



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:54 am BST

PDB ID : 3RVD
Title : Crystal structure of the binary complex, obtained by soaking, of photosynthetic a4 glyceraldehyde 3-phosphate dehydrogenase (gapdh) with cp12-2, both from arabidopsis thaliana.
Authors : Fermani, S.; Thumiger, A.; Falini, G.; Marri, L.; Sparla, F.; Trost, P.
Deposited on : 2011-05-06
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

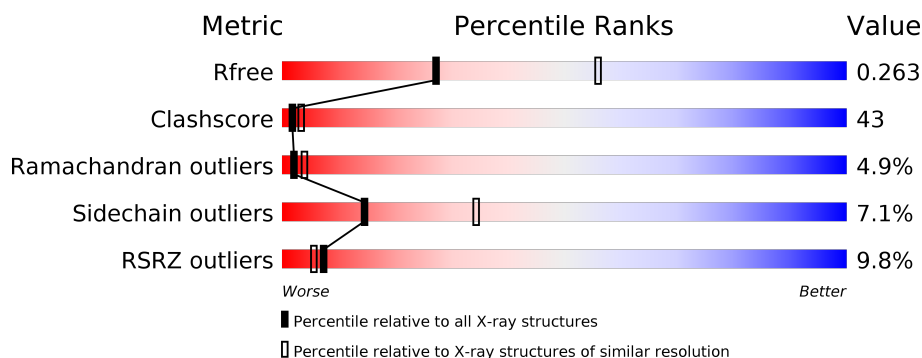
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>0%</div> <div> <div>51%</div> <div>44%</div> <div>5%</div> </div> </div>
1	B	337	<div> <div>3%</div> <div> <div>46%</div> <div>47%</div> <div>7%</div> </div> </div>
1	C	337	<div> <div>4%</div> <div> <div>51%</div> <div>42%</div> <div>7%</div> </div> </div>
1	D	337	<div> <div>7%</div> <div> <div>30%</div> <div>58%</div> <div>11%</div> </div> </div>
1	E	337	<div> <div>36%</div> <div> <div>25%</div> <div>64%</div> <div>10%</div> </div> </div>
1	F	337	<div> <div>18%</div> <div> <div>28%</div> <div>62%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	337	
1	H	337	
1	O	337	
1	Q	337	
2	I	82	
2	J	82	
2	K	82	
2	L	82	
2	M	82	
2	N	82	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27674 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	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	B	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	C	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	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	337	Total	C	N	O	S	0	0	0
			2556	1615	445	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			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	EXPRESSION TAG	UNP P25856
B	-1	ALA	-	EXPRESSION TAG	UNP P25856
C	-1	ALA	-	EXPRESSION TAG	UNP P25856
D	-1	ALA	-	EXPRESSION TAG	UNP P25856
E	-1	ALA	-	EXPRESSION TAG	UNP P25856
F	-1	ALA	-	EXPRESSION TAG	UNP P25856
G	-1	ALA	-	EXPRESSION TAG	UNP P25856
H	-1	ALA	-	EXPRESSION TAG	UNP P25856
O	-1	ALA	-	EXPRESSION TAG	UNP P25856

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-1	ALA	-	EXPRESSION TAG	UNP P25856

- Molecule 2 is a protein called Photosynthetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	22	Total	C	N	O	S	0	0	0
			182	107	29	44	2			
2	J	21	Total	C	N	O	S	0	0	0
			176	104	28	42	2			
2	K	21	Total	C	N	O	S	0	0	0
			176	104	28	42	2			
2	L	19	Total	C	N	O	S	0	0	0
			148	86	22	38	2			
2	M	22	Total	C	N	O	S	0	0	0
			182	107	29	44	2			
2	N	19	Total	C	N	O	S	0	0	0
			160	96	25	37	2			

There are 24 discrepancies between the modelled and reference sequences:

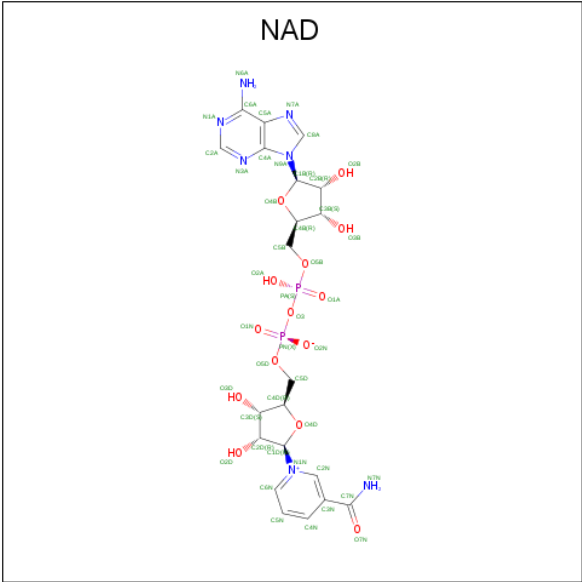
Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
I	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
I	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
I	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
J	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
J	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
J	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
J	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
K	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
K	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
K	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
K	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
L	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
L	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
L	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
L	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
M	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
M	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
M	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
M	0	MET	-	EXPRESSION TAG	UNP Q9LZP9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
N	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
N	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
N	0	MET	-	EXPRESSION TAG	UNP Q9LZP9

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		

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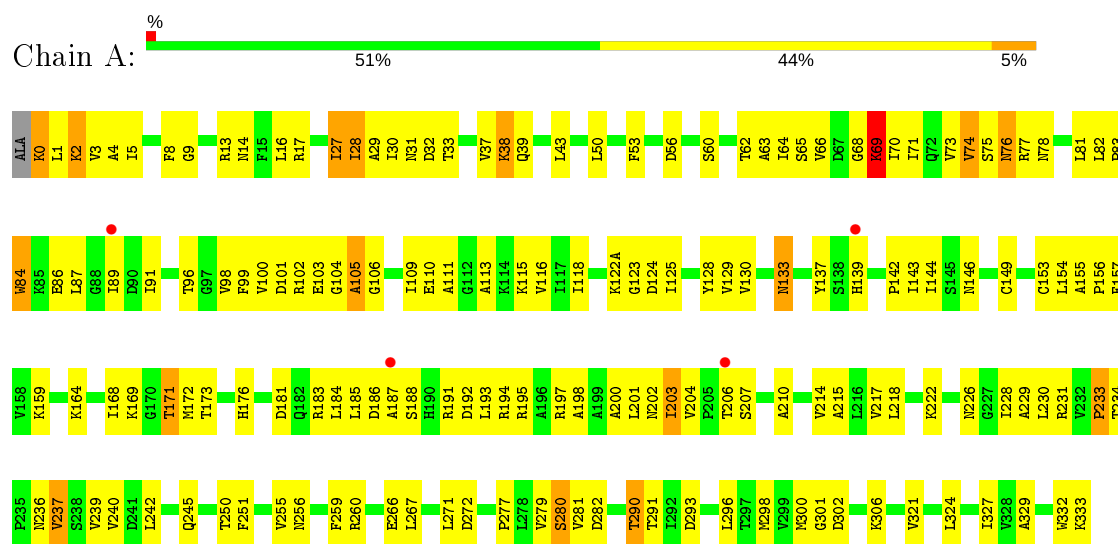
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	35	Total 35	O 35	0	0
5	C	55	Total 55	O 55	0	0
5	D	52	Total 52	O 52	0	0
5	E	42	Total 42	O 42	0	0
5	F	36	Total 36	O 36	0	0
5	G	38	Total 38	O 38	0	0
5	H	31	Total 31	O 31	0	0
5	I	3	Total 3	O 3	0	0
5	J	1	Total 1	O 1	0	0
5	K	20	Total 20	O 20	0	0
5	L	4	Total 4	O 4	0	0
5	M	6	Total 6	O 6	0	0
5	N	10	Total 10	O 10	0	0
5	O	82	Total 82	O 82	0	0
5	Q	69	Total 69	O 69	0	0

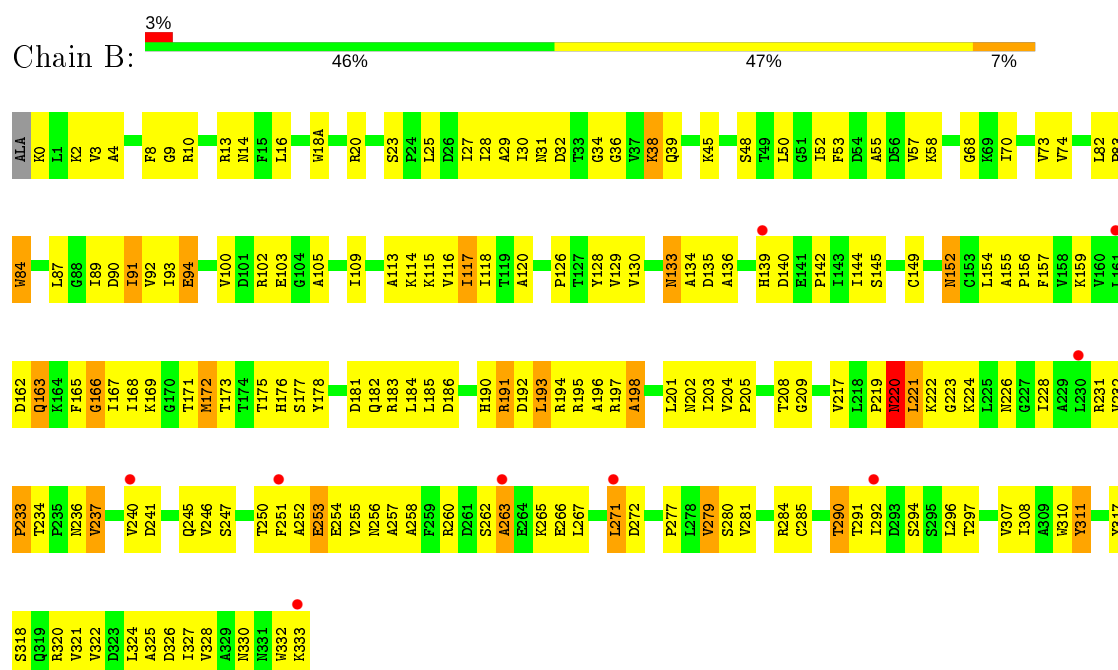
3 Residue-property plots

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

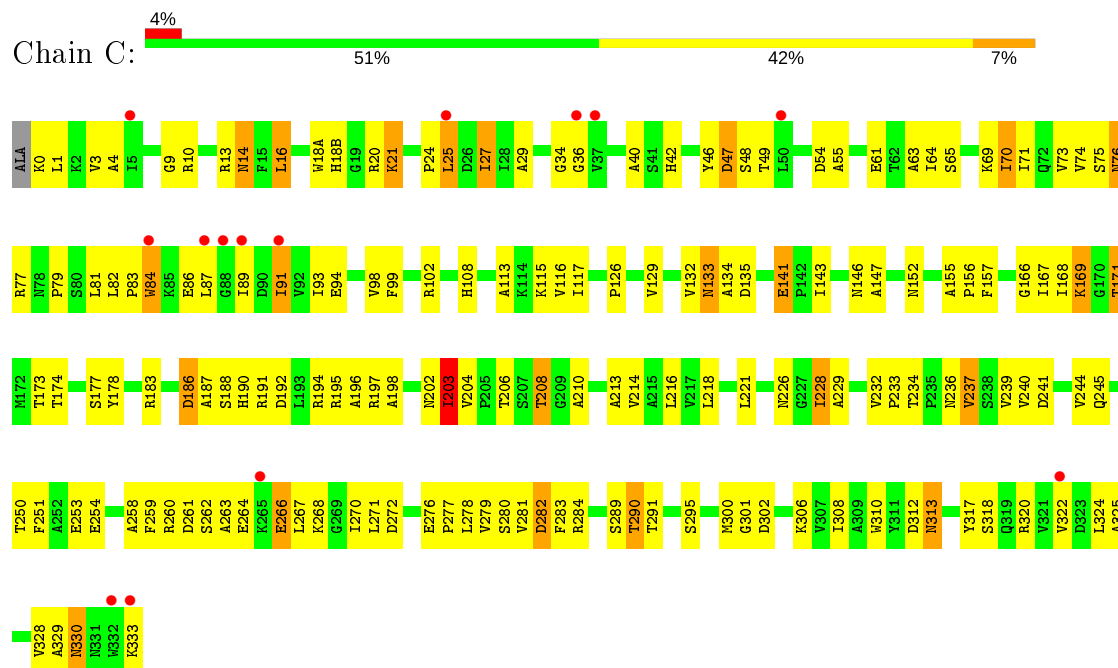
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic



