



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:43 pm BST

PDB ID : 3K2B  
Title : Crystal structure of photosynthetic A4 isoform glyceraldehyde-3-phosphate dehydrogenase complexed with NAD, from Arabidopsis thaliana  
Authors : Fermani, S.; Falini, G.; Thumiger, A.; Sparla, F.; Marri, L.; Trost, P.  
Deposited on : 2009-09-29  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

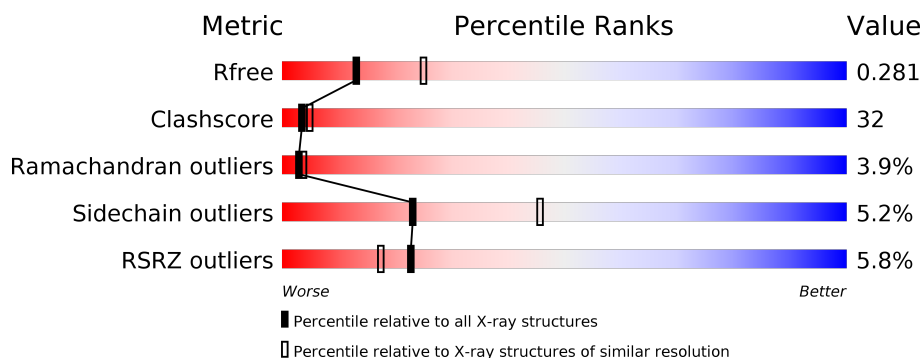
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. 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	337	<div> <div>65%</div> <div>31%</div> <div>.</div> </div>
1	B	337	<div> <div>61%</div> <div>36%</div> <div>.</div> </div>
1	C	337	<div> <div>%</div> <div>59%</div> <div>36%</div> <div>5%</div> </div>
1	D	337	<div> <div>%</div> <div>47%</div> <div>49%</div> <div>.</div> </div>
1	E	337	<div> <div>27%</div> <div>29%</div> <div>62%</div> <div>9%</div> </div>
1	F	337	<div> <div>15%</div> <div>34%</div> <div>57%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	337	<div><div></div><div>8%</div><div>42%</div><div>49%</div><div>9%</div></div>
1	H	337	<div><div></div><div>7%</div><div>38%</div><div>52%</div><div>8%</div><div>••</div></div>
1	O	337	<div><div></div><div>67%</div><div>31%</div><div>•</div></div>
1	Q	337	<div><div></div><div>59%</div><div>37%</div><div>•</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	B	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	C	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	D	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	E	336	Total	C	N	O	S	0	0	0
			2547	1609	443	486	9			
1	F	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	G	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	H	335	Total	C	N	O	S	0	0	0
			2542	1606	442	485	9			
1	O	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	Q	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			

- 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 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	F	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	G	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	H	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	O	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	Q	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	84	Total	O	0	0
			84	84		
4	C	94	Total	O	0	0
			94	94		
4	D	85	Total	O	0	0
			85	85		
4	E	79	Total	O	0	0
			79	79		
4	F	65	Total	O	0	0
			65	65		
4	G	81	Total	O	0	0
			81	81		
4	H	56	Total	O	0	0
			56	56		
4	O	129	Total	O	0	0
			129	129		

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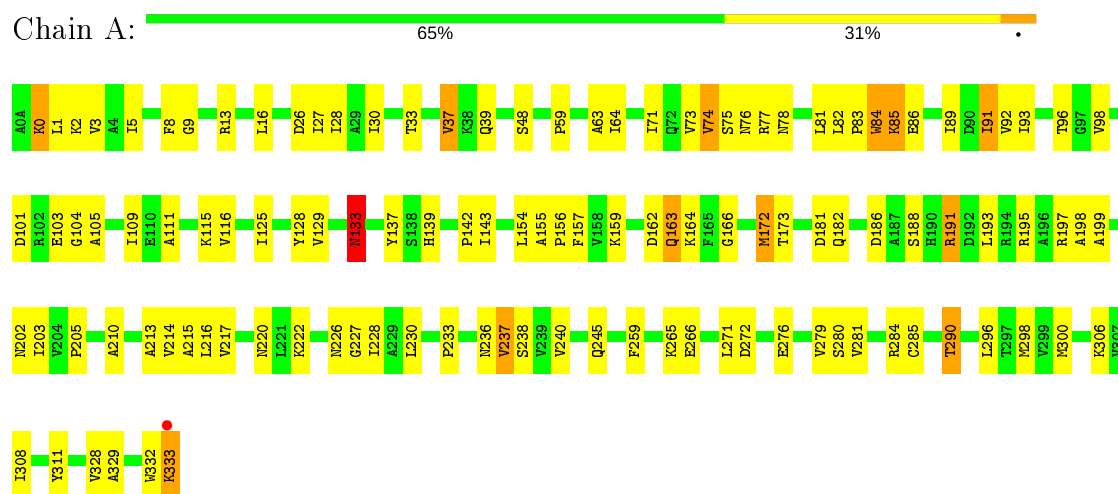
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	100	Total	O	0	0
			100	100		

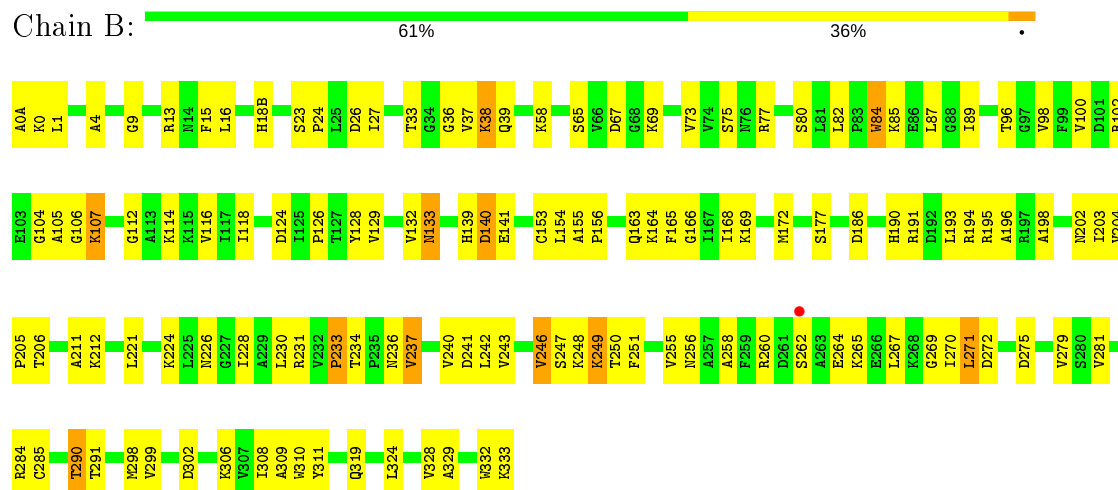
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

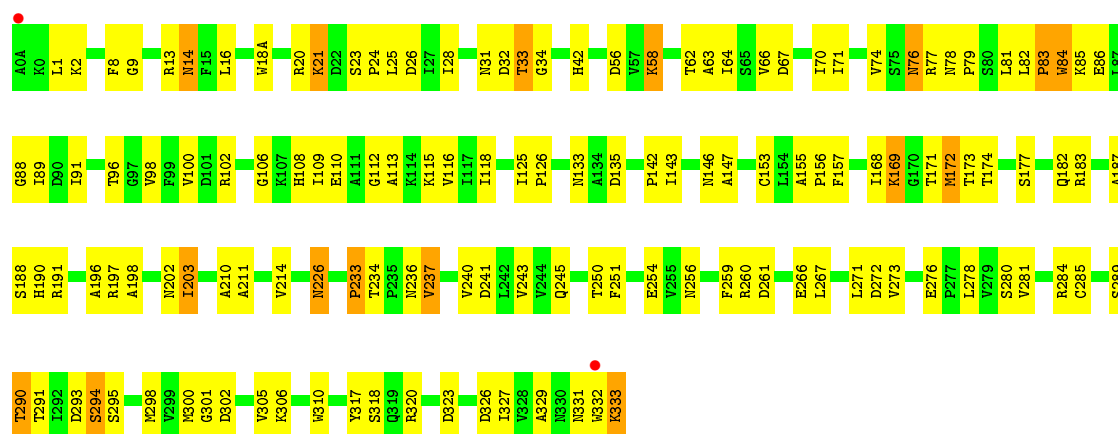


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

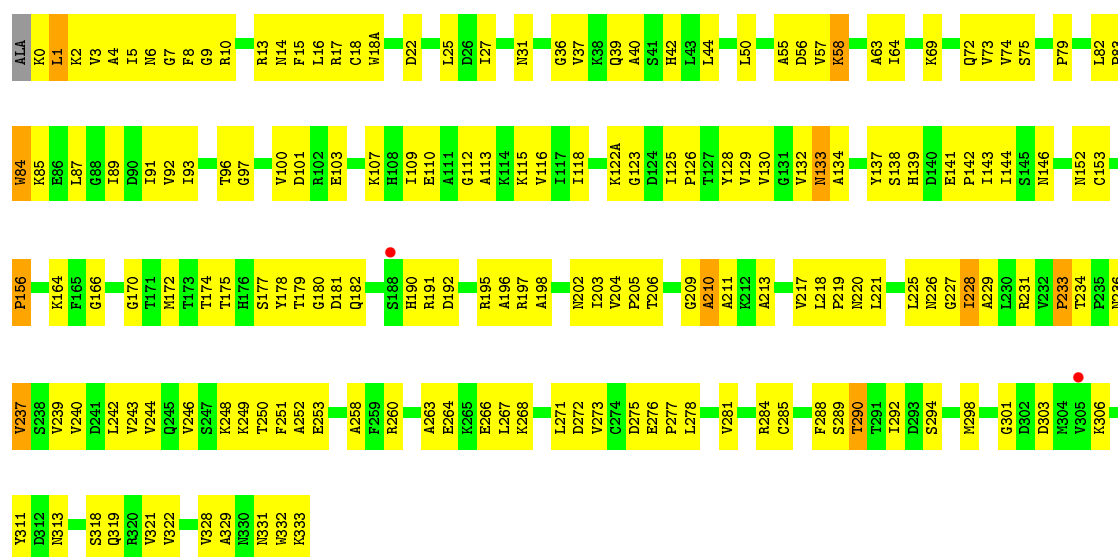


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

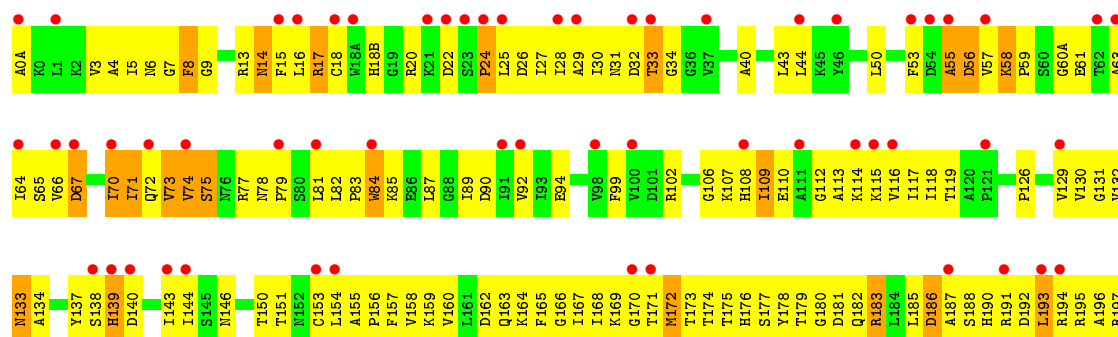


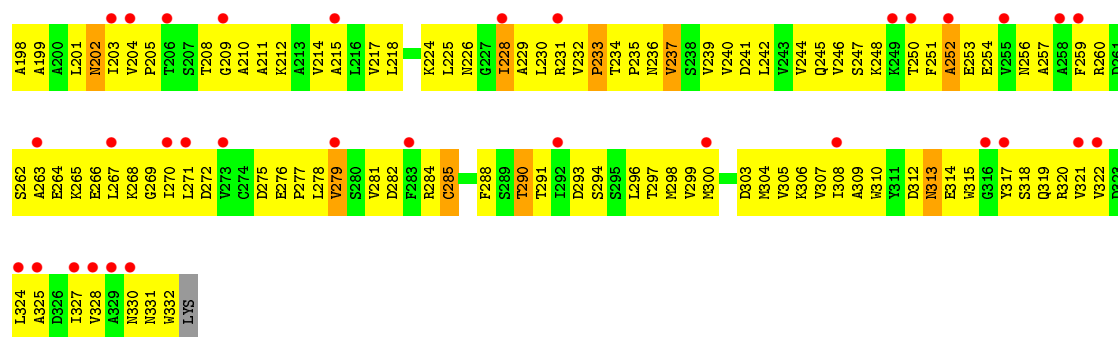


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

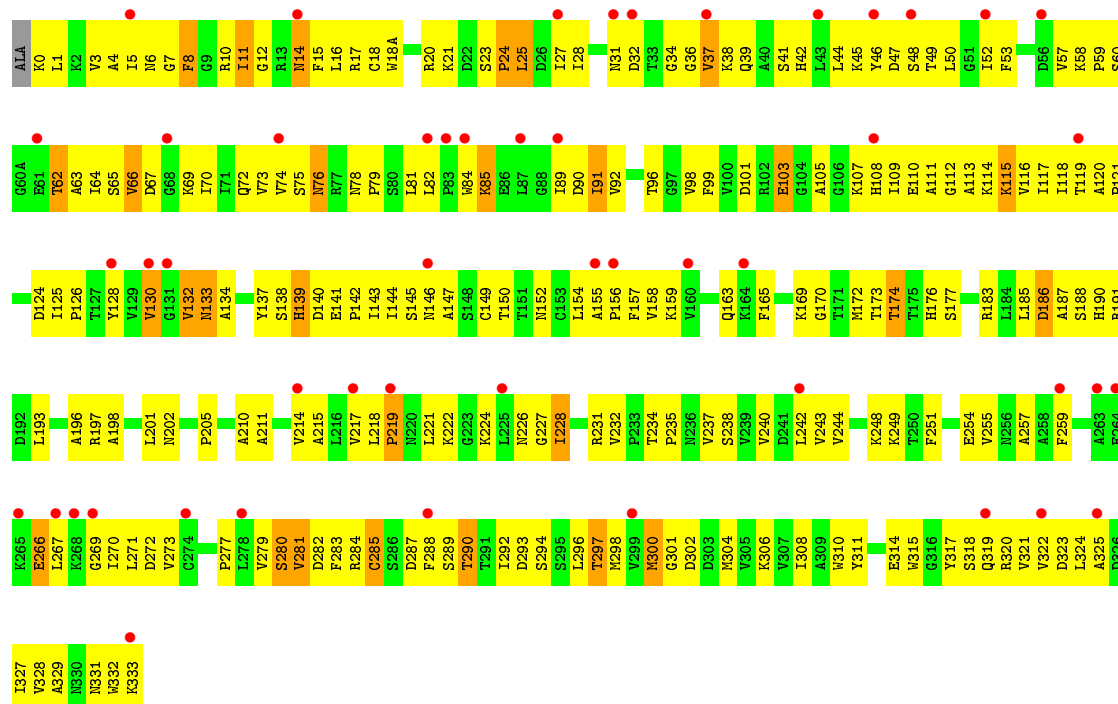


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

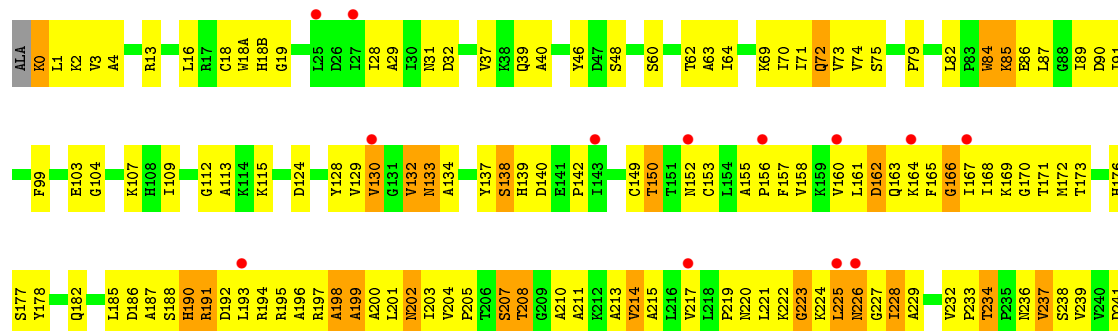
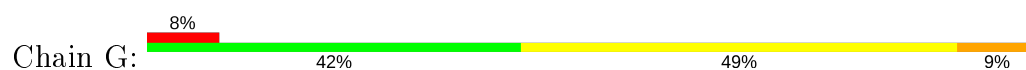


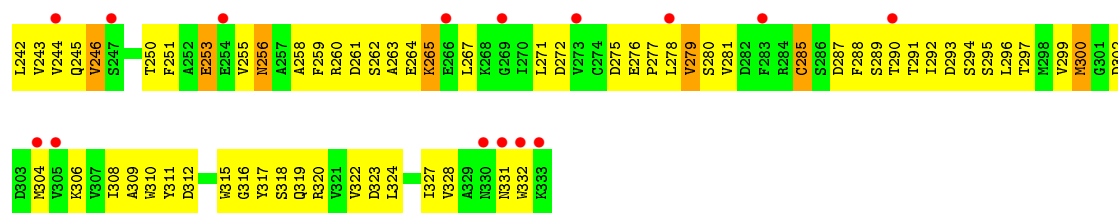


● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

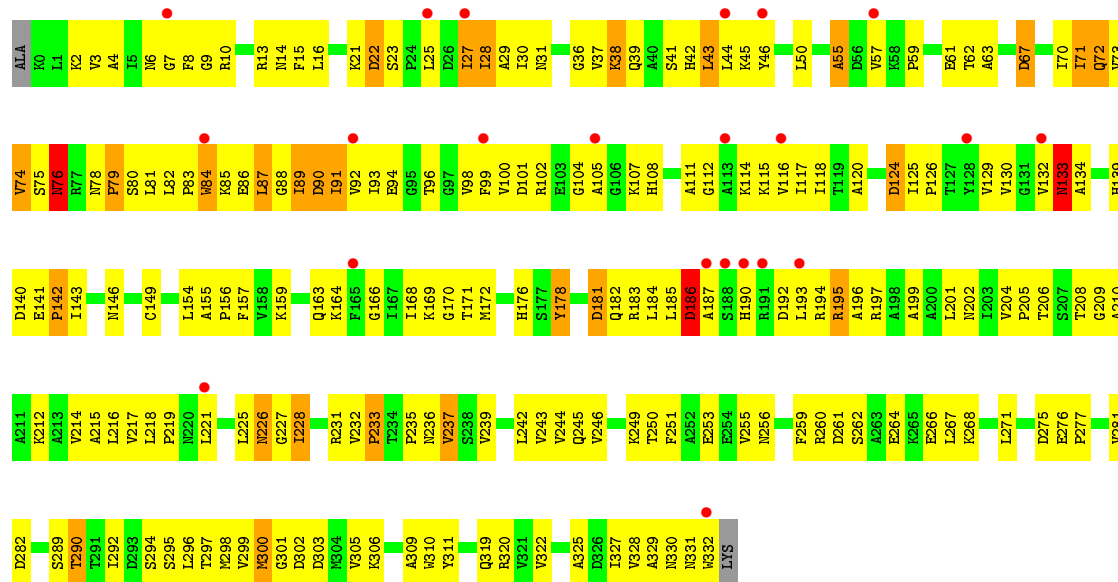


● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

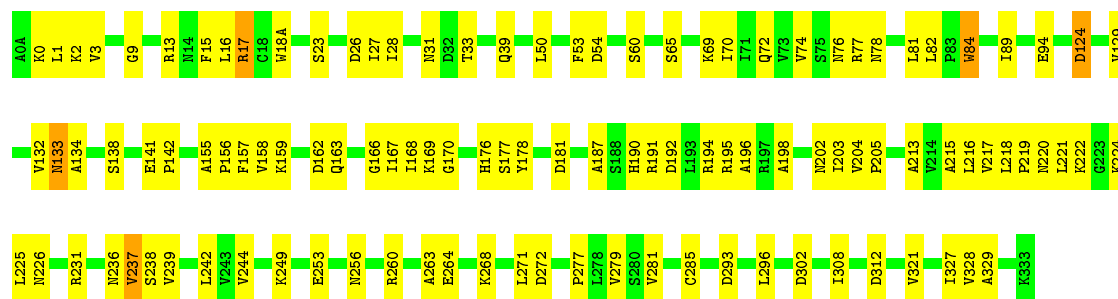




- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

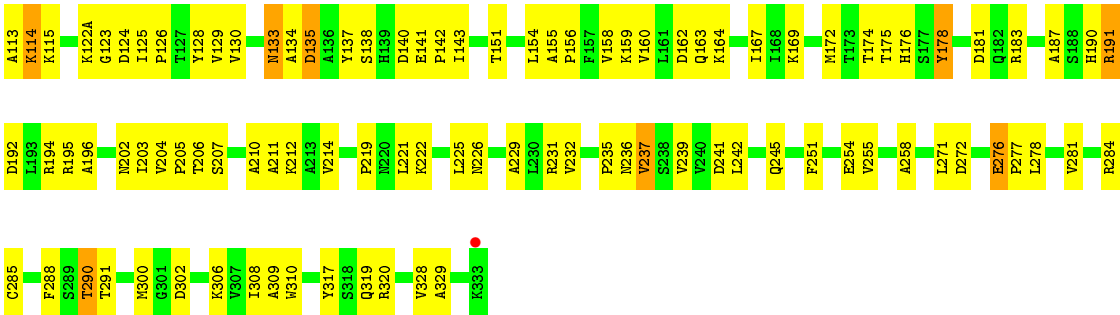


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.74Å 188.62Å 314.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.22 – 2.60 94.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (94.22-2.60) 95.9 (94.22-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.62Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.237 , 0.289 0.231 , 0.281	Depositor DCC
$R_{free}$ test set	6671 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 69.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% 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: SO4, 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	0.38	0/2601	0.66	1/3530 (0.0%)
1	B	0.38	0/2601	0.67	1/3530 (0.0%)
1	C	0.37	0/2601	0.66	1/3530 (0.0%)
1	D	0.34	0/2596	0.62	1/3523 (0.0%)
1	E	0.34	0/2591	0.60	0/3519
1	F	0.31	0/2596	0.59	0/3523
1	G	0.35	0/2596	0.62	0/3523
1	H	0.30	0/2586	0.57	0/3512
1	O	0.44	0/2601	0.72	1/3530 (0.0%)
1	Q	0.42	0/2596	0.70	1/3523 (0.0%)
All	All	0.37	0/25965	0.64	6/35243 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	203	ILE	N-CA-C	-5.86	95.18	111.00
1	D	203	ILE	N-CA-C	-5.66	95.71	111.00
1	O	203	ILE	N-CA-C	-5.62	95.82	111.00
1	A	203	ILE	N-CA-C	-5.56	95.99	111.00
1	C	203	ILE	N-CA-C	-5.42	96.35	111.00
1	B	203	ILE	N-CA-C	-5.42	96.37	111.00

