



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:49 AM GMT

PDB ID : 3DMT
Title : Structure of Glycosomal Glyceraldehyde-3-PhosphateDehydrogenase from Trypanosoma cruzi in complex with the irreversible iodoacetate inhibitor
Authors : Guido, R.V.C.; Balliano, T.L.; Andricopulo, A.D.; Oliva, G.
Deposited on : 2008-07-01
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

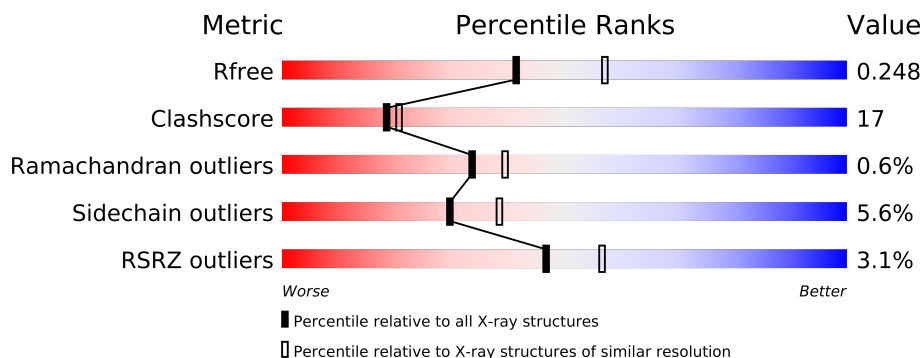
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 ≥ 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	D	359	
2	C	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
4	GOL	C	361	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12123 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.

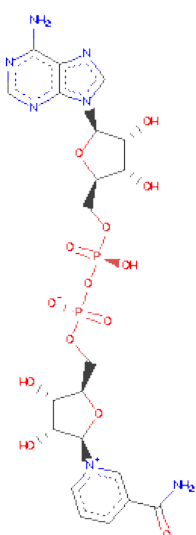
- Molecule 1 is a protein called Glyceraldehyde-3-phosphatedehydrogenase, glycosomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			
1	B	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			
1	D	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			

- Molecule 2 is a protein called Glyceraldehyde-3-phosphatedehydrogenase, glycosomal.

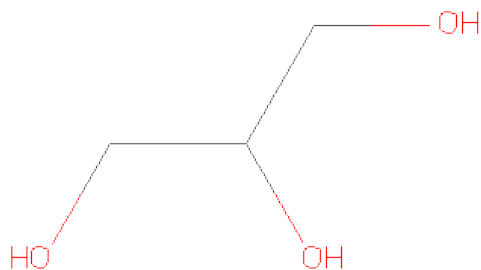
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	359	Total	C	N	O	S	0	0	0
			2737	1719	483	522	13			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

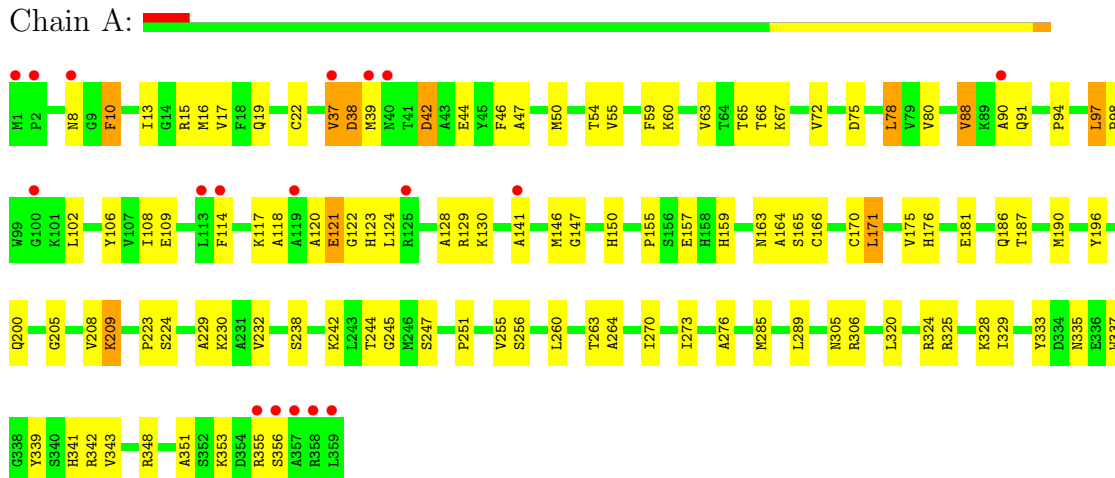
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	195	Total	O	0	0
			195	195		
5	B	294	Total	O	0	0
			294	294		
5	C	297	Total	O	0	0
			297	297		
5	D	219	Total	O	0	0
			219	219		

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.

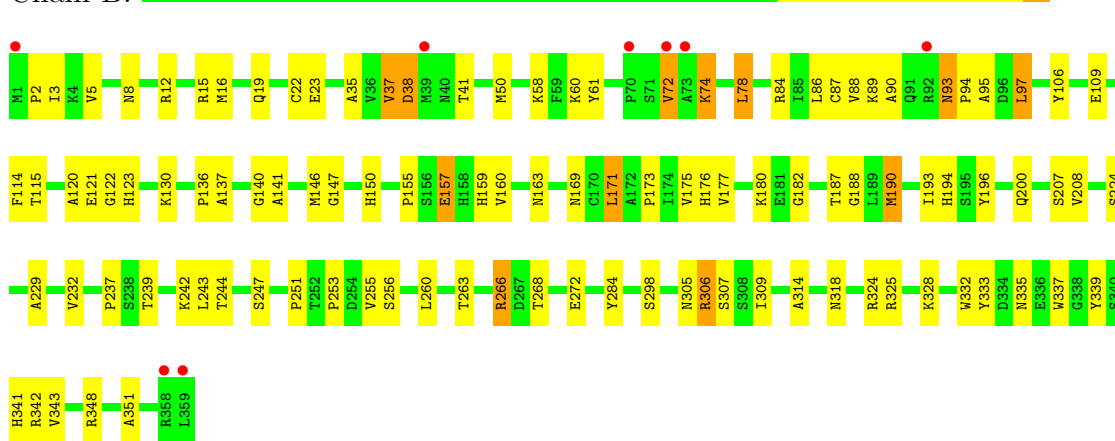
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, glycosomal

Chain A:



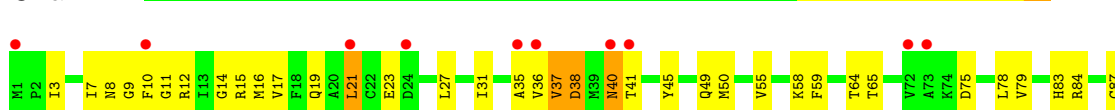
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, glycosomal

