



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:25 am GMT

PDB ID : 1P44  
Title : Targeting tuberculosis and malaria through inhibition of enoyl reductase: compound activity and structural data  
Authors : Kuo, M.R.; Morbidoni, H.R.; Alland, D.; Sneddon, S.F.; Gourlie, B.B.; Staveski, M.M.; Leonard, M.; Gregory, J.S.; Janjigian, A.D.; Yee, C.; Musser, J.M.; Kreiswirth, B.; Iwamoto, H.; Perozzo, R.; Jacobs Jr, W.R.; Sacchettini, J.C.; Fidock, D.A.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2003-04-21  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

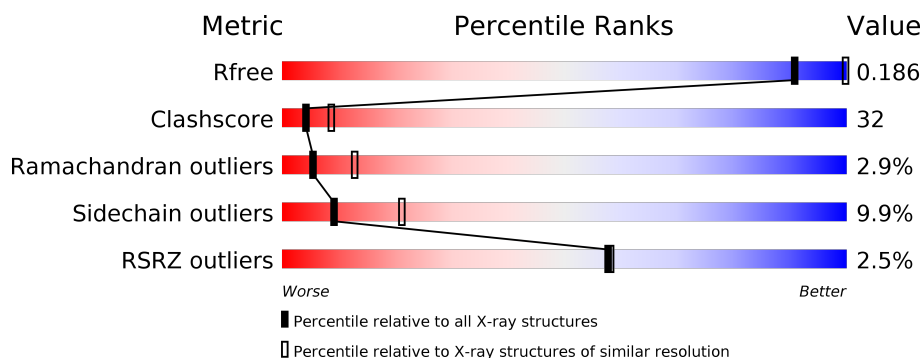
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	269	<div> <div></div> <div> <div></div> <div>53%</div> <div>41%</div> <div>6%</div> </div> </div>
1	B	269	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>5%</div> </div> </div>
1	C	269	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>44%</div> <div>9%</div> </div> </div>
1	D	269	<div> <div>5%</div> <div> <div></div> <div>41%</div> <div>53%</div> <div>6%</div> </div> </div>
1	E	269	<div> <div></div> <div> <div></div> <div>46%</div> <div>46%</div> <div>7%</div> </div> </div>
1	F	269	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>46%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GEQ	C	550	-	-	-	X

## 2 Entry composition [i](#)

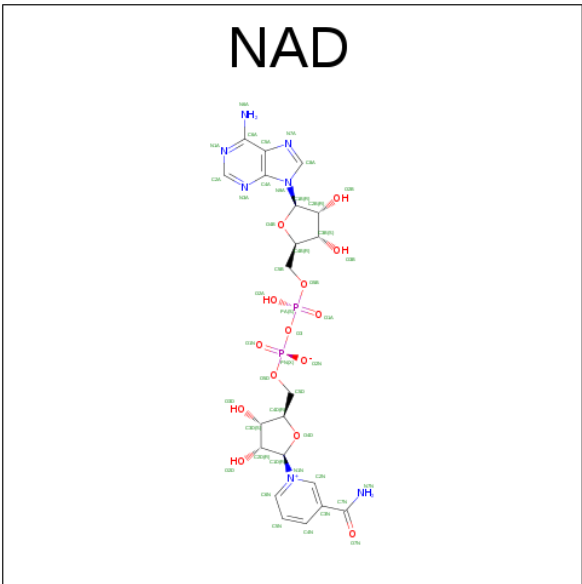
There are 4 unique types of molecules in this entry. The entry contains 12495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enoyl-[acyl-carrier-protein] reductase [NADH].

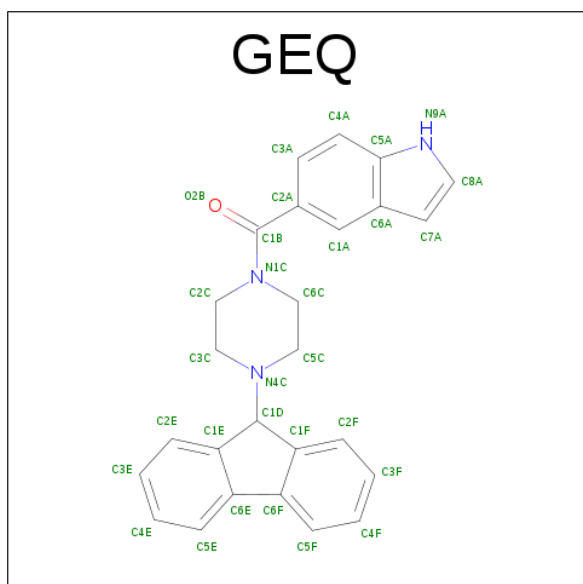
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	B	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	C	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	D	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	E	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	F	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 3 is 5-[[4-(9H-FLUOREN-9-YL)PIPERAZIN-1-YL]CARBONYL]-1H-INDOLE (three-letter code: GEQ) (formula: C<sub>26</sub>H<sub>23</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	26	3	1		
3	B	1	Total	C	N	O	0	0
			30	26	3	1		
3	C	1	Total	C	N	O	0	0
			30	26	3	1		
3	D	1	Total	C	N	O	0	0
			30	26	3	1		

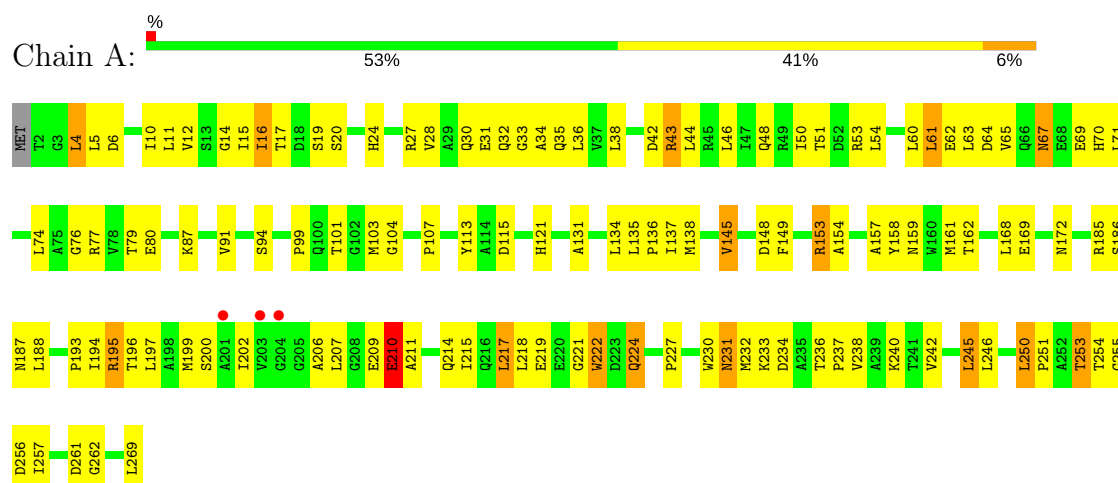
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	36	Total 36	O 36	0	0
4	C	27	Total 27	O 27	0	0
4	D	14	Total 14	O 14	0	0
4	E	21	Total 21	O 21	0	0
4	F	19	Total 19	O 19	0	0

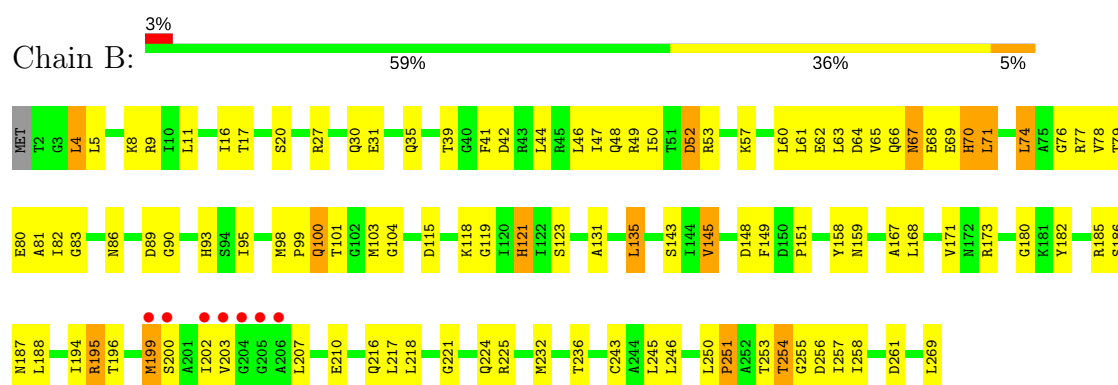
### 3 Residue-property plots

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: Enoyl-[acyl-carrier-protein] reductase [NADH]

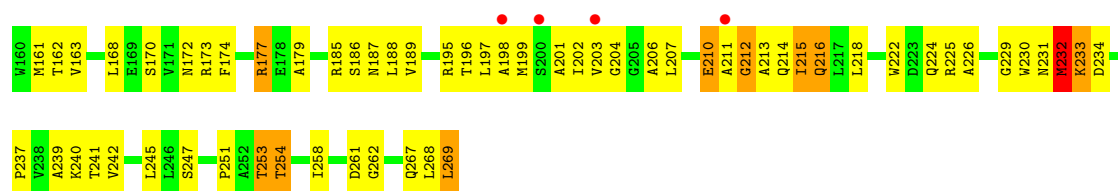


#### • Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

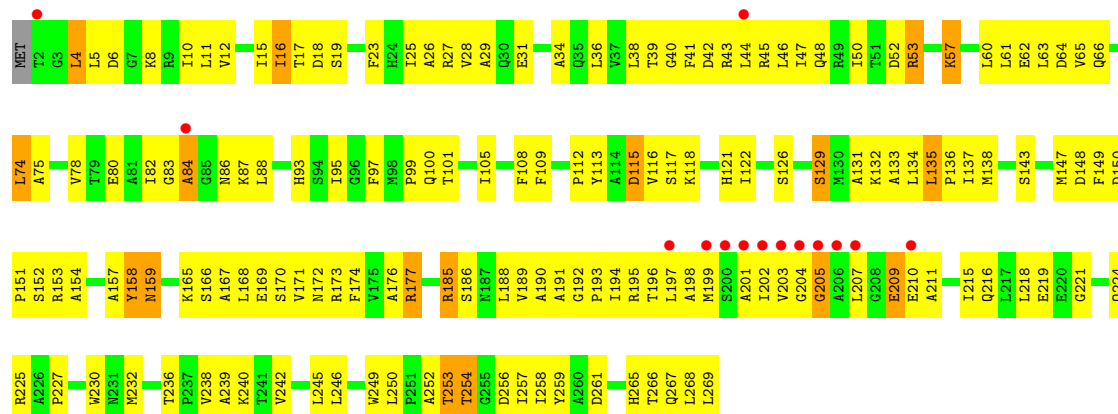


#### • Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

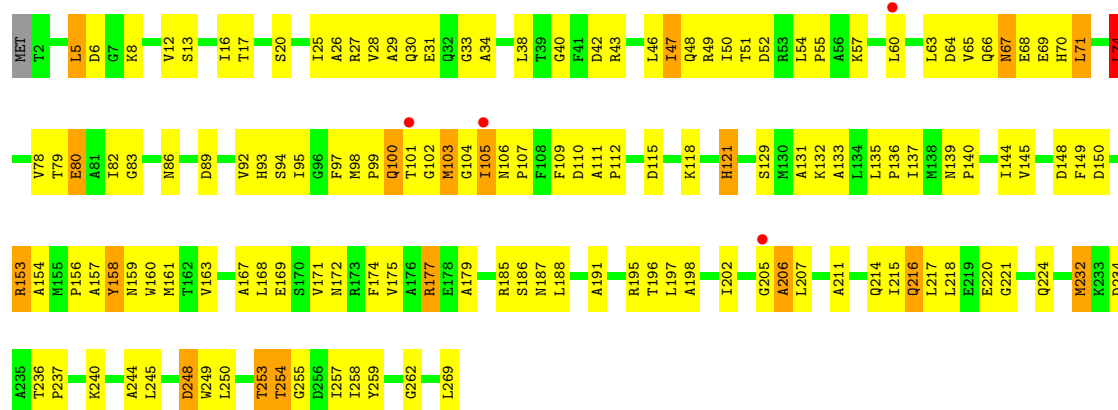




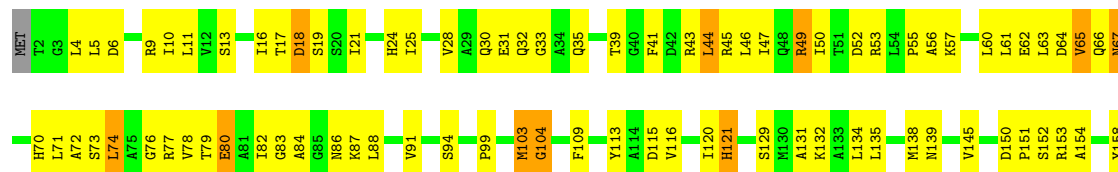
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



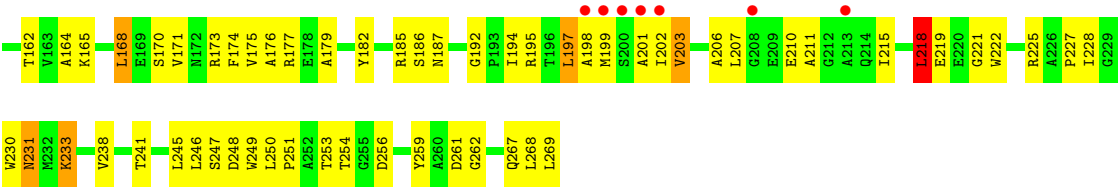
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.62Å 83.22Å 192.97Å 90.00° 94.95° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 67.9 (29.29-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.190 , 0.288 0.191 , 0.186	Depositor DCC
$R_{free}$ test set	1936 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 15.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12495	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GEQ, 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	0.43	0/2032	0.68	0/2758
1	B	0.42	0/2032	0.70	0/2758
1	C	0.35	0/2032	0.64	0/2758
1	D	0.34	0/2032	0.63	0/2758
1	E	0.35	0/2032	0.66	0/2758
1	F	0.37	0/2032	0.67	1/2758 (0.0%)
All	All	0.38	0/12192	0.67	1/16548 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	218	LEU	CA-CB-CG	6.32	129.83	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1994	0	2008	112	1
1	B	1994	0	2008	102	0
1	C	1994	0	2008	151	0
1	D	1994	0	2008	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1994	0	2008	142	0
1	F	1994	0	2008	155	0
2	A	44	0	26	8	0
2	B	44	0	26	3	0
2	C	44	0	26	3	0
2	D	44	0	26	4	0
2	E	44	0	26	4	0
2	F	44	0	26	1	0
3	A	30	0	23	2	0
3	B	30	0	23	3	0
3	C	30	0	23	1	0
3	D	30	0	23	0	0
4	A	30	0	0	2	0
4	B	36	0	0	4	0
4	C	27	0	0	4	0
4	D	14	0	0	2	0
4	E	21	0	0	2	0
4	F	19	0	0	1	0
All	All	12495	0	12296	796	1

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 32.