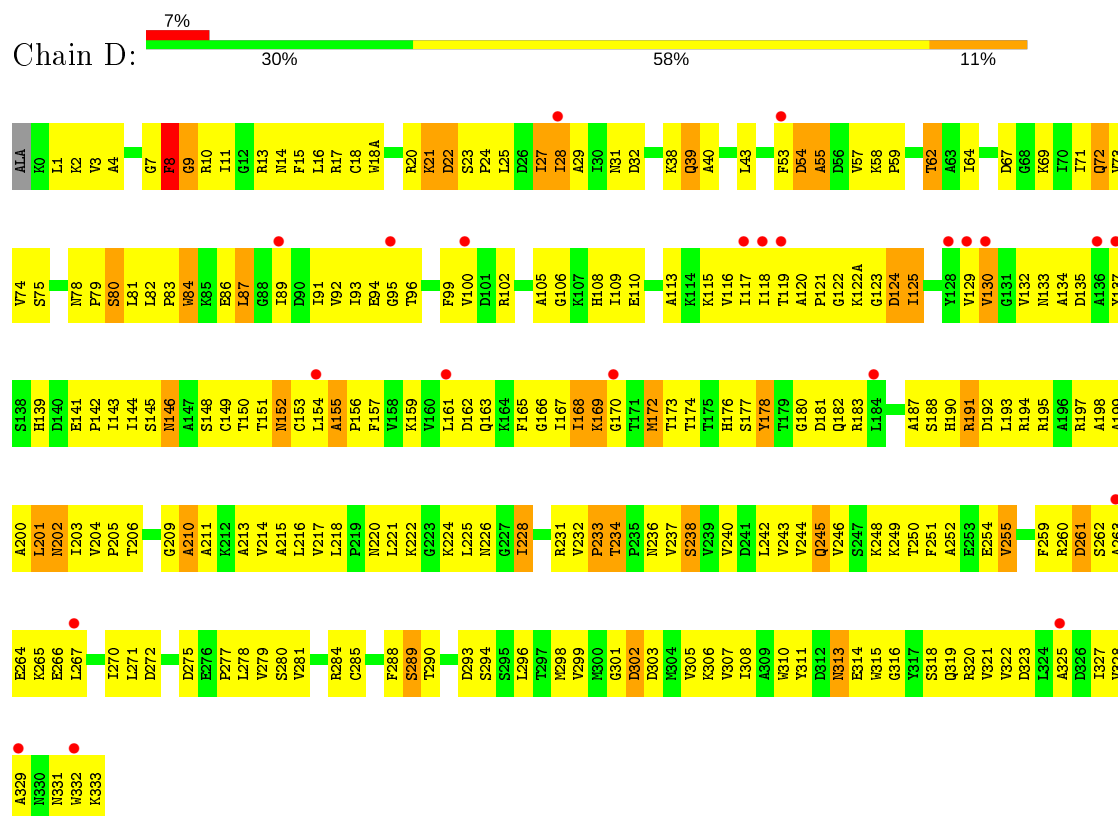
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic



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

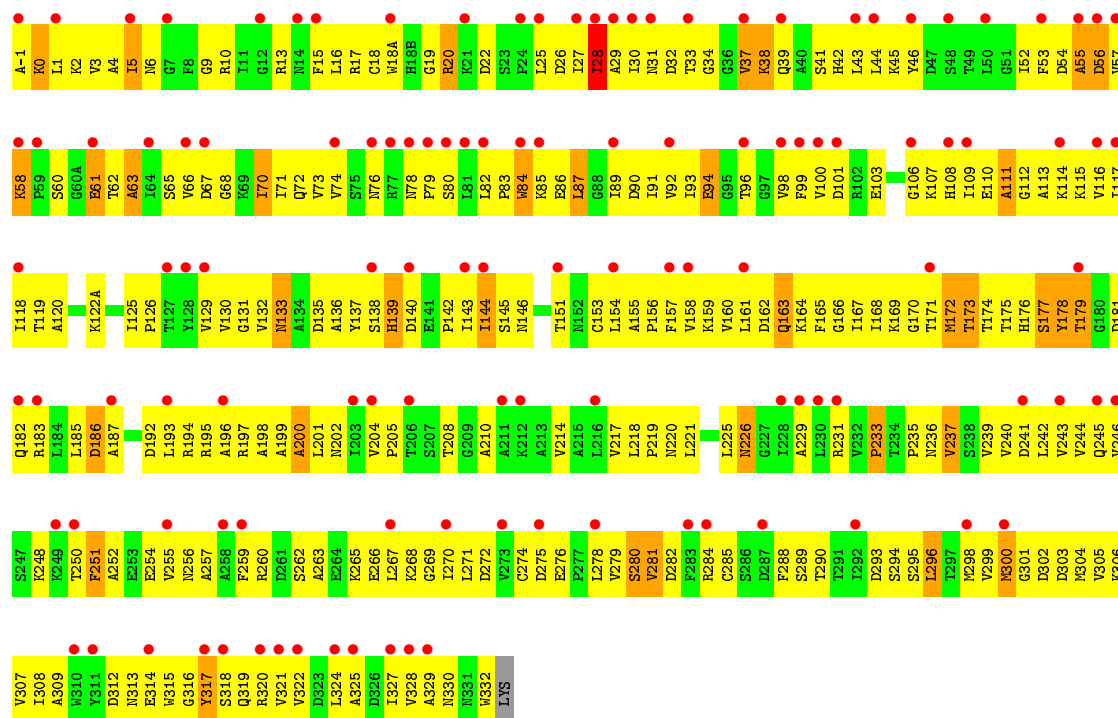


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



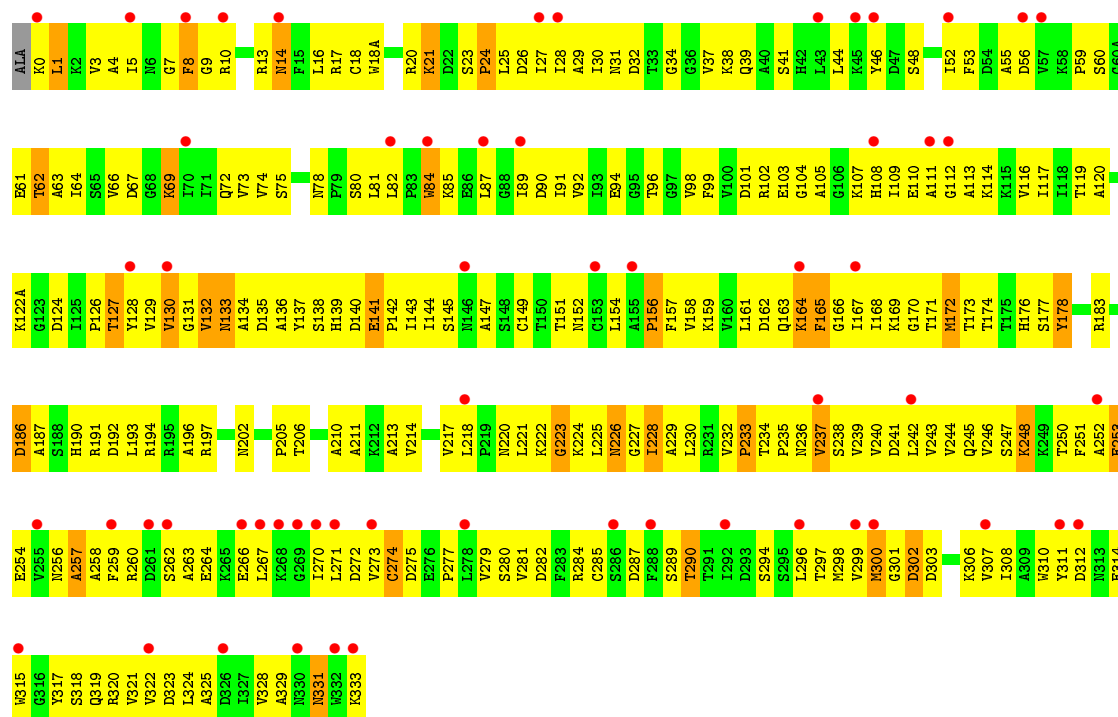
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic





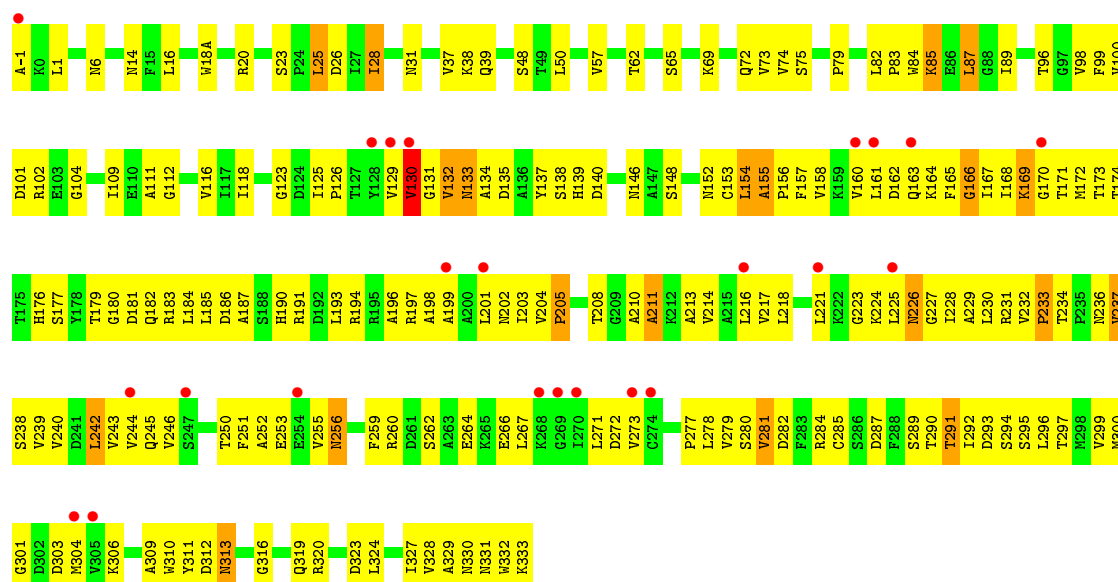
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