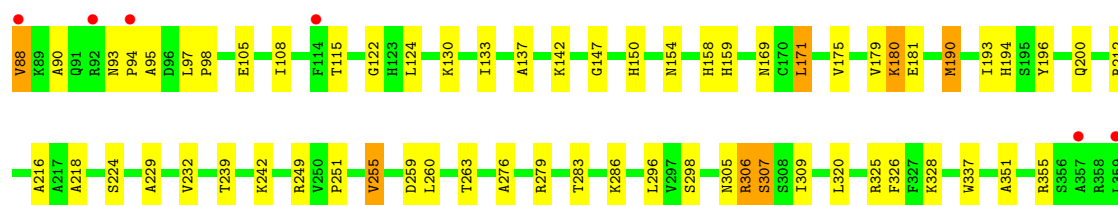
Chain B:



- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, glycosomal

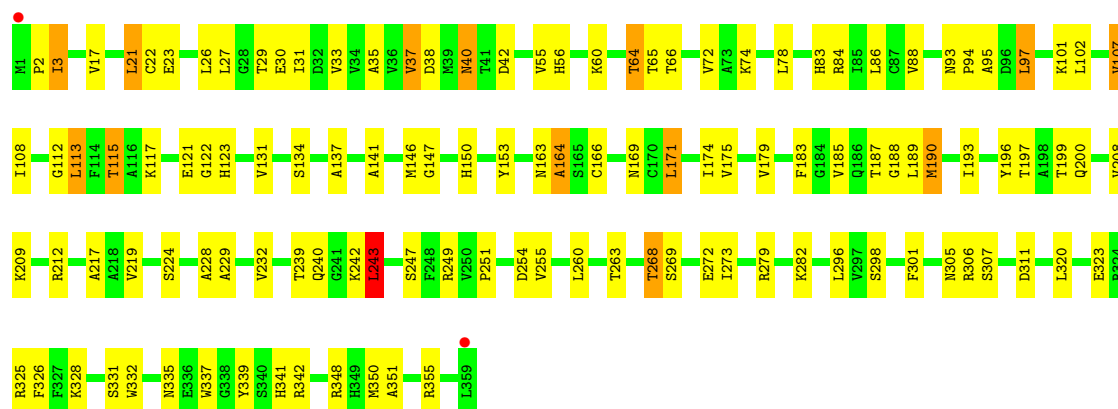
Chain D:





● Molecule 2: Glyceraldehyde-3-phosphatedehydrogenase, glycosomal

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.75Å 83.71Å 105.61Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	38.10 – 2.30 38.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.10-2.30) 96.5 (38.09-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.252 0.185 , 0.248	Depositor DCC
R_{free} test set	2987 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.6	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	2 of 58607 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12123	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GOL, CCS, 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	0.56	1/2786 (0.0%)	0.67	0/3778
1	B	0.57	0/2786	0.70	0/3778
1	D	0.54	0/2786	0.66	1/3778 (0.0%)
2	C	0.60	1/2779 (0.0%)	0.73	3/3767 (0.1%)
All	All	0.57	2/11137 (0.0%)	0.69	4/15101 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	22	CYS	CB-SG	-7.58	1.69	1.82
1	A	22	CYS	CB-SG	-5.99	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	243	LEU	CA-CB-CG	5.97	129.04	115.30
2	C	113	LEU	CA-CB-CG	5.46	127.85	115.30
2	C	279	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	21	LEU	CA-CB-CG	5.17	127.18	115.30

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	2733	0	2721	86	0
1	B	2733	0	2722	89	0
1	D	2733	0	2722	88	0
2	C	2737	0	2723	115	0
3	A	44	0	26	4	0
3	B	44	0	26	3	0
3	C	44	0	26	7	0
3	D	44	0	26	3	0
4	C	6	0	8	5	0
5	A	195	0	0	13	0
5	B	294	0	0	15	0
5	C	297	0	0	19	0
5	D	219	0	0	10	0
All	All	12123	0	11000	364	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 17.