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	2557	0	2598	126	0
1	B	2557	0	2598	117	0
1	C	2557	0	2598	125	0
1	D	2552	0	2593	168	1
1	E	2547	0	2585	348	0
1	F	2552	0	2593	266	0
1	G	2552	0	2593	250	0
1	H	2542	0	2580	255	0
1	O	2557	0	2598	98	0
1	Q	2552	0	2593	122	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	3	0
2	E	44	0	26	5	0
2	F	44	0	26	2	0
2	G	44	0	26	1	0
2	H	44	0	26	2	0
2	O	44	0	26	1	0
2	Q	44	0	26	0	0
3	A	35	0	0	0	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
3	D	15	0	0	0	0
3	E	20	0	0	3	0
3	F	15	0	0	0	0
3	G	25	0	0	0	0
3	H	15	0	0	0	0
3	O	30	0	0	0	0
3	Q	25	0	0	0	0
4	A	109	0	0	1	0
4	B	84	0	0	1	0
4	C	94	0	0	4	0
4	D	85	0	0	6	0
4	E	79	0	0	9	0
4	F	65	0	0	1	0
4	G	81	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	56	0	0	0	0
4	O	129	0	0	2	0
4	Q	100	0	0	4	0
All	All	27072	0	26189	1682	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 (1682) 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:Q:191:ARG:HB3	1:Q:191:ARG:HH11	1.22	1.04
1:G:63:ALA:HB1	1:G:70:ILE:HD11	1.34	1.04
1:E:17:ARG:HA	1:E:17:ARG:HE	1.18	1.03
1:F:90:ASP:HA	1:F:114:LYS:HD3	1.41	1.03
1:D:139:HIS:HB3	1:D:333:LYS:HE2	1.40	1.02
1:F:126:PRO:HG2	1:F:141:GLU:HG2	1.42	1.01
1:E:304:MET:HE3	1:G:245:GLN:HB2	1.45	0.98
1:G:221:LEU:HD21	1:G:225:LEU:HD11	1.46	0.98
1:O:17:ARG:NH1	1:O:53:PHE:HB2	1.79	0.98
1:H:72:GLN:H	1:H:72:GLN:NE2	1.62	0.97
1:E:226:ASN:HB3	1:G:300:MET:HE2	1.45	0.96
1:G:161:LEU:HB2	1:G:167:ILE:HD11	1.51	0.93
1:Q:38:LYS:HE3	1:Q:38:LYS:H	1.34	0.92
1:E:194:ARG:HH21	1:G:277:PRO:HA	1.34	0.91
1:G:256:ASN:HD21	1:G:297:THR:HG21	1.35	0.91
1:E:126:PRO:HB2	1:E:144:ILE:HG22	1.53	0.90
1:D:85:LYS:HG3	1:D:112:GLY:HA2	1.51	0.90
1:E:70:ILE:HD13	1:E:70:ILE:H	1.35	0.90
1:A:202:ASN:HD21	1:C:281:VAL:HG12	1.37	0.89
1:E:117:ILE:HG22	1:E:144:ILE:HD11	1.52	0.89
1:F:202:ASN:HD22	1:H:281:VAL:H	1.23	0.87
1:F:85:LYS:HG2	1:F:112:GLY:HA2	1.57	0.86
1:F:96:THR:OG1	1:F:98:VAL:HG22	1.76	0.86
1:E:154:LEU:HD21	1:E:172:MET:HG3	1.58	0.86
1:G:251:PHE:O	1:G:255:VAL:HG23	1.77	0.85
1:G:2:LYS:HD2	1:G:28:ILE:HG21	1.58	0.85
1:F:317:TYR:O	1:F:321:VAL:HG23	1.77	0.84
1:E:133:ASN:H	1:E:133:ASN:HD22	1.22	0.84
1:H:190:HIS:HB3	1:H:196:ALA:HB2	1.59	0.84
1:C:333:LYS:HE2	4:C:423:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:HIS:O	1:E:231:ARG:HA	1.78	0.82
1:E:139:HIS:CE1	1:E:332:TRP:HA	2.14	0.82
1:Q:191:ARG:HB3	1:Q:191:ARG:NH1	1.94	0.82
1:B:139:HIS:NE2	1:B:333:LYS:HD3	1.95	0.81
1:F:130:VAL:HB	1:F:320:ARG:HD3	1.61	0.81
1:F:328:VAL:O	1:F:332:TRP:HB2	1.80	0.81
1:F:31:ASN:HB2	1:F:74:VAL:HG13	1.61	0.81
1:H:96:THR:OG1	1:H:98:VAL:HG22	1.81	0.81
1:E:17:ARG:HA	1:E:17:ARG:NE	1.96	0.80
1:C:156:PRO:HB2	1:C:290:THR:HG21	1.63	0.80
1:D:129:VAL:HG23	1:D:217:VAL:HG11	1.63	0.80
1:E:232:VAL:HG21	1:G:203:ILE:HD11	1.61	0.80
1:D:264:GLU:HA	1:D:268:LYS:HE3	1.62	0.80
1:H:170:GLY:HA3	1:H:244:VAL:HG12	1.64	0.80
1:H:228:ILE:H	1:H:228:ILE:HD13	1.47	0.80
1:G:129:VAL:HG23	1:G:217:VAL:HG11	1.63	0.79
1:G:294:SER:O	1:G:297:THR:HG22	1.81	0.79
1:H:129:VAL:H	1:H:133:ASN:HD21	1.27	0.79
1:H:86:GLU:O	1:H:87:LEU:HB2	1.81	0.79
1:O:281:VAL:HB	1:Q:202:ASN:HD21	1.46	0.79
1:Q:0:LYS:HD2	1:Q:0:LYS:O	1.84	0.78
1:E:262:SER:HB3	1:E:267:LEU:HD12	1.65	0.78
1:E:203:ILE:HD11	1:G:232:VAL:HG21	1.64	0.78
1:G:211:ALA:CB	1:G:226:ASN:HA	2.14	0.78
1:H:195:ARG:HH21	1:H:206:THR:HG21	1.49	0.78
1:B:163:GLN:HE21	1:B:164:LYS:NZ	1.82	0.77
1:E:133:ASN:N	1:E:133:ASN:HD22	1.78	0.77
1:E:277:PRO:HA	1:G:194:ARG:HE	1.50	0.77
1:Q:159:LYS:HG2	1:Q:163:GLN:HE21	1.47	0.77
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.18	0.77
1:F:315:TRP:O	1:F:319:GLN:HG2	1.83	0.77
1:D:91:ILE:HA	1:D:115:LYS:O	1.85	0.77
1:E:72:GLN:HG3	1:E:73:VAL:H	1.50	0.77
1:B:226:ASN:ND2	1:D:298:MET:SD	2.58	0.77
1:E:171:THR:HB	1:G:300:MET:HG2	1.64	0.77
1:E:0(A):ALA:HB1	1:E:26:ASP:HB2	1.65	0.77
1:H:130:VAL:HA	1:H:134:ALA:HB2	1.67	0.77
1:E:169:LYS:HE3	1:G:304:MET:HB2	1.66	0.76
1:F:79:PRO:HA	1:F:82:LEU:HD12	1.65	0.76
1:E:165:PHE:HD1	1:E:248:LYS:HD2	1.50	0.76
1:Q:138:SER:HB3	1:Q:141:GLU:OE2	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ILE:HG23	1:E:73:VAL:HG21	1.67	0.76
1:A:156:PRO:HB2	1:A:290:THR:HG21	1.66	0.75
1:A:85:LYS:HE3	1:A:85:LYS:N	2.02	0.75
1:E:167:ILE:HG23	1:E:244:VAL:HB	1.68	0.75
1:Q:78:ASN:HB3	1:Q:81:LEU:HD12	1.69	0.75
1:G:293:ASP:OD1	1:G:296:LEU:HG	1.87	0.75
1:F:243:VAL:HG11	1:H:171:THR:HG21	1.69	0.75
1:B:153:CYS:HA	1:B:290:THR:HG22	1.67	0.75
1:E:194:ARG:HG2	1:G:277:PRO:O	1.86	0.75
1:F:284:ARG:O	1:F:285:CYS:HB2	1.87	0.75
1:H:38:LYS:HD2	1:H:38:LYS:H	1.51	0.75
1:F:85:LYS:HG2	1:F:112:GLY:CA	2.17	0.75
1:E:58:LYS:HB2	1:E:59:PRO:HD2	1.69	0.74
1:E:204:VAL:HB	1:E:231:ARG:HB2	1.67	0.74
1:B:233:PRO:HB2	1:D:233:PRO:HB2	1.67	0.74
1:Q:210:ALA:O	1:Q:214:VAL:HG23	1.88	0.74
1:E:256:ASN:HD21	1:E:297:THR:HB	1.51	0.74
1:A:30:ILE:HG13	1:A:71:ILE:HD11	1.67	0.74
1:O:281:VAL:HB	1:Q:202:ASN:ND2	2.01	0.74
1:D:91:ILE:HG22	1:D:115:LYS:HB3	1.69	0.73
1:H:156:PRO:HB2	1:H:290:THR:HG21	1.69	0.73
1:C:76:ASN:HD22	1:C:77:ARG:N	1.85	0.73
1:H:81:LEU:H	1:H:81:LEU:HD12	1.53	0.73
1:B:271:LEU:HD13	1:B:272:ASP:N	2.03	0.73
1:F:78:ASN:HB3	1:F:81:LEU:HD13	1.69	0.73
1:G:129:VAL:H	1:G:133:ASN:HD21	1.35	0.73
1:E:279:VAL:CG1	1:G:204:VAL:HG22	2.18	0.73
1:H:168:ILE:HD12	1:H:245:GLN:HG2	1.69	0.73
1:A:33:THR:HG22	1:A:77:ARG:HG2	1.69	0.73
1:E:156:PRO:HB2	1:E:290:THR:HG21	1.71	0.73
1:F:60:SER:H	1:F:64:ILE:HA	1.54	0.73
1:F:228:ILE:HD13	1:F:228:ILE:H	1.54	0.73
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.23	0.73
1:E:217:VAL:HG23	1:E:218:LEU:HG	1.71	0.73
1:H:183:ARG:HG2	1:H:196:ALA:HA	1.71	0.73
1:E:194:ARG:NH2	1:G:277:PRO:HA	2.03	0.73
1:H:70:ILE:HG22	1:H:71:ILE:H	1.53	0.73
1:E:7:GLY:HA2	2:E:335:NAD:H1B	1.70	0.72
1:F:267:LEU:HD22	1:F:270:ILE:HG21	1.68	0.72
1:F:222:LYS:HG2	1:F:224:LYS:HE2	1.71	0.72
1:D:153:CYS:HA	1:D:290:THR:HG22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:VAL:HA	1:G:134:ALA:HB2	1.71	0.72
1:E:20:ARG:NH2	1:E:322:VAL:HB	2.03	0.72
1:F:16:LEU:HD22	1:F:44:LEU:HD11	1.71	0.72
1:F:249:LYS:HG2	1:F:302:ASP:HB3	1.71	0.72
1:H:155:ALA:HB3	1:H:156:PRO:HD3	1.70	0.72
1:G:193:LEU:H	1:G:193:LEU:HD22	1.54	0.72
1:B:105:ALA:HB1	1:B:116:VAL:HG11	1.71	0.71
1:D:0:LYS:HD2	4:D:363:HOH:O	1.90	0.71
1:E:194:ARG:HD3	1:E:205:PRO:HG2	1.73	0.71
1:D:74:VAL:HG22	1:D:75:SER:H	1.54	0.71
1:E:3:VAL:HG21	1:E:25:LEU:HD22	1.72	0.71
1:E:235:PRO:HB3	1:H:201:LEU:HD11	1.72	0.71
1:G:62:THR:HG22	1:Q:62:THR:HG22	1.73	0.71
1:E:195:ARG:HH22	1:E:231:ARG:NH2	1.89	0.70
1:F:21:LYS:N	1:F:21:LYS:HD2	2.05	0.70
1:E:186:ASP:HB2	1:H:10:ARG:NH1	2.06	0.70
1:B:139:HIS:CD2	1:B:333:LYS:HD3	2.25	0.70
1:G:241:ASP:OD1	1:G:308:ILE:HD11	1.91	0.70
1:A:271:LEU:HD12	1:A:272:ASP:H	1.57	0.70
1:G:186:ASP:OD1	1:G:197:ARG:HA	1.92	0.70
1:H:4:ALA:HB2	1:H:89:ILE:HD12	1.72	0.70
1:E:178:TYR:HA	1:E:182:GLN:OE1	1.92	0.70
1:A:27:ILE:HG22	1:A:71:ILE:HD12	1.74	0.70
1:A:48:SER:HA	1:B:281:VAL:HG11	1.73	0.70
1:D:83:PRO:HB3	1:H:72:GLN:OE1	1.92	0.70
1:E:119:THR:HG22	1:E:321:VAL:HG11	1.74	0.70
1:F:318:SER:O	1:F:322:VAL:HG23	1.92	0.70
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.27	0.70
1:E:157:PHE:HE1	1:E:307:VAL:HG21	1.56	0.70
1:B:281:VAL:HG12	1:D:202:ASN:HD21	1.57	0.70
1:E:194:ARG:HE	1:G:277:PRO:C	1.95	0.70
1:F:11:ILE:O	1:F:11:ILE:HD13	1.92	0.70
1:H:181:ASP:HB3	1:H:195:ARG:HD3	1.74	0.70
1:H:37:VAL:HG21	1:H:62:THR:HA	1.74	0.70
1:Q:4:ALA:HB2	1:Q:89:ILE:HD12	1.74	0.70
1:E:192:ASP:HB3	1:E:195:ARG:HB2	1.73	0.69
1:F:222:LYS:HG2	1:F:224:LYS:CE	2.21	0.69
1:F:228:ILE:HG21	1:H:296:LEU:HD22	1.74	0.69
1:H:72:GLN:HE21	1:H:72:GLN:H	1.37	0.69
1:G:256:ASN:HD22	1:G:256:ASN:N	1.89	0.69
1:F:75:SER:O	1:F:76:ASN:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:MET:HG2	1:H:226:ASN:ND2	2.07	0.69
1:E:194:ARG:HH12	1:G:296:LEU:HD21	1.57	0.69
1:F:298:MET:HE3	1:F:306:LYS:HD3	1.74	0.69
1:B:212:LYS:HE3	4:B:785:HOH:O	1.91	0.69
1:D:18:CYS:HB3	1:D:319:GLN:OE1	1.92	0.69
1:G:256:ASN:HB3	1:G:260:ARG:NH1	2.07	0.69
1:F:126:PRO:HB2	1:F:144:ILE:HG22	1.74	0.69
1:H:45:LYS:HB2	1:H:57:VAL:HB	1.74	0.69
1:O:202:ASN:HD21	1:Q:281:VAL:HB	1.57	0.69
1:A:3:VAL:HG22	1:A:91:ILE:HG23	1.72	0.69
1:E:204:VAL:HG22	1:G:279:VAL:HG11	1.75	0.69
1:E:63:ALA:HA	1:E:73:VAL:HG23	1.74	0.69
1:F:133:ASN:HD21	1:F:217:VAL:HG12	1.58	0.69
1:F:21:LYS:H	1:F:21:LYS:HD2	1.59	0.69
1:F:323:ASP:O	1:F:327:ILE:HG13	1.92	0.69
1:O:159:LYS:O	1:O:163:GLN:HG3	1.92	0.69
1:A:281:VAL:CG1	1:C:202:ASN:HD21	2.06	0.68
1:E:114:LYS:HB2	1:E:332:TRP:HH2	1.57	0.68
1:F:31:ASN:HB2	1:F:74:VAL:CG1	2.23	0.68
1:G:170:GLY:HA2	1:G:243:VAL:O	1.92	0.68
1:E:154:LEU:O	1:E:158:VAL:HG23	1.94	0.68
1:F:202:ASN:HD21	1:H:281:VAL:HB	1.58	0.68
1:E:183:ARG:HD3	1:E:190:HIS:HB2	1.76	0.68
1:G:256:ASN:ND2	1:G:297:THR:HG21	2.08	0.68
1:A:202:ASN:HD21	1:C:281:VAL:CG1	2.05	0.68
1:C:115:LYS:HE2	1:C:142:PRO:HA	1.76	0.68
1:A:281:VAL:H	1:C:202:ASN:ND2	1.92	0.68
1:E:55:ALA:O	1:E:57:VAL:HG23	1.94	0.68
1:Q:169:LYS:HE3	1:Q:245:GLN:NE2	2.09	0.68
1:E:134:ALA:HB3	4:E:490:HOH:O	1.93	0.67
1:A:281:VAL:HG12	1:C:202:ASN:HD21	1.59	0.67
1:D:172:MET:O	1:D:227:GLY:HA3	1.94	0.67
1:G:0:LYS:NZ	1:G:0:LYS:HB3	2.09	0.67
1:Q:85:LYS:HB2	1:Q:112:GLY:HA3	1.75	0.67
1:A:78:ASN:ND2	1:A:81:LEU:HG	2.08	0.67
1:E:240:VAL:HG23	1:E:309:ALA:HB3	1.76	0.67
1:H:159:LYS:HE3	1:H:218:LEU:HD21	1.77	0.67
1:E:31:ASN:HA	1:E:74:VAL:CG2	2.24	0.67
1:F:272:ASP:HB2	1:F:288:PHE:CD2	2.30	0.67
1:F:5:ILE:HD13	1:F:8:PHE:HD1	1.59	0.67
1:B:240:VAL:HG22	1:B:309:ALA:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ASP:OD1	1:E:296:LEU:HG	1.93	0.67
1:F:210:ALA:O	1:F:214:VAL:HG23	1.94	0.67
1:Q:206:THR:HG22	1:Q:229:ALA:HB3	1.77	0.67
1:F:133:ASN:ND2	1:F:217:VAL:HG12	2.10	0.67
1:E:194:ARG:HE	1:G:277:PRO:CA	2.07	0.67
1:E:5:ILE:CD1	1:E:27:ILE:HD12	2.25	0.67
1:F:222:LYS:H	1:F:224:LYS:HE3	1.57	0.67
1:G:262:SER:HB3	1:G:267:LEU:HG	1.75	0.67
1:F:152:ASN:O	1:F:289:SER:HB3	1.96	0.66
1:B:38:LYS:H	1:B:38:LYS:HD2	1.60	0.66
1:G:162:ASP:HA	1:G:167:ILE:HG13	1.75	0.66
1:E:25:LEU:HD11	1:E:325:ALA:HB3	1.76	0.66
1:Q:154:LEU:O	1:Q:158:VAL:HG23	1.95	0.66
1:A:105:ALA:HB1	1:A:116:VAL:HG11	1.77	0.66
1:E:242:LEU:HB3	1:E:307:VAL:CG2	2.26	0.66
1:E:279:VAL:HG22	1:E:282:ASP:OD2	1.94	0.66
1:F:202:ASN:ND2	1:H:281:VAL:HB	2.11	0.66
1:C:58:LYS:HE2	4:C:378:HOH:O	1.96	0.66
1:D:83:PRO:O	1:D:87:LEU:HD23	1.94	0.66
1:E:126:PRO:HD2	1:E:143:ILE:O	1.95	0.66
1:E:132:VAL:HG21	1:E:155:ALA:HB1	1.77	0.66
1:F:125:ILE:H	1:F:125:ILE:HD12	1.61	0.66
1:D:109:ILE:HA	1:D:113:ALA:O	1.95	0.66
1:D:116:VAL:HB	1:D:143:ILE:HD12	1.78	0.66
1:G:211:ALA:HB1	1:G:226:ASN:HA	1.76	0.66
1:F:169:LYS:HD2	1:H:301:GLY:HA3	1.77	0.66
1:A:154:LEU:HD22	1:A:172:MET:HE3	1.77	0.66
1:F:280:SER:HB3	1:F:310:TRP:HZ3	1.61	0.66
1:E:299:VAL:HG22	1:E:305:VAL:HG22	1.76	0.66
1:F:114:LYS:N	1:F:114:LYS:HD2	2.11	0.66
1:G:187:ALA:O	1:G:196:ALA:HB1	1.95	0.66
1:E:304:MET:CE	1:G:245:GLN:HB2	2.23	0.66
1:F:266:GLU:HG3	4:F:578:HOH:O	1.96	0.66
1:G:168:ILE:HG22	1:G:169:LYS:HG3	1.77	0.65
1:H:236:ASN:O	1:H:237:VAL:HB	1.96	0.65
1:B:38:LYS:N	1:B:38:LYS:HD2	2.10	0.65
1:F:176:HIS:O	1:F:231:ARG:HA	1.95	0.65
1:H:129:VAL:HG23	1:H:217:VAL:HG11	1.78	0.65
1:A:202:ASN:ND2	1:C:281:VAL:HG12	2.11	0.65
1:E:279:VAL:HG12	1:G:204:VAL:HG22	1.76	0.65
1:B:33:THR:HG21	1:B:77:ARG:HD3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ARG:HG3	1:E:13:ARG:HH11	1.62	0.65
1:E:5:ILE:HD12	1:E:27:ILE:HD12	1.77	0.65
1:E:297:THR:HG23	1:E:306:LYS:O	1.96	0.65
1:H:204:VAL:HB	1:H:231:ARG:HB2	1.79	0.65
1:F:226:ASN:HB3	1:H:300:MET:SD	2.37	0.65
1:B:193:LEU:HD13	1:C:42:HIS:CG	2.31	0.65
1:B:80:SER:OG	1:B:107:LYS:HG2	1.97	0.65
1:E:210:ALA:O	1:E:214:VAL:HG23	1.97	0.65
1:G:155:ALA:HB3	1:G:156:PRO:HD3	1.79	0.65
1:G:285:CYS:HA	1:G:315:TRP:CD1	2.31	0.65
1:E:151:THR:HG23	1:E:214:VAL:HG22	1.79	0.65
1:E:170:GLY:N	1:E:224:LYS:O	2.30	0.65
1:F:226:ASN:ND2	1:H:298:MET:SD	2.70	0.65
1:A:1:LEU:HD22	1:A:329:ALA:CB	2.27	0.65
1:F:118:ILE:H	1:F:118:ILE:HD12	1.61	0.65
1:G:293:ASP:HB3	1:G:296:LEU:HD12	1.78	0.64
1:A:64:ILE:HG13	1:A:71:ILE:HG23	1.78	0.64
1:F:188:SER:HB2	1:G:39:GLN:OE1	1.96	0.64
1:H:182:GLN:HE22	1:H:231:ARG:HB3	1.61	0.64
1:B:168:ILE:HD11	1:B:247:SER:HB3	1.79	0.64
1:F:281:VAL:HB	1:H:202:ASN:HB3	1.79	0.64
1:F:296:LEU:HD22	1:H:228:ILE:HG21	1.79	0.64
1:F:89:ILE:O	1:F:113:ALA:HA	1.97	0.64
1:G:221:LEU:HD21	1:G:225:LEU:CD1	2.25	0.64
1:G:130:VAL:CG2	1:G:320:ARG:HD3	2.28	0.64
1:H:239:VAL:HG23	1:H:309:ALA:O	1.97	0.64
1:A:228:ILE:C	1:A:228:ILE:HD12	2.18	0.64
1:F:187:ALA:O	1:F:196:ALA:HB1	1.97	0.64
1:F:280:SER:HB3	1:F:310:TRP:CZ3	2.33	0.64
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.32	0.64
1:D:284:ARG:O	1:D:285:CYS:HB2	1.95	0.64
1:H:251:PHE:HE2	1:H:253:GLU:HB2	1.61	0.64
1:E:165:PHE:CD1	1:E:248:LYS:HD2	2.33	0.64
1:E:183:ARG:HA	1:E:183:ARG:HH11	1.62	0.64
1:E:277:PRO:CA	1:G:194:ARG:HE	2.10	0.64
1:E:328:VAL:O	1:E:332:TRP:HB2	1.97	0.64
1:G:260:ARG:O	1:G:263:ALA:HB3	1.98	0.64
1:E:79:PRO:HB2	1:E:107:LYS:HB2	1.79	0.64
1:G:124:ASP:HB2	4:G:634:HOH:O	1.97	0.64
1:G:18(A):TRP:C	1:G:19:GLY:H	1.99	0.64
1:G:64:ILE:O	1:G:70:ILE:HD12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:VAL:CG2	1:H:217:VAL:HG11	2.26	0.64
1:H:78:ASN:HB3	1:H:81:LEU:HD13	1.79	0.64
1:F:324:LEU:O	1:F:328:VAL:HG23	1.97	0.63
1:B:132:VAL:HG21	1:B:155:ALA:HB1	1.80	0.63
1:D:74:VAL:HG22	1:D:75:SER:N	2.12	0.63
1:E:176:HIS:N	1:E:230:LEU:O	2.28	0.63
1:E:250:THR:OG1	1:E:254:GLU:HB3	1.98	0.63
1:F:285:CYS:HA	1:F:315:TRP:CD1	2.33	0.63
1:B:4:ALA:HB2	1:B:89:ILE:HG12	1.80	0.63
1:E:109:ILE:HD13	1:E:109:ILE:O	1.98	0.63
1:F:59:PRO:HA	1:F:64:ILE:HA	1.81	0.63
1:G:221:LEU:HD11	1:G:225:LEU:HD21	1.79	0.63
1:H:251:PHE:CE2	1:H:253:GLU:HB2	2.34	0.63
1:F:298:MET:HE2	1:H:228:ILE:HG23	1.79	0.63
1:O:78:ASN:ND2	1:O:81:LEU:HG	2.12	0.63
1:F:118:ILE:N	1:F:118:ILE:HD12	2.12	0.63
1:H:299:VAL:HG22	1:H:305:VAL:HG22	1.81	0.63
1:H:70:ILE:HG22	1:H:71:ILE:N	2.12	0.63
1:C:77:ARG:O	1:C:79:PRO:HD3	1.99	0.63
1:E:58:LYS:NZ	1:E:58:LYS:HB3	2.13	0.63
1:G:130:VAL:HA	1:G:134:ALA:CB	2.28	0.63
1:D:272:ASP:HB2	1:D:288:PHE:CD2	2.33	0.63
1:E:79:PRO:HB2	1:E:107:LYS:CB	2.28	0.63
1:E:72:GLN:HG3	1:E:73:VAL:N	2.13	0.63
1:F:11:ILE:HD12	1:F:119:THR:HG21	1.80	0.63
1:O:17:ARG:HH11	1:O:53:PHE:HB2	1.61	0.63
1:O:202:ASN:HD21	1:Q:281:VAL:CG1	2.12	0.63
1:D:125:ILE:HD12	1:D:126:PRO:HD2	1.80	0.63
1:G:150:THR:HG23	1:G:311:TYR:OH	1.99	0.63
1:F:64:ILE:O	1:F:70:ILE:HG23	1.99	0.63
1:G:166:GLY:O	1:G:246:VAL:HA	1.98	0.63
1:O:204:VAL:HB	1:O:231:ARG:HB2	1.81	0.63
1:B:281:VAL:H	1:D:202:ASN:ND2	1.97	0.62
1:E:155:ALA:HB3	1:E:156:PRO:HD3	1.81	0.62
1:E:74:VAL:O	1:E:75:SER:HB2	1.98	0.62
1:E:208:THR:HG23	1:E:208:THR:O	1.99	0.62
1:E:250:THR:HG1	1:E:254:GLU:HB3	1.64	0.62
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.80	0.62
1:G:171:THR:O	1:G:242:LEU:HB2	2.00	0.62
1:F:27:ILE:N	1:F:27:ILE:HD12	2.15	0.62
1:C:26:ASP:O	1:C:28:ILE:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ILE:HA	1:E:71:ILE:HG12	1.82	0.62
1:H:183:ARG:HE	1:H:187:ALA:HB3	1.62	0.62
1:B:15:PHE:HE2	1:B:27:ILE:HD11	1.64	0.62
1:A:306:LYS:HD2	1:C:171:THR:OG1	2.00	0.62
1:O:33:THR:CG2	1:O:77:ARG:HG2	2.30	0.62
1:O:134:ALA:HB3	4:O:401:HOH:O	1.97	0.62
1:A:173:THR:HG23	1:A:228:ILE:HD11	1.82	0.62
1:D:318:SER:O	1:D:322:VAL:HG23	2.00	0.62
1:E:119:THR:CG2	1:E:321:VAL:HG11	2.29	0.62
1:E:270:ILE:HD11	4:E:491:HOH:O	1.99	0.62
1:G:259:PHE:CD2	1:G:292:ILE:HG21	2.34	0.62
1:O:202:ASN:ND2	1:Q:281:VAL:HB	2.14	0.62
1:Q:8:PHE:N	1:Q:32:ASP:OD2	2.31	0.62
1:E:183:ARG:CZ	1:E:187:ALA:HB3	2.30	0.62
1:B:281:VAL:H	1:D:202:ASN:HD22	1.48	0.62
1:Q:272:ASP:O	1:Q:291:THR:HA	1.99	0.62
1:B:262:SER:HB3	1:B:267:LEU:HD12	1.82	0.61
1:E:263:ALA:O	1:E:268:LYS:HA	1.99	0.61
1:F:108:HIS:O	1:F:111:ALA:HB3	1.99	0.61
1:G:239:VAL:HG23	1:G:309:ALA:O	1.99	0.61
1:A:154:LEU:HD22	1:A:172:MET:CE	2.29	0.61
1:A:281:VAL:H	1:C:202:ASN:HD22	1.47	0.61
1:E:174:THR:HB	1:E:240:VAL:HG12	1.81	0.61
1:E:260:ARG:HD2	4:E:538:HOH:O	2.01	0.61
1:D:138:SER:O	1:D:141:GLU:HG2	2.01	0.61
1:O:202:ASN:HD22	1:Q:281:VAL:H	1.46	0.61
1:E:84:TRP:CE3	1:E:89:ILE:HG13	2.35	0.61
1:H:85:LYS:HB2	1:H:111:ALA:O	2.01	0.61
1:H:84:TRP:HA	1:H:89:ILE:HG13	1.81	0.61
1:C:62:THR:HG22	1:C:62:THR:O	2.00	0.61
1:E:117:ILE:O	1:E:117:ILE:HG13	2.00	0.61
1:F:138:SER:HA	1:F:331:ASN:OD1	2.01	0.61
1:G:18:CYS:SG	1:G:319:GLN:HG2	2.41	0.61
1:G:221:LEU:HD11	1:G:225:LEU:CD2	2.30	0.61
1:E:264:GLU:HG3	4:E:535:HOH:O	2.00	0.61
1:F:279:VAL:O	1:F:281:VAL:N	2.34	0.61
1:F:38:LYS:HG3	1:F:39:GLN:N	2.16	0.61
1:C:250:THR:OG1	1:C:251:PHE:N	2.34	0.61
1:D:240:VAL:HG13	1:D:311:TYR:CE1	2.36	0.61
1:H:176:HIS:HB3	1:H:231:ARG:HD3	1.83	0.61
1:H:192:ASP:HB3	1:H:195:ARG:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:LYS:HB2	1:F:218:LEU:HD11	1.82	0.61
1:G:225:LEU:O	1:G:226:ASN:HB2	2.01	0.61
1:G:294:SER:C	1:G:296:LEU:H	2.03	0.61
1:E:265:LYS:HB2	1:E:266:GLU:OE1	2.00	0.60
1:F:6:ASN:OD1	1:F:31:ASN:ND2	2.34	0.60
1:O:224:LYS:O	1:O:225:LEU:HD23	2.01	0.60
1:H:31:ASN:OD1	1:H:74:VAL:HG23	2.01	0.60
1:A:298:MET:SD	1:C:226:ASN:OD1	2.59	0.60
1:E:209:GLY:HA3	1:E:212:LYS:HE2	1.84	0.60
1:E:270:ILE:HG13	4:E:828:HOH:O	2.00	0.60
1:G:177:SER:HB3	1:G:234:THR:O	2.01	0.60
1:A:142:PRO:HB2	1:A:143:ILE:HD12	1.82	0.60
1:E:186:ASP:O	1:H:13:ARG:NH2	2.35	0.60
1:G:162:ASP:CA	1:G:167:ILE:HG13	2.31	0.60
1:H:38:LYS:CD	1:H:38:LYS:H	2.12	0.60
1:O:202:ASN:HD21	1:Q:281:VAL:CB	2.15	0.60
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.83	0.60
1:E:6:ASN:ND2	1:E:108:HIS:HE1	1.99	0.60
1:F:251:PHE:CZ	1:F:254:GLU:HB2	2.37	0.60
1:O:124:ASP:CG	1:O:124:ASP:O	2.40	0.60
1:O:281:VAL:CB	1:Q:202:ASN:HD21	2.14	0.60
1:E:94:GLU:OE1	1:E:99:PHE:HB2	2.00	0.60
1:F:126:PRO:CG	1:F:141:GLU:HG2	2.26	0.60
1:F:243:VAL:HG22	1:F:306:LYS:HG3	1.82	0.60
1:A:5:ILE:HD11	1:A:27:ILE:HD13	1.84	0.60
1:B:281:VAL:CG1	1:D:202:ASN:HD21	2.14	0.60
1:E:320:ARG:HA	1:E:320:ARG:NE	2.17	0.60
1:G:208:THR:C	1:G:210:ALA:H	2.05	0.60
1:Q:31:ASN:OD1	1:Q:74:VAL:HG23	2.01	0.60
1:G:129:VAL:CG2	1:G:217:VAL:HG11	2.30	0.60
1:H:133:ASN:N	1:H:133:ASN:HD22	1.99	0.60
1:H:264:GLU:HA	1:H:268:LYS:HG3	1.84	0.60
1:D:133:ASN:HD22	1:D:133:ASN:C	2.05	0.59
1:F:14:ASN:ND2	1:F:314:GLU:HG2	2.17	0.59
1:H:256:ASN:O	1:H:260:ARG:HG3	2.02	0.59
1:H:27:ILE:O	1:H:28:ILE:HB	2.02	0.59
1:Q:183:ARG:NH1	4:Q:463:HOH:O	2.27	0.59
1:F:186:ASP:HA	1:F:196:ALA:O	2.02	0.59
1:F:277:PRO:HB2	1:H:194:ARG:HG3	1.84	0.59
1:H:91:ILE:HD13	1:H:91:ILE:C	2.23	0.59
1:E:31:ASN:HA	1:E:74:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLN:HE22	1:C:245:GLN:NE2	1.99	0.59
1:E:157:PHE:CE1	1:E:307:VAL:HG21	2.37	0.59
1:C:56:ASP:O	1:C:66:VAL:HA	2.02	0.59
1:E:18:CYS:O	1:E:20:ARG:HG2	2.02	0.59
1:E:190:HIS:HB3	1:E:196:ALA:HB2	1.85	0.59
1:E:194:ARG:HH11	1:E:205:PRO:HG2	1.67	0.59
1:F:267:LEU:HD22	1:F:270:ILE:CG2	2.33	0.59
1:F:149:CYS:HB3	2:F:335:NAD:H5N	1.84	0.59
1:G:168:ILE:HG22	1:G:169:LYS:HE3	1.84	0.59
1:O:129:VAL:H	1:O:133:ASN:HD21	1.48	0.59
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.83	0.59
1:A:245:GLN:HE22	1:C:245:GLN:HE22	1.51	0.59
1:A:271:LEU:HD12	1:A:272:ASP:N	2.17	0.59
1:D:164:LYS:HD2	1:D:258:ALA:HB1	1.85	0.59
1:E:195:ARG:NH2	1:E:231:ARG:NH2	2.51	0.59
1:A:281:VAL:CB	1:C:202:ASN:HD21	2.16	0.59
1:F:271:LEU:HD13	1:F:290:THR:HG23	1.84	0.59
1:Q:2:LYS:HE2	4:Q:451:HOH:O	2.02	0.59
1:E:44:LEU:O	1:E:53:PHE:HD1	1.86	0.59
1:F:271:LEU:HD13	1:F:290:THR:CG2	2.32	0.59
1:F:6:ASN:O	1:F:96:THR:HG23	2.03	0.59
1:G:205:PRO:HA	1:G:229:ALA:O	2.03	0.59
1:E:202:ASN:HD22	1:G:281:VAL:CG1	2.16	0.59
1:E:109:ILE:HA	1:E:113:ALA:O	2.03	0.59
1:E:117:ILE:HG22	1:E:144:ILE:CD1	2.31	0.59
1:E:3:VAL:CG2	1:E:25:LEU:HD22	2.32	0.59
1:F:183:ARG:NE	1:F:187:ALA:HB3	2.18	0.59
1:F:243:VAL:CG1	1:H:171:THR:HG21	2.33	0.59
1:E:318:SER:O	1:E:322:VAL:HG23	2.03	0.58
1:F:145:SER:C	1:F:147:ALA:H	2.06	0.58
1:C:241:ASP:OD1	1:C:306:LYS:HE3	2.03	0.58
1:E:157:PHE:HB2	1:E:259:PHE:CE1	2.37	0.58
1:E:159:LYS:O	1:E:163:GLN:HG3	2.03	0.58
1:E:293:ASP:CG	1:E:296:LEU:HG	2.23	0.58
1:F:271:LEU:HD11	1:F:292:ILE:HD11	1.84	0.58
1:E:279:VAL:HG22	1:G:197:ARG:NH1	2.18	0.58
1:H:108:HIS:HB2	1:H:116:VAL:HG21	1.85	0.58
1:E:199:ALA:HB2	1:H:184:LEU:HD21	1.85	0.58
1:E:228:ILE:H	1:E:228:ILE:HD13	1.68	0.58
1:G:172:MET:O	1:G:227:GLY:HA3	2.03	0.58
1:G:243:VAL:HG22	1:G:306:LYS:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:276:GLU:HB2	1:Q:278:LEU:HG	1.86	0.58
1:B:269:GLY:C	1:B:270:ILE:HD12	2.24	0.58
1:G:192:ASP:CG	1:G:195:ARG:HG3	2.24	0.58
1:G:228:ILE:H	1:G:228:ILE:HD13	1.69	0.58
1:O:1:LEU:CD1	1:O:329:ALA:HA	2.34	0.58
1:O:277:PRO:HA	1:Q:194:ARG:NH2	2.19	0.58
1:Q:129:VAL:H	1:Q:133:ASN:ND2	2.01	0.58
1:E:115:LYS:HD2	1:E:328:VAL:HG11	1.86	0.58
1:F:115:LYS:HD2	1:F:332:TRP:HZ3	1.68	0.58
1:F:154:LEU:HG	1:F:158:VAL:HG21	1.84	0.58
1:C:210:ALA:O	1:C:214:VAL:HG23	2.03	0.58
1:F:140:ASP:O	1:F:142:PRO:HD3	2.03	0.58
1:H:27:ILE:HG22	1:H:28:ILE:H	1.68	0.58
1:F:202:ASN:HD21	1:H:281:VAL:CG1	2.17	0.58
1:F:235:PRO:HB3	1:G:201:LEU:HD11	1.86	0.58
1:H:195:ARG:HH21	1:H:206:THR:CG2	2.15	0.58
1:E:183:ARG:NE	1:E:187:ALA:HB3	2.19	0.58
1:E:267:LEU:HD13	1:E:271:LEU:HD23	1.86	0.58
1:G:251:PHE:HA	1:G:299:VAL:HG21	1.86	0.58
1:H:328:VAL:O	1:H:332:TRP:HB2	2.03	0.58
1:O:33:THR:HG22	1:O:77:ARG:HG2	1.86	0.58
1:Q:123:GLY:O	1:Q:125:ILE:N	2.32	0.58
1:E:298:MET:SD	1:G:226:ASN:ND2	2.74	0.57
1:E:277:PRO:HG2	1:F:42:HIS:CE1	2.39	0.57
1:G:294:SER:O	1:G:296:LEU:N	2.37	0.57
1:F:205:PRO:HG2	1:H:310:TRP:HZ2	1.68	0.57
1:O:168:ILE:HG22	1:O:169:LYS:HG2	1.86	0.57
1:F:0:LYS:HD2	1:F:24:PRO:HA	1.85	0.57
1:G:157:PHE:O	1:G:161:LEU:HG	2.05	0.57
1:E:193:LEU:HB3	1:H:42:HIS:CD2	2.39	0.57
1:A:271:LEU:HD13	1:A:290:THR:OG1	2.04	0.57
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.86	0.57
1:E:71:ILE:HD13	1:E:72:GLN:N	2.19	0.57
1:H:38:LYS:HD2	1:H:38:LYS:N	2.19	0.57
1:D:3:VAL:HG21	1:D:25:LEU:HD22	1.86	0.57
1:D:58:LYS:HB3	1:D:58:LYS:NZ	2.20	0.57
1:E:160:VAL:O	1:E:164:LYS:HB2	2.05	0.57
1:E:203:ILE:HA	1:E:231:ARG:O	2.04	0.57
1:G:264:GLU:HG2	1:G:264:GLU:O	2.04	0.57
1:H:134:ALA:HB1	1:H:327:ILE:CD1	2.35	0.57
1:G:153:CYS:O	1:G:156:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:LEU:HD11	1:G:292:ILE:HG12	1.86	0.57
1:E:74:VAL:HG23	1:E:75:SER:N	2.18	0.57
1:Q:129:VAL:H	1:Q:133:ASN:HD21	1.53	0.57
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.05	0.57
1:D:82:LEU:HD13	1:D:84:TRP:CZ2	2.39	0.57
1:E:15:PHE:CE1	1:E:322:VAL:HG22	2.40	0.57
1:E:205:PRO:HA	1:E:229:ALA:O	2.05	0.57
1:H:246:VAL:HG22	1:H:303:ASP:O	2.05	0.57
1:H:83:PRO:HB2	1:H:86:GLU:CG	2.34	0.57
1:Q:190:HIS:HB3	1:Q:196:ALA:HB2	1.87	0.57
1:A:181:ASP:OD2	1:A:195:ARG:NH1	2.38	0.57
1:A:115:LYS:HD2	1:A:332:TRP:CZ3	2.39	0.57
1:C:172:MET:HG2	1:C:173:THR:N	2.20	0.57
1:D:4:ALA:HB2	1:D:89:ILE:HG12	1.87	0.57
1:E:24:PRO:HG2	1:E:330:ASN:HD21	1.70	0.57
1:F:16:LEU:HD23	1:F:16:LEU:C	2.24	0.57
1:B:255:VAL:O	1:B:258:ALA:HB3	2.05	0.56
1:B:38:LYS:CD	1:B:38:LYS:H	2.13	0.56
1:E:33:THR:O	1:E:33:THR:HG22	2.05	0.56
1:F:37:VAL:N	1:F:73:VAL:HG11	2.20	0.56
1:A:91:ILE:HD13	1:A:91:ILE:C	2.25	0.56
1:C:18(A):TRP:O	1:C:20:ARG:HB2	2.06	0.56
1:E:13:ARG:HG3	1:E:13:ARG:NH1	2.20	0.56
1:F:156:PRO:O	1:F:159:LYS:HB3	2.05	0.56
1:B:256:ASN:HB3	1:B:260:ARG:HH12	1.68	0.56
1:E:272:ASP:HB2	1:E:288:PHE:CD2	2.40	0.56
1:F:304:MET:HB2	1:H:169:LYS:NZ	2.19	0.56
1:B:128:TYR:HA	1:B:133:ASN:HD21	1.70	0.56
1:G:185:LEU:HA	1:G:198:ALA:HB2	1.87	0.56
1:A:281:VAL:HG12	1:C:202:ASN:ND2	2.20	0.56
1:H:91:ILE:HA	1:H:115:LYS:O	2.06	0.56
1:F:279:VAL:HG12	1:H:204:VAL:HA	1.88	0.56
1:H:21:LYS:O	1:H:22:ASP:C	2.44	0.56
1:E:64:ILE:O	1:E:70:ILE:HA	2.06	0.56
1:E:279:VAL:HG11	1:G:204:VAL:HG22	1.85	0.56
1:O:236:ASN:O	1:O:237:VAL:HB	2.04	0.56
1:C:21:LYS:HE3	1:C:21:LYS:H	1.70	0.56
1:C:243:VAL:HG22	1:C:306:LYS:HG2	1.88	0.56
1:G:28:ILE:HD11	1:G:89:ILE:CD1	2.35	0.56
1:H:132:VAL:O	1:H:133:ASN:HB3	2.05	0.56
1:Q:169:LYS:HE3	1:Q:245:GLN:HE22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:251:PHE:CZ	1:Q:254:GLU:HB2	2.40	0.56
1:Q:84:TRP:CE3	1:Q:89:ILE:HG13	2.40	0.56
1:B:15:PHE:CE2	1:B:27:ILE:HD11	2.40	0.56
1:D:209:GLY:O	1:D:211:ALA:N	2.39	0.56
1:A:103:GLU:HB2	1:G:253:GLU:OE1	2.05	0.56
1:D:133:ASN:ND2	1:D:133:ASN:C	2.58	0.56
1:H:157:PHE:HB2	1:H:259:PHE:CE1	2.41	0.56
1:B:193:LEU:HD13	1:C:42:HIS:CD2	2.41	0.56
1:E:279:VAL:CG2	1:E:281:VAL:HG12	2.36	0.56
1:F:202:ASN:HD21	1:H:281:VAL:CB	2.17	0.56
1:A:210:ALA:O	1:A:214:VAL:HG23	2.05	0.56
1:C:266:GLU:HG2	1:C:267:LEU:N	2.19	0.56
1:D:292:ILE:N	1:D:292:ILE:HD12	2.19	0.56
1:E:158:VAL:HG11	1:E:225:LEU:HD11	1.87	0.56
1:E:171:THR:HG23	1:G:306:LYS:HE3	1.88	0.56
1:F:172:MET:O	1:F:227:GLY:HA3	2.06	0.55
1:D:246:VAL:O	1:D:303:ASP:HB2	2.05	0.55
1:E:25:LEU:HD11	1:E:325:ALA:CB	2.36	0.55
1:E:241:ASP:OD1	1:E:306:LYS:HE2	2.06	0.55
1:E:4:ALA:HB3	1:E:92:VAL:HG22	1.89	0.55
1:F:37:VAL:H	1:F:73:VAL:HG11	1.71	0.55
1:G:192:ASP:OD1	1:G:195:ARG:HG3	2.07	0.55
1:B:177:SER:HB3	1:B:234:THR:O	2.07	0.55
1:F:115:LYS:HD2	1:F:332:TRP:CZ3	2.41	0.55
1:G:222:LYS:O	1:G:224:LYS:N	2.39	0.55
1:D:75:SER:HB3	1:H:61:GLU:HB3	1.87	0.55
1:E:183:ARG:HB3	1:E:187:ALA:HB3	1.88	0.55
1:F:157:PHE:HB2	1:F:259:PHE:CE1	2.41	0.55
1:F:170:GLY:HA3	1:F:244:VAL:HG12	1.88	0.55
1:H:102:ARG:NE	1:H:124:ASP:OD1	2.40	0.55
1:H:9:GLY:HA2	1:H:13:ARG:HH12	1.72	0.55
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.05	0.55
1:D:37:VAL:HG22	1:D:73:VAL:HB	1.89	0.55
1:D:79:PRO:HA	1:D:82:LEU:HD12	1.88	0.55
1:E:202:ASN:HD22	1:G:281:VAL:HG12	1.72	0.55
1:E:119:THR:HG22	1:E:321:VAL:CG1	2.36	0.55
1:H:194:ARG:C	1:H:196:ALA:H	2.10	0.55
1:A:333:LYS:C	1:A:333:LYS:HE2	2.27	0.55
1:E:85:LYS:N	1:E:112:GLY:HA3	2.21	0.55
1:E:257:ALA:HB2	4:E:537:HOH:O	2.07	0.55
1:E:276:GLU:OE2	1:E:277:PRO:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLN:HE22	1:D:231:ARG:HB3	1.72	0.55
1:E:256:ASN:HD21	1:E:297:THR:CB	2.19	0.55
1:G:193:LEU:CD2	1:G:193:LEU:H	2.20	0.55
1:H:132:VAL:HG12	1:H:132:VAL:O	2.06	0.55
1:H:181:ASP:CB	1:H:195:ARG:HD3	2.36	0.55
1:H:2:LYS:HD2	1:H:88:GLY:CA	2.37	0.55
1:A:85:LYS:H	1:A:85:LYS:HE3	1.71	0.55
1:B:172:MET:HE3	1:B:211:ALA:HB2	1.87	0.55
1:D:266:GLU:HG2	1:D:267:LEU:HG	1.89	0.55
1:D:91:ILE:CG2	1:D:115:LYS:HB3	2.35	0.55
1:H:266:GLU:HG2	1:H:267:LEU:HG	1.89	0.55
1:H:294:SER:C	1:H:296:LEU:H	2.09	0.55
1:O:192:ASP:CG	1:O:195:ARG:HG3	2.27	0.55
1:O:213:ALA:O	1:O:216:LEU:HB2	2.07	0.55
1:B:240:VAL:CG2	1:B:309:ALA:HB3	2.37	0.55
1:D:84:TRP:HB2	1:D:112:GLY:HA3	1.89	0.55
1:E:179:THR:HG22	1:E:180:GLY:N	2.22	0.55
1:F:301:GLY:HA3	1:H:169:LYS:HD2	1.89	0.55
1:G:194:ARG:HH11	1:G:205:PRO:HB2	1.72	0.55
1:H:90:ASP:O	1:H:114:LYS:HB2	2.07	0.55
1:O:162:ASP:OD2	1:O:220:ASN:ND2	2.40	0.55
1:Q:317:TYR:O	1:Q:320:ARG:HB2	2.07	0.55
1:B:193:LEU:HB3	1:C:42:HIS:CD2	2.42	0.55
1:C:243:VAL:HA	1:C:305:VAL:O	2.06	0.55
1:D:129:VAL:CG2	1:D:217:VAL:HG11	2.35	0.55
1:H:125:ILE:HD12	1:H:125:ILE:N	2.23	0.55
1:Q:78:ASN:OD1	1:Q:80:SER:HB2	2.07	0.55
1:E:210:ALA:HB2	3:E:337:SO4:O4	2.06	0.54
1:G:271:LEU:HD13	1:G:290:THR:HG23	1.89	0.54
1:A:129:VAL:H	1:A:133:ASN:ND2	2.05	0.54
1:C:272:ASP:O	1:C:291:THR:HA	2.07	0.54
1:C:85:LYS:N	1:C:112:GLY:HA3	2.22	0.54
1:E:172:MET:HG2	1:E:173:THR:N	2.23	0.54
1:Q:135:ASP:N	1:Q:135:ASP:OD2	2.36	0.54
1:Q:160:VAL:HG13	1:Q:164:LYS:HE3	1.89	0.54
1:O:202:ASN:ND2	1:Q:281:VAL:H	2.04	0.54
1:D:84:TRP:CE3	1:D:84:TRP:HA	2.42	0.54
1:E:166:GLY:O	1:E:246:VAL:HA	2.07	0.54
1:F:169:LYS:CD	1:H:301:GLY:HA3	2.37	0.54
1:H:130:VAL:HG21	1:H:320:ARG:HD3	1.90	0.54
1:O:84:TRP:CE3	1:O:84:TRP:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ASN:O	2:D:335:NAD:H4N	2.08	0.54
1:E:296:LEU:HD12	1:E:308:ILE:HG21	1.90	0.54
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.72	0.54
1:A:2:LYS:HG2	1:A:28:ILE:HD13	1.90	0.54
1:A:9:GLY:HA3	2:A:335:NAD:O5B	2.08	0.54
1:A:226:ASN:ND2	1:C:300:MET:HB2	2.22	0.54
1:E:14:ASN:HB3	1:E:318:SER:OG	2.08	0.54
1:E:70:ILE:HD13	1:E:70:ILE:N	2.16	0.54
1:E:87:LEU:HD12	1:E:87:LEU:N	2.22	0.54
1:G:201:LEU:O	1:G:233:PRO:HG2	2.07	0.54
1:H:194:ARG:HD3	1:H:205:PRO:O	2.07	0.54
1:A:91:ILE:HD11	1:A:93:ILE:HD13	1.89	0.54
1:E:169:LYS:HE2	1:E:245:GLN:CD	2.27	0.54
1:E:17:ARG:HH11	1:E:18(B):HIS:HB3	1.72	0.54
1:Q:133:ASN:HD22	1:Q:133:ASN:H	1.55	0.54
1:B:271:LEU:HD22	1:B:290:THR:OG1	2.07	0.54
1:C:76:ASN:ND2	1:C:78:ASN:H	2.06	0.54
1:F:255:VAL:C	1:F:257:ALA:H	2.10	0.54
1:G:176:HIS:HA	1:G:238:SER:OG	2.08	0.54
1:G:256:ASN:ND2	1:G:256:ASN:N	2.54	0.54
1:F:310:TRP:HZ2	1:H:205:PRO:HG2	1.72	0.54
1:E:138:SER:O	1:E:140:ASP:N	2.41	0.54
1:E:151:THR:HG23	1:E:214:VAL:CG2	2.37	0.54
1:E:209:GLY:O	1:E:212:LYS:HG2	2.07	0.54
1:E:270:ILE:O	1:E:270:ILE:HG22	2.07	0.54
1:F:38:LYS:HG3	1:F:39:GLN:H	1.72	0.54
1:F:28:ILE:HG22	1:F:89:ILE:HD11	1.90	0.54
1:G:161:LEU:O	1:G:165:PHE:HB2	2.08	0.54
1:A:30:ILE:HG13	1:A:71:ILE:CD1	2.35	0.54
1:D:152:ASN:O	1:D:289:SER:HB3	2.08	0.54
1:E:58:LYS:CG	1:E:65:SER:HB3	2.38	0.54
1:O:84:TRP:HE3	1:O:84:TRP:HA	1.73	0.54
1:B:242:LEU:O	1:B:306:LYS:HA	2.08	0.53
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.43	0.53
1:D:84:TRP:HA	1:D:84:TRP:HE3	1.72	0.53
1:E:240:VAL:CG2	1:E:309:ALA:HB3	2.38	0.53
1:G:90:ASP:HB3	1:G:332:TRP:CH2	2.43	0.53
1:H:15:PHE:CE2	1:H:93:ILE:HG13	2.44	0.53
1:Q:90:ASP:HA	1:Q:114:LYS:HG2	1.90	0.53
1:E:252:ALA:HB1	1:E:298:MET:HA	1.90	0.53
1:F:228:ILE:H	1:F:228:ILE:CD1	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:THR:CG2	1:G:310:TRP:HB2	2.39	0.53
1:F:202:ASN:ND2	1:H:281:VAL:H	1.98	0.53
1:O:192:ASP:OD2	1:O:195:ARG:HG3	2.08	0.53
1:A:281:VAL:HB	1:C:202:ASN:HD21	1.72	0.53
1:C:115:LYS:HG3	1:C:142:PRO:O	2.08	0.53
1:E:199:ALA:HB3	1:H:184:LEU:HD11	1.90	0.53
1:E:279:VAL:HB	1:G:203:ILE:O	2.08	0.53
1:E:77:ARG:CZ	1:E:77:ARG:HB3	2.38	0.53
1:Q:38:LYS:CE	1:Q:38:LYS:H	2.16	0.53
1:C:1:LEU:HD23	1:C:91:ILE:HD11	1.89	0.53
1:E:211:ALA:CB	1:E:226:ASN:HA	2.39	0.53
1:F:126:PRO:HD2	1:F:143:ILE:O	2.07	0.53
1:F:296:LEU:O	1:F:298:MET:HG3	2.08	0.53
1:H:105:ALA:HB3	1:H:143:ILE:HD13	1.91	0.53
1:O:277:PRO:HA	1:Q:194:ARG:CZ	2.38	0.53
1:A:300:MET:HE3	1:C:226:ASN:HB3	1.90	0.53
1:C:70:ILE:HD12	1:C:70:ILE:N	2.24	0.53
1:G:188:SER:O	1:G:190:HIS:HB2	2.07	0.53
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.91	0.53
1:A:191:ARG:HH11	1:A:191:ARG:HB2	1.73	0.53
1:D:263:ALA:O	1:D:268:LYS:HA	2.09	0.53
1:E:130:VAL:HA	1:E:134:ALA:HB2	1.91	0.53
1:E:317:TYR:O	1:E:321:VAL:HG23	2.09	0.53
1:F:120:ALA:O	1:F:145:SER:HB2	2.08	0.53
1:F:176:HIS:HA	1:F:238:SER:HB3	1.91	0.53
1:G:13:ARG:HH11	1:G:13:ARG:HG3	1.73	0.53
1:G:152:ASN:O	1:G:289:SER:HB3	2.09	0.53
1:O:162:ASP:HB2	1:O:167:ILE:HD12	1.91	0.53
1:C:289:SER:OG	1:C:320:ARG:HD2	2.09	0.53
1:E:153:CYS:O	1:E:156:PRO:HD2	2.08	0.53
1:A:101:ASP:OD1	1:A:103:GLU:HG3	2.09	0.53
1:F:279:VAL:HG12	1:H:205:PRO:CD	2.39	0.53
1:G:138:SER:HB2	1:G:140:ASP:OD2	2.09	0.53
1:H:81:LEU:HD12	1:H:81:LEU:N	2.21	0.53
1:O:133:ASN:HD22	1:O:133:ASN:H	1.55	0.53
1:E:242:LEU:HB3	1:E:307:VAL:HG23	1.91	0.53
1:G:31:ASN:OD1	1:G:74:VAL:HG23	2.09	0.53
1:G:79:PRO:HA	1:G:82:LEU:HD12	1.91	0.53
1:O:18(A):TRP:CD2	1:O:27:ILE:HD13	2.44	0.53
1:D:236:ASN:O	1:D:237:VAL:HB	2.09	0.53
1:D:79:PRO:HB2	1:D:107:LYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:ILE:HD12	1:H:125:ILE:H	1.72	0.53
1:H:25:LEU:HD11	1:H:325:ALA:HB1	1.91	0.53
1:H:83:PRO:O	1:H:86:GLU:HG2	2.09	0.53
1:D:251:PHE:CE2	1:D:253:GLU:HG2	2.44	0.52
1:F:198:ALA:HB1	1:F:201:LEU:HG	1.91	0.52
1:F:301:GLY:HA3	1:H:169:LYS:CD	2.39	0.52
1:H:186:ASP:OD2	1:H:197:ARG:NE	2.42	0.52
1:H:250:THR:OG1	1:H:251:PHE:N	2.42	0.52
1:H:94:GLU:OE2	1:H:99:PHE:HD2	1.92	0.52
1:B:163:GLN:HE21	1:B:164:LYS:HZ2	1.53	0.52
1:B:205:PRO:HA	1:B:230:LEU:HD23	1.92	0.52
1:E:58:LYS:HG3	1:E:65:SER:HB3	1.90	0.52
1:H:242:LEU:HD12	1:H:243:VAL:H	1.74	0.52
1:C:1:LEU:HD21	1:C:332:TRP:CE3	2.45	0.52
1:E:162:ASP:HA	1:E:167:ILE:HG13	1.91	0.52
1:F:18(A):TRP:HA	1:F:20:ARG:HG2	1.90	0.52
1:G:16:LEU:O	1:G:16:LEU:HD23	2.09	0.52
1:E:204:VAL:HG22	1:G:279:VAL:CG1	2.40	0.52
1:H:83:PRO:HB2	1:H:86:GLU:HG3	1.89	0.52
1:C:21:LYS:CE	1:C:21:LYS:H	2.23	0.52
1:E:192:ASP:OD2	1:E:195:ARG:HD2	2.10	0.52
1:E:129:VAL:HG21	1:E:217:VAL:HG11	1.91	0.52
1:G:236:ASN:O	1:G:237:VAL:HB	2.09	0.52
1:H:115:LYS:HE2	1:H:332:TRP:HZ3	1.74	0.52
1:A:16:LEU:HD23	1:A:16:LEU:O	2.10	0.52
1:B:87:LEU:HB2	1:B:89:ILE:HD13	1.91	0.52
1:E:185:LEU:HA	1:E:198:ALA:HB2	1.91	0.52
1:E:79:PRO:HA	1:E:82:LEU:HG	1.90	0.52
1:F:296:LEU:HD13	1:F:308:ILE:HG13	1.91	0.52
1:F:60:SER:N	1:F:64:ILE:HA	2.24	0.52
1:H:294:SER:O	1:H:296:LEU:N	2.41	0.52
1:O:133:ASN:N	1:O:133:ASN:HD22	2.08	0.52
1:Q:211:ALA:HB1	1:Q:226:ASN:HA	1.92	0.52
1:Q:219:PRO:O	1:Q:222:LYS:HB2	2.09	0.52
1:D:220:ASN:C	1:D:221:LEU:HD22	2.30	0.52
1:B:102:ARG:HG2	1:B:102:ARG:NH1	2.24	0.52
1:G:160:VAL:CG1	1:G:258:ALA:HB1	2.40	0.52
1:G:276:GLU:HB3	1:G:277:PRO:HD2	1.91	0.52
1:H:134:ALA:HB1	1:H:327:ILE:HD13	1.91	0.52
1:Q:156:PRO:HB2	1:Q:290:THR:HG21	1.92	0.52
1:E:183:ARG:HG2	1:E:196:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:VAL:HG22	1:G:197:ARG:HH12	1.75	0.52
1:H:129:VAL:N	1:H:133:ASN:HD21	2.04	0.52
1:O:129:VAL:H	1:O:133:ASN:ND2	2.08	0.52
1:Q:128:TYR:HA	1:Q:133:ASN:HD21	1.75	0.52
1:Q:181:ASP:OD2	1:Q:195:ARG:NH1	2.36	0.52
1:O:226:ASN:HB2	1:Q:300:MET:CE	2.40	0.52
1:C:271:LEU:HD12	1:C:290:THR:HG23	1.92	0.52
1:E:181:ASP:OD2	1:E:195:ARG:NH1	2.43	0.52
1:F:186:ASP:OD1	1:F:197:ARG:HA	2.09	0.52
1:F:243:VAL:HG11	1:H:171:THR:CG2	2.39	0.52
1:B:310:TRP:HZ2	1:D:205:PRO:HG2	1.74	0.52
1:C:64:ILE:CD1	1:C:66:VAL:HG23	2.40	0.52
1:D:218:LEU:HB3	1:D:221:LEU:HD23	1.92	0.52
1:D:4:ALA:HB3	1:D:92:VAL:HG22	1.92	0.52
1:E:115:LYS:HD2	1:E:328:VAL:CG1	2.40	0.52
1:G:137:TYR:CE2	1:G:328:VAL:HA	2.44	0.52
1:G:168:ILE:CG2	1:G:169:LYS:HE3	2.40	0.52
1:G:197:ARG:O	1:G:199:ALA:N	2.43	0.52
1:G:243:VAL:CG2	1:G:306:LYS:HE2	2.40	0.52
1:F:306:LYS:HD2	1:H:171:THR:OG1	2.09	0.52
1:Q:84:TRP:HA	1:Q:84:TRP:HE3	1.75	0.52
1:B:9:GLY:HA3	2:B:335:NAD:O5B	2.10	0.51
1:G:161:LEU:HD13	1:G:244:VAL:HG21	1.91	0.51
1:G:243:VAL:HG13	1:G:306:LYS:HB2	1.92	0.51
1:H:330:ASN:C	1:H:332:TRP:H	2.13	0.51
1:D:130:VAL:HA	1:D:134:ALA:HB2	1.90	0.51
1:F:128:TYR:HA	1:F:133:ASN:HD21	1.76	0.51
1:G:296:LEU:HD13	1:G:308:ILE:HG21	1.93	0.51
1:E:171:THR:CG2	1:G:306:LYS:HE3	2.41	0.51
1:H:72:GLN:N	1:H:72:GLN:NE2	2.46	0.51
1:C:76:ASN:C	1:C:76:ASN:HD22	2.13	0.51
1:D:101:ASP:CB	1:D:122(A):LYS:HB2	2.40	0.51
1:D:175:THR:HB	1:D:239:VAL:CG1	2.41	0.51
1:D:89:ILE:O	1:D:113:ALA:HA	2.10	0.51
1:F:4:ALA:HB3	1:F:89:ILE:HG21	1.92	0.51
1:H:14:ASN:OD1	1:H:50:LEU:HD11	2.11	0.51
1:Q:1:LEU:HG	1:Q:1:LEU:O	2.10	0.51
1:Q:86:GLU:N	1:Q:86:GLU:OE2	2.44	0.51
1:E:202:ASN:CB	1:G:280:SER:OG	2.58	0.51
1:H:264:GLU:O	1:H:268:LYS:HD2	2.11	0.51
1:H:81:LEU:CD1	1:H:81:LEU:H	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:176:HIS:HB3	1:Q:231:ARG:HD3	1.92	0.51
1:D:79:PRO:HA	1:D:82:LEU:CD1	2.40	0.51
1:E:175:THR:HB	1:E:239:VAL:HG12	1.92	0.51
1:E:203:ILE:HD11	1:G:232:VAL:CG2	2.36	0.51
1:E:320:ARG:HA	1:E:320:ARG:HE	1.75	0.51
1:E:253:GLU:HG3	3:E:334:SO4:O3	2.10	0.51
1:F:79:PRO:HB3	1:F:108:HIS:CE1	2.46	0.51
1:H:242:LEU:HD12	1:H:243:VAL:N	2.26	0.51
1:H:92:VAL:HG11	1:H:108:HIS:CE1	2.46	0.51
1:Q:84:TRP:HA	1:Q:84:TRP:CE3	2.46	0.51
1:A:83:PRO:HA	1:A:85:LYS:HE2	1.93	0.51
1:B:37:VAL:HG22	1:B:73:VAL:HB	1.93	0.51
1:D:271:LEU:HD11	1:D:292:ILE:HD11	1.93	0.51
1:F:174:THR:HB	1:F:240:VAL:HG12	1.92	0.51
1:G:137:TYR:OH	1:G:328:VAL:HG13	2.11	0.51
1:O:0:LYS:NZ	1:O:23:SER:O	2.44	0.51
1:A:172:MET:HG2	1:A:173:THR:N	2.25	0.51
1:B:221:LEU:HA	1:B:224:LYS:HD2	1.91	0.51
1:B:324:LEU:O	1:B:328:VAL:HG23	2.11	0.51
1:A:280:SER:HB3	1:C:203:ILE:HB	1.93	0.51
1:D:170:GLY:O	1:D:225:LEU:HA	2.11	0.51
1:B:228:ILE:HG23	1:D:298:MET:HE1	1.93	0.51
1:E:27:ILE:HD11	1:E:30:ILE:CG1	2.40	0.51
1:G:99:PHE:HB3	1:G:104:GLY:O	2.11	0.51
1:F:279:VAL:HG12	1:H:205:PRO:HD2	1.92	0.51
1:H:289:SER:OG	1:H:320:ARG:NH1	2.43	0.51
1:H:72:GLN:N	1:H:72:GLN:HE21	2.07	0.51
1:A:193:LEU:HD13	1:D:42:HIS:CG	2.46	0.51
1:B:114:LYS:HD2	1:B:332:TRP:HZ2	1.76	0.51
1:F:218:LEU:N	1:F:219:PRO:HD3	2.26	0.51
1:G:130:VAL:HG21	1:G:320:ARG:HD3	1.92	0.51
1:E:43:LEU:HD11	1:H:187:ALA:O	2.11	0.51
1:Q:191:ARG:HG2	1:Q:192:ASP:N	2.26	0.51
1:A:74:VAL:HG23	1:A:75:SER:N	2.26	0.51
1:C:301:GLY:O	1:C:302:ASP:HB2	2.10	0.51
1:C:64:ILE:HD11	1:C:71:ILE:HD12	1.93	0.51
1:C:76:ASN:OD1	1:C:81:LEU:HB2	2.11	0.51
1:D:16:LEU:HD23	1:D:16:LEU:O	2.11	0.51
1:E:199:ALA:CB	1:H:184:LEU:HD21	2.40	0.51
1:F:174:THR:HA	1:F:240:VAL:HA	1.93	0.51
1:E:226:ASN:CB	1:G:300:MET:HE2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD12	1:A:290:THR:O	2.11	0.51
1:A:78:ASN:HD22	1:A:81:LEU:HG	1.76	0.51
1:E:272:ASP:HB2	1:E:288:PHE:CG	2.46	0.51
1:E:32:ASP:OD2	1:E:40:ALA:HB2	2.11	0.51
1:F:157:PHE:HB2	1:F:259:PHE:HE1	1.76	0.51
1:B:0(A):ALA:HB3	1:B:23:SER:O	2.11	0.50
1:E:212:LYS:O	1:E:215:ALA:HB3	2.10	0.50
1:E:89:ILE:HG21	1:E:92:VAL:HG22	1.93	0.50
1:G:85:LYS:HG3	1:G:86:GLU:N	2.26	0.50
1:O:17:ARG:HD2	1:O:53:PHE:CD1	2.46	0.50
1:Q:1:LEU:HD23	1:Q:91:ILE:HD11	1.93	0.50
1:B:84:TRP:HA	1:B:84:TRP:CE3	2.46	0.50
1:C:9:GLY:O	1:C:13:ARG:HG3	2.11	0.50
1:E:267:LEU:HD13	1:E:271:LEU:CD2	2.41	0.50
1:F:287:ASP:OD1	1:F:319:GLN:NE2	2.44	0.50
1:F:60:SER:OG	1:F:70:ILE:HD13	2.12	0.50