Chain F: 18% 28% 62% 9%

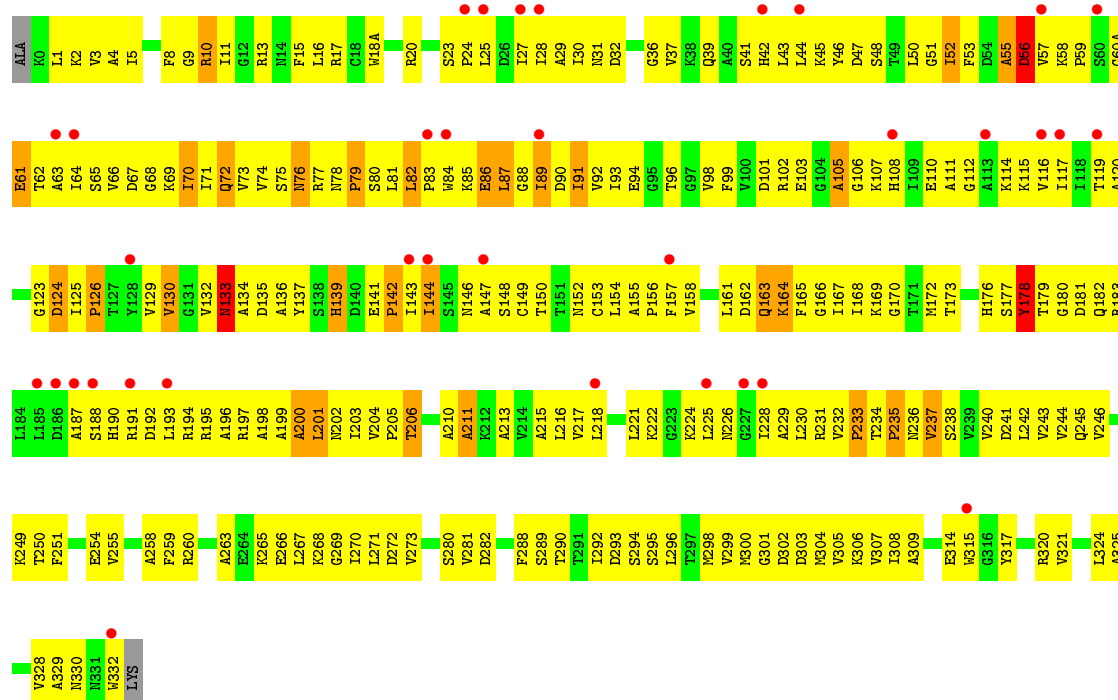


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

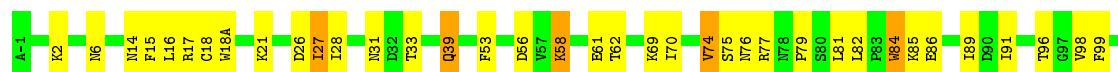
Chain G: 7% 43% 51% 6%

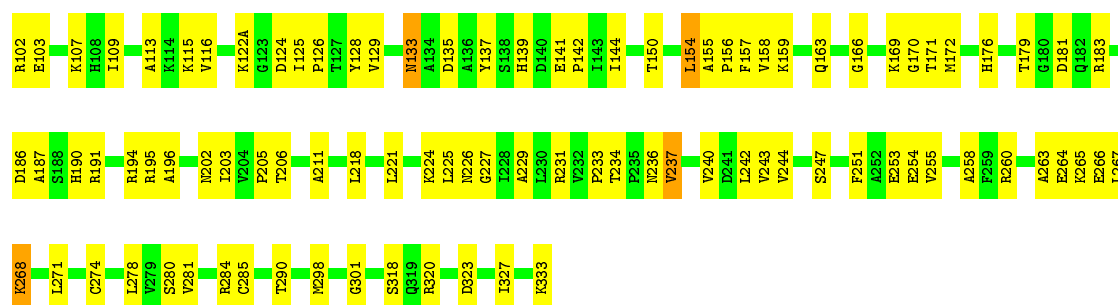


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



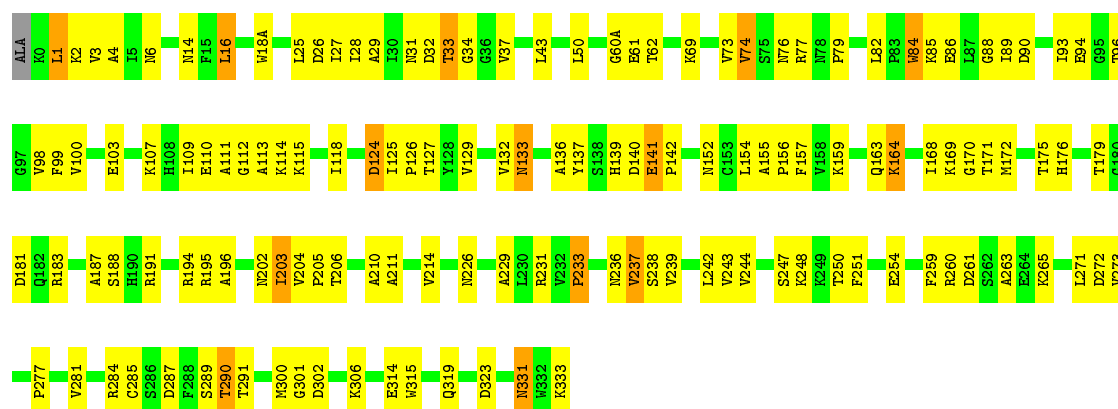
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic





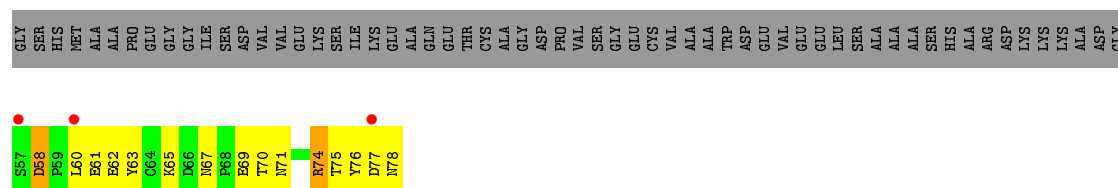
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

Chain Q: 58% 37% .



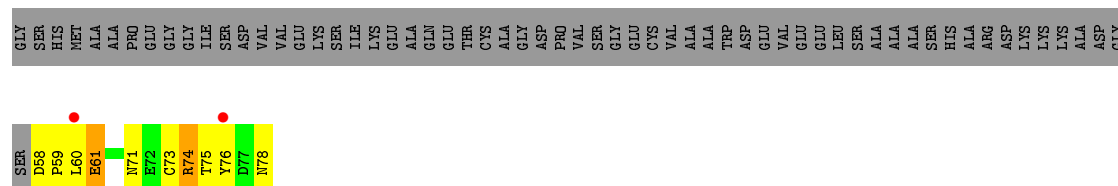
- Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)

Chain I: 4% 9% 16% . 73%



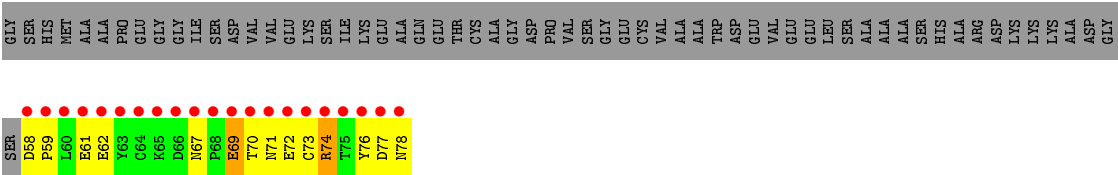
- Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)

Chain J: 2% 13% 10% . 74%

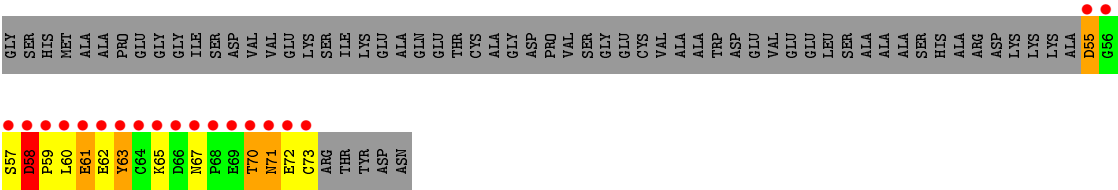


- Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)

Chain K: 26% 9% 15% . 74%



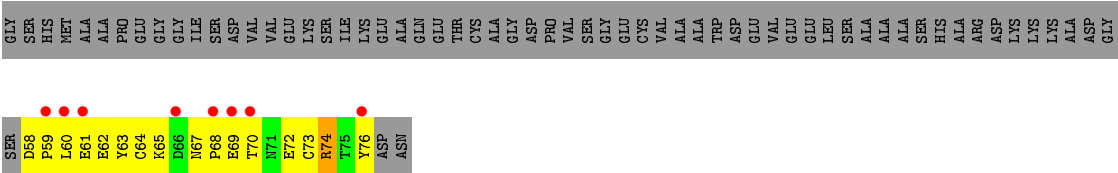
• Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)



• Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)



• Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.18Å 188.75Å 312.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.61 – 2.70 94.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (94.61-2.70) 95.8 (94.60-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.247 , 0.318 0.242 , 0.263	Depositor DCC
R_{free} test set	11850 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 86.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27674	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/2596	0.69	1/3523 (0.0%)
1	B	0.44	0/2596	0.73	2/3523 (0.1%)
1	C	0.44	0/2596	0.70	1/3523 (0.0%)
1	D	0.40	0/2596	0.66	0/3523
1	E	0.44	0/2591	0.68	0/3519
1	F	0.40	0/2596	0.64	0/3523
1	G	0.42	0/2600	0.68	0/3530
1	H	0.40	0/2586	0.65	0/3512
1	O	0.55	0/2601	0.77	1/3530 (0.0%)
1	Q	0.51	0/2596	0.77	2/3523 (0.1%)
2	I	0.75	0/185	0.64	0/251
2	J	0.84	1/179 (0.6%)	0.64	0/243
2	K	0.46	0/179	0.65	0/243
2	L	0.64	0/150	0.86	0/203
2	M	0.66	0/185	0.70	0/251
2	N	0.55	0/163	0.56	0/221
All	All	0.46	1/26995 (0.0%)	0.70	7/36641 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	61	GLU	CG-CD	5.06	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	203	ILE	N-CA-C	-6.16	94.37	111.00
1	O	203	ILE	N-CA-C	-5.87	95.16	111.00
1	B	203	ILE	N-CA-C	-5.82	95.30	111.00
1	A	203	ILE	N-CA-C	-5.62	95.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	60(A)	GLY	N-CA-C	-5.54	99.24	113.10
1	C	203	ILE	N-CA-C	-5.53	96.08	111.00
1	B	34	GLY	N-CA-C	5.52	126.89	113.10

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	2552	0	2593	200	0
1	B	2552	0	2593	218	0
1	C	2552	0	2593	198	0
1	D	2552	0	2593	318	0
1	E	2547	0	2585	369	0
1	F	2552	0	2593	312	0
1	G	2556	0	2598	264	0
1	H	2542	0	2580	338	0
1	O	2557	0	2598	135	0
1	Q	2552	0	2593	129	0
2	I	182	0	149	25	0
2	J	176	0	144	14	0
2	K	176	0	144	25	0
2	L	148	0	117	23	0
2	M	182	0	149	23	0
2	N	160	0	134	31	0
3	A	44	0	26	3	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	6	0
3	E	44	0	26	5	0
3	F	44	0	26	6	0
3	G	44	0	26	1	0
3	H	44	0	26	13	0
3	O	44	0	26	0	0
3	Q	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	0	1	0
4	B	10	0	0	1	0
4	C	25	0	0	1	0
4	D	5	0	0	1	0
4	E	15	0	0	2	0
4	F	10	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	O	10	0	0	0	0
4	Q	20	0	0	1	0
5	A	72	0	0	3	0
5	B	35	0	0	2	0
5	C	55	0	0	1	0
5	D	52	0	0	4	0
5	E	42	0	0	6	0
5	F	36	0	0	5	0
5	G	38	0	0	3	0
5	H	31	0	0	1	0
5	I	3	0	0	0	0
5	J	1	0	0	0	0
5	K	20	0	0	1	0
5	L	4	0	0	2	0
5	M	6	0	0	1	0
5	N	10	0	0	2	0
5	O	82	0	0	3	0
5	Q	69	0	0	3	1
All	All	27674	0	27016	2311	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 43.