All (364) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:MET:HG2	5:A:435:HOH:O	1.41	1.18
1:B:37:VAL:HG22	3:B:360:NAD:H2A	1.40	0.99
1:A:305:ASN:HB3	5:A:535:HOH:O	1.72	0.88
1:D:37:VAL:HG22	3:D:360:NAD:H2A	1.57	0.83
1:A:47:ALA:HA	1:A:50:MET:HE3	1.61	0.82
1:A:66:THR:HG22	5:A:480:HOH:O	1.80	0.82
2:C:311:ASP:HB2	5:C:445:HOH:O	1.79	0.81
1:A:147:GLY:H	1:A:150:HIS:HD2	1.29	0.80
1:D:16:MET:HG2	5:D:471:HOH:O	1.80	0.79
1:B:19:GLN:HG3	5:B:375:HOH:O	1.83	0.79
2:C:3:ILE:HG22	2:C:355:ARG:HH21	1.47	0.78
2:C:37:VAL:HG22	3:C:360:NAD:H2A	1.64	0.78
1:D:8:ASN:HA	1:D:37:VAL:HG13	1.66	0.77
2:C:147:GLY:H	2:C:150:HIS:HD2	1.31	0.77
2:C:171:LEU:HD13	2:C:232:VAL:HG21	1.67	0.77
2:C:190:MET:HG2	2:C:229:ALA:HB2	1.66	0.76
1:A:190:MET:HG2	1:A:229:ALA:HB2	1.68	0.76
1:B:2:PRO:HB3	5:B:531:HOH:O	1.86	0.76
1:A:186:GLN:HB2	1:A:263:THR:HG23	1.68	0.76
2:C:239:THR:HA	2:C:242:LYS:HE2	1.68	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:147:GLY:H	2:C:150:HIS:CD2	2.04	0.75
2:C:101:LYS:HG3	5:C:430:HOH:O	1.86	0.75
2:C:26:LEU:HD22	2:C:30:GLU:HG3	1.68	0.74
1:B:190:MET:HG2	1:B:229:ALA:HB2	1.68	0.74
1:A:176:HIS:HD2	5:A:425:HOH:O	1.68	0.74
1:D:147:GLY:H	1:D:150:HIS:CD2	2.06	0.74
1:B:37:VAL:CG2	3:B:360:NAD:H2A	2.17	0.74
2:C:188:GLY:HA3	2:C:243:LEU:HD13	1.70	0.73
1:B:176:HIS:HE1	5:B:411:HOH:O	1.72	0.73
1:A:147:GLY:H	1:A:150:HIS:CD2	2.05	0.73
1:A:238:SER:O	1:A:242:LYS:HE2	1.89	0.72
1:A:171:LEU:HD13	1:A:232:VAL:HG21	1.72	0.71
2:C:37:VAL:HB	2:C:88:VAL:HG22	1.71	0.71
2:C:107:VAL:HG11	2:C:123:HIS:HB3	1.71	0.71
1:B:348:ARG:HD2	5:B:510:HOH:O	1.91	0.71
2:C:268:THR:HG22	2:C:269:SER:H	1.54	0.70
2:C:199:THR:HG23	4:C:361:GOL:H32	1.71	0.70
1:B:115:THR:HG23	1:B:136:PRO:O	1.92	0.70
1:A:171:LEU:HG	1:A:190:MET:HE2	1.75	0.69
1:D:37:VAL:CG2	3:D:360:NAD:H2A	2.23	0.68
2:C:174:ILE:HD11	2:C:331:SER:HB2	1.74	0.68
1:A:190:MET:HG3	1:A:245:GLY:HA3	1.76	0.68
1:A:263:THR:HA	1:A:325:ARG:O	1.95	0.66
2:C:94:PRO:HA	2:C:97:LEU:HD22	1.78	0.66
1:D:21:LEU:HD11	1:D:31:ILE:HD13	1.78	0.65
2:C:331:SER:HA	5:C:445:HOH:O	1.96	0.65
1:D:38:ASP:O	1:D:90:ALA:HB2	1.96	0.65
1:D:171:LEU:HD22	1:D:175:VAL:HG23	1.80	0.64
1:A:42:ASP:O	1:A:46:PHE:HD1	1.80	0.64
1:B:74:LYS:HG3	5:B:410:HOH:O	1.97	0.64
1:B:182:GLY:O	1:B:266:ARG:HD3	1.97	0.64
1:A:171:LEU:HD22	1:A:175:VAL:HG23	1.80	0.64
1:D:93:ASN:OD1	1:D:95:ALA:HB3	1.98	0.63
1:B:171:LEU:HD22	1:B:175:VAL:HG23	1.81	0.63
2:C:23:GLU:OE1	5:C:650:HOH:O	2.16	0.63
2:C:117:LYS:O	2:C:121:GLU:HG3	1.98	0.63
1:B:157:GLU:HG3	5:B:459:HOH:O	1.99	0.63
1:A:8:ASN:HA	1:A:37:VAL:HG13	1.80	0.62
1:B:78:LEU:HD22	1:B:87:CYS:SG	2.38	0.62
1:B:171:LEU:HD13	1:B:232:VAL:HG21	1.81	0.62
1:A:114:PHE:O	1:A:120:ALA:HB2	2.00	0.62
1:A:117:LYS:HG3	1:A:141:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:239:THR:HB	2:C:243:LEU:HD23	1.82	0.61
1:D:169:ASN:O	1:D:307:SER:HB2	1.99	0.61
2:C:196:TYR:HA	2:C:200:GLN:NE2	2.15	0.61
2:C:171:LEU:HD22	2:C:175:VAL:HG23	1.82	0.61
1:A:47:ALA:HA	1:A:50:MET:CE	2.31	0.61
1:D:181:GLU:HG3	1:D:276:ALA:HB1	1.84	0.60
1:B:147:GLY:H	1:B:150:HIS:CD2	2.20	0.60
1:B:23:GLU:OE2	1:B:341:HIS:CE1	2.55	0.59
1:D:19:GLN:HG3	1:D:59:PHE:CE1	2.37	0.59
1:D:171:LEU:HD13	1:D:232:VAL:HG21	1.85	0.59
1:A:285:MET:HB3	1:A:289:LEU:HB3	1.84	0.59
2:C:341:HIS:HE1	5:C:650:HOH:O	1.85	0.59
1:A:50:MET:HE1	1:A:63:VAL:HG11	1.84	0.59
2:C:84:ARG:NH2	5:C:498:HOH:O	2.34	0.59
1:D:306:ARG:HB2	1:D:309:ILE:CD1	2.33	0.58
1:B:306:ARG:HB2	1:B:309:ILE:CD1	2.32	0.58
1:D:45:TYR:O	1:D:49:GLN:HG3	2.04	0.58
1:A:38:ASP:O	1:A:90:ALA:HB2	2.03	0.58
1:D:283:THR:O	1:D:286:LYS:HB2	2.04	0.58
2:C:185:VAL:O	2:C:242:LYS:HE3	2.03	0.58
1:B:137:ALA:HB3	1:B:141:ALA:HB3	1.85	0.58
1:D:224:SER:HB2	1:D:249:ARG:NH2	2.20	0.57
1:D:147:GLY:H	1:D:150:HIS:HD2	1.53	0.57
2:C:94:PRO:HA	2:C:97:LEU:CD2	2.35	0.57
1:D:64:THR:HG22	1:D:65:THR:H	1.69	0.57
2:C:107:VAL:HG11	2:C:123:HIS:CB	2.35	0.57
1:D:190:MET:HG2	1:D:229:ALA:HB2	1.87	0.56
2:C:260:LEU:O	2:C:328:LYS:HA	2.05	0.56
1:B:207:SER:HB2	5:B:542:HOH:O	2.05	0.56
1:B:266:ARG:NH2	1:B:272:GLU:OE1	2.36	0.56
2:C:351:ALA:O	2:C:355:ARG:HG2	2.06	0.56
1:B:38:ASP:O	1:B:90:ALA:HB2	2.06	0.56
2:C:196:TYR:HA	2:C:200:GLN:HE22	1.71	0.56
1:A:15:ARG:O	1:A:19:GLN:HG3	2.07	0.55
1:D:64:THR:HG22	1:D:65:THR:N	2.21	0.55
1:D:84:ARG:NH2	5:D:444:HOH:O	2.39	0.55
2:C:112:GLY:HA2	3:C:360:NAD:O3D	2.07	0.55
1:B:306:ARG:HB2	1:B:309:ILE:HD11	1.88	0.54
2:C:197:THR:OG1	4:C:361:GOL:H11	2.07	0.54
1:A:17:VAL:HG11	1:A:108:ILE:HD13	1.90	0.54
1:A:320:LEU:HD13	1:B:187:THR:HG23	1.89	0.54
1:B:150:HIS:HE1	5:B:471:HOH:O	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:LEU:HD23	1:B:88:VAL:HG12	1.89	0.54
1:A:348:ARG:HD2	5:A:422:HOH:O	2.08	0.54
2:C:171:LEU:HD12	2:C:229:ALA:HA	1.89	0.54
2:C:21:LEU:HD11	2:C:31:ILE:HD13	1.89	0.54
1:A:165:SER:HB2	5:A:511:HOH:O	2.07	0.54
2:C:197:THR:OG1	4:C:361:GOL:H31	2.08	0.54
1:A:260:LEU:O	1:A:328:LYS:HA	2.08	0.54
1:B:94:PRO:HA	1:B:97:LEU:HD22	1.90	0.54
1:A:196:TYR:HA	1:A:200:GLN:NE2	2.22	0.54
1:A:166:CYS:HB3	3:A:360:NAD:H5N	1.90	0.53
2:C:174:ILE:HD11	2:C:331:SER:CB	2.38	0.53
1:A:171:LEU:CG	1:A:190:MET:HE2	2.38	0.53
2:C:183:PHE:CD1	2:C:268:THR:HG21	2.44	0.53
2:C:282:LYS:HE2	5:C:580:HOH:O	2.08	0.53
1:B:239:THR:HA	1:B:242:LYS:HD2	1.91	0.53
1:A:118:ALA:O	1:A:121:GLU:HB2	2.09	0.53
1:A:124:LEU:HA	1:A:128:ALA:O	2.09	0.53
1:A:251:PRO:HB2	1:B:251:PRO:HB2	1.91	0.53
2:C:146:MET:HB2	2:C:342:ARG:HD3	1.90	0.53