All (796) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ARG:HB2	1:B:195:ARG:HH11	1.19	1.05
1:F:16:ILE:HG23	1:F:17:THR:HG23	1.33	1.05
1:D:186:SER:H	1:D:254:THR:HG23	1.20	1.03
1:C:245:LEU:HD21	1:C:258:ILE:HD12	1.41	1.00
1:B:186:SER:H	1:B:254:THR:HG22	1.26	0.98
1:A:16:ILE:HG23	1:A:17:THR:HG23	1.43	0.98
1:E:16:ILE:HG23	1:E:17:THR:HG23	1.42	0.97
1:F:49:ARG:NH1	1:F:49:ARG:HB3	1.81	0.95
1:C:168:LEU:HD22	1:C:188:LEU:HD21	1.46	0.95
1:B:64:ASP:H	1:B:70:HIS:HD2	1.11	0.93
1:C:196:THR:HG22	1:C:197:LEU:H	1.32	0.93
1:C:77:ARG:O	1:C:80:GLU:HG3	1.70	0.92
1:B:44:LEU:HD21	1:B:62:GLU:HG3	1.51	0.90
1:D:5:LEU:O	1:D:8:LYS:HB2	1.74	0.88
1:D:60:LEU:HD23	1:D:61:LEU:N	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:ARG:HH22	1:F:86:ASN:ND2	1.74	0.86
1:D:143:SER:HB2	1:D:185:ARG:NH1	1.91	0.85
1:A:199:MET:HA	1:A:202:ILE:HD13	1.59	0.85
1:E:135:LEU:HD21	1:E:179:ALA:HA	1.56	0.84
1:D:66:GLN:HG2	1:D:121:HIS:CD2	2.13	0.84
1:A:214:GLN:O	1:A:218:LEU:HD23	1.77	0.84
1:A:231:ASN:HD21	1:A:233:LYS:HG2	1.42	0.84
1:A:99:PRO:HB2	1:A:101:THR:HG22	1.58	0.83
1:D:108:PHE:HB2	1:D:159:ASN:ND2	1.93	0.83
1:F:49:ARG:HH11	1:F:49:ARG:HB3	1.41	0.83
1:E:109:PHE:HB3	1:F:132:LYS:HD2	1.61	0.82
1:A:202:ILE:HD12	1:A:202:ILE:H	1.44	0.82
1:D:57:LYS:O	1:D:57:LYS:HD3	1.78	0.82
1:E:202:ILE:HG13	1:E:207:LEU:HD22	1.62	0.81
1:D:16:ILE:HG13	1:D:43:ARG:HH22	1.45	0.81
1:B:202:ILE:HG23	1:B:207:LEU:HD22	1.62	0.81
1:F:195:ARG:HH12	1:F:203:VAL:HG11	1.46	0.81
1:E:38:LEU:HB2	1:E:60:LEU:HD13	1.60	0.81
1:F:231:ASN:HD21	1:F:233:LYS:NZ	1.78	0.80
1:B:17:THR:HA	1:B:50:ILE:HD13	1.61	0.80
1:F:99:PRO:HG3	1:F:115:ASP:HB3	1.61	0.80
1:D:66:GLN:HG2	1:D:121:HIS:HD2	1.46	0.80
1:F:74:LEU:O	1:F:78:VAL:HG23	1.81	0.79
1:D:27:ARG:O	1:D:31:GLU:HG3	1.83	0.79
1:E:17:THR:HA	1:E:50:ILE:HD13	1.63	0.79
1:D:186:SER:N	1:D:254:THR:HG23	1.98	0.78
1:C:174:PHE:CE2	1:D:159:ASN:HA	2.18	0.78
1:A:101:THR:HG21	1:A:115:ASP:OD1	1.84	0.78
1:A:186:SER:H	1:A:254:THR:HG23	1.48	0.77
1:D:108:PHE:HB2	1:D:159:ASN:HD22	1.49	0.77
1:D:99:PRO:HG3	1:D:115:ASP:HB2	1.67	0.77
1:C:202:ILE:HA	1:C:207:LEU:HD13	1.67	0.77
1:A:24:HIS:O	1:A:28:VAL:HG23	1.84	0.76
1:E:105:ILE:HG23	1:E:106:ASN:H	1.50	0.76
1:C:177:ARG:HA	1:F:227:PRO:HB3	1.67	0.75
1:C:105:ILE:HD13	1:C:105:ILE:O	1.87	0.75
1:F:82:ILE:HG13	1:F:83:GLY:H	1.50	0.75
1:E:27:ARG:O	1:E:31:GLU:HG3	1.87	0.74
1:B:195:ARG:HH11	1:B:195:ARG:CB	1.98	0.74
1:F:231:ASN:ND2	1:F:233:LYS:NZ	2.36	0.74
1:F:231:ASN:ND2	1:F:233:LYS:HG2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:LEU:HD13	1:D:188:LEU:HD21	1.69	0.74
1:C:186:SER:H	1:C:254:THR:CG2	2.01	0.74
1:A:231:ASN:HD21	1:A:233:LYS:CG	2.01	0.74
1:B:67:ASN:HD22	1:B:67:ASN:C	1.89	0.74
1:F:222:TRP:HE1	1:F:261:ASP:HB2	1.51	0.73
1:C:137:ILE:HG13	1:C:137:ILE:O	1.89	0.73
1:C:99:PRO:HB2	1:C:101:THR:HG22	1.71	0.73
1:F:10:ILE:HD13	1:F:246:LEU:HD13	1.70	0.73
1:C:201:ALA:O	1:C:206:ALA:HB3	1.87	0.73
1:D:143:SER:HB2	1:D:185:ARG:HH11	1.53	0.72
1:B:186:SER:H	1:B:254:THR:CG2	2.01	0.72
1:F:18:ASP:H	1:F:50:ILE:HD13	1.52	0.72
1:B:195:ARG:HB2	1:B:195:ARG:NH1	2.01	0.72
1:C:186:SER:H	1:C:254:THR:HG23	1.53	0.72
1:D:186:SER:H	1:D:254:THR:CG2	2.00	0.72
1:E:47:ILE:O	1:E:51:THR:HG23	1.90	0.72
1:F:228:ILE:HD11	1:F:262:GLY:HA2	1.71	0.71
1:A:135:LEU:HB3	1:A:136:PRO:HD3	1.72	0.71
1:C:8:LYS:HA	1:C:89:ASP:OD2	1.89	0.71
1:A:4:LEU:HB3	1:A:5:LEU:HD12	1.72	0.71
1:A:202:ILE:HA	1:A:206:ALA:HB3	1.73	0.71
1:F:99:PRO:CG	1:F:115:ASP:HB3	2.21	0.70
1:C:222:TRP:HE1	1:C:261:ASP:HB2	1.56	0.70
1:A:20:SER:HB3	2:A:300:NAD:O2A	1.92	0.70
1:D:249:TRP:HB3	1:E:244:ALA:HB2	1.72	0.70
1:C:199:MET:SD	1:C:215:ILE:HD11	2.32	0.69
1:E:171:VAL:O	1:E:175:VAL:HG23	1.93	0.69
1:D:105:ILE:HG22	1:D:211:ALA:HB3	1.75	0.69
1:D:267:GLN:OE1	1:F:154:ALA:HB3	1.92	0.69
1:A:10:ILE:HD13	1:A:246:LEU:HD13	1.74	0.69
1:C:135:LEU:HD21	1:C:179:ALA:HA	1.74	0.69
1:E:26:ALA:O	1:E:30:GLN:HG3	1.93	0.69
1:E:67:ASN:HD22	1:E:68:GLU:N	1.91	0.68
1:C:196:THR:HG22	1:C:197:LEU:N	2.08	0.68
1:E:168:LEU:HD22	1:E:188:LEU:HD21	1.76	0.68
1:F:11:LEU:HD13	1:F:134:LEU:HD11	1.76	0.68
1:F:231:ASN:HD21	1:F:233:LYS:HZ3	1.40	0.68
1:C:67:ASN:HD22	1:C:67:ASN:C	1.98	0.67
1:E:269:LEU:HD13	1:E:269:LEU:OXT	1.94	0.67
1:C:218:LEU:HD21	1:E:269:LEU:HB2	1.75	0.67
1:F:231:ASN:HD21	1:F:233:LYS:HG2	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ALA:HB3	1:D:215:ILE:HD11	1.76	0.67
1:B:167:ALA:O	1:B:171:VAL:HG23	1.94	0.67
1:D:101:THR:HG21	1:D:115:ASP:OD2	1.95	0.67
1:C:185:ARG:HG3	1:C:185:ARG:HH11	1.60	0.66
1:C:64:ASP:H	1:C:70:HIS:CD2	2.12	0.66
1:D:16:ILE:HG13	1:D:43:ARG:NH2	2.09	0.66
1:D:17:THR:HG22	1:D:19:SER:H	1.61	0.66
1:E:103:MET:HB3	1:E:105:ILE:HG22	1.78	0.66
1:E:196:THR:HG21	2:E:700:NAD:O1N	1.95	0.66
1:C:62:GLU:HG2	1:C:70:HIS:NE2	2.10	0.66
1:F:82:ILE:HG13	1:F:83:GLY:N	2.11	0.66
1:D:238:VAL:O	1:D:242:VAL:HG23	1.96	0.66
1:E:78:VAL:O	1:E:82:ILE:HG12	1.96	0.65
1:D:174:PHE:O	1:D:177:ARG:HG2	1.96	0.65
1:D:153:ARG:NH2	1:F:153:ARG:HE	1.95	0.65
1:F:9:ARG:HH22	1:F:86:ASN:HD22	1.43	0.65
1:A:6:ASP:HA	1:A:33:GLY:O	1.97	0.65
1:C:64:ASP:H	1:C:70:HIS:HD2	1.43	0.65
1:A:131:ALA:O	1:A:135:LEU:HB2	1.96	0.64
1:A:236:THR:O	1:A:240:LYS:HG3	1.97	0.64
1:B:17:THR:HA	1:B:50:ILE:CD1	2.27	0.64
1:A:202:ILE:HD12	1:A:202:ILE:N	2.13	0.64
1:D:60:LEU:HD23	1:D:61:LEU:H	1.60	0.64
1:F:268:LEU:O	1:F:269:LEU:HB3	1.97	0.64
1:D:108:PHE:HD2	1:D:159:ASN:HB3	1.62	0.64
1:B:99:PRO:HB2	1:B:101:THR:HG22	1.79	0.64
1:B:67:ASN:HD21	1:B:69:GLU:HB2	1.63	0.64
1:A:64:ASP:H	1:A:70:HIS:HD2	1.46	0.63
1:B:145:VAL:HA	1:B:187:ASN:O	1.98	0.63
1:C:78:VAL:O	1:C:82:ILE:HG12	1.98	0.63
1:A:11:LEU:HD13	1:A:134:LEU:HD13	1.81	0.63
1:B:64:ASP:H	1:B:70:HIS:CD2	2.03	0.63
1:C:21:ILE:O	1:C:25:ILE:HG13	1.98	0.63
1:F:174:PHE:O	1:F:177:ARG:HG3	1.99	0.63
1:F:215:ILE:HG22	1:F:219:GLU:OE2	1.97	0.63
1:C:25:ILE:HA	1:C:239:ALA:HB1	1.79	0.63
1:D:16:ILE:CG1	1:D:43:ARG:HH22	2.12	0.63
1:A:218:LEU:HD12	3:A:350:GEQ:H4E	1.81	0.63
1:F:30:GLN:NE2	1:F:56:ALA:HB3	2.14	0.63
1:A:5:LEU:HD12	1:A:5:LEU:N	2.14	0.63
1:F:201:ALA:O	1:F:206:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:ARG:NH2	1:F:86:ASN:HD22	1.97	0.63
1:C:39:THR:HG22	1:C:61:LEU:HB2	1.80	0.62
1:B:221:GLY:O	1:B:225:ARG:HD3	1.99	0.62
1:B:44:LEU:CD2	1:B:62:GLU:HG3	2.24	0.62
1:D:39:THR:HB	1:D:63:LEU:HB3	1.81	0.62
1:E:186:SER:H	1:E:254:THR:HG22	1.64	0.62
1:D:43:ARG:HB3	1:D:46:LEU:HB2	1.81	0.62
1:B:27:ARG:O	1:B:31:GLU:HG3	1.99	0.62
1:E:157:ALA:O	1:E:158:TYR:HB2	1.99	0.62
1:F:145:VAL:HA	1:F:187:ASN:O	2.00	0.62
1:D:218:LEU:HD12	1:F:269:LEU:HD21	1.81	0.62
1:A:197:LEU:HD22	1:A:200:SER:HB2	1.82	0.61
1:B:39:THR:HB	1:B:63:LEU:HB3	1.82	0.61
1:B:61:LEU:HD13	1:B:77:ARG:HB3	1.82	0.61
1:C:225:ARG:HH11	1:C:225:ARG:HG3	1.66	0.61
1:D:134:LEU:O	1:D:138:MET:HG3	2.00	0.61
1:C:95:ILE:HG12	2:C:500:NAD:H1B	1.81	0.61
1:C:24:HIS:O	1:C:28:VAL:HG23	2.01	0.61
1:C:132:LYS:HD2	1:D:109:PHE:HB3	1.82	0.61
1:F:39:THR:HA	1:F:61:LEU:O	2.01	0.61
1:C:269:LEU:HD11	1:E:218:LEU:HA	1.83	0.61
1:E:202:ILE:CG1	1:E:207:LEU:HD22	2.29	0.61
1:E:20:SER:HB3	2:E:700:NAD:O2A	2.01	0.61
1:F:230:TRP:CZ3	1:F:261:ASP:HA	2.35	0.61
1:A:197:LEU:HA	1:A:200:SER:OG	2.01	0.61
1:C:103:MET:O	1:C:104:GLY:O	2.19	0.60
1:F:135:LEU:HG	1:F:182:TYR:CD1	2.35	0.60
1:C:10:ILE:HG23	1:C:90:GLY:HA3	1.83	0.60
1:C:198:ALA:O	1:C:202:ILE:HD13	1.99	0.60
1:E:6:ASP:HA	1:E:33:GLY:O	2.01	0.60
1:F:231:ASN:ND2	1:F:233:LYS:HZ3	1.99	0.60
1:C:27:ARG:O	1:C:31:GLU:HG3	2.00	0.60
1:E:101:THR:HG21	1:E:112:PRO:HD2	1.84	0.60
1:D:25:ILE:O	1:D:29:ALA:HB2	2.02	0.60
1:D:195:ARG:N	1:D:232:MET:O	2.29	0.60
1:E:104:GLY:HA3	1:E:157:ALA:HA	1.82	0.60
1:B:67:ASN:ND2	1:B:69:GLU:H	2.00	0.60
1:F:21:ILE:O	1:F:25:ILE:HG13	2.01	0.60
1:D:218:LEU:CD1	1:F:269:LEU:HD21	2.32	0.60
1:A:250:LEU:N	1:A:251:PRO:HD3	2.16	0.60
1:D:168:LEU:HD13	1:D:188:LEU:CD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLY:HA3	1:C:47:ILE:CD1	2.32	0.60
1:E:13:SER:O	1:E:94:SER:HB2	2.01	0.60
1:C:11:LEU:C	1:C:11:LEU:HD23	2.22	0.59
1:D:172:ASN:CG	1:D:188:LEU:HD13	2.22	0.59
1:D:65:VAL:HB	1:D:126:SER:HB2	1.82	0.59
1:A:65:VAL:HG22	2:A:300:NAD:N1A	2.17	0.59
1:C:127:TYR:OH	1:C:144:ILE:HG22	2.01	0.59
1:A:211:ALA:HA	1:A:214:GLN:HE21	1.67	0.59
1:E:16:ILE:HB	2:E:700:NAD:O3B	2.03	0.59
1:F:225:ARG:HG2	1:F:269:LEU:HA	1.83	0.59
1:F:62:GLU:O	1:F:77:ARG:NH1	2.35	0.59
1:B:131:ALA:O	1:B:135:LEU:HB2	2.02	0.59
1:F:202:ILE:O	1:F:202:ILE:HG22	2.01	0.59
1:E:211:ALA:O	1:E:215:ILE:HG12	2.02	0.59
1:F:171:VAL:O	1:F:175:VAL:HG23	2.03	0.59
1:F:253:THR:O	1:F:253:THR:HG23	2.02	0.59
1:D:267:GLN:CD	1:F:154:ALA:HB3	2.23	0.59
1:E:198:ALA:O	1:E:202:ILE:HD13	2.03	0.59