All (2311) 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:D:117:ILE:HG23	1:D:144:ILE:HD11	1.23	1.17
1:D:78:ASN:HD22	1:D:81:LEU:HG	1.11	1.13
1:G:161:LEU:HB3	1:G:167:ILE:HD11	1.19	1.12
1:A:202:ASN:HD21	1:C:281:VAL:HG12	1.06	1.11
1:C:183:ARG:HE	1:C:187:ALA:HB3	1.12	1.11
1:B:208:THR:HG23	1:B:209:GLY:H	1.17	1.06
1:F:59:PRO:HA	1:F:64:ILE:HG22	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LYS:HD3	2:M:57:SER:HA	1.38	1.05
1:F:117:ILE:HA	1:F:144:ILE:HD11	1.35	1.04
1:E:194:ARG:HH21	1:G:277:PRO:HA	1.21	1.02
1:A:65:SER:HB3	1:A:70:ILE:HD13	1.38	1.01
1:H:2:LYS:HD2	1:H:88:GLY:HA2	1.40	1.01
1:B:139:HIS:HB3	1:B:333:LYS:HE2	1.41	1.01
1:D:299:VAL:HG22	1:D:305:VAL:HG22	1.41	1.00
1:E:169:LYS:HD2	1:G:301:GLY:HA3	1.44	1.00
1:F:176:HIS:HA	1:F:238:SER:HB3	1.43	1.00
1:G:271:LEU:HD11	1:G:292:ILE:HD13	1.45	0.99
1:E:262:SER:HB3	1:E:267:LEU:HD12	1.44	0.97
1:O:6:ASN:ND2	1:O:31:ASN:HD22	1.61	0.97
1:H:181:ASP:HB3	1:H:195:ARG:HD3	1.47	0.97
1:E:160:VAL:O	1:E:164:LYS:HB2	1.64	0.96
1:E:202:ASN:HB3	1:G:281:VAL:HG23	1.48	0.96
1:E:186:ASP:HB2	1:H:10:ARG:NH1	1.81	0.95
2:M:62:GLU:HG3	5:M:101:HOH:O	1.64	0.95
1:E:117:ILE:HG12	1:E:144:ILE:HD11	1.46	0.95
1:E:204:VAL:HB	1:E:231:ARG:HB2	1.46	0.94
1:G:221:LEU:HD11	1:G:225:LEU:HG	1.47	0.94
1:D:149:CYS:SG	2:I:78:ASN:ND2	2.42	0.93
1:F:318:SER:O	1:F:322:VAL:HG23	1.67	0.93
1:A:202:ASN:ND2	1:C:281:VAL:HG12	1.83	0.93
2:J:71:ASN:HA	2:J:74:ARG:HH21	1.31	0.92
2:K:69:GLU:HB3	1:O:98:VAL:HG11	1.49	0.92
1:F:202:ASN:HD22	1:H:281:VAL:HG23	1.33	0.91
1:H:215:ALA:HB1	1:H:222:LYS:HA	1.53	0.91
1:E:70:ILE:HD13	1:E:70:ILE:H	1.35	0.91
1:Q:331:ASN:HD22	1:Q:331:ASN:N	1.67	0.91
1:G:271:LEU:HD13	1:G:290:THR:HG23	1.54	0.90
1:D:78:ASN:HD21	1:D:80:SER:HB2	1.36	0.90
1:E:279:VAL:HG11	1:G:204:VAL:HG22	1.53	0.90
1:F:129:VAL:HG23	1:F:217:VAL:HG11	1.53	0.90
1:F:245:GLN:HE21	1:H:245:GLN:NE2	1.70	0.90
1:E:17:ARG:CZ	1:E:53:PHE:HB2	2.02	0.89
1:D:62:THR:OG1	1:H:74:VAL:HG13	1.70	0.89
1:B:233:PRO:HB2	1:D:233:PRO:HB2	1.54	0.89
1:F:5:ILE:HB	1:F:30:ILE:HG23	1.54	0.89
1:D:7:GLY:HA3	1:D:96:THR:HG22	1.53	0.89
1:E:262:SER:O	1:E:267:LEU:HB2	1.73	0.88
2:N:70:THR:HB	2:N:73:CYS:SG	2.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:O	1:H:111:ALA:HB1	1.74	0.88
1:F:250:THR:HG23	1:F:299:VAL:HG11	1.53	0.88
1:G:130:VAL:HG21	1:G:320:ARG:HD3	1.53	0.88
1:F:117:ILE:HA	1:F:144:ILE:CD1	2.04	0.87
1:H:1:LEU:HD11	1:H:90:ASP:HB2	1.52	0.87
1:A:300:MET:HB2	1:C:226:ASN:ND2	1.90	0.87
2:K:78:ASN:HD21	1:O:231:ARG:HE	1.17	0.87
1:G:130:VAL:CG2	1:G:320:ARG:HD3	2.05	0.87
1:D:83:PRO:O	1:D:87:LEU:HB2	1.75	0.86
1:Q:210:ALA:O	1:Q:214:VAL:HG23	1.75	0.86
1:C:183:ARG:NE	1:C:187:ALA:HB3	1.89	0.86
1:G:271:LEU:HD12	1:G:272:ASP:H	1.40	0.86
1:B:204:VAL:HG22	1:D:279:VAL:HG11	1.58	0.86
1:E:60:SER:OG	1:E:65:SER:HB2	1.74	0.86
3:H:401:NAD:N7A	2:N:69:GLU:HG2	1.90	0.86
1:Q:4:ALA:HB2	1:Q:89:ILE:HG12	1.56	0.86
1:E:194:ARG:HH11	1:E:205:PRO:HB2	1.40	0.86
1:O:159:LYS:O	1:O:163:GLN:HG3	1.74	0.86
1:H:299:VAL:HG22	1:H:305:VAL:HG22	1.58	0.85
1:H:126:PRO:HB2	1:H:144:ILE:HG22	1.59	0.85
1:E:173:THR:HG22	1:E:241:ASP:HB3	1.56	0.85
1:F:183:ARG:HE	1:F:187:ALA:HB3	1.41	0.85
1:Q:133:ASN:HD22	1:Q:133:ASN:H	1.25	0.84
1:O:6:ASN:HD21	1:O:31:ASN:HD22	1.23	0.84
1:F:233:PRO:HG2	1:H:234:THR:HG22	1.60	0.84
1:H:70:ILE:C	1:H:71:ILE:HD12	1.97	0.84
1:E:300:MET:HB2	1:G:169:LYS:NZ	1.92	0.83
1:G:177:SER:HB3	1:G:234:THR:O	1.77	0.83
1:G:239:VAL:HG23	1:G:309:ALA:O	1.78	0.83
1:H:231:ARG:HG3	1:H:231:ARG:HH11	1.44	0.83
1:E:210:ALA:O	1:E:214:VAL:HG23	1.78	0.83
2:K:69:GLU:CG	1:O:77:ARG:NH2	2.41	0.83
1:E:163:GLN:O	1:E:164:LYS:HD2	1.77	0.82
2:I:62:GLU:HA	2:I:65:LYS:HE3	1.60	0.82
1:H:154:LEU:HD13	1:H:240:VAL:HG11	1.61	0.82
1:F:129:VAL:H	1:F:133:ASN:HD21	1.24	0.82
1:D:129:VAL:HG23	1:D:217:VAL:HG11	1.61	0.82
1:A:100:VAL:HG12	1:A:118:ILE:HG21	1.61	0.82
1:D:3:VAL:HG21	1:D:25:LEU:HB3	1.62	0.82
1:E:154:LEU:HD23	1:E:214:VAL:HG21	1.62	0.82
1:E:4:ALA:O	1:E:93:ILE:HD12	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:ALA:HB1	1:G:226:ASN:HA	1.60	0.82
1:C:84:TRP:HA	1:C:89:ILE:HD13	1.59	0.82
1:D:16:LEU:HD23	1:D:16:LEU:O	1.80	0.82
2:L:70:THR:HG22	2:L:71:ASN:OD1	1.78	0.82
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.62	0.81
1:G:131:GLY:H	1:G:134:ALA:HB2	1.45	0.81
1:G:157:PHE:HE1	1:G:242:LEU:HD22	1.45	0.81
1:E:194:ARG:NH2	1:G:277:PRO:HA	1.95	0.81
1:G:129:VAL:H	1:G:133:ASN:HD21	1.27	0.81
1:G:231:ARG:NH2	2:M:78:ASN:HD22	1.77	0.81
1:H:91:ILE:HD13	1:H:92:VAL:N	1.96	0.81
1:H:168:ILE:HG22	1:H:169:LYS:HG2	1.63	0.81
1:G:293:ASP:HB3	1:G:296:LEU:HD12	1.63	0.80
1:A:202:ASN:HD21	1:C:281:VAL:CG1	1.92	0.80
1:G:130:VAL:HA	1:G:134:ALA:HB2	1.64	0.80
1:D:249:LYS:HD2	1:D:302:ASP:HB3	1.61	0.80
1:C:156:PRO:HB2	1:C:290:THR:HG21	1.64	0.80
1:D:170:GLY:HA3	1:D:244:VAL:HG12	1.64	0.80
1:O:260:ARG:O	1:O:264:GLU:HG3	1.80	0.80
1:D:15:PHE:CE2	1:D:93:ILE:HG13	2.17	0.80
1:E:28:ILE:HA	1:E:71:ILE:HD12	1.64	0.80
1:F:156:PRO:HB2	1:F:290:THR:HG21	1.62	0.80
1:G:79:PRO:HA	1:G:82:LEU:HD12	1.63	0.80
1:F:117:ILE:CA	1:F:144:ILE:HD11	2.11	0.80
1:G:256:ASN:HD22	1:G:256:ASN:N	1.80	0.80
1:H:164:LYS:N	1:H:164:LYS:HD2	1.97	0.80
1:F:277:PRO:HB2	1:H:194:ARG:HG3	1.65	0.80
1:F:41:SER:HB2	1:F:64:ILE:HG21	1.62	0.80
1:F:78:ASN:HB3	1:F:81:LEU:HD13	1.63	0.79
1:F:202:ASN:HD22	1:H:281:VAL:CG2	1.96	0.79
1:F:4:ALA:HB3	1:F:92:VAL:HG22	1.65	0.79
1:G:14:ASN:OD1	1:G:50:LEU:HD11	1.82	0.79
1:H:72:GLN:H	1:H:72:GLN:HE21	1.30	0.79
1:F:67:ASP:HB2	1:F:69:LYS:HE2	1.64	0.79
2:L:57:SER:OG	2:L:58:ASP:N	2.12	0.79
1:H:293:ASP:HB3	1:H:296:LEU:HD12	1.63	0.79
1:D:318:SER:O	1:D:322:VAL:HG23	1.83	0.79
1:E:119:THR:HG22	1:E:321:VAL:HG11	1.65	0.79
1:E:169:LYS:HE3	1:G:303:ASP:OD2	1.83	0.78
1:G:28:ILE:H	1:G:28:ILE:HD13	1.49	0.78
1:B:139:HIS:HB3	1:B:333:LYS:CE	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:CYS:HB3	3:F:401:NAD:H5N	1.64	0.78
1:F:301:GLY:HA3	1:H:169:LYS:HD2	1.66	0.78
1:D:20:ARG:HH21	1:D:319:GLN:NE2	1.82	0.78
1:E:84:TRP:HD1	1:E:113:ALA:HB2	1.48	0.78
2:I:58:ASP:OD1	2:I:61:GLU:HG3	1.84	0.78
1:A:37:VAL:HG21	1:A:63:ALA:H	1.48	0.78
1:C:21:LYS:H	1:C:21:LYS:HD2	1.49	0.78
1:F:271:LEU:HD12	1:F:272:ASP:H	1.48	0.78
2:N:58:ASP:HA	2:N:61:GLU:OE1	1.82	0.78
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.18	0.78