2:C:35:ALA:HB1	2:C:88:VAL:HG13	1.90	0.52
1:A:130:LYS:NZ	1:A:159:HIS:HD2	2.07	0.52
3:A:360:NAD:N7N	3:A:360:NAD:O2N	2.43	0.52
1:D:196:TYR:HA	1:D:200:GLN:NE2	2.24	0.52
2:C:55:VAL:HG22	2:C:56:HIS:CD2	2.43	0.52
1:B:196:TYR:HA	1:B:200:GLN:NE2	2.25	0.52
2:C:2:PRO:HB3	2:C:29:THR:O	2.10	0.52
1:A:320:LEU:HG	1:B:244:THR:HG22	1.90	0.52
1:D:159:HIS:HE1	5:D:485:HOH:O	1.91	0.52
2:C:337:TRP:O	2:C:341:HIS:HD2	1.93	0.52
1:A:273:ILE:HG21	1:A:329:ILE:HD11	1.92	0.52
1:B:188:GLY:HA3	1:B:243:LEU:HD23	1.92	0.52
1:A:16:MET:SD	1:A:337:TRP:HZ3	2.33	0.52
1:D:351:ALA:O	1:D:355:ARG:HD3	2.10	0.51
2:C:320:LEU:HB2	2:C:323:GLU:HB2	1.92	0.51
1:B:84:ARG:NH2	5:B:495:HOH:O	2.42	0.51
2:C:72:VAL:HG12	2:C:74:LYS:O	2.11	0.51
1:D:78:LEU:HD22	1:D:87:CYS:SG	2.50	0.51
1:A:229:ALA:HB3	1:A:244:THR:HA	1.92	0.51
2:C:323:GLU:HG2	2:C:326:PHE:O	2.10	0.51
1:A:339:TYR:O	1:A:343:VAL:HG23	2.11	0.51
2:C:166:CCS:HD2	3:C:360:NAD:C4N	2.40	0.51
2:C:17:VAL:HG11	2:C:108:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:208:VAL:HG23	5:C:408:HOH:O	2.10	0.51
2:C:326:PHE:HE1	1:D:326:PHE:CE1	2.29	0.51
1:B:208:VAL:HG22	5:B:446:HOH:O	2.11	0.51
1:B:260:LEU:O	1:B:328:LYS:HA	2.11	0.51
2:C:263:THR:HA	2:C:325:ARG:O	2.11	0.51
1:B:58:LYS:HG3	5:D:451:HOH:O	2.12	0.50
3:D:360:NAD:O2N	3:D:360:NAD:N7N	2.44	0.50
2:C:268:THR:HG22	2:C:272:GLU:HB3	1.93	0.50
2:C:193:ILE:HD12	1:D:193:ILE:HG13	1.93	0.50
2:C:33:VAL:H	2:C:83:HIS:HE1	1.58	0.50
1:B:169:ASN:O	1:B:307:SER:HB3	2.11	0.50
2:C:153:TYR:CE2	2:C:350:MET:HA	2.46	0.50
1:A:230:LYS:HE2	5:A:388:HOH:O	2.11	0.50
1:D:181:GLU:OE2	1:D:279:ARG:NH2	2.45	0.49
1:B:194:HIS:HA	1:B:256:SER:HB3	1.94	0.49
1:D:19:GLN:HG3	1:D:59:PHE:CD1	2.47	0.49
1:D:224:SER:HB2	1:D:249:ARG:CZ	2.43	0.49
1:A:121:GLU:O	1:A:124:LEU:HB2	2.13	0.49
1:D:40:ASN:H	1:D:40:ASN:ND2	2.09	0.49
1:A:50:MET:HE1	1:A:78:LEU:HG	1.94	0.49
2:C:296:LEU:O	1:D:212:ARG:HD3	2.12	0.49
1:A:91:GLN:HG2	1:A:97:LEU:HD13	1.95	0.49
1:B:314:ALA:O	1:B:318:ASN:ND2	2.41	0.49
1:D:159:HIS:CE1	5:D:485:HOH:O	2.66	0.49
2:C:224:SER:HB3	2:C:247:SER:HB3	1.95	0.49
1:B:146:MET:HB2	1:B:342:ARG:HD3	1.93	0.49
3:C:360:NAD:O2N	3:C:360:NAD:N7N	2.44	0.48
1:B:266:ARG:NH1	5:B:477:HOH:O	2.46	0.48
2:C:326:PHE:CE1	1:D:326:PHE:CE1	3.02	0.48
2:C:240:GLN:NE2	5:C:485:HOH:O	2.47	0.48
2:C:301:PHE:CZ	2:C:332:TRP:CD1	3.02	0.48
1:B:193:ILE:N	1:B:193:ILE:HD12	2.28	0.48
2:C:35:ALA:HB1	2:C:88:VAL:CG1	2.43	0.48
1:B:94:PRO:HB3	1:B:123:HIS:CE1	2.48	0.48
1:B:130:LYS:NZ	1:B:159:HIS:HD2	2.11	0.48
1:A:337:TRP:O	1:A:341:HIS:HD2	1.96	0.48
1:A:106:TYR:OH	1:A:351:ALA:HA	2.14	0.48
1:A:205:GLY:HA2	5:A:515:HOH:O	2.14	0.48
1:D:10:PHE:CE1	1:D:36:VAL:HG11	2.49	0.48
1:A:256:SER:HB2	1:A:333:TYR:CZ	2.49	0.48
1:A:129:ARG:HG3	1:A:130:LYS:HG2	1.96	0.47
1:B:23:GLU:HA	1:B:60:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:8:ASN:HA	1:B:37:VAL:HG13	1.95	0.47
1:A:37:VAL:HB	1:A:88:VAL:HG22	1.96	0.47
1:B:130:LYS:NZ	1:B:155:PRO:O	2.47	0.47
2:C:95:ALA:HA	2:C:122:GLY:O	2.13	0.47
2:C:268:THR:HG23	2:C:272:GLU:OE2	2.15	0.47
2:C:341:HIS:CE1	5:C:650:HOH:O	2.64	0.47
1:A:94:PRO:HB2	1:A:122:GLY:HA3	1.95	0.47
1:B:176:HIS:CD2	5:B:647:HOH:O	2.68	0.47
1:A:37:VAL:HG22	3:A:360:NAD:H2A	1.97	0.47
1:A:263:THR:HG21	5:A:476:HOH:O	2.14	0.47
1:D:298:SER:HB2	5:D:445:HOH:O	2.14	0.47
1:D:37:VAL:HG22	1:D:37:VAL:O	2.15	0.47
2:C:197:THR:HG21	4:C:361:GOL:H11	1.97	0.46
1:B:224:SER:HB3	1:B:247:SER:HB3	1.97	0.46
1:B:50:MET:HG2	5:B:375:HOH:O	2.15	0.46
1:D:65:THR:HB	1:D:75:ASP:HB3	1.98	0.46
1:A:209:LYS:HE3	1:A:209:LYS:HA	1.95	0.46
1:B:23:GLU:OE2	1:B:341:HIS:HE1	1.97	0.46
1:A:10:PHE:CE2	1:A:15:ARG:HG2	2.50	0.46
1:B:93:ASN:C	1:B:93:ASN:HD22	2.18	0.46
2:C:134:SER:O	3:C:360:NAD:H6N	2.16	0.46
2:C:115:THR:HG22	5:C:461:HOH:O	2.16	0.46
1:B:58:LYS:HE3	5:D:451:HOH:O	2.16	0.46
1:D:11:GLY:O	1:D:15:ARG:HB2	2.16	0.46
2:C:339:TYR:CG	3:C:360:NAD:H5N	2.50	0.46
1:B:12:ARG:HH11	1:B:15:ARG:NH2	2.13	0.46
1:D:130:LYS:NZ	1:D:159:HIS:HD2	2.13	0.46
1:D:94:PRO:HA	1:D:97:LEU:HD23	1.98	0.46
2:C:40:ASN:HD22	2:C:40:ASN:C	2.20	0.46
1:A:155:PRO:HG3	1:A:353:LYS:O	2.16	0.46
2:C:239:THR:HB	2:C:243:LEU:CD2	2.46	0.45
1:B:121:GLU:HG3	1:B:160:VAL:HG21	1.97	0.45
1:B:16:MET:SD	1:B:337:TRP:HZ3	2.40	0.45
2:C:187:THR:HG23	1:D:320:LEU:CD1	2.47	0.45
1:D:298:SER:CB	5:D:445:HOH:O	2.64	0.45
1:B:106:TYR:OH	1:B:351:ALA:HA	2.16	0.45
1:D:17:VAL:O	1:D:21:LEU:HB2	2.17	0.45
1:A:98:PRO:HG2	1:A:102:LEU:HD22	1.98	0.45
1:D:17:VAL:HG11	1:D:108:ILE:HD13	1.99	0.45
1:B:263:THR:HA	1:B:325:ARG:O	2.17	0.45
1:D:196:TYR:HA	1:D:200:GLN:HE22	1.81	0.45
1:A:54:THR:HG21	1:D:216:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:PRO:CG	1:B:332:TRP:HZ2	2.29	0.45
2:C:183:PHE:CE1	2:C:268:THR:HG21	2.51	0.45
1:A:181:GLU:HG3	1:A:276:ALA:HB1	1.98	0.45
1:B:93:ASN:C	1:B:93:ASN:ND2	2.70	0.45
1:A:170:CYS:HG	1:A:333:TYR:HD1	1.64	0.45
1:A:50:MET:O	1:A:59:PHE:HB2	2.16	0.45
2:C:348:ARG:HD2	5:C:503:HOH:O	2.17	0.45
1:A:176:HIS:CD2	5:A:425:HOH:O	2.55	0.45
1:B:3:ILE:HG22	1:B:5:VAL:HG23	1.99	0.45
2:C:188:GLY:O	2:C:243:LEU:HA	2.17	0.44
2:C:93:ASN:HD22	2:C:94:PRO:HD2	1.82	0.44
1:D:130:LYS:NZ	1:D:159:HIS:CD2	2.86	0.44
2:C:137:ALA:HB3	2:C:141:ALA:HB3	1.99	0.44
1:D:21:LEU:HD11	1:D:31:ILE:CD1	2.46	0.44
1:A:320:LEU:CD1	1:B:187:THR:CG2	2.95	0.44
1:A:109:GLU:OE2	1:A:123:HIS:NE2	2.48	0.44
1:D:21:LEU:CD1	1:D:31:ILE:HD13	2.46	0.44
1:B:16:MET:SD	1:B:337:TRP:CZ3	3.11	0.44
1:D:50:MET:O	1:D:59:PHE:HB2	2.17	0.44
2:C:187:THR:HG21	1:D:326:PHE:HB3	2.00	0.44