1:H:75:SER:O	1:H:76:ASN:HB2	2.11	0.50
1:A:143:ILE:HD12	1:A:143:ILE:N	2.27	0.50
1:G:129:VAL:H	1:G:133:ASN:ND2	2.07	0.50
1:G:168:ILE:C	1:G:169:LYS:HG3	2.32	0.50
1:O:279:VAL:HG11	1:Q:204:VAL:HG22	1.93	0.50
1:Q:107:LYS:O	1:Q:110:GLU:HB2	2.10	0.50
1:C:62:THR:O	1:C:63:ALA:HB2	2.11	0.50
1:D:103:GLU:OE1	1:D:103:GLU:N	2.41	0.50
1:E:15:PHE:CD1	1:E:322:VAL:HG22	2.47	0.50
1:F:169:LYS:HA	1:F:224:LYS:HB3	1.92	0.50
1:F:232:VAL:HG11	1:H:232:VAL:HG11	1.93	0.50
1:G:18(A):TRP:C	1:G:19:GLY:N	2.64	0.50
1:O:9:GLY:O	1:O:13:ARG:HG3	2.12	0.50
1:E:79:PRO:HA	1:E:82:LEU:CD1	2.42	0.50
1:H:129:VAL:H	1:H:133:ASN:ND2	2.03	0.50
1:O:26:ASP:OD1	1:O:69:LYS:HE2	2.11	0.50
1:A:1:LEU:HD22	1:A:329:ALA:HB2	1.94	0.50
1:E:194:ARG:NH1	1:E:205:PRO:HG2	2.26	0.50
1:G:226:ASN:ND2	1:G:227:GLY:H	2.09	0.50
1:G:256:ASN:HB3	1:G:260:ARG:HH11	1.75	0.50
1:H:8:PHE:CE1	1:H:16:LEU:HD12	2.46	0.50
1:C:187:ALA:O	1:C:196:ALA:HB1	2.11	0.50
1:B:169:LYS:CD	1:D:301:GLY:HA3	2.42	0.50
1:H:3:VAL:HG23	1:H:91:ILE:O	2.11	0.50
1:D:97:GLY:HA2	2:D:335:NAD:O3D	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:LEU:HD21	1:H:46:TYR:CZ	2.46	0.50
1:O:181:ASP:OD2	1:O:195:ARG:NH1	2.43	0.50
1:O:1:LEU:HD11	1:O:329:ALA:HA	1.94	0.50
1:A:156:PRO:HB2	1:A:290:THR:CG2	2.39	0.50
1:E:146:ASN:ND2	1:E:324:LEU:HD22	2.27	0.50
1:F:150:THR:O	1:F:150:THR:HG22	2.12	0.50
1:F:155:ALA:HB3	1:F:156:PRO:HD3	1.92	0.50
1:G:182:GLN:HB3	1:G:199:ALA:HB2	1.93	0.50
1:A:245:GLN:NE2	1:C:245:GLN:HE22	2.08	0.49
1:B:194:ARG:CZ	1:D:277:PRO:HA	2.41	0.49
1:B:39:GLN:NE2	1:C:190:HIS:H	2.09	0.49
1:D:206:THR:HG23	1:D:229:ALA:HB3	1.93	0.49
1:F:177:SER:HB3	1:F:234:THR:O	2.12	0.49
1:G:109:ILE:CD1	1:G:142:PRO:HB2	2.41	0.49
1:G:3:VAL:HG22	1:G:91:ILE:HB	1.93	0.49
1:H:55:ALA:HB1	1:H:67:ASP:OD1	2.11	0.49
1:O:219:PRO:O	1:O:222:LYS:HG2	2.12	0.49
1:A:236:ASN:O	1:A:237:VAL:HB	2.12	0.49
1:A:245:GLN:NE2	1:C:245:GLN:NE2	2.60	0.49
1:D:204:VAL:HB	1:D:231:ARG:HB2	1.94	0.49
1:E:277:PRO:HA	1:G:194:ARG:NE	2.23	0.49
1:E:312:ASP:CG	1:E:315:TRP:HB3	2.32	0.49
1:F:159:LYS:O	1:F:163:GLN:HB2	2.13	0.49
1:F:4:ALA:O	1:F:92:VAL:HG13	2.13	0.49
1:H:91:ILE:HD11	1:H:117:ILE:CG2	2.42	0.49
1:H:228:ILE:H	1:H:228:ILE:CD1	2.22	0.49
1:H:63:ALA:HA	1:H:73:VAL:HG23	1.93	0.49
1:H:82:LEU:HD13	1:H:84:TRP:CZ2	2.47	0.49
1:O:281:VAL:H	1:Q:202:ASN:HD22	1.59	0.49
1:Q:151:THR:OG1	1:Q:210:ALA:HA	2.13	0.49
1:C:251:PHE:CZ	1:C:254:GLU:HB2	2.47	0.49
1:E:109:ILE:HG12	1:E:113:ALA:O	2.12	0.49
1:E:129:VAL:HB	1:E:133:ASN:HD21	1.77	0.49
1:E:30:ILE:O	1:E:74:VAL:HG22	2.12	0.49
1:E:77:ARG:HB3	1:E:77:ARG:NH1	2.28	0.49
1:F:133:ASN:N	1:F:133:ASN:HD22	2.10	0.49
1:F:240:VAL:O	1:F:240:VAL:HG23	2.12	0.49
1:G:210:ALA:O	1:G:214:VAL:HG23	2.12	0.49
1:H:319:GLN:OE1	1:H:319:GLN:HA	2.12	0.49
1:H:84:TRP:CE3	1:H:84:TRP:HA	2.47	0.49
1:O:33:THR:HG22	1:O:77:ARG:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:LYS:HD2	1:H:88:GLY:HA2	1.94	0.49
1:C:256:ASN:OD1	1:C:294:SER:HB2	2.12	0.49
1:C:1:LEU:HD22	1:C:329:ALA:CB	2.42	0.49
1:E:211:ALA:HB1	1:E:226:ASN:HA	1.95	0.49
1:E:260:ARG:HB3	4:E:534:HOH:O	2.11	0.49
1:G:158:VAL:HG13	1:G:167:ILE:CD1	2.43	0.49
1:Q:190:HIS:CB	1:Q:196:ALA:HB2	2.42	0.49
1:B:85:LYS:HB2	1:B:112:GLY:HA3	1.94	0.49
1:B:250:THR:OG1	1:B:251:PHE:N	2.43	0.49
1:E:6:ASN:ND2	1:E:108:HIS:CE1	2.80	0.49
1:E:202:ASN:HB2	1:G:280:SER:OG	2.12	0.49
1:G:13:ARG:NH1	1:G:13:ARG:HG3	2.27	0.49
1:H:157:PHE:HE1	1:H:242:LEU:HD23	1.76	0.49
1:H:6:ASN:ND2	1:H:96:THR:HG21	2.27	0.49
1:O:129:VAL:HG23	1:O:217:VAL:HG11	1.94	0.49
1:O:221:LEU:HA	1:O:224:LYS:HD2	1.93	0.49
1:Q:109:ILE:HA	1:Q:113:ALA:O	2.12	0.49
1:Q:239:VAL:HG23	1:Q:309:ALA:O	2.12	0.49
1:B:140:ASP:OD2	1:B:140:ASP:N	2.45	0.49
1:C:1:LEU:HD23	1:C:91:ILE:CD1	2.42	0.49
1:D:172:MET:CE	1:D:211:ALA:HB2	2.43	0.49
1:E:139:HIS:CG	1:E:139:HIS:O	2.66	0.49
1:E:16:LEU:HD13	1:E:44:LEU:HD21	1.94	0.49
1:E:79:PRO:O	1:E:82:LEU:HG	2.13	0.49
1:F:32:ASP:OD2	2:F:335:NAD:H1B	2.13	0.49
1:H:28:ILE:C	1:H:71:ILE:HG13	2.32	0.49
1:Q:191:ARG:H	1:Q:191:ARG:CZ	2.26	0.49
1:Q:137:TYR:CZ	1:Q:328:VAL:HG22	2.48	0.49
1:B:0(A):ALA:N	1:B:26:ASP:HB2	2.28	0.49
1:D:123:GLY:O	1:D:125:ILE:HG22	2.12	0.49
1:E:16:LEU:HD23	1:E:16:LEU:O	2.12	0.49
1:E:232:VAL:O	1:E:234:THR:N	2.38	0.49
1:E:172:MET:HA	1:E:242:LEU:HA	1.95	0.49
1:E:70:ILE:H	1:E:70:ILE:CD1	2.15	0.49
1:F:228:ILE:HG21	1:H:296:LEU:CD2	2.43	0.49
1:F:292:ILE:HG22	1:F:293:ASP:N	2.27	0.49
1:H:182:GLN:HE22	1:H:231:ARG:CB	2.26	0.49
1:B:84:TRP:HA	1:B:84:TRP:HE3	1.78	0.49
1:C:260:ARG:HG2	1:C:273:VAL:HG21	1.95	0.49
1:C:84:TRP:CE3	1:C:84:TRP:HA	2.48	0.49
1:D:107:LYS:HA	1:D:110:GLU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LYS:HG3	1:D:112:GLY:CA	2.33	0.49
1:E:171:THR:HB	1:G:300:MET:CG	2.39	0.49
1:H:142:PRO:HG2	1:H:143:ILE:H	1.78	0.49
1:F:193:LEU:HD12	1:H:277:PRO:HG3	1.95	0.49
1:A:173:THR:HG23	1:A:228:ILE:CD1	2.43	0.49
1:B:251:PHE:C	1:B:299:VAL:HG21	2.34	0.49
1:C:109:ILE:CD1	1:C:142:PRO:HB2	2.42	0.49
1:E:252:ALA:HB2	4:E:545:HOH:O	2.12	0.49
1:G:168:ILE:HB	1:G:245:GLN:O	2.12	0.49
1:G:2:LYS:HE3	1:G:87:LEU:O	2.13	0.49
1:O:226:ASN:HB2	1:Q:300:MET:HE2	1.95	0.49
1:O:242:LEU:HD11	1:O:244:VAL:HG13	1.94	0.49
1:O:281:VAL:CG1	1:Q:202:ASN:HD21	2.25	0.49
1:A:188:SER:HA	1:D:39:GLN:OE1	2.13	0.48
1:C:108:HIS:HB2	1:C:116:VAL:HG21	1.95	0.48
1:C:317:TYR:O	1:C:320:ARG:HB2	2.13	0.48
1:D:190:HIS:HB3	1:D:196:ALA:HB2	1.95	0.48
1:F:152:ASN:O	1:F:156:PRO:HG2	2.13	0.48
1:G:0:LYS:HB3	1:G:0:LYS:HZ2	1.75	0.48
1:A:101:ASP:OD1	1:A:104:GLY:N	2.40	0.48
1:C:323:ASP:O	1:C:327:ILE:HG13	2.14	0.48
1:D:260:ARG:O	1:D:263:ALA:HB3	2.13	0.48
1:F:202:ASN:ND2	1:H:281:VAL:CB	2.76	0.48
1:H:126:PRO:HG2	1:H:141:GLU:OE2	2.13	0.48
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.48	0.48
1:A:191:ARG:NH1	4:A:770:HOH:O	2.45	0.48
1:B:270:ILE:N	1:B:270:ILE:HD12	2.27	0.48
1:C:168:ILE:HG22	1:C:169:LYS:HD3	1.95	0.48
1:D:292:ILE:H	1:D:292:ILE:HD12	1.78	0.48
1:D:44:LEU:HD23	1:D:57:VAL:CG1	2.44	0.48
1:D:84:TRP:HA	1:D:89:ILE:HD13	1.94	0.48
1:E:299:VAL:CG2	1:E:305:VAL:HG22	2.42	0.48
1:E:32:ASP:C	1:E:34:GLY:H	2.17	0.48
1:F:118:ILE:CD1	1:F:118:ILE:H	2.26	0.48
1:F:327:ILE:O	1:F:327:ILE:HG22	2.14	0.48
1:H:242:LEU:O	1:H:306:LYS:HA	2.14	0.48
1:H:84:TRP:HE3	1:H:84:TRP:HA	1.78	0.48
1:B:36:GLY:HA3	1:B:38:LYS:HE3	1.94	0.48
1:C:182:GLN:HB3	4:C:396:HOH:O	2.12	0.48
1:C:329:ALA:O	1:C:332:TRP:HB2	2.14	0.48
1:D:272:ASP:OD2	1:D:273:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ILE:HD12	1:D:93:ILE:N	2.28	0.48
1:F:17:ARG:HD3	1:F:50:LEU:HD12	1.95	0.48
1:G:79:PRO:HB2	1:G:107:LYS:HB2	1.95	0.48
1:H:249:LYS:HA	1:H:302:ASP:O	2.13	0.48
1:A:133:ASN:ND2	1:A:133:ASN:C	2.67	0.48
1:A:64:ILE:CG1	1:A:71:ILE:HG23	2.42	0.48
1:E:208:THR:C	1:E:210:ALA:H	2.15	0.48
1:E:90:ASP:OD1	1:E:114:LYS:HD2	2.14	0.48
1:G:194:ARG:HD3	1:G:205:PRO:HD2	1.94	0.48
1:B:126:PRO:HG2	1:B:141:GLU:HG2	1.95	0.48
1:C:177:SER:HB2	1:C:237:VAL:O	2.14	0.48
1:D:132:VAL:HG13	1:D:218:LEU:HD21	1.96	0.48
1:E:169:LYS:HE2	1:E:245:GLN:OE1	2.13	0.48
1:E:251:PHE:CE1	1:E:254:GLU:HB2	2.49	0.48
1:F:132:VAL:HG13	1:F:218:LEU:HD21	1.95	0.48
1:G:318:SER:O	1:G:322:VAL:HG23	2.13	0.48
1:H:16:LEU:HD23	1:H:16:LEU:O	2.13	0.48
1:H:7:GLY:CA	1:H:96:THR:HG22	2.44	0.48
1:O:1:LEU:HD12	1:O:329:ALA:CB	2.44	0.48
1:O:15:PHE:CE1	1:O:321:VAL:HG12	2.48	0.48
1:A:296:LEU:HB3	1:A:308:ILE:HD12	1.96	0.48
1:B:251:PHE:O	1:B:255:VAL:HG23	2.14	0.48
1:C:31:ASN:HB2	1:C:74:VAL:HG23	1.95	0.48
1:G:130:VAL:HG23	1:G:320:ARG:HD3	1.96	0.48
1:G:48:SER:HA	1:H:281:VAL:HG11	1.96	0.48
1:E:187:ALA:O	1:H:43:LEU:HD11	2.14	0.48
1:D:84:TRP:HB3	1:D:113:ALA:H	1.79	0.48
1:E:18:CYS:HB3	1:E:319:GLN:CD	2.34	0.48
1:H:79:PRO:HB2	1:H:107:LYS:HB3	1.95	0.48
1:A:64:ILE:HG13	1:A:71:ILE:CG2	2.43	0.48
1:G:191:ARG:HG3	1:G:192:ASP:N	2.29	0.48
1:B:228:ILE:HG23	1:D:298:MET:CE	2.44	0.48
1:C:109:ILE:HA	1:C:113:ALA:O	2.14	0.48
1:E:14:ASN:OD1	1:E:315:TRP:HA	2.13	0.48
1:E:279:VAL:HG23	1:E:281:VAL:HG12	1.95	0.48
1:E:71:ILE:HD13	1:E:72:GLN:O	2.14	0.48
1:F:144:ILE:HD12	1:F:324:LEU:HD21	1.95	0.48
1:G:250:THR:OG1	1:G:251:PHE:N	2.46	0.48
1:H:178:TYR:HA	1:H:182:GLN:OE1	2.13	0.48
1:H:28:ILE:HG23	1:H:29:ALA:N	2.29	0.48
1:C:23:SER:C	1:C:25:LEU:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:SER:HA	1:C:310:TRP:CZ3	2.48	0.47
1:D:44:LEU:HA	4:D:341:HOH:O	2.13	0.47
1:D:14:ASN:OD1	1:D:50:LEU:HD11	2.14	0.47
1:F:59:PRO:HA	1:F:64:ILE:HG22	1.95	0.47
1:H:132:VAL:HG21	1:H:155:ALA:HB1	1.96	0.47
1:H:149:CYS:HB3	2:H:335:NAD:C5N	2.44	0.47
1:H:38:LYS:HG2	1:H:39:GLN:N	2.29	0.47
1:C:236:ASN:O	1:C:237:VAL:HB	2.14	0.47
1:C:284:ARG:O	1:C:285:CYS:HB2	2.14	0.47
1:D:87:LEU:HB2	1:D:89:ILE:CD1	2.44	0.47
1:E:83:PRO:O	1:E:87:LEU:HD13	2.14	0.47
1:F:280:SER:OG	1:H:202:ASN:HB2	2.14	0.47
1:G:194:ARG:O	1:G:204:VAL:HG11	2.15	0.47
1:G:194:ARG:NH1	1:G:205:PRO:HB2	2.29	0.47
1:G:299:VAL:HG11	4:G:872:HOH:O	2.13	0.47
1:O:293:ASP:HB3	1:O:296:LEU:HD12	1.96	0.47
1:D:85:LYS:CG	1:D:112:GLY:HA2	2.33	0.47
1:E:236:ASN:CG	1:E:237:VAL:H	2.17	0.47
1:E:58:LYS:HB2	1:E:59:PRO:CD	2.39	0.47
1:F:321:VAL:O	1:F:325:ALA:HB2	2.14	0.47
1:F:62:THR:O	1:F:63:ALA:HB2	2.14	0.47
1:G:128:TYR:CZ	1:G:137:TYR:HA	2.49	0.47
1:E:226:ASN:HD22	1:G:300:MET:CE	2.26	0.47
1:G:312:ASP:HB3	1:G:316:GLY:H	1.79	0.47
1:O:9:GLY:HA3	2:O:335:NAD:O5B	2.14	0.47
1:Q:115:LYS:HG3	1:Q:142:PRO:O	2.14	0.47
1:C:331:ASN:O	1:C:333:LYS:HD3	2.15	0.47
1:D:126:PRO:HB2	1:D:144:ILE:HG22	1.95	0.47
1:E:115:LYS:HE3	1:E:137:TYR:OH	2.14	0.47
1:E:300:MET:SD	1:G:170:GLY:O	2.72	0.47
1:F:90:ASP:HA	1:F:114:LYS:CD	2.28	0.47
1:G:198:ALA:O	1:G:200:ALA:N	2.48	0.47
1:Q:126:PRO:HD2	1:Q:143:ILE:O	2.14	0.47
1:B:102:ARG:O	1:B:106:GLY:N	2.47	0.47
1:B:194:ARG:NH1	1:D:278:LEU:O	2.47	0.47
1:E:115:LYS:HE3	1:E:328:VAL:HG13	1.96	0.47
1:F:240:VAL:HG13	1:F:311:TYR:CE1	2.49	0.47
1:G:239:VAL:HB	1:G:310:TRP:CE3	2.49	0.47
1:H:15:PHE:CE1	1:H:322:VAL:HG22	2.49	0.47
1:Q:44:LEU:O	1:Q:44:LEU:HD12	2.15	0.47
1:G:62:THR:CG2	1:Q:62:THR:HG22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ALA:HA	1:A:73:VAL:HG23	1.96	0.47
1:B:195:ARG:HH21	1:B:206:THR:HG21	1.79	0.47
1:D:64:ILE:HG23	1:D:73:VAL:HG21	1.96	0.47
1:E:5:ILE:HD12	1:E:27:ILE:CD1	2.43	0.47
1:E:284:ARG:O	1:E:285:CYS:HB2	2.14	0.47
1:G:208:THR:C	1:G:210:ALA:N	2.68	0.47
1:E:194:ARG:CG	1:G:277:PRO:O	2.60	0.47
1:E:190:HIS:N	1:H:39:GLN:OE1	2.47	0.47
1:D:177:SER:HB3	1:D:234:THR:O	2.14	0.47
1:F:4:ALA:HB3	1:F:92:VAL:HG22	1.96	0.47
1:H:228:ILE:HD13	1:H:228:ILE:N	2.24	0.47
1:Q:284:ARG:O	1:Q:285:CYS:HB2	2.15	0.47
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.79	0.47
1:B:154:LEU:HD21	1:B:172:MET:HE2	1.97	0.47
1:B:165:PHE:HB3	1:B:246:VAL:HG11	1.96	0.47
1:D:0:LYS:O	1:D:1:LEU:HB2	2.15	0.47
1:E:138:SER:C	1:E:140:ASP:H	2.17	0.47
1:E:58:LYS:HB3	1:E:58:LYS:HZ2	1.79	0.47
1:G:133:ASN:N	1:G:133:ASN:HD22	2.13	0.47
1:H:192:ASP:C	1:H:194:ARG:H	2.16	0.47
1:O:28:ILE:HD11	1:O:89:ILE:HD13	1.97	0.47
1:Q:130:VAL:HA	1:Q:134:ALA:HB2	1.97	0.47
1:Q:272:ASP:HB2	1:Q:288:PHE:CD2	2.49	0.47
1:Q:28:ILE:HD12	1:Q:28:ILE:C	2.35	0.47
1:B:186:ASP:HA	1:B:196:ALA:O	2.15	0.47
1:B:240:VAL:HG13	1:B:311:TYR:CE1	2.49	0.47
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.49	0.47
1:O:187:ALA:O	1:O:196:ALA:HB1	2.15	0.47
1:D:134:ALA:HB3	4:D:396:HOH:O	2.15	0.47
1:F:255:VAL:C	1:F:257:ALA:N	2.68	0.47
1:G:260:ARG:NH2	1:G:275:ASP:OD1	2.47	0.47
1:G:294:SER:C	1:G:296:LEU:N	2.68	0.47
1:F:298:MET:CE	1:H:228:ILE:HG23	2.45	0.47
1:H:8:PHE:HE1	1:H:16:LEU:HD12	1.80	0.47
1:B:279:VAL:HG22	1:D:197:ARG:NH1	2.29	0.47
1:C:241:ASP:OD1	1:C:306:LYS:CE	2.63	0.47
1:C:84:TRP:HE3	1:C:84:TRP:HA	1.79	0.47
1:O:169:LYS:HD2	1:Q:300:MET:HG3	1.97	0.47
1:Q:183:ARG:HG3	1:Q:196:ALA:HA	1.97	0.47
1:A:226:ASN:HD21	1:C:300:MET:HB2	1.80	0.46
1:A:284:ARG:O	1:A:285:CYS:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASN:OD1	1:D:281:VAL:HB	2.16	0.46
1:C:153:CYS:SG	1:C:240:VAL:HG13	2.55	0.46
1:E:117:ILE:CG2	1:E:144:ILE:HD11	2.36	0.46
1:F:107:LYS:HA	1:F:110:GLU:HG2	1.96	0.46
1:F:177:SER:O	1:F:231:ARG:HD2	2.15	0.46
1:H:146:ASN:O	1:H:146:ASN:OD1	2.32	0.46
1:Q:18:CYS:HB3	1:Q:319:GLN:OE1	2.15	0.46
1:B:284:ARG:O	1:B:285:CYS:HB2	2.13	0.46
1:E:108:HIS:HB2	1:E:116:VAL:HG21	1.97	0.46
1:G:85:LYS:N	1:G:112:GLY:HA3	2.31	0.46
1:H:256:ASN:ND2	1:H:297:THR:OG1	2.31	0.46
1:H:149:CYS:HB3	2:H:335:NAD:H5N	1.96	0.46
1:Q:271:LEU:HD23	1:Q:271:LEU:C	2.35	0.46
1:B:133:ASN:HD22	1:B:133:ASN:H	1.61	0.46
1:E:169:LYS:HE3	1:G:304:MET:CB	2.43	0.46
1:E:179:THR:HG22	1:E:180:GLY:H	1.80	0.46
1:E:179:THR:OG1	1:E:231:ARG:NH1	2.49	0.46
1:F:301:GLY:O	1:F:302:ASP:HB2	2.15	0.46
1:F:322:VAL:O	1:F:325:ALA:HB3	2.15	0.46
1:F:85:LYS:HD2	1:F:85:LYS:HA	1.78	0.46
1:A:13:ARG:HG3	1:A:13:ARG:HH11	1.80	0.46
1:A:91:ILE:HD13	1:A:92:VAL:N	2.31	0.46
1:D:15:PHE:CE1	1:D:322:VAL:HG22	2.50	0.46
1:D:139:HIS:CB	1:D:333:LYS:HE2	2.27	0.46
1:E:251:PHE:CZ	1:E:254:GLU:HB2	2.50	0.46
1:E:79:PRO:HB2	1:E:107:LYS:HB3	1.96	0.46
1:F:65:SER:HA	1:F:70:ILE:HA	1.97	0.46
1:Q:194:ARG:HD2	1:Q:205:PRO:O	2.15	0.46
1:C:211:ALA:HB1	1:C:226:ASN:N	2.31	0.46
1:D:37:VAL:O	1:D:40:ALA:HB3	2.15	0.46
1:F:108:HIS:HB2	1:F:116:VAL:HG21	1.97	0.46
1:G:172:MET:HB2	1:G:242:LEU:CB	2.45	0.46
1:G:4:ALA:HB2	1:G:89:ILE:HD12	1.97	0.46
1:A:159:LYS:NZ	1:A:163:GLN:HE22	2.13	0.46
1:B:191:ARG:NH1	1:B:191:ARG:HB2	2.30	0.46
1:C:33:THR:HG21	1:C:77:ARG:CZ	2.45	0.46
1:E:178:TYR:CB	1:E:199:ALA:HB1	2.46	0.46
1:E:202:ASN:ND2	1:G:281:VAL:CG1	2.78	0.46
1:G:84:TRP:CE3	1:G:84:TRP:HA	2.50	0.46
1:O:253:GLU:H	1:O:253:GLU:CD	2.19	0.46
1:C:320:ARG:HA	1:C:320:ARG:NE	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:ARG:O	1:E:285:CYS:CB	2.63	0.46
1:F:18:CYS:SG	1:F:319:GLN:OE1	2.74	0.46
1:F:15:PHE:CE1	1:F:322:VAL:HG22	2.50	0.46
1:F:45:LYS:HD3	1:F:57:VAL:HB	1.97	0.46
1:G:291:THR:O	1:G:291:THR:HG23	2.16	0.46
1:H:132:VAL:O	1:H:133:ASN:CB	2.63	0.46
1:O:215:ALA:HB1	1:O:222:LYS:HD3	1.97	0.46
1:O:285:CYS:N	1:O:312:ASP:OD2	2.45	0.46
1:A:300:MET:HE3	1:C:226:ASN:CB	2.46	0.46
1:E:154:LEU:C	1:E:158:VAL:HG23	2.36	0.46
1:E:260:ARG:HD3	4:E:534:HOH:O	2.15	0.46
1:E:70:ILE:O	1:E:70:ILE:HG12	2.15	0.46
1:F:27:ILE:N	1:F:27:ILE:CD1	2.77	0.46
1:F:90:ASP:O	1:F:115:LYS:N	2.41	0.46
1:O:2:LYS:HD2	1:O:28:ILE:HD13	1.97	0.46
1:Q:271:LEU:HD23	1:Q:272:ASP:N	2.31	0.46
1:D:322:VAL:O	1:D:322:VAL:HG12	2.16	0.46
1:E:183:ARG:CG	1:E:196:ALA:HA	2.46	0.46
1:E:226:ASN:HD22	1:G:300:MET:HE1	1.81	0.46
1:H:210:ALA:O	1:H:214:VAL:HG23	2.16	0.46
1:A:84:TRP:HA	1:A:84:TRP:CE3	2.52	0.45
1:B:163:GLN:NE2	1:B:164:LYS:NZ	2.58	0.45
1:B:190:HIS:HB3	1:B:196:ALA:HB2	1.97	0.45
1:E:133:ASN:H	1:E:133:ASN:ND2	2.01	0.45
1:E:133:ASN:N	1:E:133:ASN:ND2	2.51	0.45
1:F:154:LEU:HD11	1:F:242:LEU:HD13	1.98	0.45
1:F:66:VAL:O	1:F:67:ASP:HB2	2.16	0.45
1:G:162:ASP:C	1:G:164:LYS:H	2.19	0.45
1:G:228:ILE:N	1:G:228:ILE:HD13	2.30	0.45
1:H:130:VAL:CG2	1:H:320:ARG:HD3	2.46	0.45
1:C:14:ASN:HB3	1:C:318:SER:OG	2.16	0.45
1:D:101:ASP:HB3	1:D:122(A):LYS:HB2	1.98	0.45
1:D:228:ILE:HD13	1:D:228:ILE:H	1.80	0.45
1:D:242:LEU:HG	1:D:244:VAL:HG13	1.98	0.45
1:D:83:PRO:HB2	1:D:87:LEU:HD23	1.98	0.45
1:E:17:ARG:HE	1:E:17:ARG:CA	2.05	0.45
1:E:235:PRO:HG2	1:E:236:ASN:H	1.81	0.45
1:E:63:ALA:HB2	1:E:72:GLN:OE1	2.15	0.45
1:F:109:ILE:CD1	1:F:142:PRO:HB3	2.45	0.45
1:F:139:HIS:CD2	1:F:333:LYS:HG2	2.51	0.45
1:F:145:SER:O	1:F:147:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:LEU:N	1:F:81:LEU:HD12	2.30	0.45
1:G:242:LEU:HD23	1:G:242:LEU:H	1.82	0.45
1:H:208:THR:HG23	1:H:208:THR:O	2.16	0.45
1:H:4:ALA:HB3	1:H:92:VAL:HG22	1.98	0.45
1:A:213:ALA:O	1:A:216:LEU:HB2	2.17	0.45
1:A:296:LEU:O	1:A:298:MET:HG3	2.16	0.45
1:C:82:LEU:HA	1:C:83:PRO:HD3	1.79	0.45
1:D:210:ALA:O	1:D:213:ALA:HB3	2.17	0.45
1:E:246:VAL:O	1:E:303:ASP:HB2	2.16	0.45
1:F:235:PRO:HB3	1:G:201:LEU:HD21	1.97	0.45
1:G:291:THR:HG22	1:G:310:TRP:O	2.15	0.45
1:H:105:ALA:HB1	1:H:116:VAL:HG11	1.98	0.45
1:A:215:ALA:HB2	1:A:222:LYS:HA	1.98	0.45
1:B:38:LYS:N	1:B:38:LYS:CD	2.77	0.45
1:H:88:GLY:O	1:H:89:ILE:C	2.55	0.45
1:O:279:VAL:CG1	1:Q:204:VAL:HG22	2.46	0.45
1:Q:183:ARG:CG	1:Q:196:ALA:HA	2.46	0.45
1:Q:204:VAL:HB	1:Q:231:ARG:HB2	1.98	0.45
1:A:227:GLY:N	1:C:298:MET:HE1	2.31	0.45
1:B:319:GLN:HA	1:B:319:GLN:OE1	2.16	0.45
1:D:10:ARG:HG2	4:D:377:HOH:O	2.16	0.45
1:D:181:ASP:OD1	1:D:195:ARG:NE	2.50	0.45
1:D:3:VAL:CG1	1:D:93:ILE:HD13	2.45	0.45
1:E:290:THR:HA	1:E:310:TRP:O	2.17	0.45
1:F:23:SER:C	1:F:25:LEU:H	2.20	0.45
1:F:27:ILE:CD1	1:F:27:ILE:H	2.30	0.45
1:F:47:ASP:OD1	1:F:48:SER:N	2.49	0.45
1:G:193:LEU:HD22	1:G:193:LEU:N	2.26	0.45
1:G:267:LEU:HD12	1:G:271:LEU:HD22	1.99	0.45
1:A:279:VAL:HG23	1:A:281:VAL:HG12	1.99	0.45
1:C:126:PRO:HD2	1:C:143:ILE:O	2.17	0.45
1:D:18(A):TRP:CE3	1:D:27:ILE:HD12	2.51	0.45
1:D:27:ILE:O	1:D:69:LYS:HE3	2.16	0.45
1:E:186:ASP:HB2	1:H:10:ARG:HH12	1.82	0.45
1:F:101:ASP:OD1	1:F:103:GLU:HB3	2.16	0.45
1:F:119:THR:O	1:F:120:ALA:HB2	2.16	0.45
1:F:31:ASN:ND2	1:F:82:LEU:HD11	2.31	0.45
1:F:84:TRP:CE3	1:F:84:TRP:HA	2.52	0.45
1:H:185:LEU:O	1:H:186:ASP:C	2.55	0.45
1:O:176:HIS:HA	1:O:238:SER:HB3	1.99	0.45
1:Q:178:TYR:CE1	1:Q:235:PRO:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:H	1:A:133:ASN:HD21	1.65	0.45
1:C:293:ASP:O	1:C:295:SER:N	2.49	0.45
1:C:2:LYS:HD3	1:C:28:ILE:HD13	1.98	0.45
1:E:102:ARG:O	1:E:106:GLY:N	2.50	0.45
1:F:137:TYR:CE2	1:F:328:VAL:HA	2.52	0.45
1:F:271:LEU:HA	1:F:290:THR:HG23	1.99	0.45
1:A:159:LYS:O	1:A:163:GLN:HB2	2.17	0.45
1:D:44:LEU:HD23	1:D:57:VAL:HG11	1.99	0.45
1:E:66:VAL:O	1:E:67:ASP:HB2	2.16	0.45
1:E:7:GLY:HA2	2:E:335:NAD:C1B	2.42	0.45
1:F:52:ILE:HG22	1:F:53:PHE:N	2.31	0.45
1:E:194:ARG:NH1	1:G:296:LEU:HD21	2.30	0.45
1:H:329:ALA:O	1:H:332:TRP:HB3	2.16	0.45
1:O:218:LEU:HB3	1:O:221:LEU:HD23	1.99	0.45
1:Q:69:LYS:HD3	4:Q:618:HOH:O	2.15	0.45
1:B:271:LEU:HD13	1:B:272:ASP:H	1.76	0.45
1:E:132:VAL:HG13	1:E:218:LEU:HD21	1.99	0.45
1:E:31:ASN:HA	1:E:74:VAL:HG23	1.98	0.45
1:E:9:GLY:N	2:E:335:NAD:H4B	2.31	0.45
1:F:185:LEU:O	1:F:186:ASP:C	2.55	0.45
1:F:296:LEU:O	1:F:297:THR:C	2.56	0.45
1:F:74:VAL:HG22	1:F:75:SER:N	2.32	0.45
1:G:28:ILE:HD11	1:G:89:ILE:HD13	1.98	0.45
1:H:192:ASP:OD1	1:H:194:ARG:HB2	2.16	0.45
1:H:218:LEU:HB3	1:H:221:LEU:HD23	1.99	0.45
1:H:3:VAL:HG13	1:H:27:ILE:HA	1.99	0.45
1:O:263:ALA:O	1:O:268:LYS:HA	2.17	0.45
1:B:241:ASP:HA	1:B:308:ILE:HD13	1.99	0.45
1:D:116:VAL:HB	1:D:143:ILE:CD1	2.47	0.45
1:D:74:VAL:CG2	1:D:75:SER:H	2.28	0.45
1:E:278:LEU:HD21	1:F:46:TYR:CE2	2.52	0.45
1:F:132:VAL:HG11	1:F:218:LEU:HG	1.98	0.45
1:G:79:PRO:HB2	1:G:107:LYS:CB	2.47	0.45
1:G:287:ASP:OD1	1:G:319:GLN:HG3	2.16	0.45
1:G:32:ASP:OD1	2:G:335:NAD:H1B	2.17	0.45
1:G:46:TYR:HB3	1:H:282:ASP:OD1	2.17	0.45
1:H:132:VAL:HG13	1:H:218:LEU:HD21	1.98	0.45
1:H:92:VAL:HB	1:H:116:VAL:HG22	1.99	0.45
1:Q:212:LYS:HB3	4:Q:459:HOH:O	2.15	0.45
1:Q:1:LEU:HD22	1:Q:329:ALA:CB	2.47	0.45
1:A:215:ALA:CB	1:A:222:LYS:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:O	1:B:249:LYS:C	2.55	0.44
1:E:173:THR:HG23	1:E:228:ILE:HD11	1.99	0.44
1:F:190:HIS:HB3	1:F:196:ALA:HB2	1.99	0.44
1:G:204:VAL:HA	1:G:205:PRO:HD3	1.83	0.44
1:H:133:ASN:N	1:H:133:ASN:ND2	2.65	0.44
1:H:139:HIS:C	1:H:141:GLU:H	2.20	0.44
1:H:176:HIS:HB3	1:H:231:ARG:CD	2.46	0.44
1:H:276:GLU:HB3	1:H:277:PRO:HD2	1.98	0.44
1:O:157:PHE:HE1	1:O:242:LEU:HD23	1.83	0.44
1:O:54:ASP:HB3	4:O:425:HOH:O	2.16	0.44
1:Q:133:ASN:HD22	1:Q:133:ASN:N	2.13	0.44
1:Q:320:ARG:NE	1:Q:320:ARG:HA	2.32	0.44
1:A:83:PRO:HA	1:A:85:LYS:CE	2.47	0.44
1:B:204:VAL:HB	1:B:231:ARG:HB2	2.00	0.44
1:D:191:ARG:NE	4:D:338:HOH:O	2.47	0.44
1:D:146:ASN:HD22	1:D:321:VAL:HG22	1.81	0.44
1:E:178:TYR:CA	1:E:182:GLN:OE1	2.63	0.44
1:E:28:ILE:HG12	1:E:28:ILE:O	2.17	0.44
1:F:132:VAL:HG12	1:F:133:ASN:N	2.31	0.44
1:F:215:ALA:O	1:F:219:PRO:HG3	2.18	0.44
1:F:251:PHE:CE1	1:F:254:GLU:HB2	2.52	0.44
1:G:172:MET:HA	1:G:242:LEU:HA	2.00	0.44
1:G:75:SER:HB2	1:Q:61:GLU:HG2	1.99	0.44
1:H:292:ILE:HD13	1:H:309:ALA:HB2	1.99	0.44
1:O:70:ILE:HD12	1:O:70:ILE:N	2.31	0.44
1:A:33:THR:CG2	1:A:77:ARG:HG2	2.44	0.44
1:B:298:MET:SD	1:D:226:ASN:ND2	2.90	0.44
1:D:13:ARG:HD2	4:D:341:HOH:O	2.17	0.44
1:D:197:ARG:N	1:D:197:ARG:HD2	2.32	0.44
1:E:327:ILE:HG23	3:E:338:SO4:O3	2.18	0.44
1:F:84:TRP:HE3	1:F:84:TRP:HA	1.82	0.44
1:G:185:LEU:HA	1:G:198:ALA:CB	2.47	0.44
1:G:278:LEU:HD22	1:H:46:TYR:CD2	2.52	0.44
1:H:157:PHE:CE1	1:H:242:LEU:HD23	2.53	0.44
1:Q:191:ARG:CB	1:Q:191:ARG:NH1	2.75	0.44
1:Q:1:LEU:O	1:Q:90:ASP:HB2	2.17	0.44
1:D:228:ILE:H	1:D:228:ILE:CD1	2.30	0.44
1:E:251:PHE:O	1:E:253:GLU:N	2.51	0.44
1:F:98:VAL:HG23	1:F:99:PHE:CD1	2.52	0.44
1:E:203:ILE:CD1	1:G:232:VAL:HG21	2.42	0.44
1:H:170:GLY:H	1:H:225:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:226:ASN:OD1	1:H:227:GLY:N	2.51	0.44
1:O:157:PHE:CE1	1:O:242:LEU:HD23	2.53	0.44
1:A:85:LYS:HZ2	1:A:86:GLU:HB3	1.81	0.44
1:B:272:ASP:O	1:B:291:THR:HA	2.17	0.44
1:D:17:ARG:HD3	1:D:50:LEU:HD13	2.00	0.44
1:D:221:LEU:N	1:D:221:LEU:HD22	2.33	0.44
1:D:329:ALA:O	1:D:332:TRP:HB2	2.18	0.44
1:E:170:GLY:O	1:E:225:LEU:HA	2.18	0.44
1:E:173:THR:HG23	1:E:228:ILE:CD1	2.47	0.44
1:E:197:ARG:NH1	1:G:279:VAL:HG22	2.33	0.44
1:E:50:LEU:HB2	1:E:53:PHE:CZ	2.52	0.44
1:A:205:PRO:HA	1:A:230:LEU:HD23	1.98	0.44
1:A:137:TYR:CZ	1:A:328:VAL:HG22	2.52	0.44
1:C:276:GLU:HB2	1:C:278:LEU:HG	1.99	0.44
1:D:298:MET:HE3	1:D:306:LYS:HD2	2.00	0.44
1:E:60(A):GLY:O	1:E:61:GLU:HG2	2.17	0.44
1:Q:3:VAL:HG12	1:Q:4:ALA:N	2.33	0.44
1:A:84:TRP:HA	1:A:84:TRP:HE3	1.82	0.44
1:B:133:ASN:HD22	1:B:133:ASN:N	2.15	0.44
1:C:146:ASN:O	1:C:147:ALA:HB3	2.17	0.44
1:C:16:LEU:HD23	1:C:16:LEU:C	2.38	0.44
1:D:133:ASN:OD1	1:D:217:VAL:HA	2.18	0.44
1:E:106:GLY:O	1:E:110:GLU:HG3	2.18	0.44
1:F:154:LEU:HD23	1:F:214:VAL:HG21	2.00	0.44
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.81	0.44
1:Q:255:VAL:O	1:Q:258:ALA:HB3	2.18	0.44
1:A:0:LYS:HG2	1:A:26:ASP:HB2	2.00	0.44
1:E:194:ARG:HE	1:G:277:PRO:HA	1.82	0.44
1:G:251:PHE:CA	1:G:299:VAL:HG21	2.46	0.44
1:G:37:VAL:HG21	1:G:62:THR:HA	2.00	0.44
1:H:182:GLN:HB3	1:H:199:ALA:HB2	1.99	0.44
1:C:56:ASP:N	1:C:67:ASP:OD1	2.35	0.44
1:D:175:THR:HB	1:D:239:VAL:HG13	2.00	0.44
1:E:8:PHE:CZ	1:E:13:ARG:HG2	2.53	0.44
1:E:158:VAL:O	1:E:158:VAL:HG12	2.18	0.44
1:F:259:PHE:HB3	1:F:273:VAL:HG21	1.98	0.44
1:G:211:ALA:HB1	1:G:226:ASN:CA	2.44	0.44
1:G:222:LYS:HG2	1:G:223:GLY:N	2.32	0.44
1:E:201:LEU:HD11	1:H:235:PRO:HB3	1.99	0.44
1:H:30:ILE:HG13	1:H:71:ILE:HD11	2.00	0.44
1:H:2:LYS:HD2	1:H:88:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:125:ILE:HG23	1:Q:143:ILE:O	2.17	0.44
1:Q:174:THR:O	1:Q:174:THR:HG23	2.18	0.44
1:Q:1:LEU:HD22	1:Q:329:ALA:HA	1.99	0.44
1:D:248:LYS:O	1:D:249:LYS:C	2.56	0.43
1:D:253:GLU:CD	1:D:253:GLU:H	2.21	0.43
1:D:276:GLU:HB2	1:D:278:LEU:HG	2.00	0.43
1:E:106:GLY:O	1:E:109:ILE:HG22	2.18	0.43
1:G:162:ASP:O	1:G:164:LYS:N	2.49	0.43
1:F:38:LYS:CE	1:G:193:LEU:HD21	2.48	0.43
1:O:158:VAL:HG13	1:O:167:ILE:CD1	2.48	0.43
1:Q:206:THR:HG23	1:Q:207:SER:O	2.17	0.43
1:E:153:CYS:SG	1:E:240:VAL:HG21	2.58	0.43
1:E:77:ARG:CB	1:E:77:ARG:NH1	2.81	0.43
1:F:279:VAL:O	1:F:279:VAL:HG23	2.17	0.43
1:G:153:CYS:C	1:G:156:PRO:HD2	2.39	0.43
1:H:70:ILE:CG2	1:H:71:ILE:H	2.27	0.43
1:O:236:ASN:O	1:O:237:VAL:CB	2.66	0.43
1:O:2:LYS:CD	1:O:28:ILE:HD13	2.48	0.43
1:A:227:GLY:H	1:C:298:MET:HE1	1.83	0.43
1:A:76:ASN:ND2	1:A:81:LEU:HB2	2.34	0.43
1:F:10:ARG:HH11	1:G:186:ASP:HB2	1.84	0.43
1:F:279:VAL:CG1	1:H:204:VAL:HA	2.47	0.43
1:F:301:GLY:HA3	1:H:169:LYS:CE	2.48	0.43
1:A:109:ILE:N	1:A:109:ILE:HD12	2.33	0.43
1:A:233:PRO:HB2	1:C:233:PRO:HB2	2.00	0.43
1:B:256:ASN:HB3	1:B:260:ARG:NH1	2.32	0.43
1:D:103:GLU:CD	1:D:103:GLU:H	2.19	0.43
1:E:228:ILE:HD13	1:E:228:ILE:N	2.32	0.43
1:E:266:GLU:HG2	1:E:267:LEU:N	2.33	0.43
1:E:277:PRO:HA	1:G:194:ARG:HH21	1.82	0.43
1:F:125:ILE:CG2	1:F:143:ILE:HG22	2.48	0.43
1:F:277:PRO:HG3	1:H:193:LEU:HD12	2.00	0.43
1:G:167:ILE:O	1:G:167:ILE:HG22	2.18	0.43
1:G:327:ILE:HG23	1:G:331:ASN:HD22	1.83	0.43
1:G:1:LEU:HD21	1:G:332:TRP:CE3	2.54	0.43
1:H:79:PRO:HB2	1:H:107:LYS:CB	2.47	0.43
1:B:9:GLY:O	1:B:13:ARG:HG3	2.17	0.43
1:D:174:THR:O	1:D:174:THR:HG23	2.19	0.43
1:D:209:GLY:O	1:D:210:ALA:C	2.57	0.43
1:E:177:SER:OG	1:E:237:VAL:O	2.36	0.43
1:G:64:ILE:HG23	1:G:73:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.53	0.43
1:A:101:ASP:HA	1:A:125:ILE:HD11	2.00	0.43
1:A:39:GLN:NE2	1:D:190:HIS:O	2.44	0.43
1:E:312:ASP:O	1:E:314:GLU:N	2.51	0.43
1:E:55:ALA:HB1	1:E:67:ASP:OD1	2.19	0.43
1:H:61:GLU:O	1:H:61:GLU:HG3	2.19	0.43
1:E:139:HIS:CG	1:E:331:ASN:O	2.72	0.43
1:F:304:MET:HB2	1:H:169:LYS:HZ2	1.82	0.43
1:G:69:LYS:HE3	1:G:71:ILE:HD11	2.00	0.43
1:H:37:VAL:HG22	1:H:73:VAL:HB	2.01	0.43
1:A:133:ASN:HD22	1:A:133:ASN:C	2.22	0.43
1:B:251:PHE:N	1:B:251:PHE:CD1	2.87	0.43
1:D:250:THR:OG1	1:D:251:PHE:N	2.52	0.43
1:E:79:PRO:HA	1:E:82:LEU:HD11	1.99	0.43
1:F:235:PRO:CB	1:G:201:LEU:HD11	2.48	0.43
1:F:1:LEU:HD22	1:F:329:ALA:HB2	2.01	0.43
1:O:33:THR:HG21	1:O:77:ARG:HG2	1.99	0.43
1:B:33:THR:HA	1:B:75:SER:OG	2.19	0.43
1:D:100:VAL:HA	1:D:118:ILE:HD13	2.00	0.43
1:D:84:TRP:CB	1:D:112:GLY:HA3	2.48	0.43
1:E:9:GLY:CA	2:E:335:NAD:H4B	2.48	0.43
1:F:105:ALA:HB3	1:F:143:ILE:HD13	2.01	0.43
1:G:158:VAL:HG11	1:G:221:LEU:CD2	2.49	0.43
1:G:219:PRO:O	1:G:221:LEU:N	2.52	0.43
1:H:23:SER:O	1:H:25:LEU:N	2.43	0.43
1:O:17:ARG:NH2	1:O:50:LEU:HB3	2.34	0.43
1:A:238:SER:HB2	1:A:311:TYR:CE1	2.53	0.43
1:B:236:ASN:O	1:B:237:VAL:HB	2.18	0.43
1:C:183:ARG:NH1	1:C:188:SER:O	2.52	0.43
1:D:72:GLN:HE22	1:H:83:PRO:HG3	1.84	0.43
1:G:0:LYS:HG3	4:G:597:HOH:O	2.17	0.43
1:G:18(A):TRP:O	1:G:19:GLY:N	2.52	0.43
1:G:28:ILE:HD11	1:G:89:ILE:HD11	1.99	0.43
1:H:261:ASP:OD1	1:H:262:SER:N	2.52	0.43
1:H:36:GLY:HA3	1:H:38:LYS:CD	2.49	0.43
1:H:3:VAL:O	1:H:28:ILE:HG22	2.19	0.43
1:O:202:ASN:HD21	1:Q:281:VAL:HG12	1.82	0.43
1:Q:162:ASP:HB2	1:Q:167:ILE:HD12	2.01	0.43
1:A:84:TRP:HB2	1:A:111:ALA:O	2.19	0.42
1:A:37:VAL:CG1	1:A:59:PRO:HB3	2.49	0.42
1:A:84:TRP:CE3	1:A:89:ILE:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18(B):HIS:HE1	1:B:67:ASP:OD2	2.01	0.42
1:B:240:VAL:HG23	1:B:240:VAL:O	2.19	0.42
1:B:96:THR:OG1	1:B:98:VAL:HG22	2.19	0.42
1:C:174:THR:O	1:C:174:THR:HG23	2.19	0.42
1:D:179:THR:O	1:D:181:ASP:N	2.52	0.42
1:F:173:THR:OG1	1:F:228:ILE:HD11	2.19	0.42
1:G:164:LYS:HG2	1:G:164:LYS:O	2.19	0.42
1:G:261:ASP:O	1:G:262:SER:C	2.57	0.42
1:H:195:ARG:NH2	1:H:206:THR:HG21	2.27	0.42
1:H:70:ILE:CG2	1:H:71:ILE:N	2.81	0.42
1:O:253:GLU:N	1:O:253:GLU:CD	2.72	0.42
1:A:191:ARG:NH1	1:A:191:ARG:HB2	2.34	0.42
1:E:78:ASN:HB3	1:E:81:LEU:HG	1.99	0.42
1:H:209:GLY:HA3	1:H:212:LYS:HE2	2.01	0.42
1:O:249:LYS:HB3	1:O:302:ASP:HB3	2.00	0.42
1:Q:242:LEU:O	1:Q:306:LYS:HA	2.19	0.42
1:Q:31:ASN:HA	1:Q:74:VAL:O	2.19	0.42
1:B:163:GLN:HE21	1:B:164:LYS:CE	2.32	0.42
1:C:24:PRO:HD2	1:C:326:ASP:OD1	2.19	0.42
1:C:28:ILE:HD11	1:C:89:ILE:HD13	2.01	0.42
1:D:156:PRO:HB2	1:D:290:THR:HG21	2.01	0.42
1:E:150:THR:HB	1:E:210:ALA:CB	2.49	0.42
1:E:242:LEU:HD21	1:E:244:VAL:HG13	2.00	0.42
1:E:84:TRP:C	1:E:112:GLY:HA3	2.40	0.42
1:E:29:ALA:HB1	1:E:84:TRP:HZ3	1.85	0.42
1:F:126:PRO:HB3	1:F:128:TYR:OH	2.18	0.42
1:F:154:LEU:O	1:F:158:VAL:HG23	2.19	0.42
1:F:37:VAL:HG12	1:F:38:LYS:N	2.34	0.42
1:H:154:LEU:O	1:H:155:ALA:C	2.58	0.42
1:F:234:THR:HG22	1:H:233:PRO:HG2	2.00	0.42
1:A:162:ASP:OD2	1:A:220:ASN:ND2	2.39	0.42
1:C:241:ASP:OD2	1:C:306:LYS:HE2	2.19	0.42
1:D:178:TYR:HB2	1:D:182:GLN:OE1	2.18	0.42
1:E:159:LYS:HB2	1:E:218:LEU:HD11	2.01	0.42
1:E:269:GLY:HA2	1:E:288:PHE:CE1	2.54	0.42
1:F:58:LYS:O	1:F:65:SER:N	2.52	0.42
1:G:236:ASN:O	1:G:237:VAL:CB	2.67	0.42
1:H:171:THR:HG23	1:H:243:VAL:HB	2.01	0.42
1:A:142:PRO:C	1:A:143:ILE:HD12	2.40	0.42
1:D:264:GLU:CA	1:D:268:LYS:HE3	2.43	0.42
1:D:15:PHE:CD1	1:D:322:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:NE2	1:H:83:PRO:HG3	2.34	0.42
1:D:7:GLY:HA3	1:D:96:THR:HG22	2.01	0.42
1:E:185:LEU:O	1:E:186:ASP:C	2.57	0.42
1:E:252:ALA:HA	1:E:299:VAL:HG23	2.02	0.42
1:E:79:PRO:HA	1:E:82:LEU:CG	2.49	0.42
1:F:132:VAL:C	1:F:134:ALA:H	2.23	0.42
1:F:27:ILE:HD12	1:F:27:ILE:H	1.82	0.42
1:O:132:VAL:HG21	1:O:155:ALA:HB1	2.01	0.42
1:Q:16:LEU:HD23	1:Q:16:LEU:O	2.19	0.42
1:Q:241:ASP:HA	1:Q:308:ILE:HD13	2.01	0.42
1:A:197:ARG:O	1:A:198:ALA:C	2.57	0.42
1:A:1:LEU:HD21	1:A:332:TRP:CE3	2.54	0.42
1:B:260:ARG:NH2	1:B:275:ASP:OD1	2.52	0.42
1:D:153:CYS:SG	1:D:290:THR:HB	2.59	0.42
1:D:240:VAL:HG13	1:D:311:TYR:HE1	1.82	0.42
1:E:188:SER:HA	1:H:39:GLN:OE1	2.19	0.42
1:E:194:ARG:NH1	1:E:205:PRO:CG	2.83	0.42
1:E:202:ASN:OD1	1:E:202:ASN:N	2.52	0.42
1:F:222:LYS:HG2	1:F:224:LYS:HE3	1.98	0.42
1:F:41:SER:OG	1:F:59:PRO:HD3	2.20	0.42
1:G:157:PHE:HZ	1:G:242:LEU:HD22	1.85	0.42
1:G:256:ASN:HD21	1:G:297:THR:CG2	2.18	0.42
1:O:205:PRO:HG2	1:Q:310:TRP:HZ2	1.85	0.42
1:B:129:VAL:H	1:B:133:ASN:ND2	2.18	0.42
1:B:243:VAL:HG11	1:D:243:VAL:HG11	2.00	0.42
1:D:192:ASP:HB3	1:D:195:ARG:HB2	2.01	0.42
1:E:239:VAL:HG22	1:E:240:VAL:H	1.83	0.42
1:H:251:PHE:O	1:H:255:VAL:HG23	2.19	0.42
1:H:275:ASP:OD1	1:H:294:SER:OG	2.34	0.42
1:O:194:ARG:HD2	1:O:205:PRO:O	2.18	0.42
1:O:271:LEU:HD23	1:O:271:LEU:C	2.40	0.42
1:A:182:GLN:HB3	1:A:199:ALA:HB2	2.00	0.42
1:B:191:ARG:HH11	1:B:191:ARG:HB2	1.84	0.42
1:B:65:SER:HA	1:B:69:LYS:O	2.20	0.42
1:C:177:SER:OG	1:C:234:THR:O	2.34	0.42
1:D:128:TYR:HA	1:D:133:ASN:HD21	1.85	0.42
1:E:183:ARG:CZ	1:E:187:ALA:CB	2.96	0.42
1:F:156:PRO:HB2	1:F:290:THR:HG21	2.01	0.42
1:G:291:THR:O	1:G:291:THR:CG2	2.67	0.42
1:O:60:SER:HB2	1:O:65:SER:HB2	2.02	0.42
1:Q:79:PRO:HA	1:Q:82:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:HIS:CE1	1:A:333:LYS:HG2	2.55	0.42
1:B:23:SER:HA	1:B:24:PRO:HD3	1.78	0.42
1:C:237:VAL:CG2	1:C:284:ARG:HD3	2.50	0.42
1:D:79:PRO:HB2	1:D:107:LYS:CB	2.50	0.42
1:E:137:TYR:CZ	1:E:139:HIS:HA	2.55	0.42
1:E:162:ASP:HB2	1:E:167:ILE:HD12	2.01	0.42
1:E:31:ASN:ND2	2:E:335:NAD:H2A	2.34	0.42
1:H:84:TRP:HD1	1:H:111:ALA:HB3	1.85	0.42
1:C:106:GLY:O	1:C:110:GLU:HG3	2.19	0.42
1:D:2:LYS:HZ2	1:H:87:LEU:HD13	1.85	0.42
1:D:63:ALA:HB2	1:D:72:GLN:HA	2.02	0.42
1:E:129:VAL:HB	1:E:133:ASN:ND2	2.34	0.42
1:E:291:THR:HB	1:E:310:TRP:HB2	2.02	0.42
1:H:6:ASN:HD22	1:H:96:THR:HG21	1.85	0.42
1:A:228:ILE:C	1:A:228:ILE:CD1	2.87	0.41
1:F:36:GLY:O	1:F:37:VAL:C	2.58	0.41
1:G:213:ALA:O	1:G:215:ALA:N	2.53	0.41
1:G:255:VAL:HG12	1:G:259:PHE:CE2	2.56	0.41
1:H:36:GLY:C	1:H:38:LYS:HD2	2.40	0.41
1:O:170:GLY:HA3	1:O:244:VAL:HG12	2.02	0.41
1:O:256:ASN:O	1:O:260:ARG:HG3	2.20	0.41
1:A:116:VAL:HB	1:A:143:ILE:HG13	2.02	0.41
1:A:238:SER:HB2	1:A:311:TYR:CZ	2.54	0.41
1:C:156:PRO:HB2	1:C:290:THR:CG2	2.43	0.41
1:C:271:LEU:HG	1:C:272:ASP:N	2.35	0.41
1:E:154:LEU:CD1	1:E:240:VAL:HG11	2.50	0.41
1:E:185:LEU:O	1:E:187:ALA:N	2.53	0.41
1:E:324:LEU:HD12	1:E:327:ILE:HD12	2.01	0.41
1:F:118:ILE:HD11	1:F:143:ILE:HG23	2.02	0.41
1:F:218:LEU:O	1:F:221:LEU:HD23	2.20	0.41
1:F:37:VAL:HG22	1:F:63:ALA:H	1.85	0.41
1:F:85:LYS:HE3	1:F:85:LYS:O	2.20	0.41
1:F:4:ALA:HB2	1:F:89:ILE:HD12	2.03	0.41
1:O:191:ARG:HH11	1:O:191:ARG:HG3	1.82	0.41
1:O:76:ASN:HB3	1:O:82:LEU:CD2	2.50	0.41
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.56	0.41
1:A:129:VAL:HG23	1:A:217:VAL:HG11	2.02	0.41
1:D:109:ILE:HG13	1:D:116:VAL:HG23	2.01	0.41
1:E:214:VAL:HG12	1:E:214:VAL:O	2.20	0.41
1:F:34:GLY:HA2	1:F:39:GLN:NE2	2.35	0.41
1:G:320:ARG:NE	1:G:323:ASP:OD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:LEU:HB3	1:H:57:VAL:HG11	2.02	0.41
1:H:83:PRO:HB2	1:H:86:GLU:HG2	2.03	0.41
1:Q:221:LEU:HD12	1:Q:225:LEU:HD11	2.01	0.41
1:B:100:VAL:O	1:B:118:ILE:HD13	2.20	0.41
1:E:239:VAL:HG22	1:E:240:VAL:N	2.36	0.41
1:E:30:ILE:CD1	1:E:71:ILE:HD12	2.50	0.41
1:F:17:ARG:HD3	1:F:50:LEU:CD1	2.50	0.41
1:F:202:ASN:HD21	1:H:281:VAL:HG12	1.85	0.41
1:G:170:GLY:CA	1:G:243:VAL:O	2.67	0.41
1:G:291:THR:HG22	1:G:310:TRP:HB2	2.01	0.41
1:G:39:GLN:O	1:G:40:ALA:C	2.57	0.41
1:H:115:LYS:HB2	1:H:115:LYS:HE2	1.97	0.41
1:Q:175:THR:CG2	1:Q:232:VAL:HG11	2.50	0.41
1:B:165:PHE:CB	1:B:246:VAL:HG11	2.51	0.41
1:B:262:SER:HB3	1:B:267:LEU:HB2	2.02	0.41
1:B:39:GLN:HE22	1:C:188:SER:HB2	1.86	0.41
1:C:2:LYS:HD3	1:C:28:ILE:CD1	2.50	0.41
1:F:138:SER:O	1:F:139:HIS:HB3	2.19	0.41
1:F:79:PRO:HA	1:F:82:LEU:CD1	2.43	0.41
1:G:302:ASP:HB3	4:G:651:HOH:O	2.20	0.41
1:F:310:TRP:CZ2	1:H:205:PRO:HG2	2.55	0.41
1:H:216:LEU:N	1:H:216:LEU:HD12	2.35	0.41
1:C:77:ARG:NH2	4:C:364:HOH:O	2.45	0.41
1:D:6:ASN:OD1	1:D:31:ASN:ND2	2.40	0.41
1:F:117:ILE:HD11	1:F:328:VAL:HG21	2.03	0.41
1:F:319:GLN:HA	1:F:319:GLN:OE1	2.20	0.41
1:G:109:ILE:HA	1:G:113:ALA:O	2.20	0.41
1:H:100:VAL:HG23	1:H:101:ASP:N	2.36	0.41
1:O:194:ARG:CZ	1:Q:277:PRO:HA	2.51	0.41
1:B:221:LEU:HD22	1:B:221:LEU:N	2.35	0.41
1:C:96:THR:HB	1:C:98:VAL:HG22	2.02	0.41
1:E:131:GLY:HA3	1:E:270:ILE:HG21	2.03	0.41
1:F:114:LYS:HB2	1:F:332:TRP:HH2	1.85	0.41
1:F:114:LYS:N	1:F:114:LYS:CD	2.82	0.41
1:F:128:TYR:OH	1:F:141:GLU:OE2	2.39	0.41
1:F:269:GLY:HA2	1:F:288:PHE:CE2	2.56	0.41
1:F:28:ILE:O	1:F:72:GLN:HB2	2.20	0.41
1:G:177:SER:CB	1:G:234:THR:O	2.66	0.41
1:A:96:THR:OG1	1:A:98:VAL:HG22	2.20	0.41
1:C:102:ARG:HB2	1:C:125:ILE:HD11	2.01	0.41
1:F:78:ASN:CB	1:F:81:LEU:HD13	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:THR:O	1:G:242:LEU:HA	2.19	0.41
1:G:324:LEU:O	1:G:327:ILE:HB	2.21	0.41
1:H:118:ILE:HG22	1:H:120:ALA:H	1.86	0.41
1:H:271:LEU:HD12	1:H:290:THR:O	2.21	0.41
1:H:76:ASN:HB3	1:H:82:LEU:HD23	2.03	0.41
1:O:327:ILE:O	1:O:328:VAL:C	2.59	0.41
1:B:154:LEU:O	1:B:155:ALA:C	2.57	0.41
1:C:8:PHE:O	1:C:13:ARG:NH1	2.51	0.41
1:D:9:GLY:HA3	2:D:335:NAD:O5B	2.21	0.41
1:E:168:ILE:HD11	1:E:247:SER:HB3	2.02	0.41
1:F:5:ILE:HD11	1:F:12:GLY:CA	2.51	0.41
1:F:267:LEU:HD13	1:F:271:LEU:HB2	2.03	0.41
1:G:317:TYR:O	1:G:320:ARG:HB2	2.21	0.41
1:G:28:ILE:C	1:G:71:ILE:HG23	2.41	0.41
1:G:29:ALA:HA	1:G:72:GLN:O	2.21	0.41
1:H:41:SER:O	1:H:57:VAL:HG12	2.21	0.41
1:H:85:LYS:CG	1:H:112:GLY:HA3	2.50	0.41
1:O:141:GLU:HA	1:O:142:PRO:HD2	1.92	0.41
1:O:271:LEU:HD23	1:O:272:ASP:N	2.36	0.41
1:Q:9:GLY:O	1:Q:10:ARG:C	2.59	0.41
1:B:153:CYS:O	1:B:290:THR:HG21	2.21	0.41
1:D:89:ILE:N	1:D:89:ILE:HD12	2.36	0.41
1:F:145:SER:C	1:F:147:ALA:N	2.72	0.41
1:F:249:LYS:HZ3	1:F:302:ASP:HB2	1.86	0.41
1:F:282:ASP:OD2	1:H:197:ARG:NH1	2.50	0.41
1:F:333:LYS:OXT	1:F:333:LYS:HG3	2.21	0.41
1:F:17:ARG:NH2	1:F:53:PHE:HA	2.36	0.41
1:G:207:SER:O	1:G:208:THR:HB	2.20	0.41
1:H:38:LYS:CD	1:H:38:LYS:N	2.82	0.41
1:O:190:HIS:HB3	1:O:196:ALA:HB2	2.02	0.41
1:Q:142:PRO:O	1:Q:143:ILE:HD13	2.21	0.41
1:Q:90:ASP:HA	1:Q:114:LYS:CG	2.51	0.41
1:A:76:ASN:HD21	1:A:78:ASN:HB3	1.86	0.41
1:C:100:VAL:HA	1:C:118:ILE:HD13	2.03	0.41
1:C:2:LYS:HD2	1:C:88:GLY:O	2.21	0.41
1:D:137:TYR:CE2	1:D:328:VAL:HA	2.56	0.41
1:D:243:VAL:HG22	1:D:306:LYS:HE3	2.02	0.41
1:D:5:ILE:HD11	1:D:27:ILE:HD13	2.03	0.41
1:G:132:VAL:HG12	1:G:133:ASN:N	2.36	0.41
1:G:265:LYS:HD2	1:G:265:LYS:HA	1.83	0.41
1:G:272:ASP:HB2	1:G:288:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ALA:O	1:H:219:PRO:HA	2.21	0.41
1:O:239:VAL:CG2	1:O:308:ILE:HG23	2.51	0.41
1:B:202:ASN:O	1:B:233:PRO:HD3	2.21	0.40
1:E:178:TYR:HB2	1:E:199:ALA:HB1	2.02	0.40
1:E:275:ASP:HA	1:E:294:SER:OG	2.20	0.40
1:F:165:PHE:HD1	1:F:248:LYS:HB3	1.86	0.40
1:F:283:PHE:N	1:F:283:PHE:CD2	2.89	0.40
1:F:48:SER:OG	1:G:202:ASN:ND2	2.54	0.40
1:F:31:ASN:CB	1:F:74:VAL:HG13	2.43	0.40
1:G:173:THR:O	1:G:241:ASP:N	2.54	0.40
1:H:41:SER:CB	1:H:59:PRO:HG3	2.50	0.40
1:H:79:PRO:O	1:H:80:SER:C	2.59	0.40
1:Q:115:LYS:HB2	1:Q:115:LYS:HE3	1.82	0.40
1:A:154:LEU:HD22	1:A:172:MET:HE2	2.03	0.40
1:A:139:HIS:ND1	1:A:333:LYS:HB3	2.36	0.40
1:B:264:GLU:O	1:B:265:LYS:HD3	2.21	0.40
1:C:157:PHE:HB2	1:C:259:PHE:CE1	2.56	0.40
1:C:64:ILE:HD13	1:C:66:VAL:HG23	2.04	0.40
1:D:137:TYR:CZ	1:D:328:VAL:HG22	2.57	0.40
1:E:146:ASN:O	1:E:146:ASN:OD1	2.39	0.40
1:F:139:HIS:HB2	1:F:331:ASN:O	2.22	0.40
1:G:208:THR:O	1:G:210:ALA:N	2.54	0.40
1:Q:235:PRO:O	1:Q:236:ASN:HB2	2.20	0.40
1:C:333:LYS:HA	1:C:333:LYS:HD2	1.81	0.40
1:D:142:PRO:O	1:D:143:ILE:HD13	2.21	0.40
1:D:275:ASP:HA	1:D:294:SER:OG	2.21	0.40
1:E:176:HIS:CE1	1:E:313:ASN:HD22	2.40	0.40
1:E:94:GLU:HB3	1:E:118:ILE:HG23	2.04	0.40
1:G:18(A):TRP:HH2	1:G:69:LYS:HE2	1.85	0.40
1:H:76:ASN:HB3	1:H:82:LEU:CD2	2.51	0.40
1:O:293:ASP:OD1	1:O:296:LEU:HG	2.21	0.40
1:O:31:ASN:HB2	1:O:74:VAL:HG22	2.03	0.40
1:A:279:VAL:HG22	1:C:197:ARG:NH1	2.36	0.40
1:B:1:LEU:HD22	1:B:329:ALA:HA	2.03	0.40
1:C:31:ASN:O	1:C:32:ASP:HB2	2.22	0.40
1:E:109:ILE:C	1:E:109:ILE:HD13	2.42	0.40
1:E:252:ALA:CB	1:E:298:MET:HA	2.49	0.40
1:E:275:ASP:HB3	1:E:294:SER:OG	2.21	0.40
1:F:16:LEU:O	1:F:16:LEU:HD23	2.21	0.40
1:F:3:VAL:HG22	1:F:91:ILE:HG23	2.01	0.40
1:G:232:VAL:HG23	1:G:234:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:ARG:C	1:H:196:ALA:N	2.75	0.40
1:H:239:VAL:O	1:H:239:VAL:HG13	2.22	0.40
1:B:164:LYS:HA	1:B:164:LYS:HD2	1.90	0.40
1:D:146:ASN:HD22	1:D:321:VAL:CG2	2.34	0.40
1:D:172:MET:HE3	1:D:211:ALA:HB2	2.02	0.40
1:E:242:LEU:HD21	1:E:244:VAL:CG1	2.51	0.40
1:E:27:ILE:HD11	1:E:30:ILE:HG12	2.03	0.40
1:F:240:VAL:O	1:F:240:VAL:CG2	2.70	0.40
1:F:91:ILE:HD11	1:F:117:ILE:HD12	2.03	0.40
1:H:154:LEU:HD21	1:H:172:MET:HG3	2.04	0.40
1:H:294:SER:C	1:H:296:LEU:N	2.74	0.40
1:Q:122(A):LYS:HD3	1:Q:122(A):LYS:HA	1.88	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:D:331:ASN:OD1	1:D:331:ASN:OD1[3_656]	2.18	0.02