1:B:185:LEU:HD21	1:C:178:TYR:HE1	1.48	0.78
1:B:208:THR:HG23	1:B:209:GLY:N	1.98	0.78
1:D:139:HIS:HB3	1:D:333:LYS:HE2	1.64	0.78
1:Q:126:PRO:HG2	1:Q:141:GLU:HG2	1.64	0.78
1:C:76:ASN:OD1	1:C:81:LEU:HD12	1.84	0.77
1:F:176:HIS:HA	1:F:238:SER:CB	2.13	0.77
1:C:89:ILE:H	1:C:89:ILE:HD12	1.49	0.77
1:E:153:CYS:HA	1:E:290:THR:HG22	1.67	0.77
1:F:56:ASP:HB2	1:F:67:ASP:H	1.50	0.77
2:K:58:ASP:O	2:K:62:GLU:HG3	1.83	0.77
1:F:56:ASP:O	1:F:66:VAL:HA	1.85	0.77
1:F:96:THR:OG1	1:F:98:VAL:HG22	1.83	0.77
1:H:91:ILE:HD13	1:H:92:VAL:H	1.49	0.77
2:M:57:SER:O	2:M:61:GLU:HB2	1.82	0.77
1:A:281:VAL:H	1:C:202:ASN:ND2	1.81	0.77
1:O:129:VAL:H	1:O:133:ASN:HD21	1.33	0.77
1:A:184:LEU:HG	1:A:185:LEU:HD12	1.67	0.77
1:F:126:PRO:HG2	1:F:144:ILE:HG22	1.66	0.77
1:H:2:LYS:HD2	1:H:88:GLY:CA	2.15	0.77
1:O:33:THR:HG22	1:O:77:ARG:HG2	1.65	0.77
1:B:191:ARG:HH21	2:J:61:GLU:HA	1.49	0.77
1:E:186:ASP:HB3	1:H:13:ARG:HH22	1.50	0.77
1:E:63:ALA:HA	1:E:73:VAL:HG23	1.67	0.77
1:F:245:GLN:HE21	1:H:245:GLN:HE21	1.31	0.76
1:F:38:LYS:HD3	2:M:57:SER:CA	2.14	0.76
1:A:65:SER:HB3	1:A:70:ILE:CD1	2.15	0.76
1:Q:28:ILE:HD11	1:Q:89:ILE:HD11	1.65	0.76
1:F:117:ILE:HG23	1:F:144:ILE:HD11	1.67	0.76
1:O:129:VAL:H	1:O:133:ASN:ND2	1.83	0.76
1:D:89:ILE:HG21	1:D:92:VAL:HG23	1.65	0.76
1:E:133:ASN:OD1	1:E:217:VAL:HA	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:O	1:B:163:GLN:HB2	1.87	0.75
1:C:260:ARG:O	1:C:264:GLU:HG2	1.86	0.75
1:G:155:ALA:HB3	1:G:156:PRO:HD3	1.67	0.75
1:E:109:ILE:HA	1:E:113:ALA:HB3	1.66	0.75
1:F:289:SER:OG	1:F:320:ARG:HD2	1.86	0.75
1:G:139:HIS:CE1	1:G:332:TRP:HA	2.22	0.75
2:K:69:GLU:CG	1:O:77:ARG:HH22	1.97	0.75
1:A:96:THR:OG1	1:A:98:VAL:HG22	1.87	0.75
1:G:273:VAL:HG13	1:G:292:ILE:HG22	1.69	0.75
1:C:330:ASN:HD22	1:C:330:ASN:N	1.84	0.75
1:G:323:ASP:O	1:G:327:ILE:HD13	1.87	0.75
1:H:130:VAL:HA	1:H:134:ALA:HB2	1.68	0.75
1:E:235:PRO:HG2	1:E:284:ARG:HH21	1.51	0.75
1:D:7:GLY:CA	1:D:96:THR:HG22	2.16	0.75
1:G:79:PRO:HA	1:G:82:LEU:CD1	2.17	0.75
1:E:80:SER:HB2	1:E:107:LYS:HE2	1.68	0.75
1:E:80:SER:CB	1:E:107:LYS:HE2	2.17	0.75
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.21	0.75
1:H:176:HIS:HA	1:H:238:SER:HB3	1.67	0.75
1:Q:90:ASP:HA	1:Q:114:LYS:HD2	1.69	0.75
1:B:139:HIS:CB	1:B:333:LYS:HE2	2.15	0.74
1:A:300:MET:CE	1:C:226:ASN:HD22	2.00	0.74
1:E:263:ALA:O	1:E:268:LYS:HA	1.87	0.74
1:E:267:LEU:HD13	1:E:271:LEU:HD13	1.69	0.74
1:A:156:PRO:HB2	1:A:290:THR:HG21	1.69	0.74
1:D:251:PHE:O	1:D:255:VAL:HG23	1.87	0.74
1:F:10:ARG:O	1:F:14:ASN:HB2	1.87	0.74
1:E:279:VAL:HG22	1:G:197:ARG:NH1	2.03	0.74
1:G:168:ILE:HB	1:G:245:GLN:O	1.87	0.74
1:B:181:ASP:OD2	2:J:76:TYR:HB2	1.86	0.74
1:A:203:ILE:HB	1:C:280:SER:HB3	1.69	0.74
1:F:172:MET:O	1:F:227:GLY:HA3	1.88	0.74
1:F:21:LYS:H	1:F:21:LYS:NZ	1.86	0.74
1:G:256:ASN:ND2	1:G:256:ASN:N	2.35	0.74
1:D:215:ALA:HB1	1:D:222:LYS:HA	1.70	0.74
1:D:78:ASN:HD22	1:D:81:LEU:CG	1.95	0.74
1:D:301:GLY:O	1:D:302:ASP:HB2	1.87	0.74
1:E:186:ASP:HB3	1:H:13:ARG:NH2	2.02	0.74
1:E:275:ASP:HA	1:E:294:SER:OG	1.88	0.74
2:K:71:ASN:HA	2:K:74:ARG:HH21	1.51	0.74
1:A:129:VAL:H	1:A:133:ASN:ND2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:MET:HB2	1:C:226:ASN:HD21	1.51	0.74
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.69	0.74
1:C:129:VAL:H	1:C:133:ASN:ND2	1.86	0.74
1:E:217:VAL:HG23	1:E:218:LEU:HG	1.69	0.73
1:F:129:VAL:H	1:F:133:ASN:ND2	1.86	0.73
1:H:269:GLY:HA2	1:H:288:PHE:HE2	1.53	0.73
1:F:190:HIS:HB3	1:F:196:ALA:HB2	1.70	0.73
1:D:106:GLY:O	1:D:109:ILE:HG12	1.88	0.73
1:D:194:ARG:NH1	1:D:205:PRO:HB2	2.04	0.73
1:E:318:SER:O	1:E:322:VAL:HG23	1.88	0.73
1:E:32:ASP:C	1:E:34:GLY:H	1.91	0.73
1:G:271:LEU:HD11	1:G:292:ILE:CD1	2.17	0.73
1:O:39:GLN:NE2	1:O:39:GLN:H	1.87	0.73
1:H:117:ILE:HD11	1:H:324:LEU:HD23	1.70	0.73
1:F:251:PHE:CE1	1:F:254:GLU:HB2	2.23	0.73
1:G:161:LEU:CB	1:G:167:ILE:HD11	2.09	0.73
1:H:206:THR:HG23	1:H:229:ALA:HB3	1.70	0.73
1:E:3:VAL:HG21	1:E:25:LEU:HD22	1.70	0.73
1:O:154:LEU:HD23	1:O:240:VAL:HG11	1.70	0.73
1:D:242:LEU:HD12	1:D:243:VAL:N	2.04	0.72
1:G:133:ASN:OD1	1:G:217:VAL:HG12	1.89	0.72
1:E:115:LYS:NZ	1:E:115:LYS:HB3	2.04	0.72
1:E:186:ASP:HB2	1:H:10:ARG:HH12	1.52	0.72
1:B:296:LEU:HD22	1:D:228:ILE:HG21	1.69	0.72
1:C:272:ASP:O	1:C:291:THR:HA	1.89	0.72
1:D:152:ASN:ND2	1:D:320:ARG:HG3	2.04	0.72
1:F:90:ASP:HA	1:F:114:LYS:HD3	1.72	0.72
1:G:203:ILE:HG23	1:G:232:VAL:HG12	1.72	0.72
1:G:83:PRO:O	1:G:87:LEU:HD22	1.89	0.72
1:E:84:TRP:CD1	1:E:113:ALA:HB2	2.23	0.72
1:F:187:ALA:O	1:F:196:ALA:HB1	1.88	0.72
2:L:58:ASP:N	2:L:59:PRO:HD3	2.03	0.72
1:E:32:ASP:OD2	3:E:401:NAD:H1B	1.89	0.72
1:D:176:HIS:HA	1:D:238:SER:HB3	1.70	0.72
1:C:177:SER:HB3	1:C:234:THR:O	1.89	0.72
1:D:161:LEU:HD21	1:D:259:PHE:CZ	2.25	0.71
1:H:84:TRP:CD1	1:H:111:ALA:HB3	2.25	0.71
1:O:154:LEU:O	1:O:158:VAL:HG23	1.90	0.71
1:D:78:ASN:ND2	1:D:81:LEU:HG	1.96	0.71
1:G:129:VAL:HG23	1:G:217:VAL:HG11	1.71	0.71
1:F:114:LYS:N	1:F:114:LYS:HD2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ILE:O	1:E:28:ILE:HD13	1.91	0.71
1:G:271:LEU:HD12	1:G:272:ASP:N	2.04	0.71
1:E:298:MET:SD	1:G:226:ASN:ND2	2.64	0.71
1:Q:168:ILE:HD11	1:Q:247:SER:HB3	1.73	0.71
1:D:242:LEU:HD11	1:D:244:VAL:HG13	1.72	0.71
1:A:300:MET:HE2	1:C:226:ASN:HD22	1.53	0.70
1:E:235:PRO:HG2	1:E:284:ARG:NH2	2.05	0.70
1:F:130:VAL:HB	1:F:320:ARG:HD3	1.72	0.70
1:G:202:ASN:O	1:G:233:PRO:HD3	1.90	0.70
1:O:202:ASN:HD21	1:Q:281:VAL:HG12	1.55	0.70
1:E:25:LEU:HD21	1:E:325:ALA:O	1.91	0.70
1:A:279:VAL:HG22	1:C:197:ARG:NH1	2.06	0.70
1:H:73:VAL:O	1:H:73:VAL:HG12	1.92	0.70
2:L:71:ASN:N	2:L:71:ASN:OD1	2.23	0.70
1:E:239:VAL:HG22	1:E:240:VAL:H	1.55	0.70
1:H:37:VAL:HG21	1:H:62:THR:HA	1.72	0.70
1:H:191:ARG:HG3	2:N:73:CYS:HA	1.72	0.70
1:B:93:ILE:HD13	1:B:117:ILE:CG2	2.22	0.70
1:C:102:ARG:HG3	1:C:102:ARG:HH11	1.57	0.70
1:C:63:ALA:HB1	1:C:70:ILE:HD11	1.74	0.70
1:A:14:ASN:OD1	1:A:50:LEU:HD11	1.92	0.69
1:H:155:ALA:HB3	1:H:156:PRO:HD3	1.71	0.69
1:H:231:ARG:HG3	1:H:231:ARG:NH1	2.06	0.69
1:H:249:LYS:HG2	1:H:302:ASP:HB3	1.74	0.69
1:B:202:ASN:HD21	1:D:281:VAL:HB	1.57	0.69
1:H:1:LEU:CD1	1:H:90:ASP:HB2	2.22	0.69
1:B:114:LYS:HZ3	1:B:332:TRP:HZ2	1.39	0.69
1:B:139:HIS:HB2	1:B:333:LYS:HG3	1.73	0.69
1:D:236:ASN:OD1	1:D:314:GLU:HG3	1.92	0.69
1:G:205:PRO:HB3	1:G:230:LEU:HD23	1.73	0.69