1:D:171:LEU:HD21	1:D:260:LEU:HD13	2.00	0.44
1:D:190:MET:HG3	1:D:190:MET:O	2.16	0.44
2:C:187:THR:CG2	1:D:320:LEU:CD1	2.96	0.44
1:B:196:TYR:HA	1:B:200:GLN:HE22	1.82	0.44
1:D:263:THR:HA	1:D:325:ARG:O	2.16	0.44
1:D:23:GLU:OE1	1:D:337:TRP:CZ2	2.70	0.44
1:D:259:ASP:OD1	1:D:328:LYS:HE3	2.18	0.44
2:C:200:GLN:HB3	2:C:217:ALA:HB2	1.99	0.44
2:C:115:THR:CG2	5:C:461:HOH:O	2.66	0.44
1:B:12:ARG:HH11	1:B:15:ARG:HH21	1.65	0.44
1:A:171:LEU:CD1	1:A:190:MET:HE2	2.48	0.44
1:A:320:LEU:CD1	1:B:187:THR:HG23	2.47	0.44
1:B:256:SER:HB2	1:B:333:TYR:CZ	2.53	0.44
2:C:27:LEU:HB2	5:C:469:HOH:O	2.17	0.44
1:A:13:ILE:O	1:A:17:VAL:HG23	2.18	0.44
1:A:196:TYR:HA	1:A:200:GLN:HE22	1.80	0.44
1:A:130:LYS:NZ	1:A:159:HIS:CD2	2.85	0.44
1:D:218:ALA:O	1:D:251:PRO:HB3	2.18	0.44
1:A:176:HIS:HE1	5:A:451:HOH:O	2.00	0.43
2:C:40:ASN:ND2	2:C:42:ASP:H	2.16	0.43
1:B:114:PHE:O	1:B:120:ALA:HB2	2.17	0.43
1:D:255:VAL:HG11	1:D:298:SER:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:163:ASN:O	2:C:164:ALA:HB3	2.17	0.43
2:C:212:ARG:HD3	1:D:296:LEU:O	2.18	0.43
1:A:63:VAL:HG22	1:A:80:VAL:HG22	2.01	0.43
1:D:11:GLY:O	1:D:12:ARG:C	2.56	0.43
2:C:30:GLU:OE2	2:C:348:ARG:NH1	2.51	0.43
1:B:93:ASN:HD22	1:B:94:PRO:HD2	1.83	0.43
1:D:260:LEU:O	1:D:328:LYS:HA	2.18	0.43
1:A:335:ASN:O	3:A:360:NAD:H4N	2.18	0.43
2:C:107:VAL:HG13	2:C:131:VAL:HG22	2.00	0.43
1:A:130:LYS:HZ1	1:A:159:HIS:HD2	1.66	0.43
1:B:298:SER:HB3	1:B:332:TRP:HZ3	1.84	0.43
1:D:180:LYS:N	1:D:180:LYS:HD2	2.32	0.43
2:C:64:THR:CG2	2:C:65:THR:N	2.81	0.43
2:C:335:ASN:O	3:C:360:NAD:H4N	2.18	0.42
1:A:190:MET:O	1:A:245:GLY:HA3	2.19	0.42
2:C:268:THR:CG2	2:C:269:SER:H	2.23	0.42
2:C:55:VAL:HG21	2:C:254:ASP:CB	2.49	0.42
1:A:67:LYS:HB3	1:A:72:VAL:HG22	2.01	0.42
2:C:305:ASN:HB3	5:C:393:HOH:O	2.19	0.42
2:C:101:LYS:HE3	5:C:430:HOH:O	2.19	0.42
2:C:298:SER:HB3	2:C:332:TRP:HZ3	1.84	0.42
2:C:183:PHE:CD1	2:C:273:ILE:HD13	2.54	0.42
2:C:298:SER:HB3	2:C:332:TRP:CZ3	2.54	0.42
1:A:44:GLU:HG2	5:A:429:HOH:O	2.19	0.42
1:A:65:THR:HB	1:A:75:ASP:HB3	2.01	0.42
1:B:140:GLY:HA2	5:B:636:HOH:O	2.19	0.42
1:B:237:PRO:HD2	5:B:551:HOH:O	2.19	0.42
1:B:109:GLU:OE2	1:B:123:HIS:NE2	2.37	0.42
1:B:337:TRP:O	1:B:341:HIS:HD2	2.02	0.42
2:C:83:HIS:HD2	5:C:433:HOH:O	2.02	0.42
1:D:10:PHE:CE2	1:D:15:ARG:HG3	2.55	0.42
1:B:22:CYS:O	1:B:61:TYR:HE1	2.03	0.42
2:C:190:MET:HE2	2:C:228:ALA:HB3	2.02	0.42
1:B:180:LYS:HE2	1:B:284:TYR:CE2	2.55	0.42
1:B:41:THR:HG21	1:B:89:LYS:HG2	2.02	0.42
1:D:83:HIS:HB2	5:D:546:HOH:O	2.20	0.42
1:D:239:THR:HA	1:D:242:LYS:HD2	2.01	0.42
2:C:175:VAL:O	2:C:179:VAL:HG23	2.19	0.41
1:D:142:LYS:HB2	1:D:158:HIS:CD2	2.55	0.41
2:C:209:LYS:HE2	5:C:525:HOH:O	2.20	0.41
1:B:339:TYR:O	1:B:343:VAL:HG23	2.20	0.41
1:A:16:MET:SD	1:A:337:TRP:CZ3	3.13	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:174:ILE:CD1	2:C:331:SER:HB2	2.45	0.41
1:D:79:VAL:HA	1:D:83:HIS:O	2.20	0.41
2:C:115:THR:HB	5:C:484:HOH:O	2.18	0.41
1:D:35:ALA:HB1	1:D:88:VAL:HG22	2.02	0.41
1:A:146:MET:HB2	1:A:342:ARG:HD3	2.01	0.41
1:D:175:VAL:O	1:D:179:VAL:HG23	2.19	0.41
2:C:200:GLN:NE2	2:C:249:ARG:HD2	2.36	0.41
2:C:94:PRO:HB3	2:C:123:HIS:CE1	2.55	0.41
2:C:169:ASN:O	2:C:307:SER:HB3	2.21	0.41
2:C:189:LEU:HD13	1:D:328:LYS:HB2	2.02	0.41
1:D:306:ARG:HB2	1:D:309:ILE:HD11	2.02	0.41
2:C:33:VAL:H	2:C:83:HIS:CE1	2.37	0.41
1:B:163:ASN:O	1:B:169:ASN:ND2	2.48	0.41
1:D:115:THR:HA	1:D:133:ILE:HG21	2.02	0.41
1:A:224:SER:HB3	1:A:247:SER:HB3	2.02	0.41
1:A:324:ARG:HG2	5:A:492:HOH:O	2.20	0.41
1:B:335:ASN:O	3:B:360:NAD:H4N	2.21	0.41
2:C:35:ALA:HA	2:C:86:LEU:O	2.20	0.41
1:D:21:LEU:CD1	1:D:31:ILE:CD1	2.99	0.41
1:D:124:LEU:HD21	1:D:159:HIS:HB3	2.01	0.41
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.90	0.41
1:B:253:PRO:HG3	2:C:219:VAL:HG11	2.02	0.41
1:D:23:GLU:OE1	1:D:337:TRP:HZ2	2.02	0.41
1:D:64:THR:HG21	5:D:460:HOH:O	2.21	0.41
1:B:35:ALA:HB1	1:B:88:VAL:HG13	2.01	0.41
1:B:175:VAL:CG1	1:B:239:THR:HG21	2.51	0.41
1:D:7:ILE:HB	1:D:36:VAL:HG12	2.03	0.41
1:D:9:GLY:O	1:D:14:GLY:HA3	2.21	0.41
2:C:196:TYR:CD2	2:C:251:PRO:HA	2.56	0.41
1:B:268:THR:O	1:B:324:ARG:HA	2.21	0.41
1:D:16:MET:SD	1:D:337:TRP:CZ3	3.14	0.40
1:B:93:ASN:HD22	1:B:94:PRO:N	2.19	0.40
2:C:342:ARG:NE	2:C:342:ARG:HA	2.36	0.40
1:A:163:ASN:O	1:A:164:ALA:HB3	2.21	0.40
2:C:200:GLN:CD	2:C:249:ARG:HD2	2.42	0.40
1:D:200:GLN:NE2	1:D:249:ARG:HD2	2.37	0.40
1:B:86:LEU:CD2	1:B:88:VAL:HG12	2.51	0.40
2:C:3:ILE:HD12	2:C:351:ALA:HB2	2.04	0.40
1:A:186:GLN:HG3	1:A:264:ALA:O	2.21	0.40
1:D:95:ALA:HA	1:D:122:GLY:O	2.21	0.40
2:C:196:TYR:CE2	2:C:251:PRO:HA	2.55	0.40
1:D:194:HIS:O	1:D:249:ARG:HA	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:173:PRO:O	1:B:177:VAL:HG23	2.22	0.40
1:B:196:TYR:CE2	1:B:251:PRO:HA	2.56	0.40
2:C:197:THR:CB	4:C:361:GOL:H31	2.52	0.40
1:B:196:TYR:CD2	1:B:251:PRO:HA	2.57	0.40
1:D:130:LYS:HZ1	1:D:159:HIS:CD2	2.39	0.40
1:D:97:LEU:HA	1:D:98:PRO:HD3	1.92	0.40
1:D:115:THR:O	1:D:137:ALA:HA	2.21	0.40
1:B:95:ALA:HA	1:B:122:GLY:O	2.22	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%)	337 (94%)	17 (5%)	3 (1%)	27	30
1	B	357/359 (99%)	341 (96%)	14 (4%)	2 (1%)	33	39
1	D	357/359 (99%)	337 (94%)	19 (5%)	1 (0%)	50	60
2	C	356/359 (99%)	337 (95%)	17 (5%)	2 (1%)	33	39
All	All	1427/1436 (99%)	1352 (95%)	67 (5%)	8 (1%)	33	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	SER
1	A	255	VAL
1	B	255	VAL
2	C	255	VAL
1	D	255	VAL
1	A	42	ASP
1	B	72	VAL
2	C	164	ALA

