39	1.55	1.52
2	B	1362	NAD	C2A-N1A	2.34	1.38	1.33
3	B	1166[B]	CYX	C6-C5	2.30	1.55	1.52
3	D	3166	CYX	C4-C2	2.29	1.36	1.32
2	C	1360	NAD	C2A-N1A	2.20	1.38	1.33
2	D	1361	NAD	C2A-N1A	2.19	1.38	1.33
2	D	1361	NAD	PA-O3	2.15	1.63	1.59
2	D	1361	NAD	C2B-C1B	2.12	1.56	1.53
2	B	1362	NAD	PA-O2A	-2.10	1.45	1.55
2	C	1360	NAD	PA-O2A	-2.03	1.46	1.55

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1362	NAD	C6N-C5N-C4N	4.90	127.23	119.44
2	C	1360	NAD	C6N-C5N-C4N	4.87	127.18	119.44
2	D	1361	NAD	C6N-C5N-C4N	4.83	127.11	119.44
2	D	1361	NAD	O4B-C1B-N9A	-4.78	104.00	108.44
2	C	1360	NAD	O4B-C1B-N9A	-4.77	104.00	108.44
2	B	1362	NAD	C5N-C4N-C3N	-4.61	114.33	120.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1360	NAD	C5N-C4N-C3N	-4.50	114.47	120.32
2	D	1361	NAD	C5N-C4N-C3N	-4.50	114.48	120.32
2	C	1360	NAD	O4B-C1B-C2B	-4.26	100.24	106.77
2	D	1361	NAD	O4B-C1B-C2B	-4.11	100.47	106.77
2	C	1360	NAD	C5N-C6N-N1N	-3.97	113.74	120.43
2	B	1362	NAD	C5N-C6N-N1N	-3.93	113.80	120.43
2	B	1362	NAD	C4N-C3N-C7N	-3.87	110.83	121.10
2	D	1361	NAD	C4N-C3N-C7N	-3.80	110.99	121.10
2	C	1360	NAD	C4N-C3N-C7N	-3.78	111.05	121.10
2	D	1361	NAD	C5N-C6N-N1N	-3.76	114.10	120.43
2	B	1362	NAD	N3A-C2A-N1A	-3.50	125.78	128.71
2	B	1362	NAD	C2N-C3N-C4N	3.48	122.26	118.31
2	D	1361	NAD	N3A-C2A-N1A	-3.39	125.87	128.71
2	C	1360	NAD	N3A-C2A-N1A	-3.37	125.89	128.71
2	C	1360	NAD	C2N-C3N-C4N	3.28	122.02	118.31
2	D	1361	NAD	C2N-C3N-C4N	3.26	122.00	118.31
3	C	2166[A]	CYX	C4-C2-C1	3.23	122.63	115.46
3	C	2166[B]	CYX	C4-C2-C1	3.19	122.56	115.46
3	D	3166	CYX	C4-C2-C1	3.15	122.46	115.46
3	B	1166[B]	CYX	C4-C2-C1	3.15	122.45	115.46
3	B	1166[A]	CYX	C4-C2-C1	3.13	122.41	115.46
2	B	1362	NAD	O4B-C1B-N9A	-2.95	105.69	108.44
2	B	1362	NAD	O4B-C1B-C2B	-2.76	102.54	106.77
2	D	1361	NAD	C2N-C3N-C7N	2.57	127.00	119.35
2	B	1362	NAD	C8A-N9A-C1B	2.56	131.42	126.38
2	D	1361	NAD	C4A-C5A-N7A	2.55	111.70	109.52
2	B	1362	NAD	C2N-C3N-C7N	2.54	126.91	119.35
2	C	1360	NAD	C2N-C3N-C7N	2.53	126.89	119.35
2	B	1362	NAD	O2N-PN-O3	2.51	115.55	108.79
2	C	1360	NAD	C4A-C5A-N7A	2.49	111.66	109.52
2	D	1361	NAD	C8A-N9A-C4A	-2.46	105.02	106.90
2	B	1362	NAD	C8A-N9A-C4A	-2.42	105.05	106.90