1:A:105:ALA:HB1	1:A:116:VAL:HG11	1.74	0.69
1:E:169:LYS:HD2	1:G:301:GLY:CA	2.22	0.69
1:G:251:PHE:C	1:G:299:VAL:HG21	2.12	0.69
1:F:32:ASP:OD1	3:F:401:NAD:H1B	1.92	0.69
1:F:300:MET:CG	1:H:226:ASN:HD21	2.06	0.69
1:E:60:SER:HG	1:E:65:SER:HB2	1.54	0.69
1:D:313:ASN:O	3:D:401:NAD:H4N	1.93	0.69
1:B:31:ASN:HB2	1:B:74:VAL:CG2	2.23	0.69
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.28	0.69
1:A:298:MET:HE1	1:C:226:ASN:HB2	1.75	0.69
1:D:262:SER:HB3	1:D:267:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:PHE:HE2	1:E:27:ILE:HD11	1.58	0.68
1:E:319:GLN:OE1	1:E:319:GLN:HA	1.92	0.68
1:F:154:LEU:O	1:F:158:VAL:HG23	1.93	0.68
1:H:181:ASP:HB3	1:H:195:ARG:CD	2.22	0.68
2:N:58:ASP:HB3	2:N:59:PRO:HD3	1.75	0.68
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.28	0.68
1:E:159:LYS:O	1:E:163:GLN:HB2	1.93	0.68
1:E:80:SER:HB2	1:E:107:LYS:CE	2.23	0.68
1:H:32:ASP:OD1	3:H:401:NAD:H1B	1.92	0.68
1:O:6:ASN:HD21	1:O:31:ASN:ND2	1.91	0.68
1:O:281:VAL:HG23	1:Q:202:ASN:ND2	2.08	0.68
1:H:144:ILE:H	1:H:144:ILE:HD13	1.59	0.68
1:A:0:LYS:H3	1:A:0:LYS:HE2	1.57	0.68
1:B:253:GLU:O	1:B:257:ALA:HB2	1.93	0.68
1:H:17:ARG:HG2	1:H:53:PHE:CE1	2.29	0.68
2:K:69:GLU:HG3	1:O:77:ARG:NH2	2.09	0.68
1:E:144:ILE:H	1:E:144:ILE:HD13	1.58	0.68
1:H:79:PRO:HG2	1:H:99:PHE:CZ	2.28	0.68
1:E:280:SER:HB3	1:G:203:ILE:H	1.59	0.68
1:F:279:VAL:HG23	1:F:281:VAL:HG12	1.74	0.68
1:H:272:ASP:OD2	1:H:273:VAL:N	2.26	0.68
1:A:100:VAL:HG12	1:A:118:ILE:CG2	2.24	0.68
1:B:190:HIS:HB3	1:B:196:ALA:HB2	1.75	0.68
1:D:194:ARG:HH11	1:D:205:PRO:HB2	1.59	0.68
1:B:202:ASN:HD21	1:D:281:VAL:CG1	2.07	0.68
1:F:108:HIS:HB2	1:F:116:VAL:HG21	1.75	0.68
1:G:157:PHE:CE1	1:G:242:LEU:HD22	2.29	0.68
1:B:186:ASP:HB2	1:C:10:ARG:HH11	1.57	0.68
1:F:210:ALA:HA	1:F:213:ALA:HB3	1.75	0.68
1:B:126:PRO:HG2	1:B:144:ILE:HG22	1.75	0.67
1:C:169:LYS:HE2	1:C:245:GLN:OE1	1.94	0.67
1:B:220:ASN:O	1:B:222:LYS:N	2.25	0.67
1:E:106:GLY:O	1:E:110:GLU:HG2	1.94	0.67
1:H:65:SER:HA	1:H:70:ILE:HA	1.76	0.67
1:O:202:ASN:HD21	1:Q:281:VAL:CG1	2.07	0.67
1:D:156:PRO:HB2	1:D:290:THR:HG21	1.76	0.67
1:G:324:LEU:O	1:G:328:VAL:HG23	1.93	0.67
1:F:183:ARG:NE	1:F:187:ALA:HB3	2.10	0.67
1:H:36:GLY:H	1:H:39:GLN:NE2	1.92	0.67
1:D:155:ALA:HB3	1:D:156:PRO:HD3	1.76	0.67
1:E:55:ALA:O	1:E:57:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:VAL:HA	1:G:118:ILE:HD13	1.77	0.67
1:O:122(A):LYS:HD2	5:O:535:HOH:O	1.93	0.67
1:O:226:ASN:HB2	1:Q:300:MET:HE3	1.76	0.67
1:D:124:ASP:O	1:D:125:ILE:HB	1.92	0.67
1:E:117:ILE:HD11	1:E:328:VAL:HG21	1.76	0.67
1:E:63:ALA:CB	1:E:72:GLN:HA	2.24	0.67
1:F:39:GLN:HE22	2:M:60:LEU:HD23	1.59	0.67
1:B:271:LEU:HD13	1:B:272:ASP:N	2.09	0.67
1:F:159:LYS:HB2	1:F:218:LEU:HD11	1.76	0.67
1:F:280:SER:OG	1:H:202:ASN:HB2	1.94	0.67
1:H:2:LYS:HD3	1:H:28:ILE:HD12	1.76	0.67
1:H:215:ALA:CB	1:H:222:LYS:HA	2.24	0.67
1:H:45:LYS:HB2	1:H:57:VAL:HB	1.76	0.67
1:F:194:ARG:HD2	1:F:205:PRO:O	1.94	0.67
1:O:281:VAL:H	1:Q:202:ASN:HD22	1.42	0.67
1:D:272:ASP:HB2	1:D:288:PHE:CD2	2.29	0.66
1:F:0:LYS:HD2	1:F:24:PRO:HA	1.77	0.66
1:F:234:THR:HG22	1:H:233:PRO:HG2	1.75	0.66
2:K:71:ASN:HA	2:K:74:ARG:NH2	2.09	0.66
1:O:126:PRO:HG2	1:O:141:GLU:HG2	1.76	0.66
1:E:139:HIS:CE1	1:E:332:TRP:HA	2.30	0.66
2:L:63:TYR:OH	2:L:70:THR:HB	1.94	0.66
1:E:31:ASN:OD1	1:E:74:VAL:HG23	1.96	0.66
1:F:245:GLN:NE2	1:H:245:GLN:HE21	1.92	0.66
1:Q:331:ASN:ND2	1:Q:331:ASN:N	2.41	0.66
1:A:125:ILE:HG21	1:A:143:ILE:HG22	1.78	0.66
1:A:210:ALA:O	1:A:214:VAL:HG23	1.95	0.66
1:E:239:VAL:HG22	1:E:240:VAL:N	2.10	0.66
1:F:37:VAL:HG22	1:F:73:VAL:HB	1.76	0.66
1:H:60(A):GLY:O	1:H:61:GLU:HG2	1.96	0.66
1:Q:272:ASP:O	1:Q:291:THR:HA	1.96	0.66
1:A:168:ILE:HG22	1:A:169:LYS:HG2	1.77	0.66
1:A:271:LEU:HD12	1:A:272:ASP:N	2.10	0.66
1:E:154:LEU:O	1:E:158:VAL:HG23	1.94	0.66
1:E:296:LEU:HD23	1:E:296:LEU:N	2.11	0.66
1:Q:2:LYS:HD2	1:Q:88:GLY:O	1.96	0.66
1:D:215:ALA:O	1:D:216:LEU:HD23	1.96	0.66
1:F:108:HIS:O	1:F:111:ALA:HB3	1.96	0.66
1:H:102:ARG:HH21	1:H:124:ASP:HB3	1.60	0.66
1:A:139:HIS:HB3	1:A:333:LYS:HE2	1.78	0.66
1:B:133:ASN:OD1	1:B:217:VAL:HA	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASN:HD21	1:D:281:VAL:CB	2.08	0.66
1:F:37:VAL:HG13	1:F:64:ILE:HG23	1.78	0.66
1:F:117:ILE:HG23	1:F:144:ILE:CD1	2.26	0.66
1:F:133:ASN:OD1	1:F:217:VAL:HG12	1.95	0.66
1:G:158:VAL:HG11	1:G:221:LEU:CD2	2.25	0.66
1:H:76:ASN:HD22	1:H:77:ARG:N	1.94	0.66
1:A:78:ASN:ND2	1:A:81:LEU:HG	2.10	0.66
1:E:115:LYS:HE3	1:E:137:TYR:OH	1.96	0.66
1:H:181:ASP:CG	2:N:76:TYR:H	1.99	0.66
1:B:279:VAL:CG1	1:D:204:VAL:HG13	2.26	0.65
1:D:59:PRO:HA	1:D:64:ILE:HA	1.78	0.65
1:E:183:ARG:NE	1:E:187:ALA:HB3	2.11	0.65
1:G:129:VAL:H	1:G:133:ASN:ND2	1.93	0.65
1:O:190:HIS:HB3	1:O:196:ALA:HB2	1.78	0.65
1:B:284:ARG:HD2	5:B:520:HOH:O	1.97	0.65
1:C:168:ILE:HG22	1:C:169:LYS:HD2	1.76	0.65
1:F:129:VAL:N	1:F:133:ASN:HD21	1.94	0.65
1:G:161:LEU:HD13	1:G:244:VAL:HG21	1.78	0.65
1:H:205:PRO:HA	1:H:230:LEU:HD23	1.78	0.65
3:H:401:NAD:C8A	2:N:69:GLU:HG2	2.26	0.65
1:B:277:PRO:HA	1:D:194:ARG:HH21	1.62	0.65
1:B:202:ASN:ND2	1:D:281:VAL:H	1.95	0.65
1:D:303:ASP:O	1:D:305:VAL:HG23	1.96	0.65
1:G:-1:ALA:HB2	5:G:513:HOH:O	1.97	0.65
1:E:202:ASN:CB	1:G:281:VAL:HG23	2.24	0.65
1:H:83:PRO:HB2	1:H:86:GLU:HG2	1.79	0.65
1:Q:129:VAL:H	1:Q:133:ASN:HD21	1.44	0.65
1:D:323:ASP:C	1:D:325:ALA:H	1.99	0.65
1:D:64:ILE:HG23	1:D:73:VAL:HG21	1.78	0.65
1:H:85:LYS:CA	1:H:112:GLY:HA3	2.26	0.65
1:A:115:LYS:HD2	1:A:332:TRP:CZ3	2.31	0.65
1:D:89:ILE:HG21	1:D:92:VAL:CG2	2.27	0.65
1:F:242:LEU:HD21	1:F:244:VAL:HG13	1.78	0.65
1:E:296:LEU:HD21	1:G:194:ARG:NH2	2.11	0.65
1:A:129:VAL:H	1:A:133:ASN:HD21	1.42	0.65
1:C:190:HIS:HB3	1:C:196:ALA:HB2	1.78	0.65
1:E:328:VAL:O	1:E:332:TRP:HB2	1.96	0.65
1:B:208:THR:CG2	1:B:209:GLY:H	2.00	0.65
1:D:144:ILE:HD12	1:D:145:SER:N	2.11	0.65
1:E:133:ASN:N	1:E:133:ASN:HD22	1.95	0.65
1:H:170:GLY:HA3	1:H:244:VAL:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ASN:ND2	1:H:281:VAL:HG23	2.11	0.65
1:O:102:ARG:NH2	1:O:124:ASP:O	2.30	0.65
1:B:281:VAL:HG12	1:D:202:ASN:HD21	1.61	0.64
1:D:89:ILE:CG2	1:D:92:VAL:HG23	2.26	0.64
1:G:179:THR:C	1:G:181:ASP:H	1.99	0.64
1:B:10:ARG:HH11	1:C:186:ASP:HB2	1.63	0.64
1:E:3:VAL:HG22	1:E:91:ILE:HG23	1.77	0.64
1:F:0:LYS:NZ	1:F:24:PRO:HG3	2.13	0.64
1:G:204:VAL:O	1:G:231:ARG:N	2.29	0.64