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	293/296 (99%)	276 (94%)	17 (6%)	28	36
1	B	293/296 (99%)	280 (96%)	13 (4%)	39	51
1	D	293/296 (99%)	276 (94%)	17 (6%)	28	36
2	C	292/295 (99%)	273 (94%)	19 (6%)	24	30
All	All	1171/1183 (99%)	1105 (94%)	66 (6%)	30	38

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	37	VAL
1	A	38	ASP
1	A	39	MET
1	A	55	VAL
1	A	60	LYS
1	A	78	LEU
1	A	88	VAL
1	A	97	LEU
1	A	121	GLU
1	A	157	GLU
1	A	171	LEU
1	A	187	THR
1	A	208	VAL
1	A	209	LYS
1	A	306	ARG
1	A	355	ARG
1	B	37	VAL
1	B	38	ASP
1	B	72	VAL
1	B	74	LYS
1	B	78	LEU
1	B	93	ASN
1	B	97	LEU
1	B	157	GLU
1	B	171	LEU

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Mol	Chain	Res	Type
1	B	190	MET
1	B	266	ARG
1	B	305	ASN
1	B	306	ARG
2	C	3	ILE
2	C	21	LEU
2	C	37	VAL
2	C	38	ASP
2	C	40	ASN
2	C	60	LYS
2	C	64	THR
2	C	66	THR
2	C	78	LEU
2	C	97	LEU
2	C	102	LEU
2	C	107	VAL
2	C	113	LEU
2	C	115	THR
2	C	171	LEU
2	C	190	MET
2	C	243	LEU
2	C	268	THR
2	C	306	ARG
1	D	3	ILE
1	D	27	LEU
1	D	37	VAL
1	D	38	ASP
1	D	40	ASN
1	D	41	THR
1	D	55	VAL
1	D	58	LYS
1	D	88	VAL
1	D	105	GLU
1	D	154	ASN
1	D	171	LEU
1	D	180	LYS
1	D	190	MET
1	D	305	ASN
1	D	306	ARG
1	D	307	SER