1:F:176:ALA:HB1	1:F:254:THR:HG22	1.83	0.59
1:C:101:THR:HG21	1:C:115:ASP:OD2	2.02	0.59
1:C:16:ILE:HG23	1:C:17:THR:HG23	1.84	0.59
1:F:49:ARG:CB	1:F:49:ARG:HH11	2.13	0.59
1:B:67:ASN:HD22	1:B:68:GLU:N	2.01	0.59
1:D:108:PHE:CB	1:D:159:ASN:HD22	2.15	0.59
1:F:46:LEU:O	1:F:46:LEU:HD23	2.02	0.59
1:C:134:LEU:O	1:C:138:MET:HG3	2.02	0.58
1:D:26:ALA:O	1:D:29:ALA:HB3	2.04	0.58
1:E:245:LEU:HD22	1:E:258:ILE:HD12	1.85	0.58
1:C:158:TYR:CD1	1:C:162:THR:OG1	2.56	0.58
1:B:67:ASN:ND2	1:B:69:GLU:N	2.52	0.58
1:E:236:THR:O	1:E:240:LYS:HG2	2.03	0.58
1:F:186:SER:H	1:F:254:THR:HG23	1.69	0.58
1:B:16:ILE:HG23	1:B:17:THR:HG23	1.85	0.58
1:B:93:HIS:CE1	1:B:95:ILE:HB	2.39	0.58
1:D:253:THR:HB	1:E:259:TYR:O	2.04	0.58
4:C:800:HOH:O	1:E:269:LEU:HD12	2.02	0.58
1:F:231:ASN:ND2	1:F:233:LYS:HZ2	2.02	0.58
1:B:67:ASN:HD21	1:B:69:GLU:CB	2.16	0.58
1:B:101:THR:HG21	1:B:115:ASP:OD1	2.03	0.58
1:E:107:PRO:HB2	1:E:110:ASP:OD1	2.04	0.58
1:A:27:ARG:HG2	1:A:31:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HB3	1:A:137:ILE:O	2.03	0.57
1:A:74:LEU:HD13	1:A:134:LEU:HD21	1.87	0.57
1:B:218:LEU:HG	3:B:450:GEQ:H4E	1.86	0.57
1:D:48:GLN:HG2	1:D:60:LEU:HD13	1.85	0.57
1:C:210:GLU:CD	1:C:210:GLU:H	2.06	0.57
1:C:43:ARG:HD2	1:C:46:LEU:CD1	2.34	0.57
1:E:156:PRO:HD3	1:F:177:ARG:HH12	1.68	0.57
1:B:83:GLY:O	1:B:86:ASN:HB2	2.05	0.57
1:F:16:ILE:HG23	1:F:17:THR:CG2	2.22	0.57
1:F:9:ARG:NH2	1:F:86:ASN:ND2	2.50	0.57
1:F:173:ARG:O	1:F:176:ALA:HB3	2.05	0.57
1:F:215:ILE:HA	1:F:218:LEU:CD1	2.35	0.57
1:B:64:ASP:N	1:B:70:HIS:HD2	1.93	0.56
1:D:157:ALA:CB	1:D:215:ILE:HD11	2.35	0.56
1:B:199:MET:HE3	1:B:199:MET:O	2.04	0.56
1:A:202:ILE:CD1	1:A:202:ILE:H	2.16	0.56
1:A:209:GLU:C	1:A:211:ALA:H	2.06	0.56
1:C:225:ARG:HD2	1:C:267:GLN:O	2.06	0.56
1:C:189:VAL:HG21	1:C:242:VAL:HG22	1.87	0.56
1:E:157:ALA:CB	1:E:214:GLN:HB3	2.35	0.56
1:F:53:ARG:HH11	1:F:53:ARG:HG2	1.68	0.56
1:C:174:PHE:O	1:C:177:ARG:HG2	2.05	0.56
1:D:27:ARG:HH11	1:D:27:ARG:HG2	1.69	0.56
1:F:6:ASP:HA	1:F:33:GLY:O	2.06	0.56
1:A:231:ASN:ND2	1:A:233:LYS:HG2	2.16	0.56
1:F:195:ARG:NH1	1:F:203:VAL:HG11	2.16	0.56
1:B:98:MET:HE2	1:B:119:GLY:HA3	1.87	0.56
1:D:202:ILE:HG12	1:D:207:LEU:HB2	1.88	0.56
1:E:131:ALA:O	1:E:135:LEU:HB2	2.06	0.56
1:E:185:ARG:HA	1:E:254:THR:HG23	1.87	0.55
1:D:42:ASP:OD2	1:D:43:ARG:HG3	2.06	0.55
1:E:172:ASN:CG	1:E:188:LEU:HD13	2.27	0.55
1:E:5:LEU:CB	1:E:34:ALA:HB2	2.35	0.55
1:E:167:ALA:O	1:E:171:VAL:HG23	2.06	0.55
1:F:5:LEU:HD23	1:F:32:GLN:CB	2.36	0.55
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.72	0.55
1:E:100:GLN:HA	1:E:103:MET:HB2	1.88	0.55
1:A:169:GLU:OE2	1:A:257:ILE:HD13	2.06	0.55
1:B:98:MET:CE	1:B:119:GLY:HA3	2.35	0.55
1:C:148:ASP:OD2	1:C:149:PHE:N	2.40	0.55
1:F:18:ASP:N	1:F:50:ILE:HD13	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:GLU:OE2	1:E:257:ILE:HD13	2.06	0.55
1:A:250:LEU:HD23	1:A:253:THR:HG21	1.89	0.55
1:B:8:LYS:HA	1:B:89:ASP:OD1	2.06	0.55
1:D:245:LEU:HD21	1:D:258:ILE:HG13	1.89	0.55
1:D:47:ILE:HG22	1:D:60:LEU:HD11	1.88	0.55
1:C:153:ARG:NH2	1:E:153:ARG:CZ	2.70	0.55
1:F:17:THR:HA	1:F:50:ILE:HD12	1.89	0.55
1:D:266:THR:HG21	1:E:255:GLY:O	2.07	0.55
1:F:24:HIS:O	1:F:28:VAL:HG23	2.06	0.55
1:B:199:MET:SD	3:B:450:GEQ:H5C2	2.47	0.55
1:E:69:GLU:CD	1:E:69:GLU:H	2.10	0.55
1:D:227:PRO:HB3	1:E:177:ARG:HA	1.89	0.55
1:E:156:PRO:HD3	1:F:177:ARG:NH1	2.21	0.55
1:F:202:ILE:HG22	1:F:215:ILE:HG13	1.87	0.55
1:C:45:ARG:HH11	1:C:45:ARG:HG2	1.72	0.54
1:C:43:ARG:O	1:C:47:ILE:HG23	2.07	0.54
1:A:217:LEU:HD12	1:A:217:LEU:C	2.28	0.54
1:A:231:ASN:ND2	1:A:233:LYS:H	2.05	0.54
1:B:64:ASP:HB3	1:B:70:HIS:CD2	2.42	0.54
1:C:231:ASN:OD1	1:C:233:LYS:HG2	2.07	0.54
1:E:30:GLN:OE1	1:E:55:PRO:HG2	2.07	0.54
1:D:209:GLU:C	1:D:211:ALA:H	2.10	0.54
1:E:186:SER:H	1:E:254:THR:CG2	2.20	0.54
1:D:112:PRO:O	1:D:115:ASP:OD1	2.26	0.54
1:A:194:ILE:HD11	1:A:230:TRP:CZ2	2.43	0.54
1:A:12:VAL:HG23	1:A:36:LEU:HD22	1.89	0.54
1:C:60:LEU:O	1:C:61:LEU:HD23	2.06	0.54
1:F:66:GLN:HE21	1:F:121:HIS:CD2	2.26	0.54
1:A:43:ARG:HD2	1:A:46:LEU:HD13	1.89	0.54
1:B:250:LEU:N	1:B:251:PRO:CD	2.71	0.54
1:E:139:ASN:OD1	1:E:140:PRO:HD2	2.07	0.54
1:D:259:TYR:O	1:E:253:THR:HG22	2.06	0.54
1:D:44:LEU:H	1:D:44:LEU:HD22	1.72	0.54
1:D:47:ILE:O	1:D:47:ILE:HG22	2.06	0.54
1:A:209:GLU:O	1:A:211:ALA:N	2.40	0.54
1:E:49:ARG:O	1:E:52:ASP:HB3	2.08	0.54
1:A:113:TYR:CE2	1:B:121:HIS:HB2	2.42	0.54
1:B:16:ILE:O	1:B:50:ILE:HD12	2.08	0.54
1:C:206:ALA:C	1:C:207:LEU:HD12	2.29	0.54
1:D:53:ARG:HE	1:D:53:ARG:CA	2.21	0.54
1:E:234:ASP:OD1	1:E:237:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ASP:OD2	1:E:43:ARG:HG3	2.08	0.54
1:F:215:ILE:O	1:F:218:LEU:HD13	2.07	0.53
1:A:158:TYR:HD1	1:A:162:THR:HG1	1.52	0.53
1:F:192:GLY:O	1:F:194:ILE:HD12	2.07	0.53
1:F:231:ASN:HD21	1:F:233:LYS:CG	2.19	0.53
1:C:4:LEU:HB3	1:C:5:LEU:HD12	1.89	0.53
1:D:170:SER:HA	1:D:173:ARG:NH1	2.24	0.53
1:C:268:LEU:HD23	1:C:269:LEU:HD23	1.90	0.53
1:C:47:ILE:O	1:C:50:ILE:HB	2.09	0.53
1:C:153:ARG:CZ	1:E:153:ARG:CZ	2.86	0.53
1:F:5:LEU:HD23	1:F:32:GLN:HB2	1.91	0.53
1:A:157:ALA:HB3	1:A:215:ILE:HD11	1.91	0.53
1:A:135:LEU:CB	1:A:136:PRO:HD3	2.38	0.53
1:B:46:LEU:HD11	1:B:49:ARG:NH2	2.23	0.53
1:C:2:THR:O	1:C:3:GLY:O	2.26	0.53
1:C:113:TYR:CE2	1:C:117:SER:HB2	2.43	0.53
1:D:95:ILE:HD13	2:D:600:NAD:N3A	2.24	0.53
1:C:199:MET:O	1:C:203:VAL:HG23	2.09	0.53
1:D:27:ARG:HH12	1:D:28:VAL:HG22	1.74	0.53
1:E:154:ALA:HB2	1:F:173:ARG:HB3	1.91	0.53
1:D:192:GLY:HA3	1:D:230:TRP:CZ2	2.43	0.53
1:C:172:ASN:CG	1:C:188:LEU:HD13	2.29	0.52
1:B:195:ARG:HG2	1:B:200:SER:HB3	1.90	0.52
1:C:43:ARG:HD2	1:C:46:LEU:HD13	1.92	0.52
1:D:108:PHE:HD2	1:D:159:ASN:HD22	1.55	0.52
1:F:199:MET:HE1	1:F:215:ILE:HG21	1.90	0.52
1:A:14:GLY:HA3	1:A:94:SER:O	2.09	0.52
1:D:202:ILE:HG22	1:D:215:ILE:HG13	1.90	0.52
1:D:47:ILE:O	1:D:47:ILE:CG2	2.57	0.52
1:D:63:LEU:HD22	1:D:74:LEU:HD11	1.91	0.52
1:E:57:LYS:HD3	1:E:57:LYS:N	2.24	0.52
1:F:250:LEU:N	1:F:251:PRO:HD3	2.23	0.52
1:A:236:THR:HB	1:A:237:PRO:HD3	1.92	0.52
1:A:67:ASN:ND2	1:A:69:GLU:H	2.07	0.52
1:B:100:GLN:N	1:B:100:GLN:HE21	2.07	0.52
1:F:71:LEU:CD2	1:F:129:SER:HB3	2.40	0.52
1:A:5:LEU:HD23	1:A:10:ILE:HD12	1.91	0.52
1:D:99:PRO:O	1:D:101:THR:N	2.43	0.52
1:D:218:LEU:HD23	1:D:218:LEU:C	2.30	0.52
1:E:54:LEU:HB3	1:E:55:PRO:HD2	1.92	0.52
1:F:61:LEU:HD13	1:F:77:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:300:NAD:H71N	3:A:350:GEQ:H3A	1.74	0.52
1:D:44:LEU:HD11	1:D:62:GLU:HG3	1.90	0.52
1:D:93:HIS:HE1	1:D:95:ILE:O	1.92	0.52
1:E:135:LEU:HD21	1:E:179:ALA:CA	2.34	0.52
1:E:145:VAL:HA	1:E:187:ASN:O	2.10	0.52
1:F:199:MET:O	1:F:203:VAL:HB	2.10	0.52
1:A:250:LEU:N	1:A:251:PRO:CD	2.73	0.51
1:B:103:MET:HE3	1:B:158:TYR:CE2	2.45	0.51
1:A:48:GLN:HE21	1:A:60:LEU:HD23	1.75	0.51
1:E:104:GLY:CA	1:E:157:ALA:HA	2.40	0.51
1:A:44:LEU:HD11	1:A:62:GLU:HG3	1.93	0.51
1:B:185:ARG:HA	1:B:254:THR:CG2	2.40	0.51
1:B:99:PRO:HB2	1:B:101:THR:CG2	2.40	0.51
1:D:15:ILE:HD12	1:D:38:LEU:HD13	1.90	0.51
1:A:154:ALA:HB2	1:B:173:ARG:HB3	1.91	0.51
1:A:76:GLY:O	1:A:79:THR:HB	2.11	0.51
1:F:11:LEU:HD13	1:F:134:LEU:CD1	2.38	0.51
1:F:21:ILE:HD11	1:F:194:ILE:HD13	1.93	0.51
1:F:211:ALA:O	1:F:215:ILE:HG12	2.09	0.51
1:F:218:LEU:HD22	1:F:219:GLU:N	2.25	0.51
1:A:215:ILE:O	1:A:219:GLU:HG3	2.10	0.51
1:D:265:HIS:CE1	1:D:266:THR:HG23	2.46	0.51
1:F:71:LEU:O	1:F:73:SER:N	2.44	0.51
1:B:243:CYS:HA	1:B:246:LEU:HD12	1.92	0.51
1:C:233:LYS:HD2	1:C:233:LYS:H	1.75	0.51
1:D:201:ALA:HB1	1:D:205:GLY:HA3	1.93	0.51
1:E:5:LEU:HB3	1:E:34:ALA:HB2	1.91	0.51
1:A:16:ILE:HB	2:A:300:NAD:O3B	2.11	0.51
1:B:4:LEU:HD22	1:B:4:LEU:O	2.10	0.51
1:E:80:GLU:HB2	4:E:828:HOH:O	2.11	0.51
1:F:185:ARG:HH11	1:F:185:ARG:HG3	1.76	0.51
1:C:198:ALA:C	1:C:202:ILE:HD13	2.31	0.51
1:C:269:LEU:CD1	1:E:218:LEU:HA	2.40	0.51
1:D:254:THR:C	1:D:256:ASP:H	2.13	0.51
1:F:254:THR:HG21	4:F:776:HOH:O	2.11	0.51
1:F:57:LYS:HB3	1:F:57:LYS:NZ	2.26	0.51
1:D:44:LEU:N	1:D:44:LEU:HD22	2.26	0.50
1:F:43:ARG:HD2	1:F:46:LEU:HD22	1.92	0.50
1:A:193:PRO:O	1:A:194:ILE:HD13	2.10	0.50
1:D:176:ALA:HB1	1:D:254:THR:HG22	1.94	0.50
1:E:245:LEU:CD2	1:E:258:ILE:HD12	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ARG:O	1:F:47:ILE:HG13	2.11	0.50
1:A:11:LEU:HD13	1:A:134:LEU:CD1	2.40	0.50
1:A:193:PRO:HA	2:A:300:NAD:O7N	2.12	0.50
1:A:238:VAL:O	1:A:242:VAL:HG23	2.11	0.50
1:B:90:GLY:HA2	1:B:143:SER:O	2.11	0.50
1:C:163:VAL:HA	1:D:170:SER:OG	2.11	0.50
1:C:3:GLY:O	1:C:6:ASP:OD1	2.30	0.50
1:E:97:PHE:CE2	1:E:99:PRO:HD3	2.47	0.50
1:F:4:LEU:HD11	1:F:247:SER:HB3	1.93	0.50
1:D:16:ILE:CD1	1:D:43:ARG:HH22	2.25	0.50
1:C:240:LYS:HG2	1:F:249:TRP:CZ3	2.46	0.50
1:D:74:LEU:HD13	1:D:134:LEU:HD21	1.93	0.50