1:E:240:VAL:CG2	1:E:309:ALA:HB3	2.28	0.64
1:E:17:ARG:NH2	1:E:53:PHE:HB2	2.12	0.64
1:C:276:GLU:HB2	1:C:278:LEU:HG	1.80	0.64
1:G:28:ILE:HD11	1:G:89:ILE:CD1	2.26	0.64
1:H:190:HIS:HB3	1:H:196:ALA:HB2	1.77	0.64
1:A:154:LEU:HD22	1:A:172:MET:HE3	1.78	0.64
1:A:63:ALA:HA	1:A:73:VAL:HG23	1.80	0.64
1:B:130:VAL:HB	1:B:320:ARG:HD3	1.80	0.64
1:G:129:VAL:CG2	1:G:217:VAL:HG11	2.26	0.64
1:G:62:THR:HG22	1:Q:62:THR:HG22	1.80	0.64
1:H:164:LYS:H	1:H:164:LYS:HD2	1.60	0.64
1:G:273:VAL:HG22	1:G:292:ILE:HB	1.79	0.64
1:H:72:GLN:H	1:H:72:GLN:NE2	1.95	0.64
1:O:181:ASP:OD2	1:O:195:ARG:NH1	2.30	0.64
1:A:1:LEU:HD23	1:A:91:ILE:HD11	1.80	0.64
1:A:84:TRP:CE3	1:A:89:ILE:HG13	2.33	0.64
1:E:300:MET:HB2	1:G:169:LYS:HZ3	1.62	0.64
1:G:251:PHE:O	1:G:255:VAL:HG23	1.97	0.64
1:E:42:HIS:CG	1:H:193:LEU:HD13	2.32	0.64
1:H:263:ALA:O	1:H:268:LYS:HA	1.97	0.64
1:A:76:ASN:HD22	1:A:77:ARG:N	1.96	0.64
1:B:0:LYS:N	5:B:526:HOH:O	2.31	0.64
1:B:221:LEU:HA	1:B:224:LYS:HD2	1.80	0.64
1:E:132:VAL:HG21	1:E:155:ALA:HB1	1.79	0.64
1:A:9:GLY:HA3	3:A:401:NAD:O5B	1.98	0.64
1:B:90:ASP:HA	1:B:114:LYS:HZ2	1.62	0.64
1:C:271:LEU:HD12	1:C:272:ASP:H	1.63	0.64
1:B:18(A):TRP:CE2	1:B:27:ILE:HD13	2.32	0.63
1:D:251:PHE:CZ	1:D:254:GLU:HB2	2.33	0.63
1:D:87:LEU:HD12	1:D:89:ILE:HD13	1.79	0.63
1:F:52:ILE:HD12	1:F:52:ILE:H	1.62	0.63
1:C:34:GLY:HA2	2:J:60:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:LEU:HD11	1:E:244:VAL:CG1	2.27	0.63
1:F:113:ALA:C	1:F:114:LYS:HD2	2.19	0.63
1:E:194:ARG:HE	1:G:277:PRO:CA	2.10	0.63
1:F:301:GLY:HA3	1:H:169:LYS:CD	2.28	0.63
1:B:165:PHE:O	1:B:246:VAL:HB	1.98	0.63
1:D:18(A):TRP:CH2	1:D:69:LYS:HE2	2.32	0.63
1:B:202:ASN:HD22	1:D:281:VAL:H	1.45	0.63
1:D:275:ASP:HA	1:D:294:SER:OG	1.98	0.63
1:E:242:LEU:HD11	1:E:244:VAL:HG13	1.78	0.63
1:D:18(A):TRP:HH2	1:D:69:LYS:HE2	1.63	0.63
1:E:109:ILE:HA	1:E:113:ALA:O	1.98	0.63
1:F:21:LYS:HZ1	1:F:21:LYS:H	1.44	0.63
1:F:87:LEU:HB2	1:F:89:ILE:HG12	1.79	0.63
1:G:133:ASN:N	1:G:133:ASN:HD22	1.96	0.63
1:O:98:VAL:HG23	1:O:99:PHE:CE2	2.33	0.63
1:C:262:SER:HA	1:C:266:GLU:OE1	1.99	0.63
1:E:9:GLY:O	1:E:13:ARG:HG3	1.98	0.63
1:F:307:VAL:C	1:F:308:ILE:HD12	2.19	0.63
1:O:2:LYS:HD3	1:O:28:ILE:HD13	1.79	0.63
1:B:91:ILE:HG13	1:B:92:VAL:N	2.13	0.63
1:D:100:VAL:HG23	1:D:122(A):LYS:HB2	1.81	0.63
1:D:54:ASP:O	1:D:55:ALA:HB2	1.98	0.63
1:E:70:ILE:H	1:E:70:ILE:CD1	2.10	0.63
1:F:38:LYS:CD	2:M:57:SER:HA	2.23	0.63
1:O:39:GLN:HE21	1:O:39:GLN:H	1.45	0.63
1:B:70:ILE:HD12	1:B:70:ILE:N	2.14	0.63
1:B:10:ARG:NH1	1:C:186:ASP:HB2	2.14	0.63
1:A:271:LEU:HD12	1:A:272:ASP:H	1.64	0.63
1:B:105:ALA:HB1	1:B:116:VAL:HG11	1.81	0.63
1:D:95:GLY:HA2	1:D:119:THR:OG1	1.99	0.63
1:E:20:ARG:NH2	1:E:322:VAL:HB	2.13	0.63
1:F:233:PRO:HB2	1:H:233:PRO:HB2	1.80	0.63
1:H:176:HIS:HA	1:H:238:SER:CB	2.28	0.63
2:L:63:TYR:HE2	2:L:72:GLU:HG3	1.63	0.63
1:A:28:ILE:HG22	1:A:69:LYS:CE	2.29	0.63
1:C:129:VAL:H	1:C:133:ASN:HD21	1.44	0.63
1:D:28:ILE:HD11	1:D:89:ILE:HD11	1.81	0.63
1:E:117:ILE:HG22	1:E:117:ILE:O	1.99	0.63
1:B:0:LYS:HE3	1:B:23:SER:O	1.99	0.62
1:H:3:VAL:HG21	1:H:93:ILE:HD11	1.81	0.62
1:A:159:LYS:HB2	1:A:218:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LYS:N	1:C:21:LYS:HD2	2.11	0.62
1:C:83:PRO:HB2	1:C:86:GLU:HB3	1.81	0.62
1:E:202:ASN:HB2	1:G:280:SER:OG	1.99	0.62
1:E:299:VAL:HG22	1:E:305:VAL:HA	1.80	0.62
1:B:168:ILE:HB	1:B:245:GLN:O	1.99	0.62
1:A:191:ARG:HG2	1:A:191:ARG:HH11	1.65	0.62
1:C:115:LYS:HE3	1:C:141:GLU:O	1.99	0.62
1:D:130:VAL:HA	1:D:134:ALA:HB2	1.81	0.62
1:Q:152:ASN:O	1:Q:289:SER:HB3	1.99	0.62
1:B:324:LEU:O	1:B:328:VAL:HG23	1.99	0.62
1:B:281:VAL:H	1:D:202:ASN:HD21	1.46	0.62
1:E:186:ASP:HB2	1:H:10:ARG:HH11	1.64	0.62
1:F:14:ASN:ND2	1:F:314:GLU:HG2	2.15	0.62
1:B:176:HIS:NE2	2:J:78:ASN:HB3	2.14	0.62
1:H:66:VAL:C	1:H:68:GLY:H	2.02	0.62
2:L:71:ASN:HB2	1:Q:183:ARG:NH1	2.14	0.62
1:Q:33:THR:HG21	1:Q:77:ARG:NH1	2.15	0.62
1:G:217:VAL:HG23	1:G:218:LEU:HG	1.80	0.62
1:A:171:THR:O	1:A:242:LEU:HD12	1.99	0.62
1:D:152:ASN:HD21	1:D:320:ARG:HG3	1.65	0.62
1:D:177:SER:HB3	1:D:234:THR:O	2.00	0.62
1:E:32:ASP:C	1:E:34:GLY:N	2.52	0.62
1:F:129:VAL:O	1:F:131:GLY:N	2.33	0.62
1:H:265:LYS:HE2	1:H:265:LYS:HA	1.82	0.62
1:H:79:PRO:CG	1:H:99:PHE:CZ	2.83	0.62
1:A:234:THR:HG21	1:C:203:ILE:HG12	1.80	0.62
1:D:123:GLY:HA2	5:D:528:HOH:O	1.99	0.62
1:B:90:ASP:HA	1:B:114:LYS:NZ	2.15	0.61
1:C:210:ALA:O	1:C:214:VAL:HG23	1.99	0.61
1:B:169:LYS:HD3	1:D:301:GLY:HA3	1.82	0.61
1:E:202:ASN:HB3	1:G:281:VAL:CG2	2.26	0.61
1:E:322:VAL:HG12	1:E:322:VAL:O	1.99	0.61
1:F:324:LEU:O	1:F:328:VAL:HG23	1.99	0.61
1:F:60:SER:N	1:F:64:ILE:HA	2.15	0.61
1:G:205:PRO:HA	1:G:229:ALA:O	1.99	0.61
1:F:310:TRP:HZ2	1:H:205:PRO:HG2	1.64	0.61
1:E:183:ARG:HH22	2:N:74:ARG:HH12	1.48	0.61
1:A:37:VAL:CG2	1:A:63:ALA:H	2.13	0.61
1:F:56:ASP:HB2	1:F:67:ASP:N	2.15	0.61
1:E:170:GLY:O	1:G:300:MET:HG2	2.00	0.61
1:H:24:PRO:C	1:H:25:LEU:HD12	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:CYS:O	1:A:156:PRO:HD2	2.00	0.61
1:D:159:LYS:O	1:D:163:GLN:HG2	2.00	0.61
1:E:214:VAL:O	1:E:217:VAL:HG22	1.99	0.61
1:E:153:CYS:O	1:E:290:THR:HG21	2.01	0.61
1:G:221:LEU:HD12	1:G:224:LYS:HB2	1.81	0.61
1:H:195:ARG:HB2	1:H:195:ARG:HH11	1.64	0.61
1:D:242:LEU:HD12	1:D:243:VAL:H	1.66	0.61
1:E:115:LYS:HB3	1:E:115:LYS:HZ2	1.64	0.61
1:O:21:LYS:HG2	5:O:580:HOH:O	1.99	0.61
1:B:193:LEU:HD13	1:C:42:HIS:CG	2.36	0.61
1:F:101:ASP:OD2	1:F:103:GLU:HB3	1.99	0.61
2:L:63:TYR:O	2:L:67:ASN:HB2	2.01	0.61
1:F:18(A):TRP:HA	1:F:20:ARG:HG2	1.82	0.61
1:H:246:VAL:HG22	1:H:303:ASP:O	2.01	0.61
1:H:255:VAL:O	1:H:258:ALA:HB3	2.00	0.61
1:B:18(A):TRP:CD2	1:B:27:ILE:HD13	2.35	0.61
1:F:211:ALA:HB3	5:F:501:HOH:O	2.00	0.61
1:Q:191:ARG:HG3	1:Q:191:ARG:HH11	1.65	0.61
1:B:130:VAL:HA	1:B:134:ALA:HB2	1.83	0.61
1:B:281:VAL:H	1:D:202:ASN:ND2	1.99	0.61
1:E:169:LYS:CE	1:G:303:ASP:OD2	2.48	0.61
1:F:227:GLY:HA2	1:H:298:MET:CE	2.31	0.61
1:A:280:SER:HB3	1:C:203:ILE:HD12	1.82	0.61
1:B:279:VAL:HG12	1:D:204:VAL:HA	1.82	0.61
1:B:31:ASN:HB2	1:B:74:VAL:HG23	1.83	0.61
1:D:264:GLU:O	1:D:265:LYS:HD2	2.01	0.61
1:F:133:ASN:N	1:F:133:ASN:HD22	1.99	0.61
1:F:280:SER:HB3	1:H:203:ILE:HB	1.83	0.61
2:M:76:TYR:N	2:M:76:TYR:CD1	2.69	0.61
1:Q:86:GLU:N	1:Q:86:GLU:OE2	2.30	0.61
1:A:281:VAL:H	1:C:202:ASN:HD21	1.48	0.60
1:B:204:VAL:HG22	1:D:279:VAL:CG1	2.30	0.60