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	93	ASN
1	A	150	HIS
1	A	159	HIS
1	A	176	HIS
1	A	186	GLN
1	A	200	GLN
1	B	8	ASN
1	B	83	HIS
1	B	93	ASN
1	B	150	HIS
1	B	151	HIS
1	B	159	HIS
1	B	176	HIS
1	B	200	GLN
1	B	305	ASN
1	B	341	HIS
2	C	19	GLN
2	C	40	ASN
2	C	83	HIS
2	C	93	ASN
2	C	150	HIS
2	C	151	HIS
2	C	176	HIS
2	C	200	GLN
2	C	240	GLN
2	C	341	HIS
1	D	8	ASN
1	D	150	HIS
1	D	154	ASN
1	D	159	HIS
1	D	200	GLN
1	D	305	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CCS	C	166	2	9,9,10	6.07	2 (22%)	8,10,12	2.40	2 (25%)

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	CCS	C	166	2	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	166	CCS	O-C	17.77	1.23	1.11
2	C	166	CCS	CD-SG	-3.03	1.76	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	166	CCS	C-CA-N	-5.95	107.89	113.83
2	C	166	CCS	CB-SG-CD	2.27	105.65	101.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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	NAD	A	360	-	48,48,48	1.01	3 (6%)	73,73,73	1.51	9 (12%)
3	NAD	B	360	-	48,48,48	1.03	3 (6%)	73,73,73	1.53	10 (13%)
3	NAD	C	360	-	48,48,48	1.05	2 (4%)	73,73,73	2.05	14 (19%)
4	GOL	C	361	-	5,5,5	0.26	0	5,5,5	0.22	0
3	NAD	D	360	-	48,48,48	1.11	4 (8%)	73,73,73	1.63	10 (13%)