1:C:66:GLN:HE22	1:C:118:LYS:HG3	1.75	0.49
1:A:67:ASN:HD21	1:A:69:GLU:HB3	1.77	0.49
1:D:167:ALA:O	1:D:171:VAL:HG23	2.13	0.49
1:D:17:THR:HG22	1:D:18:ASP:N	2.27	0.49
1:E:43:ARG:O	1:E:47:ILE:HG13	2.11	0.49
1:C:30:GLN:NE2	1:C:36:LEU:HD12	2.26	0.49
1:A:61:LEU:HD23	1:A:61:LEU:N	2.26	0.49
1:B:101:THR:HG21	1:B:115:ASP:CG	2.33	0.49
1:C:27:ARG:HG2	1:C:27:ARG:HH11	1.77	0.49
1:D:99:PRO:CG	1:D:115:ASP:HB2	2.38	0.49
1:E:80:GLU:C	1:E:80:GLU:CD	2.70	0.49
1:D:99:PRO:HB2	1:D:101:THR:HG22	1.94	0.49
1:D:147:MET:O	1:D:165:LYS:NZ	2.45	0.49
1:D:53:ARG:HA	1:D:53:ARG:HE	1.78	0.49
1:D:65:VAL:HG21	1:D:122:ILE:HG23	1.94	0.49
1:A:254:THR:HG21	4:A:851:HOH:O	2.13	0.49
1:C:201:ALA:C	1:C:206:ALA:HB3	2.32	0.49
1:E:25:ILE:O	1:E:29:ALA:HB2	2.12	0.49
1:F:71:LEU:HD21	1:F:129:SER:HB3	1.93	0.49
1:C:214:GLN:HB3	4:C:800:HOH:O	2.12	0.49
1:F:195:ARG:HH12	1:F:203:VAL:HG21	1.78	0.49
1:F:76:GLY:O	1:F:80:GLU:HG3	2.12	0.49
1:D:193:PRO:HA	2:D:600:NAD:O7N	2.13	0.49
1:D:196:THR:O	1:D:197:LEU:HD23	2.13	0.49
1:D:25:ILE:HA	1:D:239:ALA:HB1	1.95	0.49
1:E:60:LEU:HD22	1:E:60:LEU:N	2.28	0.49
1:F:13:SER:O	1:F:94:SER:HB3	2.12	0.49
1:F:228:ILE:CD1	1:F:262:GLY:HA2	2.42	0.49
1:A:210:GLU:CD	1:A:210:GLU:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:N	1:C:44:LEU:HD22	2.27	0.49
1:C:67:ASN:HD22	1:C:68:GLU:N	2.10	0.49
1:B:196:THR:HG21	2:B:400:NAD:O1N	2.12	0.48
1:D:154:ALA:HB3	1:F:267:GLN:OE1	2.12	0.48
1:D:5:LEU:HD22	1:D:5:LEU:N	2.28	0.48
1:C:4:LEU:C	1:C:5:LEU:HD12	2.34	0.48
1:D:135:LEU:N	1:D:136:PRO:CD	2.77	0.48
1:F:129:SER:O	1:F:132:LYS:HB3	2.14	0.48
1:B:16:ILE:HG23	1:B:17:THR:N	2.28	0.48
1:D:112:PRO:HB2	1:D:115:ASP:OD1	2.13	0.48
1:E:174:PHE:O	1:E:177:ARG:HG2	2.13	0.48
1:C:135:LEU:N	1:C:136:PRO:CD	2.75	0.48
1:C:60:LEU:HD12	1:C:61:LEU:H	1.78	0.48
1:F:131:ALA:O	1:F:135:LEU:HB2	2.14	0.48
1:B:68:GLU:HG3	4:B:866:HOH:O	2.12	0.48
1:C:25:ILE:HA	1:C:239:ALA:CB	2.41	0.48
1:D:10:ILE:HD12	1:D:34:ALA:HB1	1.95	0.48
1:D:129:SER:O	1:D:132:LYS:HE2	2.14	0.48
1:D:254:THR:HG21	4:D:833:HOH:O	2.12	0.48
1:C:153:ARG:CZ	1:E:153:ARG:NH1	2.76	0.48
1:B:41:PHE:HE1	1:B:64:ASP:CG	2.17	0.48
1:C:158:TYR:HD1	1:C:162:THR:OG1	1.95	0.48
1:C:226:ALA:HA	1:C:262:GLY:O	2.14	0.48
1:C:4:LEU:HD22	1:C:247:SER:HB2	1.96	0.48
1:E:216:GLN:HB2	1:E:216:GLN:HE21	1.54	0.48
1:E:214:GLN:O	1:E:218:LEU:HB2	2.13	0.48
1:F:4:LEU:HD21	1:F:249:TRP:CD1	2.48	0.48
1:A:197:LEU:HA	1:A:200:SER:CB	2.44	0.48
1:C:102:GLY:O	1:C:159:ASN:HB2	2.14	0.48
1:C:17:THR:HG21	1:C:197:LEU:HD23	1.95	0.48
1:D:195:ARG:HG3	1:D:232:MET:HG3	1.96	0.48
1:E:65:VAL:CG1	1:E:95:ILE:HD13	2.44	0.48
1:F:17:THR:C	1:F:19:SER:H	2.17	0.48
1:B:200:SER:O	1:B:203:VAL:HG12	2.13	0.48
1:C:149:PHE:O	1:C:150:ASP:C	2.52	0.48
1:F:67:ASN:HB3	1:F:70:HIS:CD2	2.48	0.48
1:D:40:GLY:N	1:D:61:LEU:O	2.46	0.47
1:F:71:LEU:C	1:F:73:SER:H	2.18	0.47
1:F:87:LYS:HB2	1:F:139:ASN:ND2	2.29	0.47
1:B:67:ASN:O	1:B:71:LEU:HD22	2.14	0.47
1:D:196:THR:OG1	1:D:197:LEU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:VAL:O	1:F:31:GLU:HB2	2.14	0.47
1:C:101:THR:O	1:C:111:ALA:HB2	2.14	0.47
1:C:230:TRP:CD1	1:C:232:MET:HB3	2.50	0.47
1:C:186:SER:N	1:C:254:THR:HG23	2.25	0.47
1:D:75:ALA:HB2	1:D:133:ALA:O	2.14	0.47
1:F:151:PRO:HB3	1:F:162:THR:CG2	2.44	0.47
1:F:71:LEU:O	1:F:74:LEU:HB2	2.14	0.47
1:A:101:THR:HG21	1:A:115:ASP:CB	2.45	0.47
1:B:20:SER:HB3	2:B:400:NAD:O2A	2.13	0.47
1:D:169:GLU:OE2	1:D:257:ILE:HD13	2.15	0.47
1:D:4:LEU:HB3	1:D:5:LEU:HD22	1.96	0.47
1:C:11:LEU:HD23	1:C:12:VAL:N	2.30	0.47
1:C:21:ILE:HG22	1:C:25:ILE:HG13	1.96	0.47
1:D:65:VAL:HG22	2:D:600:NAD:N1A	2.29	0.47
1:E:248:ASP:OD2	1:E:248:ASP:N	2.47	0.47
1:F:91:VAL:HG23	1:F:138:MET:CE	2.45	0.47
1:F:9:ARG:HH12	1:F:86:ASN:CB	2.28	0.47
1:E:157:ALA:O	1:E:158:TYR:CB	2.61	0.47
1:F:30:GLN:OE1	1:F:55:PRO:HG2	2.14	0.47
1:F:64:ASP:H	1:F:70:HIS:CD2	2.33	0.47
1:E:67:ASN:C	1:E:67:ASN:HD22	2.17	0.47
1:F:44:LEU:HD13	1:F:44:LEU:O	2.15	0.47
1:A:254:THR:HG22	1:A:255:GLY:N	2.30	0.47
1:B:199:MET:HA	1:B:202:ILE:HD13	1.97	0.47
1:C:67:ASN:C	1:C:67:ASN:ND2	2.66	0.47
1:C:215:ILE:HD13	1:C:215:ILE:C	2.35	0.46
1:C:66:GLN:CD	1:C:122:ILE:HD11	2.35	0.46
1:F:165:LYS:HA	1:F:168:LEU:HB2	1.97	0.46
1:B:76:GLY:O	1:B:80:GLU:HG3	2.15	0.46
1:E:82:ILE:O	1:E:86:ASN:ND2	2.49	0.46
1:F:198:ALA:O	1:F:202:ILE:HG13	2.15	0.46
1:B:79:THR:C	1:B:81:ALA:N	2.68	0.46
1:C:149:PHE:HD1	1:C:158:TYR:CE1	2.33	0.46
1:C:218:LEU:HD21	1:E:269:LEU:CB	2.45	0.46
1:E:148:ASP:OD1	1:E:169:GLU:OE2	2.33	0.46
1:C:201:ALA:C	1:C:203:VAL:H	2.19	0.46
1:D:48:GLN:C	1:D:50:ILE:H	2.18	0.46
1:E:67:ASN:HB3	1:E:70:HIS:HD2	1.80	0.46
1:F:164:ALA:O	1:F:168:LEU:N	2.48	0.46
1:F:195:ARG:NH1	1:F:203:VAL:HG21	2.31	0.46
1:B:256:ASP:OD1	1:B:257:ILE:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASN:ND2	1:B:67:ASN:C	2.62	0.46
1:D:151:PRO:HB2	1:D:166:SER:OG	2.14	0.46
1:F:49:ARG:HH11	1:F:50:ILE:N	2.14	0.46
1:B:216:GLN:HA	4:B:876:HOH:O	2.16	0.46
1:C:43:ARG:HD2	1:C:46:LEU:HD12	1.98	0.46
1:C:51:THR:C	1:C:53:ARG:H	2.17	0.46
1:D:203:VAL:HG13	1:D:216:GLN:HB2	1.97	0.46
1:E:191:ALA:O	2:E:700:NAD:H5N	2.16	0.46
1:F:4:LEU:HD22	1:F:4:LEU:O	2.15	0.46
1:A:28:VAL:O	1:A:32:GLN:HG2	2.16	0.46
1:C:231:ASN:CG	1:C:233:LYS:HD3	2.35	0.46
1:E:66:GLN:HE22	1:E:118:LYS:HD2	1.81	0.46
1:F:74:LEU:HD22	1:F:134:LEU:HD21	1.97	0.46
1:D:97:PHE:HE2	1:D:118:LYS:HZ1	1.61	0.46
1:E:5:LEU:HB2	1:E:34:ALA:HB2	1.97	0.46
1:B:49:ARG:HH11	1:B:49:ARG:HG3	1.81	0.46
1:C:5:LEU:HD12	1:C:5:LEU:N	2.31	0.46
1:B:42:ASP:O	1:B:44:LEU:HG	2.16	0.46
1:D:15:ILE:HG22	1:D:16:ILE:N	2.31	0.46
1:E:65:VAL:HG11	1:E:95:ILE:HD13	1.98	0.46
1:A:12:VAL:HB	1:A:38:LEU:CD2	2.46	0.45
1:C:211:ALA:C	1:C:213:ALA:H	2.19	0.45
1:F:248:ASP:O	1:F:251:PRO:HG3	2.16	0.45
1:A:202:ILE:HA	1:A:206:ALA:CB	2.42	0.45
1:B:100:GLN:CA	1:B:100:GLN:HE21	2.29	0.45
1:C:185:ARG:HH11	1:C:185:ARG:CG	2.26	0.45
1:C:201:ALA:C	1:C:203:VAL:N	2.68	0.45
1:C:195:ARG:HH12	1:C:203:VAL:HG11	1.81	0.45
1:F:201:ALA:HB1	1:F:206:ALA:HB3	1.99	0.45
1:C:225:ARG:O	1:C:267:GLN:HG3	2.17	0.45
1:D:203:VAL:CG1	1:D:216:GLN:HB2	2.47	0.45
1:F:79:THR:HG23	1:F:84:ALA:HA	1.98	0.45
1:A:148:ASP:OD2	1:A:149:PHE:N	2.50	0.45
1:B:71:LEU:O	1:B:74:LEU:HB2	2.16	0.45
1:C:197:LEU:HD22	4:C:830:HOH:O	2.15	0.45
1:A:145:VAL:HA	1:A:187:ASN:O	2.17	0.45
1:A:197:LEU:O	1:A:197:LEU:HD13	2.17	0.45
1:D:203:VAL:HG22	1:D:216:GLN:HB2	1.99	0.45
1:A:227:PRO:HD2	1:A:262:GLY:O	2.16	0.45
1:C:231:ASN:C	1:C:233:LYS:H	2.20	0.45
1:B:254:THR:HG21	4:B:845:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLU:OE2	1:C:68:GLU:HA	2.17	0.45
1:E:5:LEU:HD22	1:E:5:LEU:H	1.80	0.45
1:E:68:GLU:HB3	1:E:69:GLU:OE2	2.17	0.45
1:F:91:VAL:HG23	1:F:138:MET:HE3	1.99	0.45
1:C:233:LYS:N	1:C:233:LYS:HD2	2.32	0.45
1:D:18:ASP:HA	1:D:23:PHE:CD2	2.52	0.45
1:D:87:LYS:HB3	1:D:137:ILE:O	2.17	0.45
1:B:119:GLY:O	1:B:123:SER:HB2	2.17	0.45
1:C:269:LEU:HD13	1:E:217:LEU:HD12	1.99	0.45
1:D:66:GLN:HG3	1:D:122:ILE:HG12	1.99	0.45
1:D:203:VAL:CG2	1:D:216:GLN:HB2	2.47	0.45
1:E:249:TRP:O	1:E:250:LEU:HG	2.17	0.45
1:F:135:LEU:HD21	1:F:179:ALA:HA	1.99	0.45
1:A:15:ILE:HG22	1:A:16:ILE:N	2.31	0.45
1:C:113:TYR:CZ	1:C:117:SER:HB2	2.52	0.45
1:C:196:THR:CG2	1:C:197:LEU:H	2.15	0.45
1:D:112:PRO:O	1:D:116:VAL:HG23	2.17	0.45
1:E:132:LYS:HG3	1:F:109:PHE:HB3	1.99	0.45
1:C:156:PRO:HG3	4:C:800:HOH:O	2.17	0.44
2:C:500:NAD:O3	3:C:550:GEQ:H4A	2.17	0.44
1:D:4:LEU:HD21	1:D:249:TRP:CD1	2.52	0.44
1:C:269:LEU:CD1	1:E:217:LEU:HD12	2.47	0.44
1:A:67:ASN:ND2	1:A:69:GLU:HB3	2.32	0.44
1:B:65:VAL:HG13	2:B:400:NAD:C2A	2.47	0.44
1:D:15:ILE:HG13	4:D:814:HOH:O	2.15	0.44
1:D:45:ARG:HG3	1:D:45:ARG:NH1	2.32	0.44
1:F:103:MET:O	1:F:104:GLY:C	2.56	0.44
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.81	0.44
1:D:215:ILE:O	1:D:219:GLU:HB2	2.17	0.44
1:E:46:LEU:O	1:E:47:ILE:C	2.56	0.44
1:E:196:THR:O	1:E:197:LEU:C	2.55	0.44
1:D:221:GLY:HA2	1:D:224:GLN:CD	2.38	0.44
1:D:252:ALA:O	1:E:262:GLY:N	2.46	0.44
1:D:83:GLY:HA3	1:D:86:ASN:HD22	1.83	0.44
1:F:199:MET:HE1	1:F:215:ILE:CG2	2.47	0.44
1:A:5:LEU:CD1	1:A:5:LEU:N	2.80	0.44
1:C:185:ARG:HB3	1:C:254:THR:HG23	1.99	0.44
1:A:91:VAL:HG23	1:A:138:MET:CE	2.47	0.44
1:A:158:TYR:CZ	1:A:161:MET:HG3	2.53	0.44
1:C:212:GLY:O	1:C:216:GLN:HB2	2.18	0.44
1:D:88:LEU:N	1:D:137:ILE:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASP:OD1	1:D:169:GLU:OE2	2.35	0.44
1:D:215:ILE:O	1:D:215:ILE:HG22	2.17	0.44
1:E:137:ILE:O	1:E:137:ILE:HG13	2.17	0.44
1:F:238:VAL:O	1:F:241:THR:HB	2.17	0.44
1:F:63:LEU:HD12	1:F:64:ASP:N	2.32	0.44
1:B:39:THR:HA	1:B:61:LEU:O	2.18	0.44
1:D:250:LEU:HB3	1:D:253:THR:CG2	2.48	0.44
1:E:42:ASP:CG	1:E:43:ARG:N	2.68	0.44