## 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	335/337 (99%)	292 (87%)	36 (11%)	7 (2%)	7	13
1	B	335/337 (99%)	293 (88%)	34 (10%)	8 (2%)	6	10
1	C	335/337 (99%)	293 (88%)	34 (10%)	8 (2%)	6	10
1	D	334/337 (99%)	269 (80%)	52 (16%)	13 (4%)	3	4
1	E	334/337 (99%)	260 (78%)	57 (17%)	17 (5%)	2	2
1	F	334/337 (99%)	244 (73%)	67 (20%)	23 (7%)	1	1
1	G	334/337 (99%)	257 (77%)	55 (16%)	22 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	333/337 (99%)	248 (74%)	61 (18%)	24 (7%)	1	1
1	O	335/337 (99%)	308 (92%)	24 (7%)	3 (1%)	17	35
1	Q	334/337 (99%)	298 (89%)	31 (9%)	5 (2%)	10	21
All	All	3343/3370 (99%)	2762 (83%)	451 (14%)	130 (4%)	3	4

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	SER
1	D	1	LEU
1	D	210	ALA
1	E	75	SER
1	E	237	VAL
1	E	313	ASN
1	F	37	VAL
1	F	76	ASN
1	F	280	SER
1	G	198	ALA
1	G	202	ASN
1	G	208	THR
1	G	225	LEU
1	G	295	SER
1	H	27	ILE
1	H	28	ILE
1	H	71	ILE
1	H	87	LEU
1	H	89	ILE
1	H	133	ASN
1	Q	2	LYS
1	Q	124	ASP
1	A	237	VAL
1	B	0	LYS
1	B	166	GLY
1	B	237	VAL
1	B	302	ASP
1	C	237	VAL
1	D	36	GLY
1	D	166	GLY
1	D	180	GLY
1	D	237	VAL
1	E	55	ALA