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	NAD	A	360	-	-	0/30/62/62	0/3/5/5
3	NAD	B	360	-	-	0/30/62/62	0/3/5/5
3	NAD	C	360	-	-	0/30/62/62	0/3/5/5
4	GOL	C	361	-	-	0/4/4/4	0/0/0/0
3	NAD	D	360	-	-	0/30/62/62	0/3/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	360	NAD	C2N-N1N	4.10	1.40	1.35
3	A	360	NAD	C2N-N1N	3.77	1.40	1.35
3	B	360	NAD	C2N-N1N	3.50	1.39	1.35
3	D	360	NAD	C4A-N9A	-3.40	1.32	1.37
3	B	360	NAD	C4A-N9A	-3.14	1.33	1.37
3	D	360	NAD	C2N-N1N	3.07	1.39	1.35
3	C	360	NAD	C4A-N9A	-3.01	1.33	1.37
3	D	360	NAD	O4B-C1B	2.93	1.45	1.41
3	A	360	NAD	C4A-N9A	-2.83	1.33	1.37
3	B	360	NAD	O4D-C1D	2.33	1.44	1.41
3	D	360	NAD	O4D-C1D	2.21	1.44	1.41
3	A	360	NAD	O4D-C1D	2.11	1.44	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	360	NAD	N3A-C2A-N1A	-9.29	120.94	128.71
3	D	360	NAD	N3A-C2A-N1A	-8.97	121.21	128.71
3	C	360	NAD	O4D-C1D-N1N	-8.50	99.25	107.95
3	A	360	NAD	N3A-C2A-N1A	-7.96	122.06	128.71
3	B	360	NAD	N3A-C2A-N1A	-7.55	122.40	128.71
3	C	360	NAD	N3A-C4A-N9A	4.78	134.06	125.43
3	C	360	NAD	O4B-C1B-N9A	-4.19	104.55	108.44
3	A	360	NAD	N3A-C4A-N9A	4.08	132.80	125.43
3	D	360	NAD	N3A-C4A-N9A	3.71	132.14	125.43
3	B	360	NAD	N3A-C4A-N9A	3.64	132.01	125.43
3	A	360	NAD	O4B-C1B-N9A	-3.55	105.14	108.44
3	B	360	NAD	C4A-C5A-N7A	-3.44	106.57	109.52
3	D	360	NAD	C3N-C7N-N7N	-3.26	114.06	117.77
3	B	360	NAD	C4B-O4B-C1B	-2.99	106.50	109.75
3	C	360	NAD	C5A-C4A-N3A	-2.93	119.32	125.70
3	B	360	NAD	C3N-C7N-N7N	-2.93	114.44	117.77
3	C	360	NAD	O4B-C1B-C2B	-2.89	102.33	106.77
3	D	360	NAD	O4D-C1D-N1N	-2.88	105.01	107.95
3	C	360	NAD	C8A-N9A-C4A	2.80	109.04	106.90
3	C	360	NAD	C4B-O4B-C1B	-2.79	106.72	109.75
3	A	360	NAD	PN-O3-PA	-2.72	121.28	132.95
3	D	360	NAD	C4D-O4D-C1D	-2.70	106.82	109.75
3	C	360	NAD	O4D-C1D-C2D	-2.67	102.68	106.77
3	B	360	NAD	C5A-C4A-N3A	-2.62	120.00	125.70
3	C	360	NAD	C4A-C5A-N7A	-2.62	107.28	109.52
3	D	360	NAD	C5A-C4A-N3A	-2.59	120.06	125.70
3	A	360	NAD	C5A-C4A-N3A	-2.55	120.14	125.70
3	D	360	NAD	O4B-C1B-C2B	-2.54	102.88	106.77
3	C	360	NAD	C2A-N3A-C4A	2.52	121.18	114.01
3	D	360	NAD	C4A-C5A-N7A	-2.34	107.52	109.52
3	D	360	NAD	C2A-N3A-C4A	2.34	120.66	114.01
3	A	360	NAD	C4A-C5A-N7A	-2.30	107.56	109.52
3	A	360	NAD	C6N-N1N-C2N	-2.18	119.58	122.04
3	B	360	NAD	PN-O3-PA	-2.17	123.61	132.95
3	A	360	NAD	C4B-O4B-C1B	-2.15	107.41	109.75
3	C	360	NAD	N7A-C8A-N9A	-2.08	108.46	114.36
3	D	360	NAD	C4B-O4B-C1B	-2.05	107.52	109.75
3	B	360	NAD	O4D-C1D-C2D	-2.05	103.64	106.77
3	C	360	NAD	PN-O3-PA	-2.03	124.23	132.95
3	C	360	NAD	O4D-C4D-C5D	-2.03	102.13	109.36
3	A	360	NAD	C2A-N3A-C4A	2.02	119.77	114.01
3	B	360	NAD	C5B-C4B-C3B	-2.01	107.15	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	360	NAD	C2A-N3A-C4A	2.01	119.73	114.01

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, 95th 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 ²)	Q<0.9
1	A	359/359 (100%)	0.24	18 (5%) 28 38	6, 19, 38, 43	24 (6%)
1	B	359/359 (100%)	-0.09	8 (2%) 59 69	6, 16, 28, 39	7 (1%)
1	D	359/359 (100%)	0.20	16 (4%) 32 42	8, 20, 40, 48	14 (3%)
2	C	359/359 (100%)	-0.22	2 (0%) 86 92	7, 16, 28, 51	3 (0%)
All	All	1436/1436 (100%)	0.03	44 (3%) 47 56	6, 17, 38, 51	48 (3%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	VAL	28.0
1	B	359	LEU	26.5
1	A	1	MET	16.6
1	A	357	ALA	15.5
1	A	2	PRO	14.2
1	B	358	ARG	14.1
1	A	356	SER	13.2
1	A	359	LEU	8.3
1	A	355	ARG	7.9
1	B	72	VAL	6.4
1	D	1	MET	6.3
1	A	358	ARG	5.9
2	C	359	LEU	4.5
1	B	73	ALA	4.2
1	D	357	ALA	3.9
1	D	359	LEU	3.6
1	A	37	VAL	3.4
1	D	92	ARG	3.4
1	B	92	ARG	3.3
1	D	21	LEU	3.2
1	D	36	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	90	ALA	2.9
1	B	1	MET	2.7
1	A	119	ALA	2.7
1	A	113	LEU	2.7
1	A	8	ASN	2.6
1	B	39	MET	2.5
1	A	114	PHE	2.5
1	D	88	VAL	2.5
1	D	24	ASP	2.4
1	A	40	ASN	2.4
2	C	1	MET	2.4
1	A	39	MET	2.3
1	D	114	PHE	2.3
1	B	70	PRO	2.2
1	D	10	PHE	2.2
1	D	41	THR	2.2
1	A	141	ALA	2.2
1	D	40	ASN	2.2
1	D	73	ALA	2.1
1	A	125	ARG	2.1
1	A	100	GLY	2.1
1	D	94	PRO	2.1
1	D	35	ALA	2.0

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

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, 95th 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 ²)	Q<0.9
2	CCS	C	166	10/11	0.15	1.64	12,12,16,18	0

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, 95th 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 ²)	Q<0.9
4	GOL	C	361	6/6	1.02	37.24	43,47,48,49	6
3	NAD	A	360	44/44	0.21	0.53	20,31,33,33	0
3	NAD	B	360	44/44	0.13	-0.20	18,23,29,29	0
3	NAD	D	360	44/44	0.13	-0.45	16,24,31,32	0
3	NAD	C	360	44/44	0.10	-0.84	10,13,17,20	0

6.5 Other polymers

There are no such residues in this entry.