1:F:219:GLU:C	1:F:221:GLY:H	2.21	0.44
1:F:49:ARG:HH11	1:F:49:ARG:C	2.21	0.44
1:F:53:ARG:HG2	1:F:53:ARG:NH1	2.31	0.44
1:F:65:VAL:HG22	2:F:750:NAD:N1A	2.32	0.44
1:A:113:TYR:CZ	1:B:121:HIS:HB2	2.53	0.44
1:B:66:GLN:HE22	1:B:118:LYS:HG3	1.82	0.44
1:B:9:ARG:HA	1:B:35:GLN:O	2.18	0.44
1:C:44:LEU:HD13	1:C:47:ILE:HD11	1.99	0.44
1:D:11:LEU:C	1:D:11:LEU:HD23	2.38	0.44
1:D:236:THR:O	1:D:240:LYS:HG3	2.18	0.44
1:E:168:LEU:C	1:E:168:LEU:HD23	2.38	0.44
1:E:221:GLY:HA2	1:E:224:GLN:HB3	1.99	0.44
1:A:197:LEU:C	1:A:197:LEU:HD13	2.39	0.43
1:D:202:ILE:CG2	1:D:215:ILE:HG13	2.48	0.43
1:D:12:VAL:O	1:D:38:LEU:HA	2.17	0.43
1:A:221:GLY:O	1:A:224:GLN:HB3	2.19	0.43
1:B:148:ASP:OD2	1:B:149:PHE:N	2.48	0.43
1:E:70:HIS:O	1:E:74:LEU:HB2	2.17	0.43
1:E:83:GLY:HA3	1:E:86:ASN:HD22	1.83	0.43
1:A:148:ASP:O	2:A:300:NAD:H5N	2.19	0.43
1:A:193:PRO:O	1:A:232:MET:HB2	2.18	0.43
1:A:194:ILE:O	1:A:196:THR:N	2.52	0.43
1:A:51:THR:C	1:A:53:ARG:H	2.22	0.43
1:D:199:MET:HA	1:D:202:ILE:HD12	2.00	0.43
1:B:46:LEU:HD11	1:B:49:ARG:HH22	1.83	0.43
1:C:65:VAL:HA	1:C:71:LEU:HD21	1.99	0.43
1:D:199:MET:HA	1:D:202:ILE:HB	2.00	0.43
1:E:38:LEU:HD12	1:E:60:LEU:HD11	2.00	0.43
1:A:135:LEU:HB3	1:A:136:PRO:CD	2.46	0.43
1:A:4:LEU:HB3	1:A:5:LEU:CD1	2.46	0.43
1:A:30:GLN:OE1	1:A:54:LEU:HB3	2.18	0.43
1:B:78:VAL:O	1:B:82:ILE:HG23	2.19	0.43
1:D:259:TYR:CD2	1:D:265:HIS:CD2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PRO:CB	1:B:101:THR:HG22	2.48	0.43
1:D:149:PHE:CD1	1:D:158:TYR:CE1	3.06	0.43
1:C:225:ARG:NH1	1:C:225:ARG:HG3	2.32	0.43
1:D:132:LYS:O	1:D:132:LYS:HG2	2.18	0.43
1:D:195:ARG:CG	1:D:232:MET:HG3	2.49	0.43
1:E:93:HIS:CE1	1:E:95:ILE:HB	2.53	0.43
1:A:158:TYR:HD1	1:A:162:THR:OG1	2.00	0.43
1:C:4:LEU:HB3	1:C:5:LEU:CD1	2.49	0.43
1:D:15:ILE:CD1	1:D:38:LEU:HD13	2.49	0.43
1:C:145:VAL:HA	1:C:187:ASN:O	2.19	0.43
1:D:113:TYR:CZ	1:D:117:SER:HB2	2.53	0.43
1:E:28:VAL:HA	1:E:31:GLU:OE1	2.19	0.43
1:E:121:HIS:HB2	1:F:113:TYR:CZ	2.54	0.43
1:F:88:LEU:O	1:F:138:MET:HA	2.19	0.43
1:F:194:ILE:N	1:F:194:ILE:HD12	2.34	0.43
1:B:254:THR:O	1:B:256:ASP:N	2.52	0.43
1:B:261:ASP:C	1:B:261:ASP:OD2	2.56	0.43
1:C:16:ILE:HD12	1:C:47:ILE:HG22	2.00	0.43
1:E:79:THR:HG22	1:E:79:THR:O	2.18	0.43
1:F:215:ILE:HA	1:F:218:LEU:HD13	2.01	0.43
1:B:149:PHE:O	1:B:151:PRO:HD3	2.19	0.42
1:B:245:LEU:HD12	1:B:250:LEU:HD13	2.01	0.42
1:D:99:PRO:C	1:D:101:THR:N	2.72	0.42
1:E:205:GLY:O	1:E:206:ALA:HB3	2.18	0.42
1:C:253:THR:HG22	1:F:259:TYR:O	2.19	0.42
1:A:195:ARG:HB2	1:A:232:MET:HG3	2.01	0.42
1:B:199:MET:HG2	3:B:450:GEQ:H5C2	2.00	0.42
1:D:4:LEU:O	1:D:5:LEU:HD13	2.19	0.42
1:E:67:ASN:CB	1:E:70:HIS:HD2	2.31	0.42
1:F:9:ARG:HD3	1:F:35:GLN:HB2	2.01	0.42
1:B:254:THR:O	1:B:256:ASP:HB2	2.19	0.42
1:B:47:ILE:HD11	1:B:60:LEU:HD21	2.01	0.42
1:F:202:ILE:HG23	1:F:207:LEU:HD12	2.01	0.42
1:F:60:LEU:HG	1:F:60:LEU:O	2.19	0.42
1:F:67:ASN:C	1:F:67:ASN:HD22	2.21	0.42
1:A:215:ILE:O	1:A:218:LEU:HB2	2.19	0.42
2:A:300:NAD:H52N	2:A:300:NAD:H52A	2.00	0.42
1:D:132:LYS:HE2	1:D:132:LYS:HB3	1.90	0.42
1:D:44:LEU:HD11	1:D:62:GLU:CG	2.49	0.42
1:C:153:ARG:NH2	1:E:153:ARG:NE	2.68	0.42
1:C:173:ARG:HB3	1:D:154:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HB	2:C:500:NAD:O3B	2.19	0.42
1:E:158:TYR:CD1	1:E:158:TYR:O	2.72	0.42
1:E:160:TRP:CE3	1:E:163:VAL:HG21	2.54	0.42
1:A:199:MET:SD	1:A:199:MET:O	2.77	0.42
1:A:210:GLU:CD	1:A:210:GLU:H	2.21	0.42
1:D:221:GLY:CA	1:D:224:GLN:NE2	2.82	0.42
1:D:78:VAL:O	1:D:82:ILE:HG23	2.19	0.42
1:E:63:LEU:HD22	1:E:74:LEU:HD11	2.00	0.42
1:C:241:THR:HG23	1:F:250:LEU:HD23	2.01	0.42
1:C:13:SER:O	1:C:22:ALA:HB1	2.19	0.42
1:D:135:LEU:HA	1:D:135:LEU:HD12	1.80	0.42
1:F:49:ARG:HB3	1:F:49:ARG:CZ	2.45	0.42
1:A:185:ARG:HG3	1:A:185:ARG:HH11	1.84	0.42
1:B:245:LEU:CD1	1:B:250:LEU:HD13	2.49	0.42
1:E:99:PRO:HG2	1:E:115:ASP:HB3	2.00	0.42
1:F:11:LEU:C	1:F:11:LEU:HD23	2.39	0.42
1:F:197:LEU:HD22	1:F:197:LEU:O	2.19	0.42
1:F:4:LEU:CD1	1:F:247:SER:HB3	2.49	0.42
1:A:48:GLN:HE21	1:A:60:LEU:CD2	2.32	0.42
1:C:15:ILE:HD11	1:C:23:PHE:HA	2.01	0.42
1:C:230:TRP:CZ3	1:C:261:ASP:HA	2.55	0.42
1:C:66:GLN:HG3	1:C:122:ILE:HG12	2.02	0.42
1:D:191:ALA:HB3	2:D:600:NAD:C5N	2.49	0.42
1:E:105:ILE:HG12	1:E:106:ASN:N	2.35	0.42
1:E:66:GLN:NE2	1:E:118:LYS:HD2	2.35	0.42
1:E:195:ARG:HG3	1:E:195:ARG:NH1	2.35	0.42
1:A:77:ARG:O	1:A:80:GLU:HB2	2.20	0.42
1:D:147:MET:HE2	1:D:189:VAL:HB	2.01	0.42
1:D:148:ASP:O	1:D:190:ALA:HA	2.20	0.42
1:D:194:ILE:HD11	1:D:238:VAL:HG21	2.01	0.42
1:D:41:PHE:HE1	1:D:64:ASP:CG	2.23	0.42
1:E:185:ARG:HA	1:E:254:THR:CG2	2.49	0.42
1:F:201:ALA:HB1	1:F:206:ALA:CB	2.50	0.42
1:A:63:LEU:HB3	4:A:751:HOH:O	2.20	0.41
1:C:105:ILE:CD1	1:C:105:ILE:O	2.65	0.41
1:C:27:ARG:HG2	1:C:27:ARG:NH1	2.35	0.41
1:D:221:GLY:O	1:D:224:GLN:HB2	2.19	0.41
1:D:242:VAL:O	1:D:246:LEU:HG	2.20	0.41
1:D:74:LEU:HD22	1:D:78:VAL:HG23	2.03	0.41
1:E:132:LYS:HB2	1:F:109:PHE:CD1	2.55	0.41
1:A:185:ARG:HD3	1:A:251:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:CG1	1:A:207:LEU:HD13	2.50	0.41
1:A:202:ILE:HG13	1:A:207:LEU:HD13	2.02	0.41
1:B:143:SER:HB2	4:B:778:HOH:O	2.21	0.41
1:B:180:GLY:C	1:B:182:TYR:H	2.22	0.41
1:B:11:LEU:HD21	1:B:39:THR:HG23	2.02	0.41
1:B:99:PRO:C	1:B:101:THR:H	2.23	0.41
1:C:71:LEU:HD13	1:C:74:LEU:HD12	2.01	0.41
1:D:221:GLY:HA3	1:D:224:GLN:NE2	2.35	0.41
1:E:217:LEU:HA	1:E:220:GLU:HB3	2.02	0.41
1:E:40:GLY:HA2	4:E:812:HOH:O	2.20	0.41
1:E:57:LYS:HD3	1:E:57:LYS:H	1.85	0.41
1:C:231:ASN:OD1	1:C:233:LYS:HD3	2.20	0.41
1:C:38:LEU:HD13	1:C:51:THR:HG21	2.02	0.41
1:E:102:GLY:HA3	1:E:160:TRP:HB2	2.02	0.41
1:E:186:SER:O	1:E:255:GLY:N	2.51	0.41
1:A:157:ALA:CB	1:A:215:ILE:HD11	2.49	0.41
1:A:245:LEU:HA	1:A:245:LEU:HD12	1.75	0.41
1:A:5:LEU:HB2	1:A:34:ALA:HB2	2.02	0.41
1:B:250:LEU:N	1:B:251:PRO:HD3	2.35	0.41
1:B:67:ASN:ND2	1:B:69:GLU:HB2	2.31	0.41
1:C:185:ARG:NH1	1:C:185:ARG:CG	2.84	0.41
1:C:201:ALA:O	1:C:203:VAL:N	2.53	0.41
1:D:131:ALA:O	1:D:135:LEU:HB2	2.20	0.41
1:D:225:ARG:O	1:D:227:PRO:HD3	2.19	0.41
1:D:267:GLN:NE2	1:F:154:ALA:HB3	2.34	0.41
1:D:99:PRO:C	1:D:101:THR:H	2.24	0.41
1:F:17:THR:HA	1:F:50:ILE:CD1	2.51	0.41
1:C:46:LEU:O	1:C:50:ILE:HG12	2.19	0.41
1:A:42:ASP:N	1:A:42:ASP:OD2	2.52	0.41
1:B:60:LEU:HD13	1:B:61:LEU:N	2.35	0.41
1:D:74:LEU:HD22	1:D:78:VAL:CG2	2.51	0.41
1:E:105:ILE:HG23	1:E:106:ASN:N	2.27	0.41
1:E:101:THR:HB	1:E:111:ALA:CB	2.50	0.41
1:E:195:ARG:HH11	1:E:195:ARG:HG3	1.85	0.41
1:E:68:GLU:OE1	1:E:68:GLU:HA	2.19	0.41
1:A:12:VAL:HB	1:A:38:LEU:HD22	2.03	0.41
1:D:194:ILE:O	1:D:199:MET:HE3	2.21	0.41
1:E:129:SER:O	1:E:133:ALA:N	2.54	0.41
1:E:71:LEU:HD12	1:E:133:ALA:HB2	2.03	0.41
1:E:232:MET:CE	1:E:232:MET:H	2.34	0.41
1:F:49:ARG:NH1	1:F:50:ILE:HG13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HA	1:B:254:THR:HG23	2.02	0.41
1:C:153:ARG:NH1	1:E:153:ARG:NH2	2.68	0.41
1:C:45:ARG:HG2	1:C:45:ARG:NH1	2.33	0.41
1:E:8:LYS:HA	1:E:89:ASP:OD2	2.20	0.41
1:D:209:GLU:O	1:D:211:ALA:N	2.54	0.41
1:D:261:ASP:OD1	1:D:265:HIS:CD2	2.74	0.41
1:B:194:ILE:HA	1:B:232:MET:O	2.21	0.41
1:C:135:LEU:HD21	1:C:179:ALA:CA	2.48	0.41
1:D:10:ILE:O	1:D:36:LEU:HA	2.20	0.41
1:E:135:LEU:N	1:E:136:PRO:CD	2.83	0.41
1:D:19:SER:O	1:D:196:THR:HG22	2.20	0.41
1:D:198:ALA:O	1:D:202:ILE:HG13	2.21	0.41
1:E:97:PHE:CG	1:E:98:MET:N	2.89	0.41
1:F:116:VAL:O	1:F:120:ILE:HG13	2.20	0.41
1:F:150:ASP:CG	1:F:152:SER:HG	2.23	0.41
1:B:67:ASN:HD22	1:B:69:GLU:H	1.69	0.40
1:C:155:MET:HB2	1:C:156:PRO:HD2	2.04	0.40
1:C:185:ARG:HD3	1:C:251:PRO:O	2.21	0.40
1:D:5:LEU:HB2	1:D:34:ALA:HB2	2.03	0.40
1:E:207:LEU:HD12	1:E:207:LEU:N	2.36	0.40
1:F:71:LEU:C	1:F:73:SER:N	2.75	0.40
1:C:203:VAL:HG12	1:C:203:VAL:O	2.19	0.40
1:F:49:ARG:O	1:F:52:ASP:HB2	2.21	0.40
1:A:148:ASP:OD1	1:A:169:GLU:OE2	2.40	0.40
1:A:202:ILE:O	1:A:202:ILE:HG22	2.22	0.40
1:B:48:GLN:O	1:B:52:ASP:HB2	2.21	0.40
1:B:60:LEU:C	1:B:60:LEU:HD13	2.42	0.40
1:C:234:ASP:O	1:C:237:PRO:HD2	2.22	0.40
1:D:11:LEU:HD23	1:D:12:VAL:N	2.36	0.40
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.84	0.40
1:D:53:ARG:HE	1:D:53:ARG:N	2.20	0.40
1:E:135:LEU:HD13	1:E:144:ILE:HD11	2.03	0.40
1:A:46:LEU:HD23	1:A:50:ILE:HD13	2.03	0.40
1:B:66:GLN:NE2	1:B:118:LYS:HG3	2.36	0.40
1:C:93:HIS:CD2	1:C:127:TYR:HA	2.56	0.40
1:D:25:ILE:HG12	1:D:239:ALA:HA	2.03	0.40
1:D:83:GLY:O	1:D:84:ALA:C	2.59	0.40
1:E:64:ASP:HB3	1:E:67:ASN:HB2	2.04	0.40
1:E:12:VAL:HA	1:E:92:VAL:HB	2.03	0.40
1:E:163:VAL:HA	1:F:170:SER:OG	2.21	0.40
1:F:253:THR:O	1:F:253:THR:CG2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:CB	2:A:300:NAD:O2A	2.67	0.40
1:F:17:THR:O	1:F:19:SER:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH1	1:A:153:ARG:NH1[2_555]	1.51	0.69