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Mol	Chain	Res	Type
1	E	74	VAL
1	E	139	HIS
1	E	186	ASP
1	E	233	PRO
1	E	252	ALA
1	F	49	THR
1	F	69	LYS
1	F	130	VAL
1	F	146	ASN
1	F	266	GLU
1	F	297	THR
1	G	132	VAL
1	G	163	GLN
1	G	166	GLY
1	G	199	ALA
1	G	220	ASN
1	G	223	GLY
1	G	226	ASN
1	G	237	VAL
1	H	22	ASP
1	H	104	GLY
1	H	186	ASP
1	H	237	VAL
1	H	295	SER
1	O	237	VAL
1	Q	302	ASP
1	A	8	PHE
1	A	133	ASN
1	B	233	PRO
1	C	33	THR
1	C	34	GLY
1	C	198	ALA
1	D	55	ALA
1	E	56	ASP
1	F	8	PHE
1	F	132	VAL
1	F	211	ALA
1	F	237	VAL
1	G	18(B)	HIS
1	G	214	VAL
1	G	285	CYS
1	H	43	LEU

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Mol	Chain	Res	Type
1	H	76	ASN
1	H	140	ASP
1	Q	237	VAL
1	B	198	ALA
1	B	249	LYS
1	C	133	ASN
1	D	233	PRO
1	D	252	ALA
1	E	22	ASP
1	E	33	THR
1	E	73	VAL
1	E	193	LEU
1	E	285	CYS
1	F	186	ASP
1	F	285	CYS
1	F	294	SER
1	G	60	SER
1	G	162	ASP
1	G	190	HIS
1	G	207	SER
1	G	246	VAL
1	H	55	ALA
1	H	195	ARG
1	H	226	ASN
1	H	233	PRO
1	O	198	ALA
1	D	22	ASP
1	D	198	ALA
1	F	103	GLU
1	F	139	HIS
1	G	139	HIS
1	H	163	GLN
1	H	166	GLY
1	H	331	ASN
1	O	166	GLY
1	A	0	LYS
1	A	186	ASP
1	F	7	GLY
1	F	24	PRO
1	H	79	PRO
1	E	24	PRO
1	E	279	VAL