2	C	1360	NAD	C8A-N9A-C1B	2.41	131.13	126.38
2	C	1360	NAD	C8A-N9A-C4A	-2.37	105.09	106.90
2	B	1362	NAD	C4A-C5A-N7A	2.23	111.43	109.52
2	D	1361	NAD	C8A-N9A-C1B	2.11	130.55	126.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	359/359 (100%)	-0.31	8 (2%) 59 61	6, 23, 45, 67	6 (1%)
1	B	359/359 (100%)	-0.07	15 (4%) 35 36	5, 26, 66, 89	17 (4%)
1	C	359/359 (100%)	0.32	38 (10%) 7 6	11, 35, 87, 101	31 (8%)
1	D	359/359 (100%)	-0.42	3 (0%) 83 84	9, 22, 41, 58	5 (1%)
All	All	1436/1436 (100%)	-0.12	64 (4%) 32 33	5, 25, 67, 101	59 (4%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.3
1	C	359	LEU	5.6
1	C	71	SER	5.3
1	C	72	VAL	4.8
1	C	113	LEU	4.6
1	A	1	MET	4.5
1	B	71	SER	4.4
1	C	120	ALA	4.2
1	C	357	ALA	4.1
1	C	73	ALA	4.1
1	D	1	MET	4.1
1	C	119	ALA	4.0
1	C	97	LEU	3.5
1	A	70	PRO	3.4
1	B	92	ARG	3.3
1	C	90	ALA	3.3
1	A	359	LEU	3.2
1	C	125	ARG	3.2
1	C	128	ALA	3.2
1	C	70	PRO	3.2
1	C	138	SER	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	357	ALA	3.1
1	C	1	MET	3.1
1	B	72	VAL	3.1
1	C	156	SER	3.0
1	C	100	GLY	3.0
1	B	356	SER	2.9
1	C	7	ILE	2.9
1	C	104	VAL	2.9
1	C	118	ALA	2.8
1	B	124	LEU	2.8
1	C	103	GLY	2.8
1	A	73	ALA	2.8
1	B	70	PRO	2.7
1	A	355	ARG	2.7
1	C	116	ALA	2.6
1	C	68	SER	2.6
1	C	3	ILE	2.6
1	C	66	THR	2.6
1	C	99	TRP	2.6
1	D	359	LEU	2.5
1	B	100	GLY	2.5
1	B	2	PRO	2.5
1	C	108	ILE	2.4
1	A	69	SER	2.4
1	B	359	LEU	2.4
1	A	71	SER	2.4
1	B	69	SER	2.4
1	C	36	VAL	2.3
1	C	115	THR	2.3
1	C	2	PRO	2.2
1	C	29	THR	2.2
1	B	208	VAL	2.2
1	C	107	VAL	2.2
1	C	39	MET	2.1
1	D	140	GLY	2.1
1	B	156	SER	2.1
1	C	5	VAL	2.1
1	A	39	MET	2.1
1	C	96	ASP	2.1
1	C	98	PRO	2.0
1	C	92	ARG	2.0
1	B	103	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	124	LEU	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CYX	C	2166[B]	10/10	0.33	12.33	35,38,40,41	10
3	CYX	B	1166[A]	10/10	0.39	7.81	30,32,36,38	10
3	CYX	C	2166[A]	10/10	0.33	7.79	42,45,48,48	10
3	CYX	B	1166[B]	10/10	0.39	6.71	43,48,54,54	10
3	CYX	D	3166	10/10	0.27	5.64	39,44,50,51	0
2	NAD	B	1362	44/44	0.38	2.97	30,49,56,56	43
2	NAD	C	1360	44/44	0.28	0.99	22,28,31,33	44
2	NAD	D	1361	44/44	0.11	-0.30	22,26,29,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.