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/269 (99%)	233 (88%)	25 (9%)	8 (3%)	5	12
1	B	266/269 (99%)	233 (88%)	28 (10%)	5 (2%)	9	23
1	C	266/269 (99%)	224 (84%)	32 (12%)	10 (4%)	4	8
1	D	266/269 (99%)	222 (84%)	36 (14%)	8 (3%)	5	12
1	E	266/269 (99%)	234 (88%)	24 (9%)	8 (3%)	5	12
1	F	266/269 (99%)	232 (87%)	27 (10%)	7 (3%)	6	15
All	All	1596/1614 (99%)	1378 (86%)	172 (11%)	46 (3%)	5	13

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLY
1	A	195	ARG
1	A	210	GLU
1	B	210	GLU
1	C	104	GLY
1	E	158	TYR

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Mol	Chain	Res	Type
1	E	159	ASN
1	F	104	GLY
1	A	159	ASN
1	A	234	ASP
1	B	104	GLY
1	C	3	GLY
1	D	16	ILE
1	D	100	GLN
1	D	210	GLU
1	E	105	ILE
1	F	18	ASP
1	F	72	ALA
1	B	159	ASN
1	C	16	ILE
1	C	159	ASN
1	C	232	MET
1	D	84	ALA
1	D	159	ASN
1	E	100	GLN
1	A	43	ARG
1	A	107	PRO
1	B	199	MET
1	B	255	GLY
1	E	206	ALA
1	F	65	VAL
1	A	16	ILE
1	C	46	LEU
1	D	150	ASP
1	E	74	LEU
1	E	150	ASP
1	F	103	MET
1	C	150	ASP
1	C	204	GLY
1	C	212	GLY
1	F	41	PHE
1	D	204	GLY
1	C	229	GLY
1	D	205	GLY
1	F	203	VAL
1	E	47	ILE