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Mol	Chain	Res	Type
1	F	66	VAL
1	B	104	GLY
1	C	83	PRO
1	D	219	PRO
1	F	281	VAL
1	A	166	GLY
1	C	233	PRO
1	D	156	PRO
1	F	219	PRO
1	H	74	VAL
1	A	37	VAL
1	H	142	PRO
1	Q	34	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/279 (100%)	264 (95%)	15 (5%)	22	44
1	B	279/279 (100%)	268 (96%)	11 (4%)	32	58
1	C	279/279 (100%)	265 (95%)	14 (5%)	24	47
1	D	279/279 (100%)	272 (98%)	7 (2%)	47	73
1	E	278/279 (100%)	260 (94%)	18 (6%)	17	34
1	F	279/279 (100%)	264 (95%)	15 (5%)	22	44
1	G	279/279 (100%)	259 (93%)	20 (7%)	14	29
1	H	278/279 (100%)	261 (94%)	17 (6%)	18	38
1	O	279/279 (100%)	266 (95%)	13 (5%)	26	50
1	Q	279/279 (100%)	263 (94%)	16 (6%)	20	41
All	All	2788/2790 (100%)	2642 (95%)	146 (5%)	23	46

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	84	TRP
1	A	85	LYS
1	A	91	ILE
1	A	133	ASN
1	A	163	GLN
1	A	164	LYS
1	A	172	MET
1	A	191	ARG
1	A	240	VAL
1	A	265	LYS
1	A	266	GLU
1	A	276	GLU
1	A	290	THR
1	A	333	LYS
1	B	16	LEU
1	B	38	LYS
1	B	58	LYS
1	B	84	TRP
1	B	107	LYS
1	B	124	ASP
1	B	133	ASN
1	B	140	ASP
1	B	246	VAL
1	B	271	LEU
1	B	290	THR
1	C	14	ASN
1	C	21	LYS
1	C	58	LYS
1	C	76	ASN
1	C	84	TRP
1	C	86	GLU
1	C	135	ASP
1	C	169	LYS
1	C	172	MET
1	C	191	ARG
1	C	226	ASN
1	C	261	ASP
1	C	290	THR
1	C	333	LYS
1	D	8	PHE
1	D	56	ASP
1	D	58	LYS

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Mol	Chain	Res	Type
1	D	84	TRP
1	D	133	ASN
1	D	228	ILE
1	D	290	THR
1	E	8	PHE
1	E	14	ASN
1	E	17	ARG
1	E	56	ASP
1	E	58	LYS
1	E	67	ASP
1	E	70	ILE
1	E	71	ILE
1	E	84	TRP
1	E	109	ILE
1	E	133	ASN
1	E	172	MET
1	E	183	ARG
1	E	191	ARG
1	E	202	ASN
1	E	228	ILE
1	E	233	PRO
1	E	290	THR
1	F	11	ILE
1	F	14	ASN
1	F	25	LEU
1	F	62	THR
1	F	85	LYS
1	F	91	ILE
1	F	115	LYS
1	F	121	PRO
1	F	124	ASP
1	F	133	ASN
1	F	174	THR
1	F	191	ARG
1	F	228	ILE
1	F	290	THR
1	F	300	MET
1	G	0	LYS
1	G	72	GLN
1	G	84	TRP
1	G	85	LYS
1	G	103	GLU

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Mol	Chain	Res	Type
1	G	115	LYS
1	G	130	VAL
1	G	133	ASN
1	G	138	SER
1	G	149	CYS
1	G	150	THR
1	G	178	TYR
1	G	191	ARG
1	G	228	ILE
1	G	234	THR
1	G	253	GLU
1	G	256	ASN
1	G	265	LYS
1	G	279	VAL
1	G	300	MET
1	H	38	LYS
1	H	67	ASP
1	H	72	GLN
1	H	76	ASN
1	H	84	TRP
1	H	90	ASP
1	H	91	ILE
1	H	124	ASP
1	H	133	ASN
1	H	164	LYS
1	H	178	TYR
1	H	181	ASP
1	H	186	ASP
1	H	228	ILE
1	H	290	THR
1	H	300	MET
1	H	311	TYR
1	O	3	VAL
1	O	16	LEU
1	O	17	ARG
1	O	39	GLN
1	O	72	GLN
1	O	84	TRP
1	O	94	GLU
1	O	124	ASP
1	O	133	ASN
1	O	138	SER

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Mol	Chain	Res	Type
1	O	177	SER
1	O	178	TYR
1	O	264	GLU
1	Q	8	PHE
1	Q	38	LYS
1	Q	39	GLN
1	Q	56	ASP
1	Q	76	ASN
1	Q	84	TRP
1	Q	103	GLU
1	Q	114	LYS
1	Q	133	ASN
1	Q	135	ASP
1	Q	140	ASP
1	Q	172	MET
1	Q	178	TYR
1	Q	191	ARG
1	Q	276	GLU
1	Q	290	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	78	ASN
1	A	133	ASN
1	A	152	ASN
1	A	163	GLN
1	A	202	ASN
1	A	245	GLN
1	A	256	ASN
1	A	330	ASN
1	B	18(B)	HIS
1	B	39	GLN
1	B	133	ASN
1	B	152	ASN
1	B	163	GLN
1	B	226	ASN
1	B	256	ASN
1	B	330	ASN
1	C	39	GLN
1	C	42	HIS

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Mol	Chain	Res	Type
1	C	72	GLN
1	C	76	ASN
1	C	133	ASN
1	C	152	ASN
1	C	202	ASN
1	C	226	ASN
1	C	256	ASN
1	C	330	ASN
1	D	72	GLN
1	D	133	ASN
1	D	139	HIS
1	D	146	ASN
1	D	202	ASN
1	D	226	ASN
1	D	256	ASN
1	D	330	ASN
1	E	18(B)	HIS
1	E	42	HIS
1	E	108	HIS
1	E	133	ASN
1	E	146	ASN
1	E	152	ASN
1	E	202	ASN
1	E	226	ASN
1	E	245	GLN
1	E	256	ASN
1	E	330	ASN
1	F	42	HIS
1	F	133	ASN
1	F	139	HIS
1	F	152	ASN
1	F	202	ASN
1	F	256	ASN
1	F	330	ASN
1	G	72	GLN
1	G	133	ASN
1	G	152	ASN
1	G	202	ASN
1	G	256	ASN
1	G	330	ASN
1	G	331	ASN
1	H	42	HIS

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Mol	Chain	Res	Type
1	H	72	GLN
1	H	76	ASN
1	H	133	ASN
1	H	146	ASN
1	H	152	ASN
1	H	202	ASN
1	H	220	ASN
1	H	256	ASN
1	H	330	ASN
1	H	331	ASN
1	O	18(B)	HIS
1	O	72	GLN
1	O	78	ASN
1	O	133	ASN
1	O	152	ASN
1	O	202	ASN
1	O	256	ASN
1	Q	133	ASN
1	Q	152	ASN
1	Q	163	GLN
1	Q	202	ASN
1	Q	245	GLN
1	Q	256	ASN
1	Q	330	ASN
1	Q	331	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

55 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	335	-	42,48,48	1.51	10 (23%)	50,73,73	1.94	13 (26%)
3	SO4	F	334	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	Q	336	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	B	334	-	4,4,4	0.31	0	6,6,6	0.05	0
2	NAD	O	335	-	42,48,48	1.41	6 (14%)	50,73,73	1.88	14 (28%)
3	SO4	A	338	-	4,4,4	0.26	0	6,6,6	0.09	0
2	NAD	H	335	-	42,48,48	1.66	8 (19%)	50,73,73	1.97	13 (26%)
3	SO4	B	337	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	B	339	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	Q	338	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	O	340	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO4	A	341	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	B	338	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	F	336	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	A	337	-	4,4,4	0.32	0	6,6,6	0.14	0
2	NAD	G	335	-	42,48,48	1.65	6 (14%)	50,73,73	1.93	13 (26%)
2	NAD	D	335	-	42,48,48	1.61	8 (19%)	50,73,73	1.89	13 (26%)
2	NAD	F	335	-	42,48,48	1.69	8 (19%)	50,73,73	1.94	14 (28%)
2	NAD	C	335	-	42,48,48	1.74	8 (19%)	50,73,73	1.90	12 (24%)
2	NAD	B	335	-	42,48,48	1.51	7 (16%)	50,73,73	1.93	12 (24%)
3	SO4	D	337	-	4,4,4	0.27	0	6,6,6	0.06	0
3	SO4	F	337	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	E	338	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	Q	337	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	E	336	-	4,4,4	0.31	0	6,6,6	0.04	0
3	SO4	B	336	-	4,4,4	0.27	0	6,6,6	0.11	0
2	NAD	Q	335	-	42,48,48	1.68	10 (23%)	50,73,73	1.85	11 (22%)
3	SO4	A	336	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	C	337	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	E	337	-	4,4,4	0.25	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	E	334	-	4,4,4	0.26	0	6,6,6	0.13	0
3	SO4	O	338	-	4,4,4	0.27	0	6,6,6	0.05	0
3	SO4	G	337	-	4,4,4	0.29	0	6,6,6	0.06	0
3	SO4	O	334	-	4,4,4	0.26	0	6,6,6	0.14	0
3	SO4	H	334	-	4,4,4	0.27	0	6,6,6	0.07	0
2	NAD	E	335	-	42,48,48	1.58	7 (16%)	50,73,73	2.03	15 (30%)
3	SO4	G	338	-	4,4,4	0.27	0	6,6,6	0.05	0
3	SO4	A	340	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	O	337	-	4,4,4	0.29	0	6,6,6	0.20	0
3	SO4	D	336	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	Q	339	-	4,4,4	0.27	0	6,6,6	0.06	0
3	SO4	C	336	-	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	G	339	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	O	336	-	4,4,4	0.27	0	6,6,6	0.16	0
3	SO4	H	336	-	4,4,4	0.31	0	6,6,6	0.06	0
3	SO4	G	334	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	C	334	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	A	334	-	4,4,4	0.27	0	6,6,6	0.13	0
3	SO4	C	338	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	D	334	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	O	339	-	4,4,4	0.29	0	6,6,6	0.12	0
3	SO4	G	336	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	H	337	-	4,4,4	0.28	0	6,6,6	0.05	0
3	SO4	Q	334	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	A	339	-	4,4,4	0.24	0	6,6,6	0.07	0

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	335	-	-	9/26/62/62	0/5/5/5
2	NAD	F	335	-	-	10/26/62/62	0/5/5/5
2	NAD	C	335	-	-	9/26/62/62	0/5/5/5
2	NAD	B	335	-	-	6/26/62/62	0/5/5/5
2	NAD	O	335	-	-	5/26/62/62	0/5/5/5
2	NAD	H	335	-	-	11/26/62/62	0/5/5/5
2	NAD	E	335	-	-	13/26/62/62	0/5/5/5
2	NAD	Q	335	-	-	9/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	G	335	-	-	11/26/62/62	0/5/5/5
2	NAD	D	335	-	-	8/26/62/62	0/5/5/5

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	335	NAD	C3N-C7N	5.01	1.58	1.50
2	G	335	NAD	C3N-C7N	4.92	1.58	1.50
2	H	335	NAD	C3N-C7N	4.82	1.57	1.50
2	C	335	NAD	C3N-C7N	4.75	1.57	1.50
2	Q	335	NAD	C3N-C7N	4.75	1.57	1.50
2	D	335	NAD	C3N-C7N	4.48	1.57	1.50
2	C	335	NAD	C2N-N1N	4.42	1.40	1.35
2	E	335	NAD	C3N-C7N	4.31	1.57	1.50
2	G	335	NAD	C2N-N1N	4.02	1.39	1.35
2	D	335	NAD	C6N-N1N	4.00	1.45	1.35
2	F	335	NAD	C6N-N1N	3.97	1.45	1.35
2	H	335	NAD	C2N-N1N	3.92	1.39	1.35
2	E	335	NAD	C2N-N1N	3.87	1.39	1.35
2	B	335	NAD	C6N-N1N	3.86	1.44	1.35
2	E	335	NAD	C6N-N1N	3.84	1.44	1.35
2	Q	335	NAD	C6N-N1N	3.84	1.44	1.35
2	H	335	NAD	C6N-N1N	3.80	1.44	1.35
2	F	335	NAD	C2N-N1N	3.79	1.39	1.35
2	C	335	NAD	C6N-N1N	3.71	1.44	1.35
2	G	335	NAD	C6N-N1N	3.70	1.44	1.35
2	A	335	NAD	C6N-N1N	3.65	1.44	1.35
2	Q	335	NAD	C2N-N1N	3.61	1.39	1.35
2	O	335	NAD	C6N-N1N	3.51	1.44	1.35
2	O	335	NAD	C3N-C7N	3.48	1.55	1.50
2	A	335	NAD	C2N-N1N	3.43	1.39	1.35
2	Q	335	NAD	C4N-C3N	3.40	1.45	1.39
2	C	335	NAD	C4N-C3N	3.37	1.45	1.39
2	B	335	NAD	C3N-C7N	3.33	1.55	1.50
2	F	335	NAD	C4N-C3N	3.30	1.45	1.39
2	Q	335	NAD	O4B-C1B	3.24	1.45	1.41
2	C	335	NAD	O4B-C1B	3.21	1.45	1.41
2	H	335	NAD	O4B-C1B	3.19	1.45	1.41
2	D	335	NAD	C4N-C3N	3.17	1.44	1.39
2	B	335	NAD	C2N-N1N	3.15	1.38	1.35
2	B	335	NAD	O4B-C1B	3.00	1.45	1.41
2	E	335	NAD	C4N-C3N	2.96	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	335	NAD	C4N-C3N	2.95	1.44	1.39
2	D	335	NAD	C2N-N1N	2.92	1.38	1.35
2	A	335	NAD	O4B-C1B	2.88	1.45	1.41
2	O	335	NAD	O4B-C1B	2.87	1.45	1.41
2	G	335	NAD	O4B-C1B	2.84	1.45	1.41
2	Q	335	NAD	C4A-N3A	2.81	1.39	1.35
2	H	335	NAD	C4N-C3N	2.81	1.44	1.39
2	G	335	NAD	C4A-N3A	2.77	1.39	1.35
2	A	335	NAD	C3N-C7N	2.74	1.54	1.50
2	D	335	NAD	C4A-N3A	2.74	1.39	1.35
2	G	335	NAD	C4N-C3N	2.73	1.44	1.39
2	O	335	NAD	C4N-C3N	2.70	1.43	1.39
2	F	335	NAD	O4B-C1B	2.63	1.44	1.41
2	B	335	NAD	C4N-C3N	2.61	1.43	1.39
2	E	335	NAD	C4A-N3A	2.48	1.39	1.35
2	H	335	NAD	C4A-N3A	2.44	1.39	1.35
2	C	335	NAD	C2A-N3A	2.41	1.36	1.32
2	A	335	NAD	C4A-N3A	2.40	1.39	1.35
2	O	335	NAD	C2A-N3A	2.40	1.36	1.32
2	C	335	NAD	O3D-C3D	2.36	1.48	1.43
2	F	335	NAD	C2D-C1D	-2.35	1.50	1.53
2	Q	335	NAD	C2A-N3A	2.33	1.35	1.32
2	F	335	NAD	C4A-N3A	2.32	1.38	1.35
2	B	335	NAD	O5B-C5B	2.23	1.53	1.44
2	D	335	NAD	O4B-C1B	2.22	1.44	1.41
2	H	335	NAD	C2A-N3A	2.20	1.35	1.32
2	B	335	NAD	C4A-N3A	2.20	1.38	1.35
2	H	335	NAD	O5B-C5B	2.20	1.53	1.44
2	E	335	NAD	O4B-C1B	2.19	1.44	1.41
2	E	335	NAD	O5B-C5B	2.19	1.53	1.44
2	A	335	NAD	C2A-N3A	2.19	1.35	1.32
2	D	335	NAD	O3D-C3D	2.16	1.48	1.43
2	Q	335	NAD	O5B-C5B	2.15	1.53	1.44
2	A	335	NAD	C5N-C4N	2.15	1.43	1.38
2	Q	335	NAD	O3D-C3D	2.10	1.47	1.43
2	F	335	NAD	O5B-C5B	2.09	1.52	1.44
2	C	335	NAD	O5B-C5B	2.08	1.52	1.44
2	A	335	NAD	C7N-N7N	-2.06	1.29	1.33
2	A	335	NAD	O3D-C3D	2.05	1.47	1.43
2	D	335	NAD	C2B-C1B	-2.03	1.50	1.53
2	O	335	NAD	C2N-N1N	2.03	1.37	1.35
2	Q	335	NAD	C7N-N7N	-2.01	1.29	1.33

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	335	NAD	C5N-C6N-N1N	-5.61	112.35	120.40
2	B	335	NAD	C5N-C6N-N1N	-5.53	112.48	120.40
2	O	335	NAD	C5N-C6N-N1N	-5.42	112.63	120.40
2	G	335	NAD	C5N-C6N-N1N	-5.40	112.66	120.40
2	D	335	NAD	C5N-C6N-N1N	-5.40	112.66	120.40
2	C	335	NAD	C6N-N1N-C2N	5.38	126.88	121.97
2	Q	335	NAD	C5N-C6N-N1N	-5.36	112.72	120.40
2	E	335	NAD	C5N-C6N-N1N	-5.34	112.74	120.40
2	A	335	NAD	C6N-N1N-C2N	5.34	126.84	121.97
2	F	335	NAD	C5N-C6N-N1N	-5.33	112.76	120.40
2	H	335	NAD	C5N-C6N-N1N	-5.25	112.87	120.40
2	C	335	NAD	C5N-C6N-N1N	-5.22	112.92	120.40
2	F	335	NAD	C6N-N1N-C2N	5.14	126.67	121.97
2	Q	335	NAD	C6N-N1N-C2N	5.11	126.63	121.97
2	D	335	NAD	C6N-N1N-C2N	4.96	126.50	121.97
2	E	335	NAD	C6N-N1N-C2N	4.95	126.49	121.97
2	O	335	NAD	C6N-N1N-C2N	4.91	126.45	121.97
2	G	335	NAD	C6N-N1N-C2N	4.80	126.35	121.97
2	B	335	NAD	C6N-N1N-C2N	4.61	126.18	121.97
2	H	335	NAD	C6N-N1N-C2N	4.59	126.16	121.97
2	B	335	NAD	C6N-C5N-C4N	4.17	125.51	119.44
2	H	335	NAD	C6N-C5N-C4N	4.17	125.49	119.44
2	G	335	NAD	C6N-C5N-C4N	4.14	125.45	119.44
2	H	335	NAD	C4N-C3N-C7N	-4.13	109.99	121.04
2	E	335	NAD	C4N-C3N-C7N	-4.12	110.01	121.04
2	C	335	NAD	C3N-C2N-N1N	-4.05	116.46	120.43
2	A	335	NAD	C6N-C5N-C4N	4.03	125.30	119.44
2	E	335	NAD	C6N-C5N-C4N	4.01	125.27	119.44
2	C	335	NAD	C4N-C3N-C7N	-3.99	110.36	121.04
2	F	335	NAD	C6N-C5N-C4N	3.93	125.16	119.44
2	Q	335	NAD	C6N-C5N-C4N	3.91	125.12	119.44
2	D	335	NAD	C6N-C5N-C4N	3.89	125.10	119.44
2	G	335	NAD	C4N-C3N-C7N	-3.89	110.64	121.04
2	O	335	NAD	C6N-C5N-C4N	3.87	125.07	119.44
2	H	335	NAD	C3N-C7N-N7N	3.80	122.31	117.75
2	F	335	NAD	C4N-C3N-C7N	-3.72	111.07	121.04
2	C	335	NAD	C6N-C5N-C4N	3.70	124.81	119.44
2	A	335	NAD	C4N-C3N-C7N	-3.62	111.35	121.04
2	B	335	NAD	C4N-C3N-C7N	-3.62	111.36	121.04
2	G	335	NAD	C3N-C7N-N7N	3.58	122.04	117.75
2	E	335	NAD	C3N-C7N-N7N	3.57	122.04	117.75
2	D	335	NAD	C4N-C3N-C7N	-3.54	111.58	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	335	NAD	C3N-C2N-N1N	-3.53	116.98	120.43
2	O	335	NAD	C4N-C3N-C7N	-3.51	111.65	121.04
2	Q	335	NAD	C4N-C3N-C7N	-3.50	111.66	121.04
2	F	335	NAD	C3N-C2N-N1N	-3.50	117.00	120.43
2	F	335	NAD	C3N-C7N-N7N	3.47	121.92	117.75
2	O	335	NAD	C5N-C4N-C3N	-3.41	116.31	120.34
2	H	335	NAD	C3N-C2N-N1N	-3.37	117.14	120.43
2	G	335	NAD	C3N-C2N-N1N	-3.34	117.16	120.43
2	H	335	NAD	C3D-C2D-C1D	3.30	105.94	100.98
2	Q	335	NAD	C3N-C2N-N1N	-3.29	117.21	120.43
2	B	335	NAD	C5N-C4N-C3N	-3.24	116.51	120.34
2	A	335	NAD	C3N-C2N-N1N	-3.23	117.27	120.43
2	D	335	NAD	C3N-C2N-N1N	-3.17	117.33	120.43
2	A	335	NAD	C5N-C4N-C3N	-3.14	116.62	120.34
2	B	335	NAD	C2N-C3N-C4N	3.12	121.80	118.26
2	O	335	NAD	C2N-C3N-C4N	3.12	121.79	118.26
2	H	335	NAD	C2N-C3N-C7N	3.12	128.51	119.46
2	C	335	NAD	C2N-C3N-C7N	3.07	128.36	119.46
2	E	335	NAD	C2N-C3N-C7N	3.05	128.31	119.46
2	E	335	NAD	C2N-C3N-C4N	3.02	121.68	118.26
2	G	335	NAD	C2N-C3N-C7N	3.00	128.16	119.46
2	B	335	NAD	C3N-C2N-N1N	-2.96	117.53	120.43
2	A	335	NAD	C2N-C3N-C4N	2.96	121.62	118.26
2	H	335	NAD	C5N-C4N-C3N	-2.96	116.84	120.34
2	B	335	NAD	O3D-C3D-C4D	-2.96	102.50	111.05
2	E	335	NAD	C5N-C4N-C3N	-2.95	116.85	120.34
2	B	335	NAD	C3N-C7N-N7N	2.91	121.24	117.75
2	C	335	NAD	C5A-C6A-N6A	2.90	124.76	120.35
2	F	335	NAD	C2N-C3N-C7N	2.87	127.78	119.46
2	D	335	NAD	C5N-C4N-C3N	-2.86	116.95	120.34
2	H	335	NAD	C2N-C3N-C4N	2.86	121.50	118.26
2	D	335	NAD	C5A-C6A-N6A	2.86	124.69	120.35
2	D	335	NAD	C2N-C3N-C4N	2.83	121.46	118.26
2	E	335	NAD	C5A-C6A-N6A	2.82	124.64	120.35
2	O	335	NAD	C3N-C7N-N7N	2.82	121.13	117.75
2	A	335	NAD	C5A-C6A-N6A	2.81	124.63	120.35
2	Q	335	NAD	C5N-C4N-C3N	-2.78	117.05	120.34
2	D	335	NAD	C3N-C7N-N7N	2.74	121.04	117.75
2	O	335	NAD	C3N-C2N-N1N	-2.74	117.75	120.43
2	C	335	NAD	O3D-C3D-C4D	-2.73	103.14	111.05
2	A	335	NAD	C3N-C7N-N7N	2.73	121.03	117.75
2	E	335	NAD	C2B-C3B-C4B	2.70	107.89	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	335	NAD	C5N-C4N-C3N	-2.68	117.17	120.34
2	F	335	NAD	C5A-C6A-N6A	2.68	124.43	120.35
2	Q	335	NAD	C3N-C7N-N7N	2.66	120.94	117.75
2	C	335	NAD	C2N-C3N-C4N	2.66	121.27	118.26
2	Q	335	NAD	C2N-C3N-C4N	2.65	121.27	118.26
2	C	335	NAD	C3N-C7N-N7N	2.65	120.92	117.75
2	G	335	NAD	C5A-C6A-N6A	2.63	124.35	120.35
2	Q	335	NAD	C2N-C3N-C7N	2.62	127.07	119.46
2	A	335	NAD	O5B-C5B-C4B	-2.62	99.98	108.99
2	B	335	NAD	C5A-C6A-N6A	2.62	124.33	120.35
2	A	335	NAD	C2N-C3N-C7N	2.61	127.03	119.46
2	F	335	NAD	C5N-C4N-C3N	-2.60	117.27	120.34
2	G	335	NAD	C2N-C3N-C4N	2.60	121.20	118.26
2	D	335	NAD	C2N-C3N-C7N	2.58	126.96	119.46
2	D	335	NAD	C1B-N9A-C4A	-2.58	122.10	126.64
2	F	335	NAD	C2N-C3N-C4N	2.55	121.15	118.26
2	G	335	NAD	O3D-C3D-C4D	-2.55	103.68	111.05
2	B	335	NAD	C2N-C3N-C7N	2.54	126.85	119.46
2	E	335	NAD	O3D-C3D-C4D	-2.53	103.74	111.05
2	H	335	NAD	C5A-C6A-N6A	2.53	124.19	120.35
2	O	335	NAD	O3D-C3D-C4D	-2.51	103.78	111.05
2	O	335	NAD	C2N-C3N-C7N	2.45	126.56	119.46
2	O	335	NAD	O5B-C5B-C4B	-2.43	100.64	108.99
2	E	335	NAD	O7N-C7N-C3N	-2.41	116.75	119.63
2	Q	335	NAD	C5A-C6A-N6A	2.41	124.01	120.35
2	Q	335	NAD	O3D-C3D-C4D	-2.40	104.10	111.05
2	F	335	NAD	C3D-C2D-C1D	2.36	104.53	100.98
2	H	335	NAD	O7N-C7N-C3N	-2.36	116.81	119.63
2	A	335	NAD	O3D-C3D-C4D	-2.33	104.30	111.05
2	F	335	NAD	O3D-C3D-C4D	-2.33	104.30	111.05
2	D	335	NAD	C3D-C2D-C1D	2.31	104.45	100.98
2	O	335	NAD	C5A-C6A-N6A	2.27	123.81	120.35
2	C	335	NAD	C5N-C4N-C3N	-2.27	117.65	120.34
2	G	335	NAD	O5B-C5B-C4B	-2.25	101.24	108.99
2	H	335	NAD	O3D-C3D-C4D	-2.20	104.68	111.05
2	A	335	NAD	C1B-N9A-C4A	-2.20	122.77	126.64
2	G	335	NAD	C3D-C2D-C1D	2.19	104.28	100.98
2	F	335	NAD	O5B-C5B-C4B	-2.17	101.52	108.99
2	F	335	NAD	C1B-N9A-C4A	-2.17	122.83	126.64
2	E	335	NAD	C1B-N9A-C4A	-2.16	122.84	126.64
2	B	335	NAD	C1B-N9A-C4A	-2.15	122.86	126.64
2	E	335	NAD	C3D-C2D-C1D	2.15	104.22	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	335	NAD	O3D-C3D-C4D	-2.12	104.93	111.05
2	O	335	NAD	O7N-C7N-C3N	-2.11	117.10	119.63
2	C	335	NAD	O5B-C5B-C4B	-2.09	101.80	108.99
2	O	335	NAD	C1B-N9A-C4A	-2.03	123.07	126.64

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	335	NAD	O4D-C1D-N1N-C2N
2	A	335	NAD	O4D-C1D-N1N-C6N
2	A	335	NAD	C2D-C1D-N1N-C2N
2	A	335	NAD	C2D-C1D-N1N-C6N
2	O	335	NAD	O4D-C1D-N1N-C2N
2	O	335	NAD	O4D-C1D-N1N-C6N
2	O	335	NAD	C2D-C1D-N1N-C2N
2	O	335	NAD	C2D-C1D-N1N-C6N
2	H	335	NAD	O4D-C1D-N1N-C2N
2	H	335	NAD	O4D-C1D-N1N-C6N
2	G	335	NAD	C5B-O5B-PA-O1A
2	G	335	NAD	O4D-C1D-N1N-C2N
2	G	335	NAD	O4D-C1D-N1N-C6N
2	D	335	NAD	C5B-O5B-PA-O1A
2	D	335	NAD	O4D-C1D-N1N-C2N
2	F	335	NAD	O4D-C1D-N1N-C2N
2	C	335	NAD	O4D-C1D-N1N-C2N
2	C	335	NAD	O4D-C1D-N1N-C6N
2	C	335	NAD	C2D-C1D-N1N-C2N
2	C	335	NAD	C2D-C1D-N1N-C6N
2	B	335	NAD	O4D-C1D-N1N-C2N
2	B	335	NAD	O4D-C1D-N1N-C6N
2	B	335	NAD	C2D-C1D-N1N-C2N
2	B	335	NAD	C2D-C1D-N1N-C6N
2	Q	335	NAD	O4D-C1D-N1N-C2N
2	Q	335	NAD	O4D-C1D-N1N-C6N
2	Q	335	NAD	C2D-C1D-N1N-C2N
2	Q	335	NAD	C2D-C1D-N1N-C6N
2	E	335	NAD	C5B-O5B-PA-O2A
2	E	335	NAD	C5B-O5B-PA-O3
2	E	335	NAD	C3B-C4B-C5B-O5B
2	E	335	NAD	O4D-C1D-N1N-C2N
2	E	335	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	E	335	NAD	C2D-C1D-N1N-C2N
2	E	335	NAD	C2D-C1D-N1N-C6N
2	E	335	NAD	C2N-C3N-C7N-O7N
2	E	335	NAD	C2N-C3N-C7N-N7N
2	E	335	NAD	C4N-C3N-C7N-O7N
2	E	335	NAD	C4N-C3N-C7N-N7N
2	G	335	NAD	O4B-C4B-C5B-O5B
2	H	335	NAD	C2N-C3N-C7N-O7N
2	H	335	NAD	C2N-C3N-C7N-N7N
2	H	335	NAD	C4N-C3N-C7N-N7N
2	Q	335	NAD	O4B-C4B-C5B-O5B
2	H	335	NAD	C4N-C3N-C7N-O7N
2	E	335	NAD	O4B-C4B-C5B-O5B
2	C	335	NAD	O4B-C4B-C5B-O5B
2	A	335	NAD	PN-O3-PA-O1A
2	D	335	NAD	O4B-C4B-C5B-O5B
2	F	335	NAD	PN-O3-PA-O5B
2	H	335	NAD	C5B-O5B-PA-O3
2	G	335	NAD	C5B-O5B-PA-O3
2	D	335	NAD	C5B-O5B-PA-O3
2	F	335	NAD	C5B-O5B-PA-O3
2	Q	335	NAD	C5B-O5B-PA-O3
2	F	335	NAD	O4D-C4D-C5D-O5D
2	F	335	NAD	PA-O3-PN-O2N
2	H	335	NAD	C5B-O5B-PA-O2A
2	G	335	NAD	C5B-O5B-PA-O2A
2	D	335	NAD	C5B-O5B-PA-O2A
2	F	335	NAD	C5B-O5B-PA-O1A
2	F	335	NAD	C5B-O5B-PA-O2A
2	Q	335	NAD	C5B-O5B-PA-O2A
2	B	335	NAD	O4B-C4B-C5B-O5B
2	A	335	NAD	C4N-C3N-C7N-O7N
2	E	335	NAD	PN-O3-PA-O2A
2	F	335	NAD	C4B-C5B-O5B-PA
2	A	335	NAD	C4N-C3N-C7N-N7N
2	O	335	NAD	O4B-C4B-C5B-O5B
2	F	335	NAD	O4B-C4B-C5B-O5B
2	F	335	NAD	C3D-C4D-C5D-O5D
2	D	335	NAD	PA-O3-PN-O2N
2	Q	335	NAD	PA-O3-PN-O2N
2	G	335	NAD	C3B-C4B-C5B-O5B
2	Q	335	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	H	335	NAD	O4B-C4B-C5B-O5B
2	H	335	NAD	C2D-C1D-N1N-C2N
2	H	335	NAD	C2D-C1D-N1N-C6N
2	G	335	NAD	C2D-C1D-N1N-C2N
2	G	335	NAD	C2D-C1D-N1N-C6N
2	C	335	NAD	C5B-O5B-PA-O3
2	A	335	NAD	PN-O3-PA-O2A
2	G	335	NAD	PA-O3-PN-O1N
2	G	335	NAD	PA-O3-PN-O2N
2	D	335	NAD	PA-O3-PN-O1N
2	C	335	NAD	PA-O3-PN-O2N
2	B	335	NAD	PA-O3-PN-O2N
2	C	335	NAD	C5B-O5B-PA-O2A
2	A	335	NAD	O4B-C4B-C5B-O5B
2	D	335	NAD	C3B-C4B-C5B-O5B
2	C	335	NAD	C3B-C4B-C5B-O5B

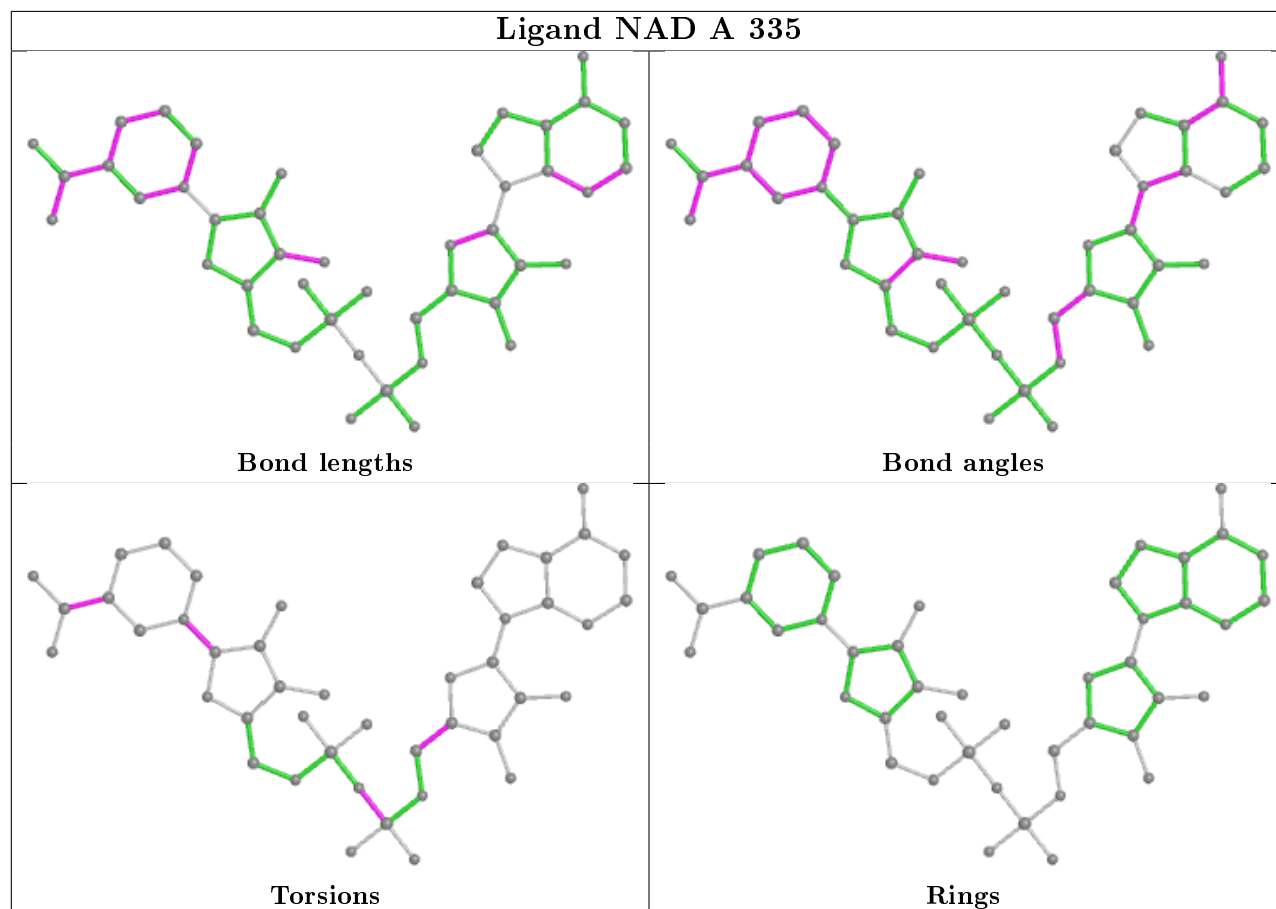
There are no ring outliers.

11 monomers are involved in 19 short contacts:

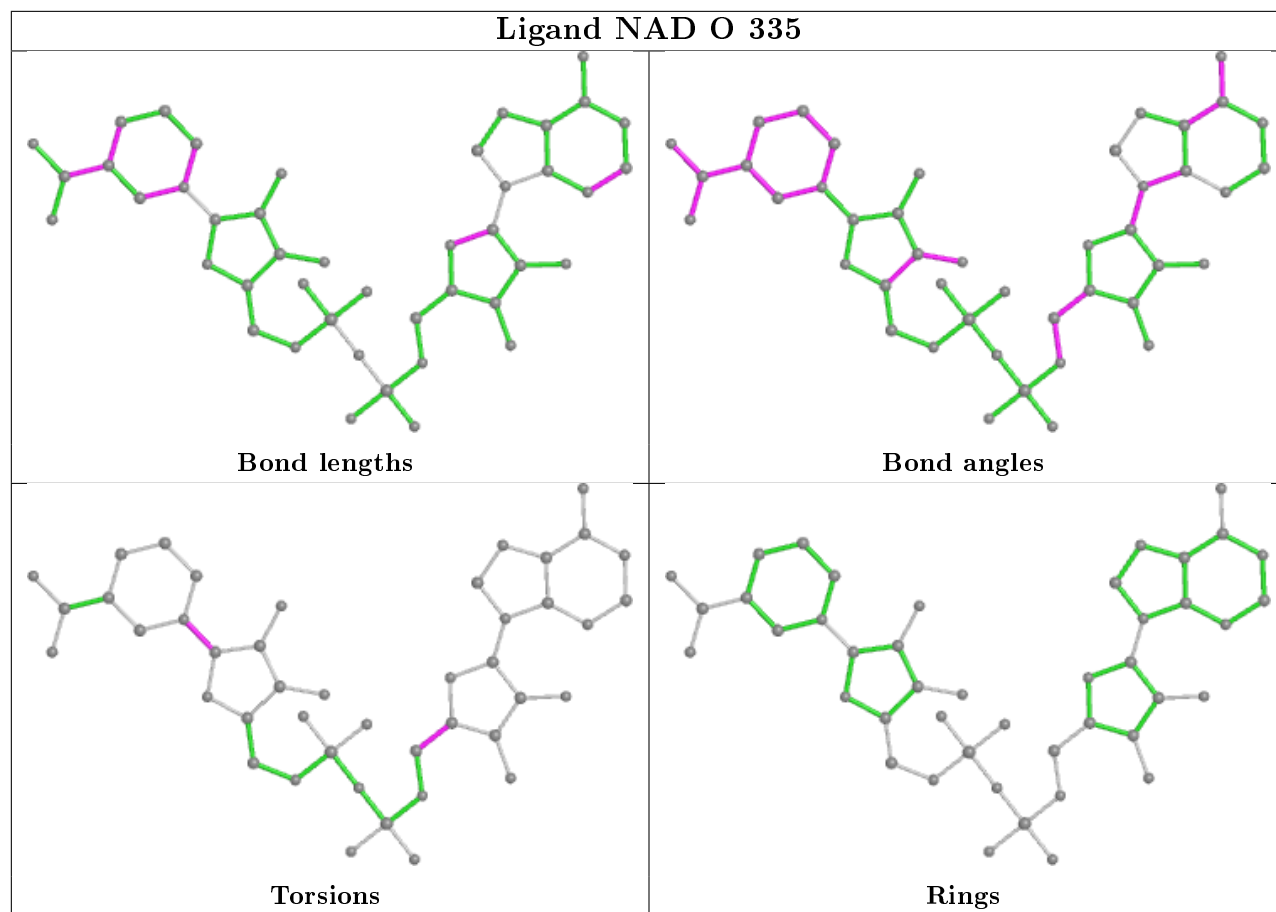
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	335	NAD	1	0
2	O	335	NAD	1	0
2	H	335	NAD	2	0
2	G	335	NAD	1	0
2	D	335	NAD	3	0
2	F	335	NAD	2	0
2	B	335	NAD	1	0
3	E	338	SO4	1	0
3	E	337	SO4	1	0
3	E	334	SO4	1	0
2	E	335	NAD	5	0

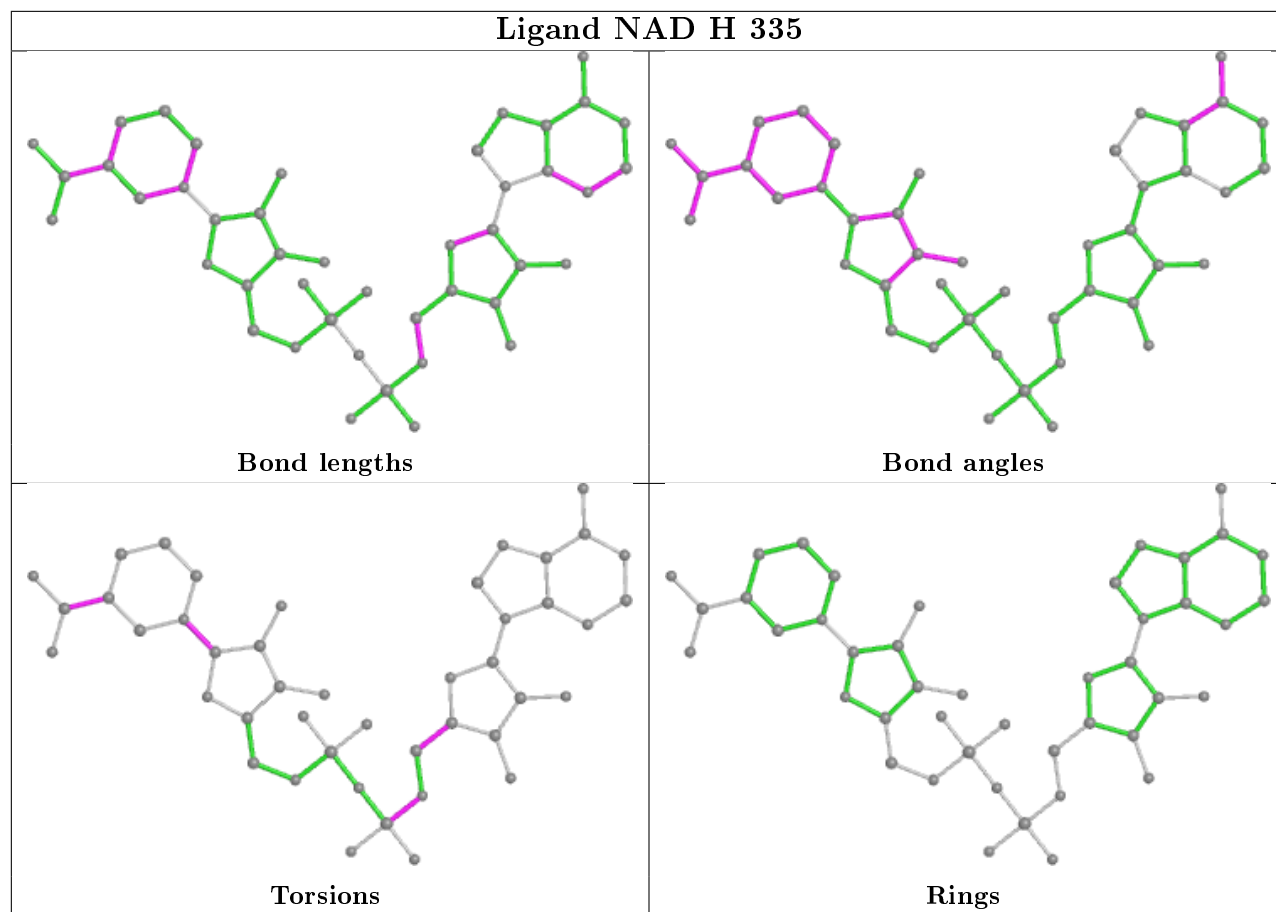
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

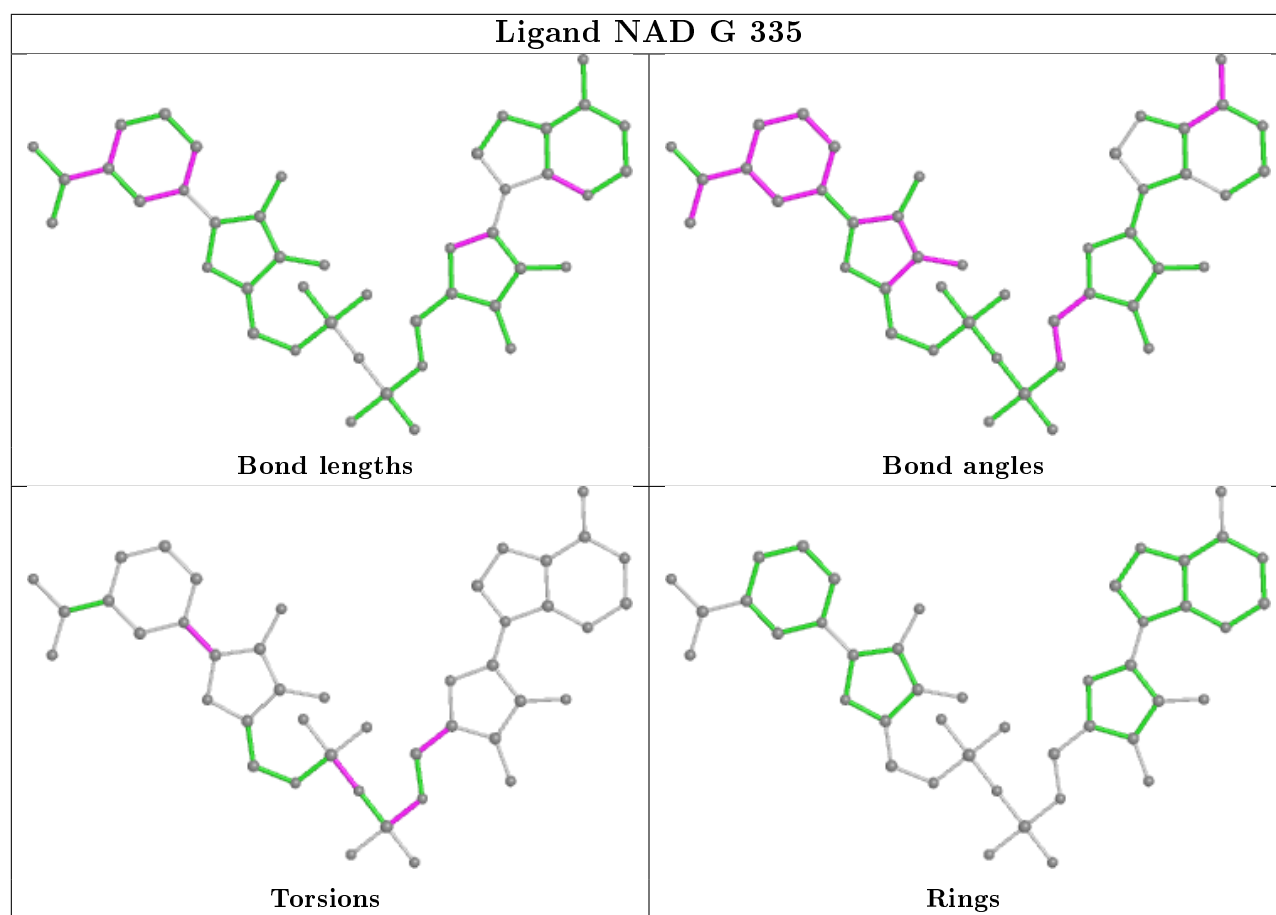
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