### 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	203/205 (99%)	180 (89%)	23 (11%)	7	16
1	B	203/205 (99%)	178 (88%)	25 (12%)	5	13
1	C	203/205 (99%)	182 (90%)	21 (10%)	8	19
1	D	203/205 (99%)	184 (91%)	19 (9%)	10	23
1	E	203/205 (99%)	186 (92%)	17 (8%)	13	29
1	F	203/205 (99%)	187 (92%)	16 (8%)	14	33
All	All	1218/1230 (99%)	1097 (90%)	121 (10%)	9	21

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	SER
1	A	35	GLN
1	A	61	LEU
1	A	67	ASN
1	A	71	LEU
1	A	103	MET
1	A	121	HIS
1	A	145	VAL
1	A	153	ARG
1	A	168	LEU
1	A	172	ASN
1	A	188	LEU
1	A	210	GLU
1	A	217	LEU
1	A	222	TRP
1	A	224	GLN
1	A	231	ASN
1	A	245	LEU
1	A	250	LEU
1	A	253	THR
1	A	256	ASP

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Mol	Chain	Res	Type
1	A	269	LEU
1	B	4	LEU
1	B	5	LEU
1	B	30	GLN
1	B	52	ASP
1	B	53	ARG
1	B	57	LYS
1	B	67	ASN
1	B	70	HIS
1	B	71	LEU
1	B	74	LEU
1	B	100	GLN
1	B	121	HIS
1	B	135	LEU
1	B	145	VAL
1	B	168	LEU
1	B	188	LEU
1	B	195	ARG
1	B	217	LEU
1	B	224	GLN
1	B	236	THR
1	B	251	PRO
1	B	253	THR
1	B	254	THR
1	B	258	ILE
1	B	269	LEU
1	C	4	LEU
1	C	60	LEU
1	C	67	ASN
1	C	70	HIS
1	C	74	LEU
1	C	80	GLU
1	C	105	ILE
1	C	115	ASP
1	C	121	HIS
1	C	161	MET
1	C	170	SER
1	C	177	ARG
1	C	210	GLU
1	C	215	ILE
1	C	216	GLN
1	C	224	GLN

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Mol	Chain	Res	Type
1	C	232	MET
1	C	233	LYS
1	C	253	THR
1	C	254	THR
1	C	269	LEU
1	D	4	LEU
1	D	6	ASP
1	D	52	ASP
1	D	53	ARG
1	D	57	LYS
1	D	74	LEU
1	D	80	GLU
1	D	115	ASP
1	D	129	SER
1	D	135	LEU
1	D	152	SER
1	D	158	TYR
1	D	177	ARG
1	D	185	ARG
1	D	209	GLU
1	D	253	THR
1	D	254	THR
1	D	268	LEU
1	D	269	LEU
1	E	5	LEU
1	E	48	GLN
1	E	67	ASN
1	E	71	LEU
1	E	74	LEU
1	E	80	GLU
1	E	103	MET
1	E	121	HIS
1	E	149	PHE
1	E	153	ARG
1	E	161	MET
1	E	177	ARG
1	E	216	GLN
1	E	232	MET
1	E	248	ASP
1	E	253	THR
1	E	254	THR
1	F	44	LEU

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Mol	Chain	Res	Type
1	F	45	ARG
1	F	49	ARG
1	F	67	ASN
1	F	74	LEU
1	F	80	GLU
1	F	121	HIS
1	F	158	TYR
1	F	168	LEU
1	F	197	LEU
1	F	210	GLU
1	F	218	LEU
1	F	231	ASN
1	F	233	LYS
1	F	245	LEU
1	F	256	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	48	GLN
1	A	67	ASN
1	A	70	HIS
1	A	86	ASN
1	A	214	GLN
1	A	224	GLN
1	A	231	ASN
1	B	67	ASN
1	B	70	HIS
1	B	100	GLN
1	B	224	GLN
1	C	66	GLN
1	C	67	ASN
1	C	70	HIS
1	C	214	GLN
1	C	224	GLN
1	D	30	GLN
1	D	70	HIS
1	D	86	ASN
1	D	121	HIS
1	D	139	ASN
1	D	224	GLN

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Mol	Chain	Res	Type
1	D	265	HIS
1	E	67	ASN
1	E	70	HIS
1	E	86	ASN
1	E	159	ASN
1	E	216	GLN
1	F	35	GLN
1	F	66	GLN
1	F	67	ASN
1	F	70	HIS
1	F	86	ASN
1	F	139	ASN
1	F	224	GLN
1	F	231	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	300	-	41,48,48	1.79	8 (19%)	43,73,73	2.34	11 (25%)
3	GEQ	A	350	-	33,35,35	2.03	19 (57%)	46,51,51	1.59	7 (15%)
2	NAD	B	400	-	41,48,48	1.85	8 (19%)	43,73,73	2.36	12 (27%)
3	GEQ	B	450	-	33,35,35	2.02	17 (51%)	46,51,51	1.66	9 (19%)
2	NAD	C	500	-	41,48,48	1.77	9 (21%)	43,73,73	2.32	11 (25%)
3	GEQ	C	550	-	33,35,35	2.05	16 (48%)	46,51,51	1.63	8 (17%)
2	NAD	D	600	-	41,48,48	1.87	8 (19%)	43,73,73	2.35	13 (30%)
3	GEQ	D	650	-	33,35,35	1.97	17 (51%)	46,51,51	1.60	7 (15%)
2	NAD	E	700	-	41,48,48	1.75	6 (14%)	43,73,73	2.44	11 (25%)
2	NAD	F	750	-	41,48,48	1.80	8 (19%)	43,73,73	2.33	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	300	-	-	0/22/62/62	0/5/5/5
3	GEQ	A	350	-	-	0/12/34/34	0/6/6/6
2	NAD	B	400	-	-	0/22/62/62	0/5/5/5
3	GEQ	B	450	-	-	0/12/34/34	0/6/6/6
2	NAD	C	500	-	-	0/22/62/62	0/5/5/5
3	GEQ	C	550	-	-	0/12/34/34	0/6/6/6
2	NAD	D	600	-	-	0/22/62/62	0/5/5/5
3	GEQ	D	650	-	-	0/12/34/34	0/6/6/6
2	NAD	E	700	-	-	0/22/62/62	0/5/5/5
2	NAD	F	750	-	-	0/22/62/62	0/5/5/5

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	450	GEQ	C6F-C6E	-2.80	1.39	1.46
2	C	500	NAD	O4B-C4B	-2.63	1.39	1.45
2	D	600	NAD	O4B-C4B	-2.56	1.39	1.45
3	A	350	GEQ	C6F-C6E	-2.48	1.40	1.46
2	F	750	NAD	O4B-C4B	-2.44	1.39	1.45
2	B	400	NAD	O4B-C4B	-2.41	1.39	1.45
3	C	550	GEQ	C6F-C6E	-2.41	1.40	1.46
3	D	650	GEQ	C6F-C6E	-2.40	1.40	1.46
3	A	350	GEQ	C2A-C1B	2.02	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	650	GEQ	C4F-C3F	2.02	1.42	1.38
3	D	650	GEQ	C4E-C3E	2.02	1.42	1.38
3	A	350	GEQ	C4F-C3F	2.04	1.43	1.38
3	D	650	GEQ	C3E-C2E	2.05	1.42	1.38
3	B	450	GEQ	C4F-C3F	2.08	1.43	1.38
3	D	650	GEQ	C4F-C5F	2.09	1.42	1.38
3	A	350	GEQ	C4E-C3E	2.11	1.43	1.38
3	B	450	GEQ	C3E-C2E	2.11	1.42	1.38
3	A	350	GEQ	C4E-C5E	2.12	1.42	1.38
3	C	550	GEQ	C4F-C3F	2.13	1.43	1.38
3	B	450	GEQ	C3F-C2F	2.13	1.43	1.38
3	B	450	GEQ	C5F-C6F	2.15	1.43	1.39
3	B	450	GEQ	C4E-C5E	2.16	1.43	1.38
3	D	650	GEQ	C3F-C2F	2.16	1.43	1.38
2	A	300	NAD	C2D-C1D	2.18	1.57	1.53
2	C	500	NAD	C2A-N3A	2.20	1.35	1.32
3	C	550	GEQ	C5F-C6F	2.20	1.43	1.39
3	C	550	GEQ	C3E-C2E	2.20	1.43	1.38
3	C	550	GEQ	C4E-C3E	2.20	1.43	1.38
3	C	550	GEQ	C4F-C5F	2.22	1.43	1.38
3	B	450	GEQ	C4E-C3E	2.22	1.43	1.38
2	C	500	NAD	C2D-C1D	2.26	1.57	1.53
2	B	400	NAD	C2A-N3A	2.26	1.36	1.32
3	A	350	GEQ	C4F-C5F	2.27	1.43	1.38
3	B	450	GEQ	C4F-C5F	2.27	1.43	1.38
3	C	550	GEQ	C3F-C2F	2.28	1.43	1.38
3	A	350	GEQ	C3E-C2E	2.30	1.43	1.38
3	A	350	GEQ	C3F-C2F	2.30	1.43	1.38
3	D	650	GEQ	C5F-C6F	2.32	1.43	1.39
3	A	350	GEQ	C5F-C6F	2.32	1.43	1.39
3	D	650	GEQ	C1F-C1D	2.35	1.56	1.52
3	D	650	GEQ	C2A-C1B	2.36	1.53	1.50
3	B	450	GEQ	C3C-N4C	2.37	1.51	1.47
3	A	350	GEQ	C4A-C3A	2.37	1.41	1.36
3	D	650	GEQ	C2E-C1E	2.38	1.42	1.39
3	A	350	GEQ	C2E-C1E	2.39	1.42	1.39
2	A	300	NAD	O3D-C3D	2.40	1.48	1.43
3	B	450	GEQ	C3A-C2A	2.40	1.43	1.39
3	C	550	GEQ	C3C-N4C	2.42	1.51	1.47
2	D	600	NAD	C2A-N3A	2.43	1.36	1.32
3	C	550	GEQ	C2E-C1E	2.45	1.42	1.39
3	A	350	GEQ	C1B-N1C	2.45	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	350	GEQ	C1F-C1D	2.49	1.56	1.52
2	A	300	NAD	C2A-N3A	2.54	1.36	1.32
2	C	500	NAD	O3D-C3D	2.58	1.48	1.43
2	F	750	NAD	O3D-C3D	2.58	1.48	1.43
3	A	350	GEQ	C3A-C2A	2.60	1.43	1.39
3	A	350	GEQ	C5C-N4C	2.62	1.52	1.47
3	B	450	GEQ	C2E-C1E	2.65	1.43	1.39
2	F	750	NAD	O2B-C2B	2.66	1.49	1.43
2	B	400	NAD	O3D-C3D	2.67	1.49	1.43
2	D	600	NAD	O3D-C3D	2.68	1.49	1.43
3	B	450	GEQ	C5C-N4C	2.70	1.52	1.47
3	D	650	GEQ	C3C-N4C	2.71	1.52	1.47
3	C	550	GEQ	C4A-C3A	2.71	1.42	1.36
3	C	550	GEQ	C1F-C1D	2.72	1.56	1.52
3	A	350	GEQ	C3C-N4C	2.72	1.52	1.47
3	D	650	GEQ	C2F-C1F	2.73	1.43	1.39
2	E	700	NAD	O2B-C2B	2.73	1.49	1.43
2	C	500	NAD	O2B-C2B	2.75	1.49	1.43
2	F	750	NAD	C2A-N3A	2.75	1.36	1.32
3	C	550	GEQ	C3A-C2A	2.75	1.43	1.39
2	D	600	NAD	O2B-C2B	2.76	1.49	1.43
3	D	650	GEQ	C4A-C3A	2.77	1.42	1.36
3	D	650	GEQ	C5C-N4C	2.79	1.52	1.47
3	B	450	GEQ	C4A-C3A	2.79	1.42	1.36
2	E	700	NAD	C2A-N3A	2.81	1.36	1.32
2	A	300	NAD	O2B-C2B	2.89	1.49	1.43
2	B	400	NAD	O2B-C2B	2.90	1.49	1.43
3	B	450	GEQ	C1F-C1D	2.90	1.57	1.52
3	D	650	GEQ	C3A-C2A	2.91	1.44	1.39
3	C	550	GEQ	C5C-N4C	2.99	1.53	1.47
3	D	650	GEQ	C1D-N4C	3.06	1.53	1.48
3	A	350	GEQ	C1D-N4C	3.11	1.53	1.48
3	C	550	GEQ	C1D-N4C	3.13	1.53	1.48
3	C	550	GEQ	C2F-C1F	3.32	1.44	1.39
2	C	500	NAD	C2B-C1B	3.32	1.58	1.53
3	B	450	GEQ	C2F-C1F	3.33	1.44	1.39
3	B	450	GEQ	C1D-N4C	3.34	1.53	1.48
3	B	450	GEQ	C1A-C2A	3.39	1.43	1.37
3	A	350	GEQ	C2F-C1F	3.40	1.44	1.39
2	E	700	NAD	C2N-C3N	3.41	1.44	1.39
2	E	700	NAD	C4N-C3N	3.41	1.44	1.39
3	A	350	GEQ	C1A-C2A	3.46	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	650	GEQ	C1A-C2A	3.60	1.43	1.37
2	F	750	NAD	C2N-C3N	3.69	1.44	1.39
3	C	550	GEQ	C1A-C2A	3.71	1.43	1.37
2	A	300	NAD	C4N-C3N	3.72	1.45	1.39
2	C	500	NAD	C4N-C3N	3.81	1.45	1.39
2	F	750	NAD	C2B-C1B	3.91	1.59	1.53
2	C	500	NAD	C2N-C3N	3.92	1.44	1.39
2	B	400	NAD	C4N-C3N	3.98	1.45	1.39
2	D	600	NAD	C2B-C1B	3.98	1.60	1.53
2	A	300	NAD	C2N-C3N	3.99	1.45	1.39
2	B	400	NAD	C2B-C1B	4.04	1.60	1.53
2	F	750	NAD	C4N-C3N	4.15	1.46	1.39
2	D	600	NAD	C4N-C3N	4.16	1.46	1.39
2	A	300	NAD	C2B-C1B	4.19	1.60	1.53
2	E	700	NAD	C2B-C1B	4.27	1.60	1.53
2	B	400	NAD	C2N-C3N	4.60	1.46	1.39
2	F	750	NAD	C4A-N3A	4.87	1.42	1.35
2	D	600	NAD	C2N-C3N	4.87	1.46	1.39
2	B	400	NAD	C4A-N3A	4.97	1.42	1.35
2	C	500	NAD	C4A-N3A	4.99	1.42	1.35
2	A	300	NAD	C4A-N3A	5.02	1.43	1.35
2	D	600	NAD	C4A-N3A	5.14	1.43	1.35
2	E	700	NAD	C4A-N3A	5.55	1.43	1.35