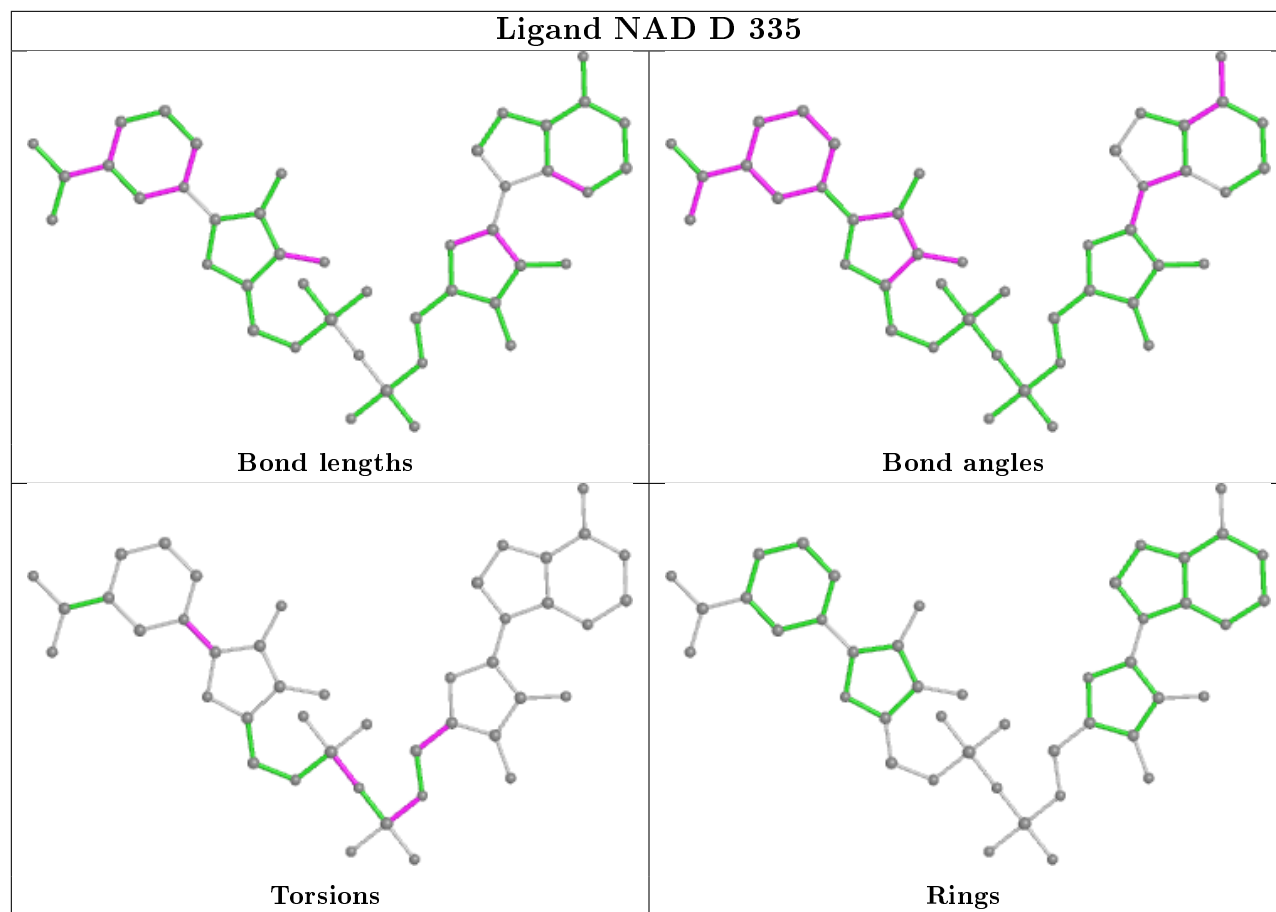


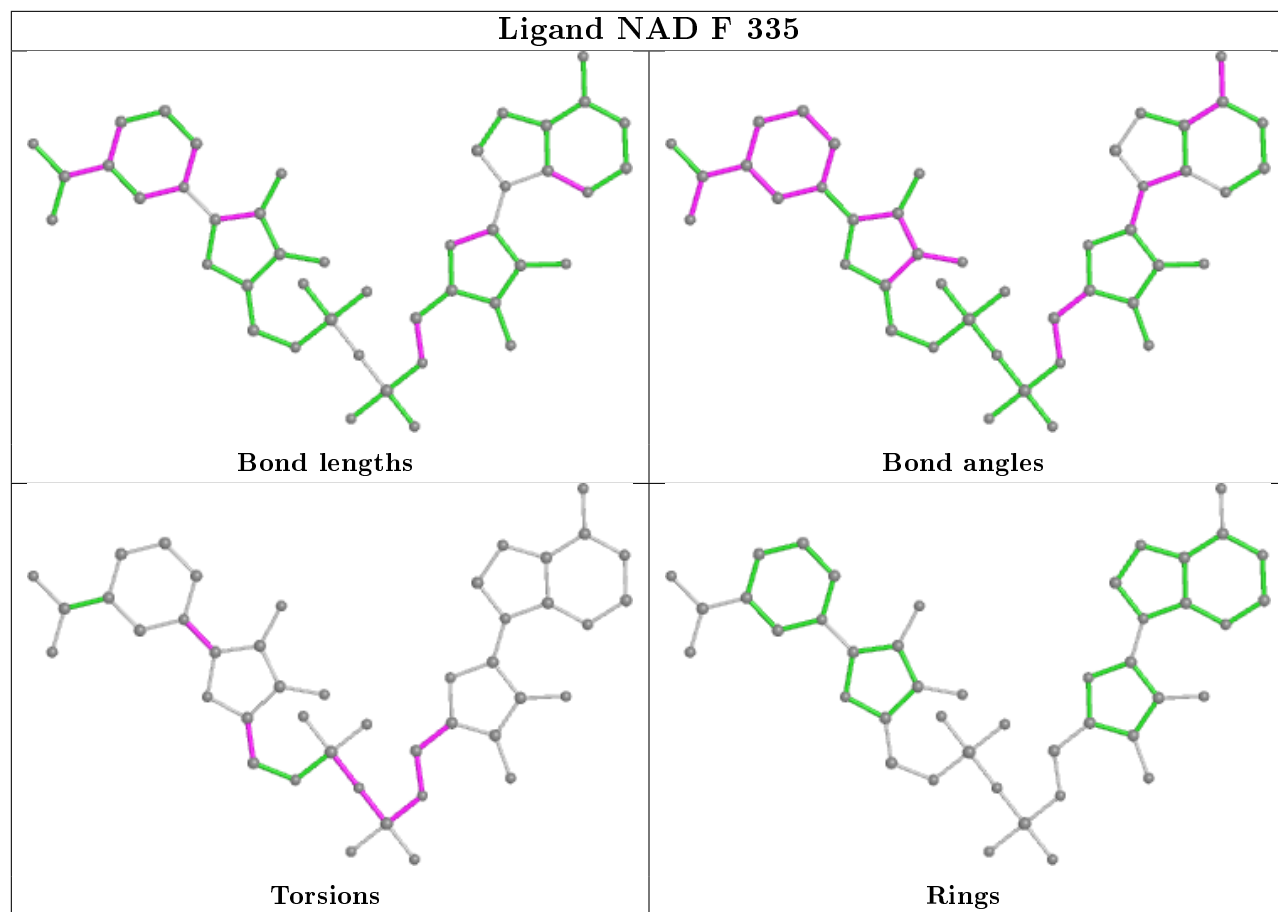


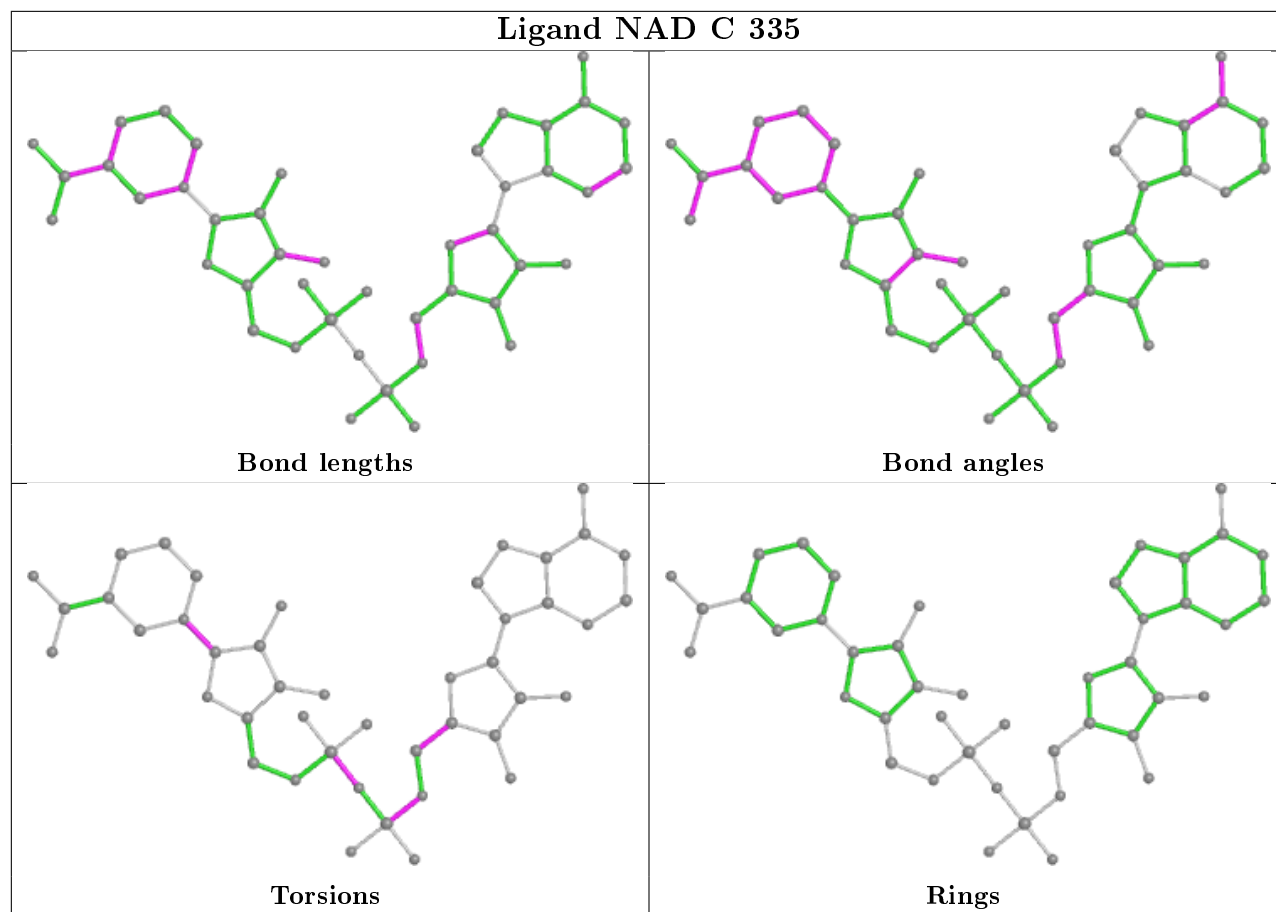


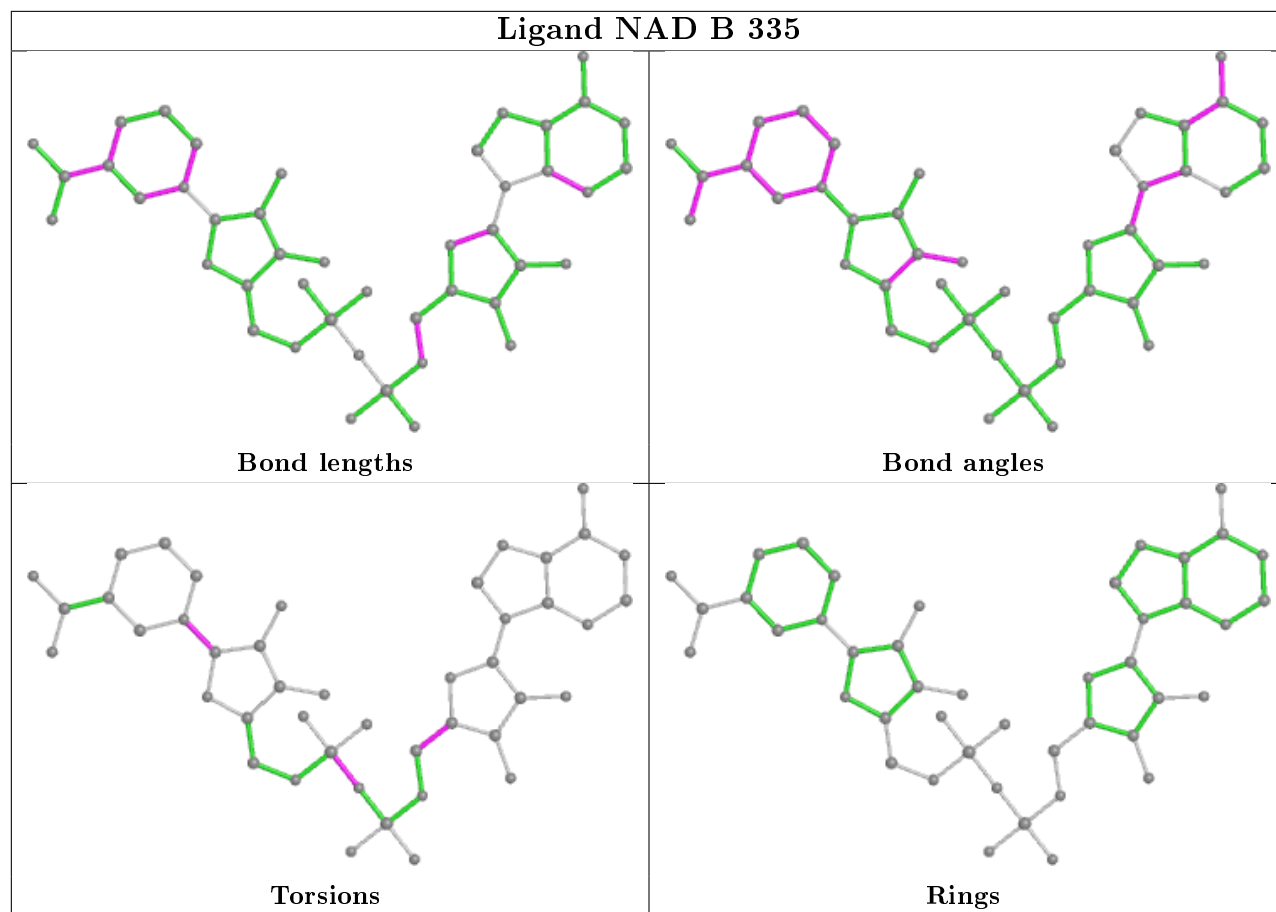


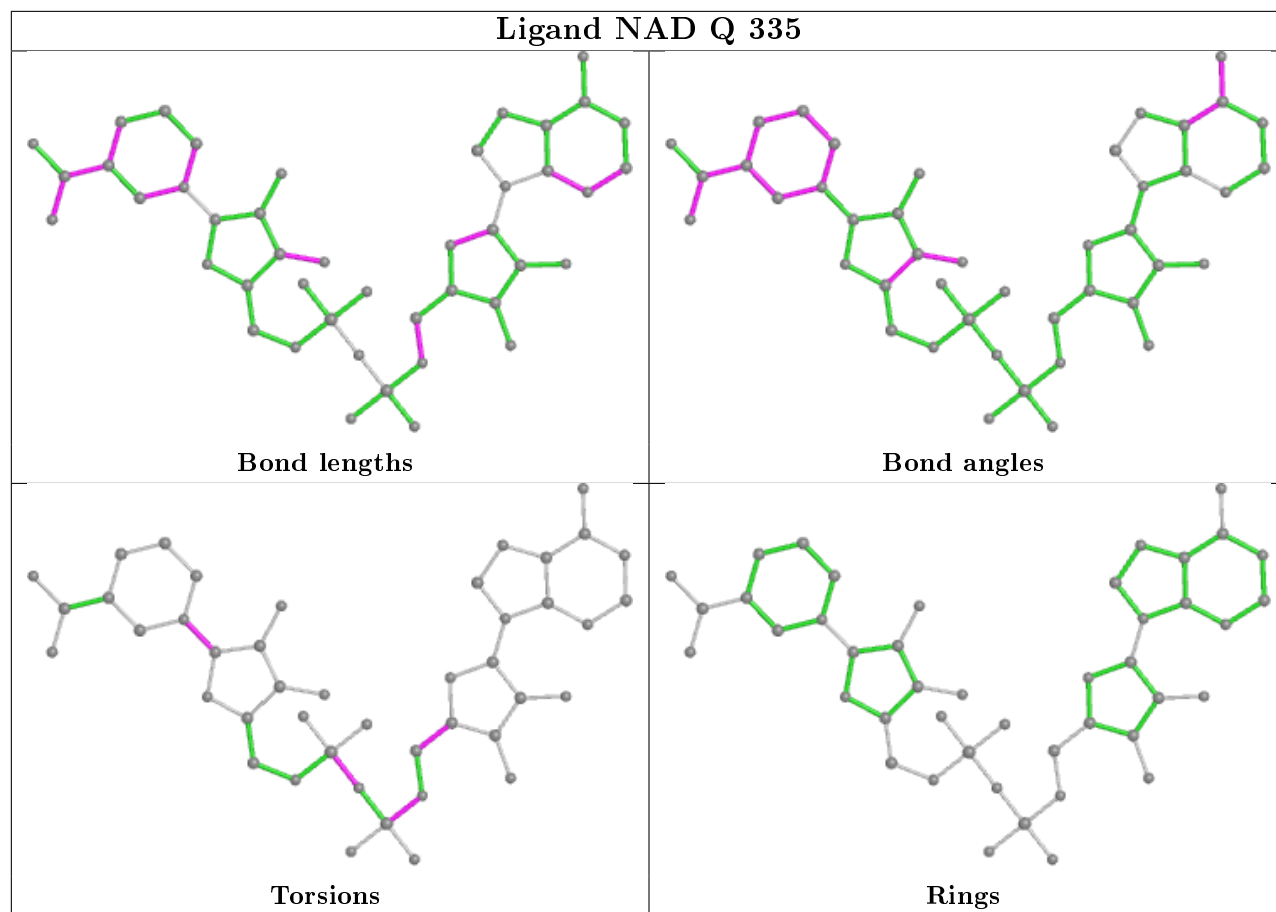




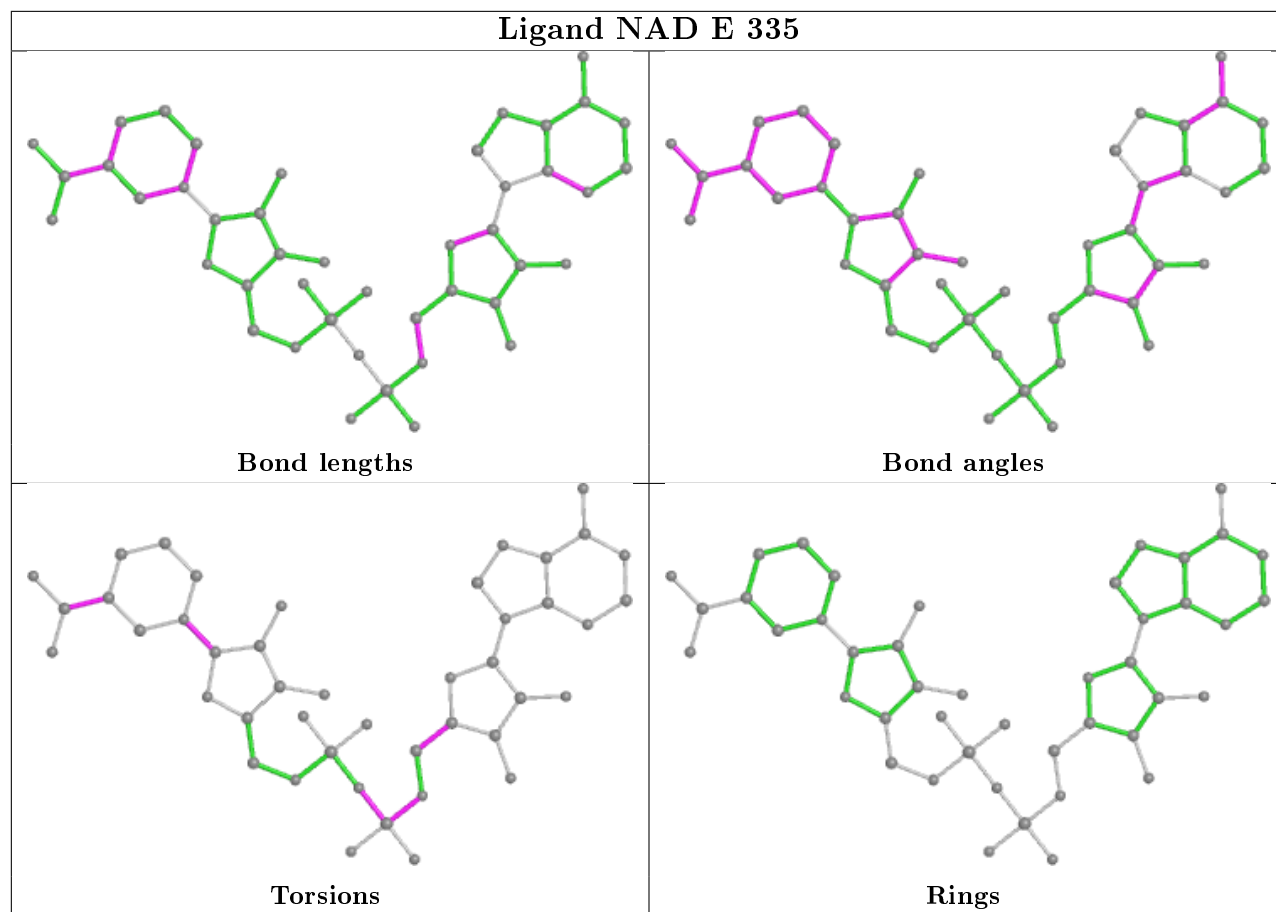












## 5.7 Other polymers [i](#)

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	337/337 (100%)	-0.11	1 (0%) 94 93	29, 42, 59, 80	0
1	B	337/337 (100%)	-0.09	1 (0%) 94 93	31, 46, 63, 71	0
1	C	337/337 (100%)	-0.02	2 (0%) 89 88	31, 48, 69, 81	0
1	D	336/337 (99%)	-0.00	2 (0%) 89 88	35, 62, 79, 96	0
1	E	336/337 (99%)	1.44	90 (26%) 0 0	55, 87, 108, 114	0
1	F	336/337 (99%)	0.81	49 (14%) 2 1	43, 88, 105, 113	0
1	G	336/337 (99%)	0.63	28 (8%) 11 8	34, 69, 91, 101	0
1	H	335/337 (99%)	0.47	22 (6%) 18 13	48, 83, 103, 114	0
1	O	337/337 (100%)	-0.07	0 100 100	19, 31, 45, 56	0
1	Q	336/337 (99%)	-0.09	1 (0%) 94 93	21, 39, 58, 81	0
All	All	3363/3370 (99%)	0.30	196 (5%) 23 17	19, 56, 99, 114	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	187	ALA	7.6
1	E	29	ALA	6.9
1	E	25	LEU	6.6
1	E	270	ILE	6.1
1	E	228	ILE	6.0
1	E	28	ILE	5.7
1	F	214	VAL	5.4
1	E	15	PHE	5.3
1	E	0(A)	ALA	5.2
1	E	79	PRO	5.2
1	E	116	VAL	5.1
1	E	66	VAL	5.0
1	F	119	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	273	VAL	4.6
1	G	269	GLY	4.6
1	E	255	VAL	4.6
1	E	328	VAL	4.6
1	E	129	VAL	4.5
1	E	92	VAL	4.4
1	E	32	ASP	4.3
1	E	267	LEU	4.3
1	C	0(A)	ALA	4.2
1	F	128	TYR	4.2
1	E	64	ILE	4.1
1	E	1	LEU	4.1
1	F	84	TRP	4.0
1	E	53	PHE	4.0
1	F	87	LEU	4.0
1	F	108	HIS	4.0
1	E	63	ALA	4.0
1	G	244	VAL	3.9
1	E	72	GLN	3.9
1	E	84	TRP	3.8
1	H	193	LEU	3.8
1	H	191	ARG	3.8
1	H	332	TRP	3.8
1	C	332	TRP	3.7
1	F	89	ILE	3.7
1	E	100	VAL	3.7
1	F	263	ALA	3.7
1	F	131	GLY	3.5
1	E	18(A)	TRP	3.5
1	E	271	LEU	3.5
1	F	46	TYR	3.4
1	E	55	ALA	3.4
1	E	98	VAL	3.4
1	G	290	THR	3.4
1	E	44	LEU	3.3
1	F	322	VAL	3.3
1	F	155	ALA	3.3
1	F	74	VAL	3.3
1	E	316	GLY	3.2
1	F	259	PHE	3.2
1	G	156	PRO	3.2
1	E	62	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	215	ALA	3.2
1	E	24	PRO	3.1
1	F	288	PHE	3.1
1	F	268	LYS	3.1
1	E	23	SER	3.1
1	F	5	ILE	3.1
1	G	160	VAL	3.1
1	Q	333	LYS	3.1
1	E	321	VAL	3.0
1	E	292	ILE	3.0
1	F	52	ILE	3.0
1	E	330	ASN	3.0
1	E	300	MET	3.0
1	E	259	PHE	3.0
1	G	130	VAL	2.9
1	G	273	VAL	2.9
1	F	217	VAL	2.9
1	F	14	ASN	2.9
1	E	108	HIS	2.9
1	E	327	ILE	2.9
1	E	322	VAL	2.9
1	E	22	ASP	2.8
1	E	209	GLY	2.8
1	E	16	LEU	2.8
1	F	82	LEU	2.7
1	G	254	GLU	2.7
1	E	74	VAL	2.7
1	E	324	LEU	2.7
1	H	221	LEU	2.7
1	E	91	ILE	2.7
1	H	46	TYR	2.7
1	E	70	ILE	2.7
1	E	154	LEU	2.7
1	F	225	LEU	2.7
1	F	278	LEU	2.7
1	E	67	ASP	2.7
1	F	32	ASP	2.7
1	E	114	LYS	2.7
1	E	325	ALA	2.7
1	F	27	ILE	2.6
1	H	92	VAL	2.6
1	G	152	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	225	LEU	2.6
1	G	330	ASN	2.6
1	F	156	PRO	2.6
1	G	305	VAL	2.6
1	G	217	VAL	2.6
1	H	84	TRP	2.6
1	E	193	LEU	2.6
1	F	61	GLU	2.6
1	E	139	HIS	2.6
1	E	37	VAL	2.6
1	F	267	LEU	2.6
1	E	144	ILE	2.5
1	E	206	THR	2.5
1	E	249	LYS	2.5
1	E	283	PHE	2.5
1	G	283	PHE	2.5
1	F	264	GLU	2.5
1	F	299	VAL	2.5
1	E	171	THR	2.5
1	E	258	ALA	2.5
1	G	27	ILE	2.5
1	F	48	SER	2.5
1	E	143	ILE	2.5
1	H	188	SER	2.5
1	G	266	GLU	2.4
1	E	138	SER	2.4
1	E	231	ARG	2.4
1	H	105	ALA	2.4
1	G	143	ILE	2.4
1	A	333	LYS	2.4
1	E	21	LYS	2.4
1	F	37	VAL	2.4
1	F	164	LYS	2.4
1	E	111	ALA	2.4
1	F	83	PRO	2.4
1	F	274	CYS	2.4
1	F	269	GLY	2.4
1	E	57	VAL	2.4
1	G	333	LYS	2.4
1	H	132	VAL	2.4
1	G	331	ASN	2.3
1	E	153	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	128	TYR	2.3
1	E	81	LEU	2.3
1	F	242	LEU	2.3
1	F	146	ASN	2.3
1	H	187	ALA	2.3
1	E	115	LYS	2.3
1	E	263	ALA	2.3
1	E	317	TYR	2.3
1	F	319	GLN	2.3
1	H	116	VAL	2.3
1	G	278	LEU	2.2
1	E	54	ASP	2.2
1	H	7	GLY	2.2
1	E	252	ALA	2.2
1	E	121	PRO	2.2
1	E	329	ALA	2.2
1	G	304	MET	2.2
1	F	68	GLY	2.2
1	E	203	ILE	2.2
1	E	308	ILE	2.2
1	E	18	CYS	2.2
1	E	194	ARG	2.2
1	B	262	SER	2.2
1	E	250	THR	2.2
1	H	25	LEU	2.2
1	F	130	VAL	2.2
1	H	57	VAL	2.2
1	F	219	PRO	2.2
1	G	25	LEU	2.2
1	H	190	HIS	2.2
1	F	56	ASP	2.2
1	E	33	THR	2.1
1	F	265	LYS	2.1
1	E	46	TYR	2.1
1	E	204	VAL	2.1
1	E	279	VAL	2.1
1	G	193	LEU	2.1
1	F	31	ASN	2.1
1	E	191	ARG	2.1
1	F	160	VAL	2.1
1	G	226	ASN	2.1
1	G	247	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	140	ASP	2.1
1	H	44	LEU	2.1
1	G	167	ILE	2.1
1	D	188	SER	2.1
1	H	165	PHE	2.1
1	F	333	LYS	2.0
1	G	164	LYS	2.0
1	F	43	LEU	2.0
1	F	325	ALA	2.0
1	H	113	ALA	2.0
1	E	170	GLY	2.0
1	H	99	PHE	2.0
1	D	305	VAL	2.0
1	H	27	ILE	2.0
1	G	332	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	341	5/5	0.74	0.23	108,108,109,109	5
3	SO4	D	336	5/5	0.78	0.28	84,84,85,86	5
3	SO4	E	337	5/5	0.81	0.21	116,117,117,117	5
3	SO4	O	334	5/5	0.84	0.19	74,74,75,77	5
3	SO4	B	334	5/5	0.84	0.19	91,91,92,92	5
3	SO4	G	334	5/5	0.84	0.34	87,87,88,89	5
3	SO4	G	339	5/5	0.85	0.17	114,114,114,114	5
3	SO4	F	334	5/5	0.86	0.14	111,111,111,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	H	336	5/5	0.87	0.21	77,77,78,78	5
3	SO4	A	334	5/5	0.87	0.20	79,79,80,81	5
3	SO4	A	339	5/5	0.87	0.28	104,104,105,106	5
3	SO4	G	337	5/5	0.88	0.24	101,102,102,102	5
3	SO4	O	340	5/5	0.88	0.22	68,68,69,70	5
3	SO4	H	334	5/5	0.88	0.21	79,80,80,81	5
3	SO4	O	338	5/5	0.89	0.23	88,89,90,90	5
3	SO4	G	338	5/5	0.89	0.19	96,96,97,97	5
3	SO4	O	337	5/5	0.89	0.32	72,74,75,75	5
3	SO4	Q	339	5/5	0.90	0.15	88,88,90,90	5
2	NAD	E	335	44/44	0.90	0.23	87,97,102,104	0
3	SO4	O	339	5/5	0.90	0.23	87,87,88,88	5
3	SO4	D	337	5/5	0.90	0.15	89,90,90,90	5
2	NAD	F	335	44/44	0.91	0.19	67,73,81,81	0
3	SO4	F	336	5/5	0.91	0.19	56,56,59,59	5
3	SO4	F	337	5/5	0.91	0.18	85,86,86,87	5
3	SO4	H	337	5/5	0.91	0.14	80,81,82,82	5
3	SO4	E	336	5/5	0.91	0.14	78,79,79,80	5
3	SO4	Q	334	5/5	0.92	0.21	73,75,75,75	5
2	NAD	H	335	44/44	0.92	0.21	83,87,95,96	0
3	SO4	B	338	5/5	0.93	0.14	75,75,76,76	5
3	SO4	C	334	5/5	0.94	0.17	79,80,80,80	5
3	SO4	E	338	5/5	0.94	0.15	87,87,88,88	5
3	SO4	C	338	5/5	0.94	0.18	62,63,64,65	5
3	SO4	D	334	5/5	0.94	0.16	75,76,76,76	5
3	SO4	B	339	5/5	0.95	0.18	69,70,71,71	5
3	SO4	G	336	5/5	0.95	0.14	67,68,68,69	5
3	SO4	B	336	5/5	0.95	0.17	52,53,53,53	5
2	NAD	Q	335	44/44	0.95	0.15	41,48,50,51	0
2	NAD	D	335	44/44	0.95	0.17	50,53,55,56	0
2	NAD	B	335	44/44	0.96	0.17	36,44,50,51	0
2	NAD	G	335	44/44	0.96	0.18	43,47,51,52	0
3	SO4	E	334	5/5	0.96	0.14	60,60,61,62	5
3	SO4	C	336	5/5	0.97	0.15	67,67,68,68	0
3	SO4	Q	336	5/5	0.97	0.15	69,71,72,72	0
3	SO4	O	336	5/5	0.97	0.16	60,62,63,63	0
2	NAD	C	335	44/44	0.97	0.16	40,45,50,51	0
3	SO4	A	337	5/5	0.97	0.19	64,65,66,68	0
3	SO4	B	337	5/5	0.97	0.17	59,60,61,61	5
2	NAD	A	335	44/44	0.97	0.17	37,41,47,50	0
2	NAD	O	335	44/44	0.98	0.17	19,23,26,29	0
3	SO4	A	338	5/5	0.98	0.14	55,56,57,58	5

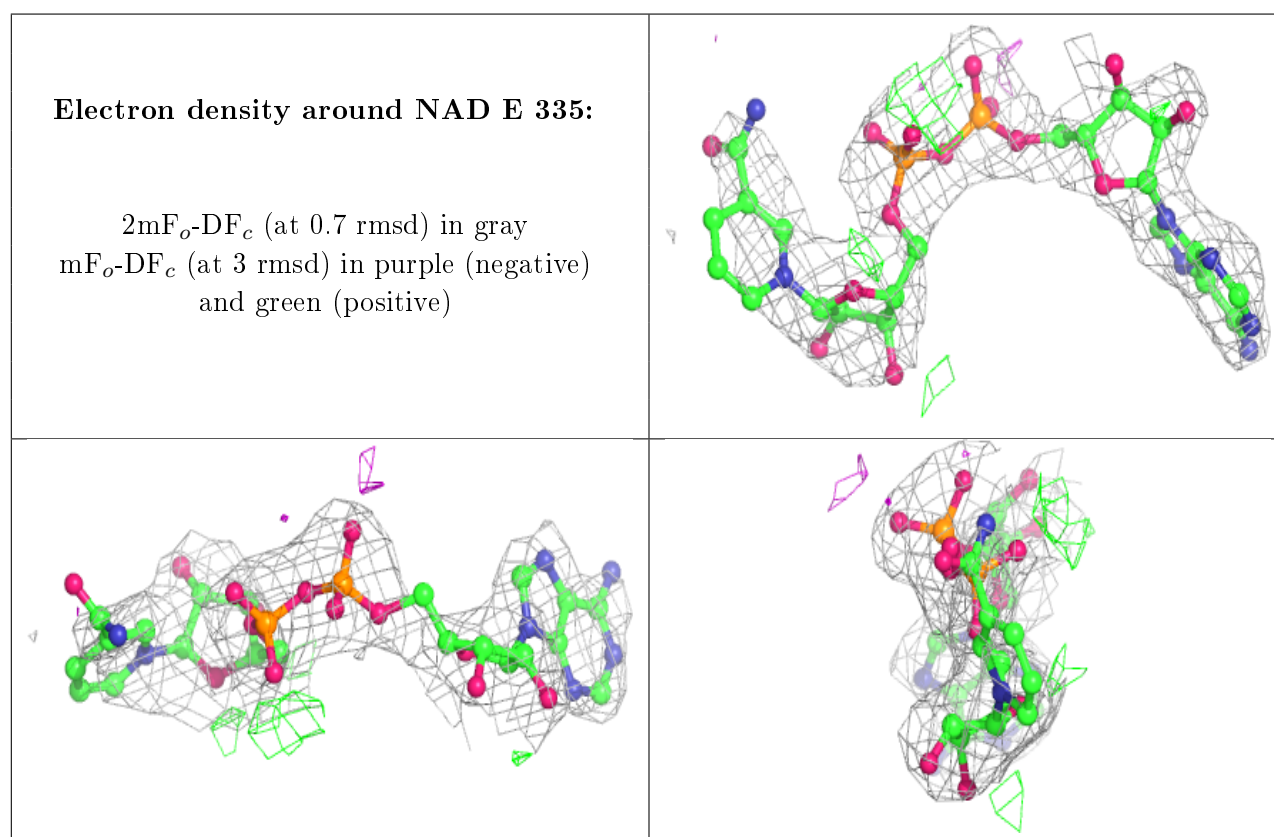
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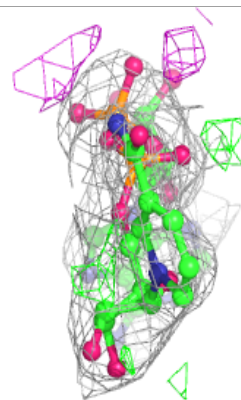
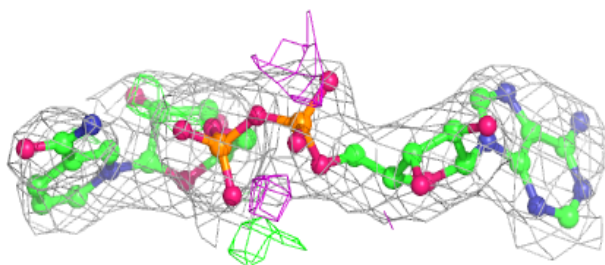
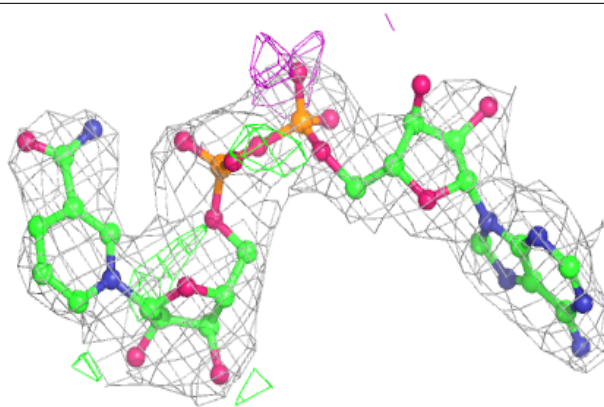
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	340	5/5	0.98	0.16	59,59,61,62	0
3	SO4	Q	337	5/5	0.98	0.19	58,58,59,59	5
3	SO4	C	337	5/5	0.99	0.15	49,49,50,50	0
3	SO4	Q	338	5/5	0.99	0.18	46,47,48,51	0
3	SO4	A	336	5/5	0.99	0.14	50,50,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

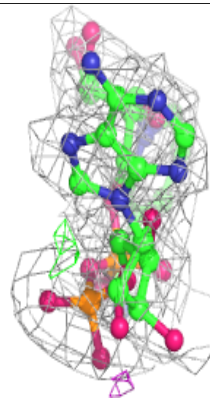
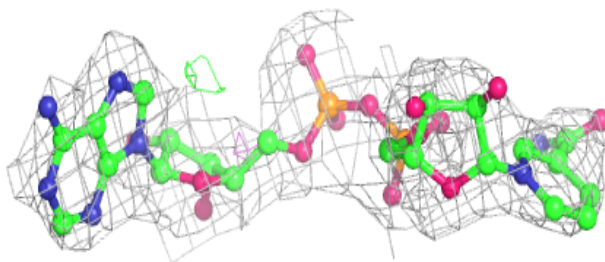
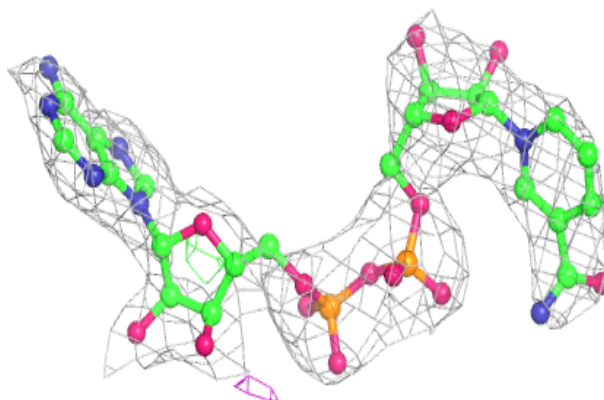


**Electron density around NAD F 335:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

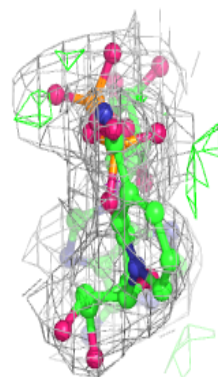
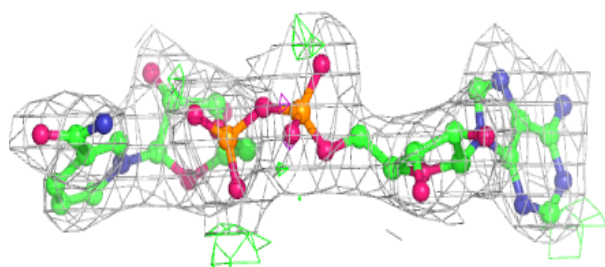
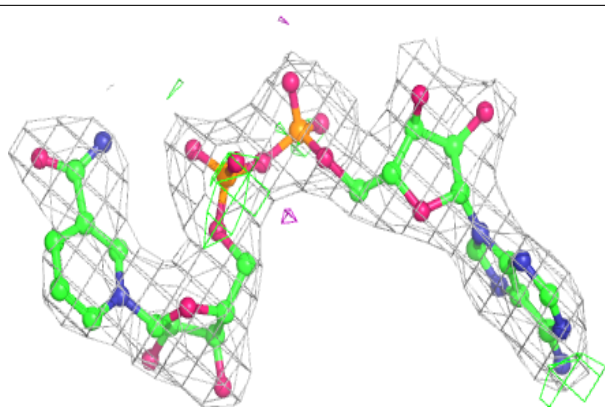
**Electron density around NAD H 335:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

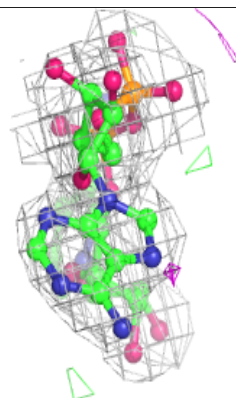
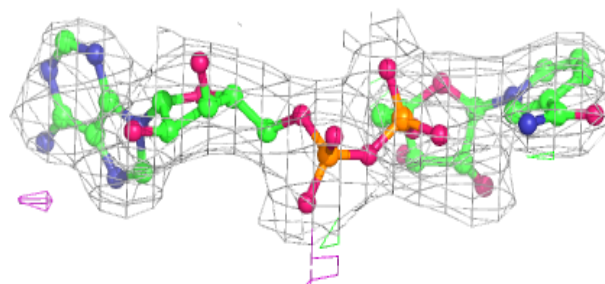
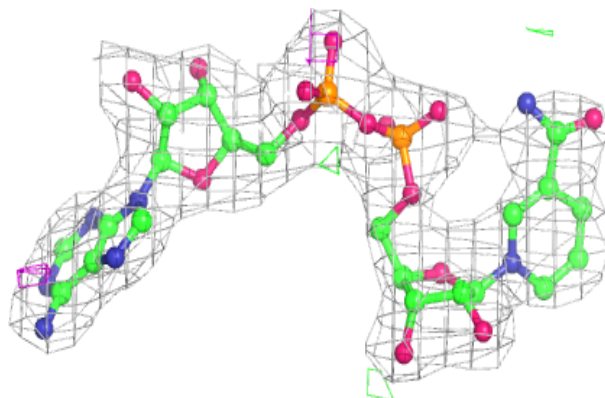


**Electron density around NAD Q 335:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

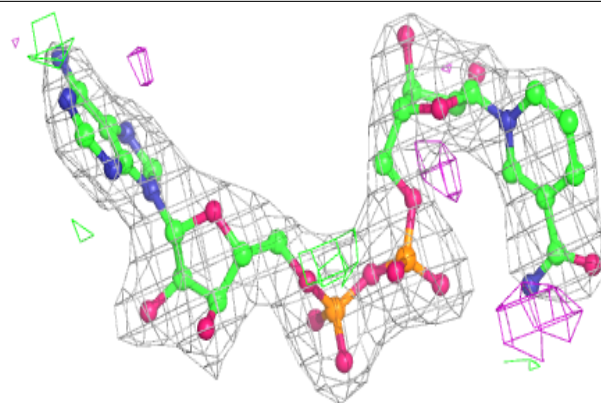
**Electron density around NAD D 335:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

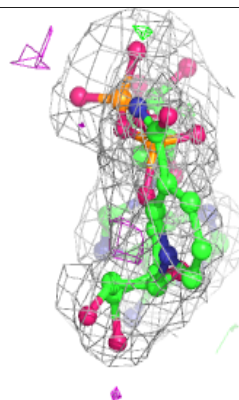
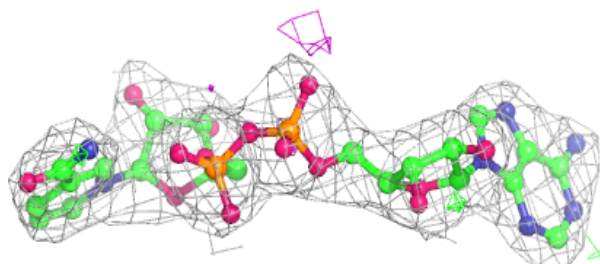
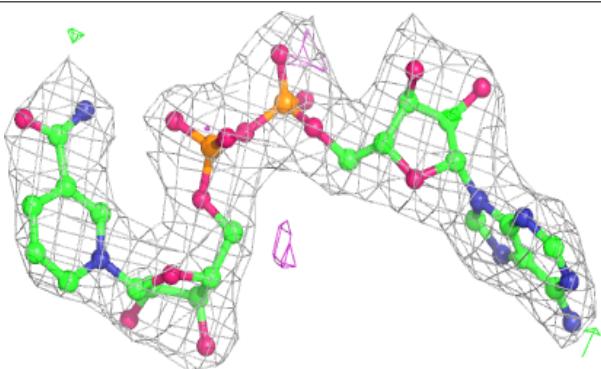


**Electron density around NAD B 335:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAD G 335:**

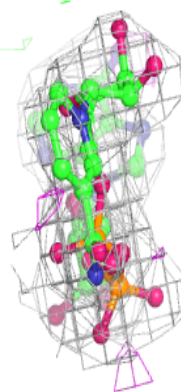
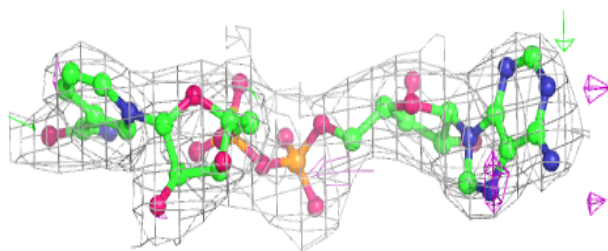
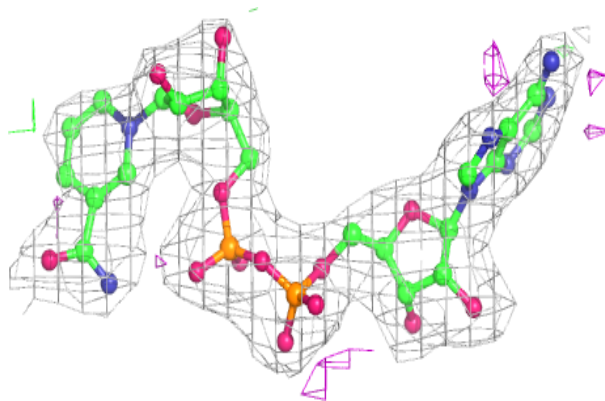
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



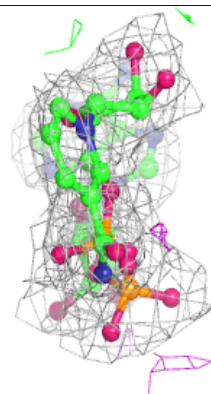
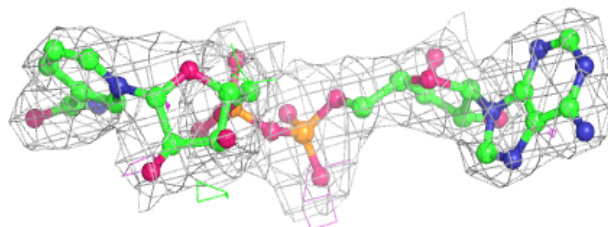
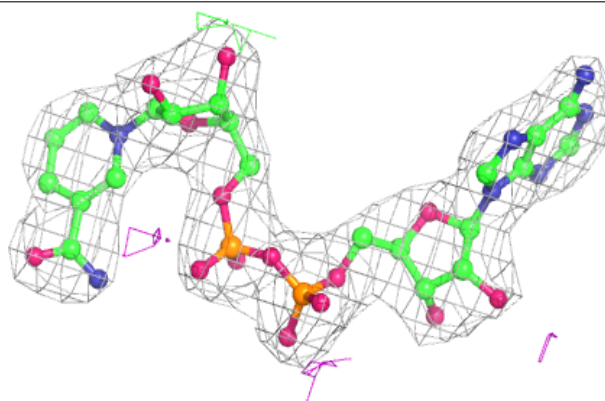


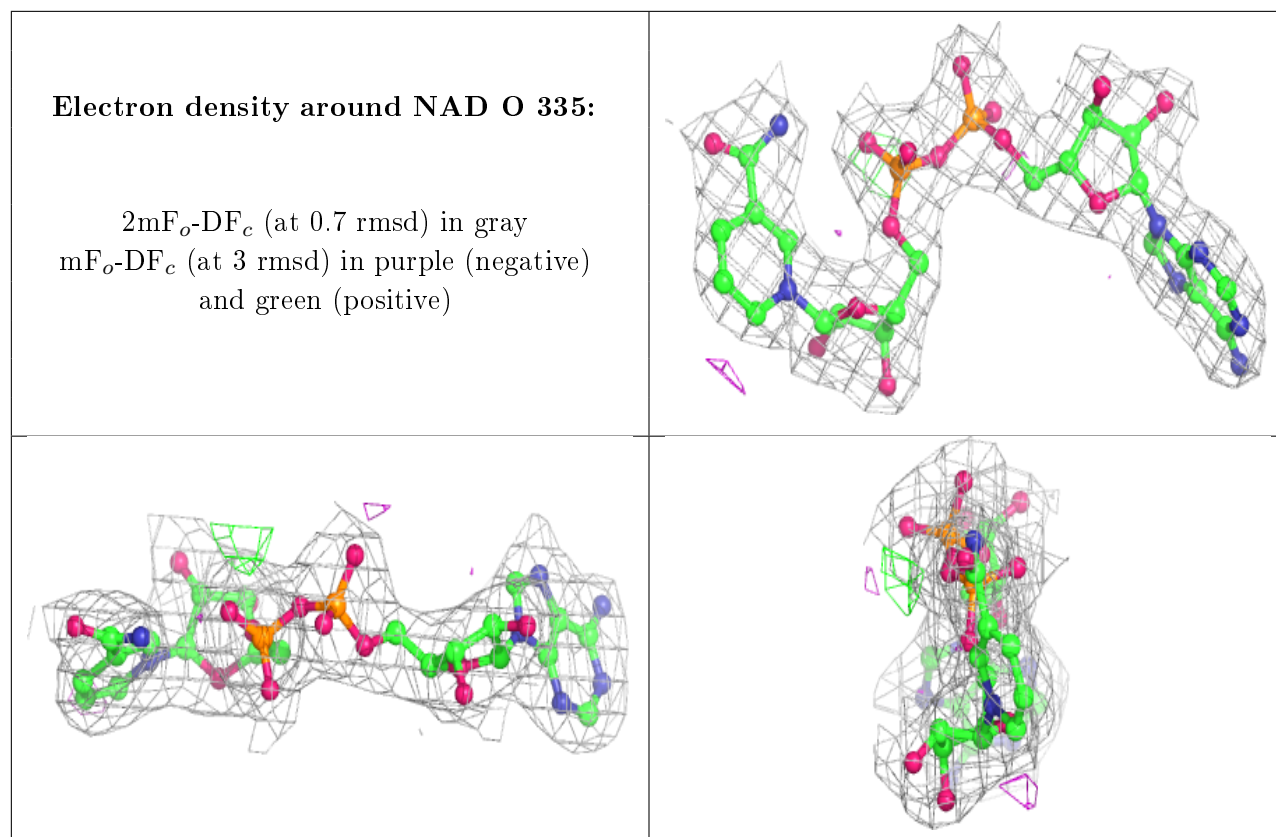
**Electron density around NAD C 335:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAD A 335:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.