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	NAD	N3A-C2A-N1A	-6.65	123.07	128.86
2	B	400	NAD	N3A-C2A-N1A	-6.58	123.13	128.86
2	E	700	NAD	N3A-C2A-N1A	-6.55	123.15	128.86
2	F	750	NAD	N3A-C2A-N1A	-6.52	123.18	128.86
2	E	700	NAD	C4B-O4B-C1B	-6.41	102.95	109.77
2	A	300	NAD	N3A-C2A-N1A	-6.37	123.31	128.86
2	D	600	NAD	N3A-C2A-N1A	-6.37	123.31	128.86
2	A	300	NAD	C4B-O4B-C1B	-5.83	103.56	109.77
2	B	400	NAD	C4B-O4B-C1B	-5.77	103.63	109.77
2	D	600	NAD	C4B-O4B-C1B	-5.65	103.75	109.77
2	C	500	NAD	C4B-O4B-C1B	-5.62	103.78	109.77
2	E	700	NAD	O7N-C7N-N7N	-5.39	114.91	122.58
2	D	600	NAD	O7N-C7N-N7N	-5.25	115.11	122.58
2	F	750	NAD	C4B-O4B-C1B	-5.20	104.23	109.77
2	B	400	NAD	O7N-C7N-N7N	-5.18	115.21	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NAD	O7N-C7N-N7N	-5.17	115.23	122.58
2	F	750	NAD	O7N-C7N-N7N	-5.05	115.39	122.58
2	C	500	NAD	O7N-C7N-N7N	-5.01	115.45	122.58
2	D	600	NAD	N6A-C6A-N1A	-4.24	110.36	118.77
2	E	700	NAD	N6A-C6A-N1A	-4.23	110.38	118.77
2	A	300	NAD	N6A-C6A-N1A	-4.18	110.48	118.77
2	F	750	NAD	N6A-C6A-N1A	-4.16	110.52	118.77
2	C	500	NAD	N6A-C6A-N1A	-4.03	110.78	118.77
2	B	400	NAD	N6A-C6A-N1A	-4.01	110.81	118.77
3	A	350	GEQ	O2B-C1B-C2A	-3.19	114.23	120.21
2	E	700	NAD	O5D-PN-O1N	-3.15	96.55	109.25
3	A	350	GEQ	C3A-C4A-C5A	-3.02	117.14	120.84
3	B	450	GEQ	O2B-C1B-C2A	-3.00	114.58	120.21
3	B	450	GEQ	C3A-C4A-C5A	-3.00	117.17	120.84
3	C	550	GEQ	O2B-C1B-C2A	-2.98	114.62	120.21
3	D	650	GEQ	C3A-C4A-C5A	-2.98	117.19	120.84
2	B	400	NAD	O5D-PN-O1N	-2.85	97.74	109.25
3	D	650	GEQ	O2B-C1B-C2A	-2.70	115.16	120.21
3	C	550	GEQ	C3A-C4A-C5A	-2.67	117.57	120.84
2	A	300	NAD	O5D-PN-O1N	-2.55	98.95	109.25
2	C	500	NAD	O5D-PN-O1N	-2.52	99.07	109.25
2	F	750	NAD	O4B-C4B-C3B	-2.50	100.19	105.17
2	B	400	NAD	O4B-C4B-C3B	-2.39	100.42	105.17
2	D	600	NAD	O5D-PN-O1N	-2.36	99.71	109.25
2	D	600	NAD	O4B-C4B-C3B	-2.33	100.53	105.17
2	F	750	NAD	O5D-PN-O1N	-2.32	99.90	109.25
2	A	300	NAD	O4B-C4B-C3B	-2.28	100.63	105.17
2	E	700	NAD	O4B-C4B-C3B	-2.24	100.71	105.17
2	C	500	NAD	O4B-C4B-C3B	-2.22	100.76	105.17
3	B	450	GEQ	C1A-C2A-C1B	-2.12	116.52	120.43
2	C	500	NAD	C1B-N9A-C4A	-2.06	123.07	126.64
2	F	750	NAD	C2D-C3D-C4D	-2.06	98.60	102.62
2	E	700	NAD	C1B-N9A-C4A	-2.02	123.14	126.64
2	D	600	NAD	C2N-C3N-C7N	2.01	125.18	119.34
3	B	450	GEQ	C6C-C5C-N4C	2.03	114.70	110.63
2	A	300	NAD	C3N-C7N-N7N	2.05	120.11	117.77
2	B	400	NAD	C3N-C7N-N7N	2.07	120.14	117.77
2	C	500	NAD	C3N-C7N-N7N	2.11	120.18	117.77
2	B	400	NAD	O3D-C3D-C2D	2.15	118.71	111.83
2	D	600	NAD	C3N-C7N-N7N	2.17	120.25	117.77
2	D	600	NAD	O2D-C2D-C3D	2.17	118.78	111.83
3	C	550	GEQ	C6C-C5C-N4C	2.18	115.00	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	NAD	O3D-C3D-C2D	2.18	118.82	111.83
2	A	300	NAD	O2D-C2D-C3D	2.26	119.07	111.83
2	E	700	NAD	O2D-C2D-C3D	2.43	119.60	111.83
2	B	400	NAD	O2D-C2D-C3D	2.43	119.62	111.83
2	F	750	NAD	O3D-C3D-C2D	2.44	119.65	111.83
3	C	550	GEQ	C6F-C1F-C1D	2.61	111.75	110.06
2	F	750	NAD	O2D-C2D-C3D	2.66	120.36	111.83
3	A	350	GEQ	C6F-C1F-C1D	2.74	111.83	110.06
3	B	450	GEQ	C6F-C1F-C1D	2.76	111.84	110.06
2	E	700	NAD	O2B-C2B-C3B	2.76	120.67	111.83
3	D	650	GEQ	C6F-C1F-C1D	2.88	111.92	110.06
2	A	300	NAD	O2B-C2B-C3B	2.96	121.31	111.83
3	A	350	GEQ	C5C-N4C-C3C	3.03	114.57	109.07
3	D	650	GEQ	C5C-N4C-C3C	3.06	114.63	109.07
2	D	600	NAD	O2B-C2B-C3B	3.21	122.13	111.83
2	C	500	NAD	O2B-C2B-C3B	3.28	122.35	111.83
2	B	400	NAD	O2B-C2B-C3B	3.31	122.42	111.83
2	F	750	NAD	O2B-C2B-C3B	3.33	122.50	111.83
3	B	450	GEQ	C5C-N4C-C3C	3.34	115.14	109.07
3	A	350	GEQ	C6C-N1C-C2C	3.55	119.31	112.61
3	C	550	GEQ	C5C-N4C-C3C	3.61	115.63	109.07
3	C	550	GEQ	C6C-N1C-C2C	3.62	119.45	112.61
3	C	550	GEQ	C6E-C1E-C1D	3.67	112.43	110.06
3	B	450	GEQ	C6C-N1C-C2C	3.69	119.59	112.61
3	A	350	GEQ	C6E-C1E-C1D	3.75	112.48	110.06
3	B	450	GEQ	C6E-C1E-C1D	3.84	112.54	110.06
3	D	650	GEQ	C6E-C1E-C1D	3.96	112.62	110.06
3	D	650	GEQ	C6C-N1C-C2C	4.01	120.18	112.61
3	D	650	GEQ	C2A-C1B-N1C	4.02	123.97	118.77
2	C	500	NAD	O7N-C7N-C3N	4.06	124.37	119.62
3	B	450	GEQ	C2A-C1B-N1C	4.06	124.02	118.77
3	A	350	GEQ	C2A-C1B-N1C	4.11	124.08	118.77
2	F	750	NAD	O7N-C7N-C3N	4.29	124.64	119.62
2	D	600	NAD	O7N-C7N-C3N	4.29	124.64	119.62
2	B	400	NAD	O7N-C7N-C3N	4.30	124.65	119.62
2	A	300	NAD	O7N-C7N-C3N	4.31	124.66	119.62
3	C	550	GEQ	C2A-C1B-N1C	4.36	124.41	118.77
2	F	750	NAD	O3B-C3B-C4B	4.57	124.44	111.09
2	B	400	NAD	O3B-C3B-C4B	4.59	124.49	111.09
2	E	700	NAD	O3B-C3B-C4B	4.62	124.58	111.09
2	D	600	NAD	O3B-C3B-C4B	4.71	124.84	111.09
2	A	300	NAD	O3B-C3B-C4B	4.74	124.93	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	700	NAD	O7N-C7N-C3N	4.79	125.23	119.62
2	C	500	NAD	O3B-C3B-C4B	4.94	125.50	111.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NAD	8	0
3	A	350	GEQ	2	0
2	B	400	NAD	3	0
3	B	450	GEQ	3	0
2	C	500	NAD	3	0
3	C	550	GEQ	1	0
2	D	600	NAD	4	0
2	E	700	NAD	4	0
2	F	750	NAD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	268/269 (99%)	-0.49	3 (1%) 80 81	3, 12, 54, 87	0
1	B	268/269 (99%)	-0.47	7 (2%) 56 56	3, 13, 53, 80	0
1	C	268/269 (99%)	-0.21	5 (1%) 67 68	9, 30, 61, 70	0
1	D	268/269 (99%)	0.06	14 (5%) 28 26	13, 34, 82, 102	0
1	E	268/269 (99%)	-0.32	4 (1%) 74 75	8, 28, 55, 68	0
1	F	268/269 (99%)	-0.16	7 (2%) 56 56	6, 26, 59, 88	0
All	All	1608/1614 (99%)	-0.26	40 (2%) 58 58	3, 25, 61, 102	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	GLY	17.3
1	D	203	VAL	7.8
1	D	207	LEU	7.2
1	F	199	MET	6.0
1	E	101	THR	5.4
1	B	204	GLY	5.4
1	A	201	ALA	4.9
1	B	199	MET	4.5
1	D	206	ALA	4.2
1	F	201	ALA	4.2
1	B	202	ILE	4.1
1	F	198	ALA	4.0
1	A	204	GLY	3.8
1	D	197	LEU	3.6
1	D	199	MET	3.6
1	D	200	SER	3.6
1	C	2	THR	3.5
1	B	203	VAL	3.2
1	D	205	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	202	ILE	3.1
1	E	205	GLY	2.9
1	C	200	SER	2.7
1	D	201	ALA	2.6
1	B	200	SER	2.6
1	F	213	ALA	2.6
1	D	210	GLU	2.6
1	C	198	ALA	2.5
1	F	202	ILE	2.5
1	B	205	GLY	2.4
1	A	203	VAL	2.4
1	D	2	THR	2.3
1	C	203	VAL	2.3
1	E	60	LEU	2.3
1	D	84	ALA	2.3
1	B	206	ALA	2.2
1	F	200	SER	2.1
1	F	208	GLY	2.1
1	D	44	LEU	2.1
1	E	105	ILE	2.1
1	C	211	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GEQ	C	550	30/30	0.75	0.33	2.56	57,61,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GEQ	A	350	30/30	0.84	0.23	1.97	42,52,56,56	0
2	NAD	B	400	44/44	0.91	0.19	1.29	34,42,45,45	0
3	GEQ	D	650	30/30	0.76	0.39	1.21	58,62,71,72	0
2	NAD	C	500	44/44	0.90	0.21	0.97	47,53,56,57	0
2	NAD	D	600	44/44	0.84	0.22	0.67	54,64,72,73	0
3	GEQ	B	450	30/30	0.81	0.22	0.52	46,51,57,58	0
2	NAD	A	300	44/44	0.94	0.15	0.44	29,37,47,48	0
2	NAD	F	750	44/44	0.92	0.15	0.32	43,47,49,51	0
2	NAD	E	700	44/44	0.94	0.16	0.24	19,34,39,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.