1:H:126:PRO:HD2	1:H:143:ILE:O	2.00	0.60
1:C:133:ASN:C	1:C:135:ASP:H	2.05	0.60
1:A:279:VAL:HG11	1:C:204:VAL:HG22	1.82	0.60
1:G:190:HIS:HB3	1:G:196:ALA:HB2	1.81	0.60
1:H:115:LYS:HG2	1:H:142:PRO:HA	1.82	0.60
1:H:1:LEU:HD12	1:H:2:LYS:H	1.66	0.60
1:A:76:ASN:ND2	1:A:78:ASN:H	2.00	0.60
1:E:20:ARG:NH1	1:E:322:VAL:HG12	2.16	0.60
1:F:27:ILE:N	1:F:27:ILE:HD12	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:LEU:HD13	1:G:271:LEU:HB3	1.82	0.60
1:O:195:ARG:HH12	1:O:231:ARG:NH2	1.99	0.60
1:O:6:ASN:ND2	1:O:31:ASN:ND2	2.44	0.60
1:Q:6:ASN:ND2	1:Q:94:GLU:OE2	2.31	0.60
1:B:284:ARG:CZ	1:B:284:ARG:HB3	2.30	0.60
1:B:83:PRO:HG2	1:B:87:LEU:HD12	1.83	0.60
1:E:58:LYS:NZ	1:E:58:LYS:HB3	2.16	0.60
1:F:117:ILE:CG2	1:F:144:ILE:HD11	2.31	0.60
1:F:271:LEU:HD12	1:F:272:ASP:N	2.14	0.60
1:G:250:THR:O	1:G:299:VAL:HG11	2.02	0.60
1:C:133:ASN:O	1:C:135:ASP:N	2.35	0.60
1:A:298:MET:CE	1:C:226:ASN:HB2	2.30	0.60
1:D:167:ILE:HG23	1:D:244:VAL:HB	1.84	0.60
1:E:116:VAL:HB	1:E:143:ILE:HD13	1.83	0.60
1:E:239:VAL:HA	1:E:309:ALA:O	2.01	0.60
1:A:101:ASP:HB3	1:A:122(A):LYS:HB3	1.84	0.60
1:A:28:ILE:HG22	1:A:69:LYS:HE2	1.84	0.60
1:E:83:PRO:HA	1:E:86:GLU:OE1	2.01	0.60
1:H:1:LEU:HD12	1:H:2:LYS:N	2.17	0.60
1:O:243:VAL:HG11	1:Q:243:VAL:HG11	1.82	0.60
1:E:32:ASP:O	1:E:34:GLY:N	2.34	0.60
1:G:129:VAL:O	1:G:129:VAL:HG12	2.02	0.60
1:E:251:PHE:CE1	1:E:254:GLU:HB2	2.36	0.60
1:E:37:VAL:HG23	1:E:38:LYS:HE2	1.84	0.60
1:F:23:SER:C	1:F:25:LEU:H	2.05	0.60
1:F:299:VAL:HG12	1:F:299:VAL:O	2.02	0.60
1:G:170:GLY:HA3	1:G:244:VAL:HA	1.84	0.60
1:G:287:ASP:HB3	5:G:501:HOH:O	2.01	0.60
2:M:58:ASP:HB3	2:M:59:PRO:HD3	1.84	0.60
1:B:117:ILE:O	1:B:117:ILE:HG23	2.02	0.59
1:B:140:ASP:O	1:B:142:PRO:HD3	2.02	0.59
1:B:271:LEU:HD13	1:B:272:ASP:H	1.67	0.59
1:E:117:ILE:CG1	1:E:144:ILE:HD11	2.28	0.59
2:K:72:GLU:CD	2:K:72:GLU:H	2.05	0.59
1:Q:96:THR:OG1	1:Q:98:VAL:HG22	2.02	0.59
1:A:204:VAL:HB	1:A:231:ARG:HB2	1.84	0.59
1:B:250:THR:OG1	1:B:251:PHE:N	2.34	0.59
1:E:25:LEU:HD11	1:E:325:ALA:HB3	1.84	0.59
1:F:137:TYR:CE2	1:F:328:VAL:HA	2.37	0.59
1:F:169:LYS:HE3	1:H:304:MET:HB2	1.83	0.59
1:H:36:GLY:H	1:H:39:GLN:HE21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:ILE:CD1	1:O:116:VAL:HG23	2.32	0.59
1:O:172:MET:CE	1:O:211:ALA:HB2	2.32	0.59
1:Q:133:ASN:ND2	1:Q:133:ASN:H	1.98	0.59
1:C:102:ARG:HG3	1:C:102:ARG:NH1	2.17	0.59
1:E:192:ASP:HB3	1:E:195:ARG:HB2	1.84	0.59
1:G:16:LEU:O	1:G:16:LEU:HD23	2.01	0.59
1:E:16:LEU:HD13	1:E:44:LEU:HD21	1.85	0.59
1:Q:133:ASN:HD22	1:Q:133:ASN:N	1.92	0.59
1:B:317:TYR:O	1:B:321:VAL:HG23	2.02	0.59
1:D:83:PRO:O	1:D:87:LEU:CB	2.49	0.59
1:H:85:LYS:N	1:H:112:GLY:HA3	2.18	0.59
1:D:146:ASN:ND2	1:D:321:VAL:HG23	2.17	0.59
1:D:209:GLY:O	1:D:211:ALA:N	2.35	0.59
1:E:276:GLU:HG2	5:E:534:HOH:O	2.03	0.59
1:H:85:LYS:O	1:H:85:LYS:HD3	2.02	0.59
1:C:241:ASP:OD1	1:C:306:LYS:HE3	2.03	0.59
1:D:133:ASN:HD21	1:D:217:VAL:HG12	1.67	0.59
1:D:167:ILE:HA	1:D:246:VAL:HG12	1.84	0.59
1:F:227:GLY:HA2	1:H:298:MET:HE1	1.83	0.59
1:A:229:ALA:O	1:A:230:LEU:HD23	2.03	0.59
1:B:272:ASP:O	1:B:291:THR:HA	2.03	0.59
1:B:93:ILE:HD13	1:B:117:ILE:HG21	1.84	0.59
1:C:21:LYS:H	1:C:21:LYS:CD	2.14	0.59
1:C:89:ILE:HD12	1:C:89:ILE:N	2.16	0.59
1:E:157:PHE:HB2	1:E:259:PHE:CE1	2.38	0.59
1:F:171:THR:HG23	1:F:171:THR:O	2.02	0.59
1:A:101:ASP:HA	1:A:125:ILE:HD11	1.85	0.59
1:E:301:GLY:O	1:E:303:ASP:N	2.35	0.59
1:E:279:VAL:HG12	1:G:205:PRO:HD2	1.85	0.59
1:G:272:ASP:O	1:G:291:THR:HA	2.03	0.59
1:B:194:ARG:NH1	1:D:278:LEU:O	2.36	0.59
1:D:150:THR:OG1	2:I:78:ASN:HB2	2.01	0.59
1:D:211:ALA:HB1	1:D:226:ASN:CA	2.33	0.59
1:E:130:VAL:HB	1:E:320:ARG:HD3	1.85	0.59
1:E:279:VAL:HG22	1:G:197:ARG:HH12	1.66	0.59
1:F:178:TYR:HE1	1:G:185:LEU:HD21	1.68	0.59
1:Q:319:GLN:HA	1:Q:319:GLN:OE1	2.02	0.59
1:A:139:HIS:HB3	1:A:333:LYS:CE	2.33	0.58
1:D:115:LYS:HG3	1:D:142:PRO:HA	1.85	0.58
1:D:162:ASP:HA	1:D:167:ILE:HG13	1.85	0.58
1:E:119:THR:CG2	1:E:321:VAL:HG11	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:THR:HG23	1:F:145:SER:OG	2.03	0.58
1:F:270:ILE:N	1:F:270:ILE:HD12	2.18	0.58
1:H:79:PRO:HB2	1:H:107:LYS:HB3	1.84	0.58
1:H:84:TRP:HA	1:H:89:ILE:HG13	1.84	0.58
1:A:100:VAL:HA	1:A:118:ILE:HD13	1.85	0.58
1:D:133:ASN:C	1:D:135:ASP:H	2.06	0.58
1:H:203:ILE:O	1:H:205:PRO:HD3	2.03	0.58
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.04	0.58
1:A:1:LEU:HD22	1:A:329:ALA:CB	2.34	0.58
1:C:18(A):TRP:O	1:C:20:ARG:HB2	2.04	0.58
1:B:279:VAL:CG2	1:D:197:ARG:HG3	2.32	0.58
1:D:94:GLU:HG3	1:D:94:GLU:O	2.03	0.58
1:E:160:VAL:CG2	1:E:267:LEU:HD11	2.34	0.58
1:E:79:PRO:HB3	1:E:108:HIS:CE1	2.39	0.58
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.39	0.58
1:F:130:VAL:HG21	1:F:320:ARG:O	2.04	0.58
1:G:162:ASP:CA	1:G:167:ILE:HG12	2.33	0.58
1:H:71:ILE:N	1:H:71:ILE:HD12	2.19	0.58
1:Q:14:ASN:OD1	1:Q:50:LEU:HD11	2.03	0.58
1:E:172:MET:HG2	1:E:173:THR:N	2.19	0.58
1:F:132:VAL:HG12	1:F:133:ASN:N	2.18	0.58
1:E:300:MET:HB3	1:G:169:LYS:HD3	1.85	0.58
1:B:87:LEU:HB2	1:B:89:ILE:HD13	1.85	0.58
1:C:98:VAL:HG23	1:C:99:PHE:CD2	2.38	0.58
1:E:300:MET:HB2	1:G:169:LYS:HZ2	1.67	0.58
1:C:228:ILE:HD13	1:C:228:ILE:H	1.68	0.58
1:D:211:ALA:HB1	1:D:226:ASN:HA	1.85	0.58
1:E:185:LEU:O	1:E:187:ALA:N	2.36	0.58
1:F:211:ALA:CB	1:F:226:ASN:HA	2.34	0.58
1:H:42:HIS:O	1:H:46:TYR:HB2	2.03	0.58
1:C:91:ILE:HD13	1:C:91:ILE:C	2.23	0.58
1:D:9:GLY:HA3	3:D:401:NAD:O5B	2.03	0.58
1:E:129:VAL:H	1:E:133:ASN:ND2	2.02	0.58
1:E:146:ASN:ND2	1:E:324:LEU:HD22	2.19	0.58
1:F:165:PHE:HD1	1:F:248:LYS:HB3	1.69	0.58
1:H:163:GLN:OE1	1:H:164:LYS:HE3	2.03	0.58
1:H:4:ALA:HB2	1:H:89:ILE:CD1	2.34	0.58
1:G:231:ARG:HH21	2:M:78:ASN:HD22	1.49	0.58
1:H:191:ARG:CG	2:N:73:CYS:HA	2.34	0.58
1:B:9:GLY:O	1:B:13:ARG:HG3	2.03	0.58
1:D:139:HIS:CD2	1:D:333:LYS:HD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:VAL:HG13	1:D:159:LYS:HD2	1.85	0.57
1:E:241:ASP:OD1	1:E:306:LYS:HE2	2.04	0.57
1:H:17:ARG:NE	1:H:53:PHE:HD1	2.01	0.57
2:N:60:LEU:O	2:N:60:LEU:HD23	2.04	0.57
1:F:101:ASP:O	1:F:104:GLY:N	2.36	0.57
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.86	0.57
1:B:197:ARG:NH2	1:C:46:TYR:HB3	2.18	0.57
1:D:20:ARG:HH21	1:D:319:GLN:HE22	1.53	0.57
1:E:60:SER:HB2	1:E:63:ALA:O	2.04	0.57
1:E:169:LYS:CD	1:G:301:GLY:HA3	2.27	0.57
2:I:70:THR:O	2:I:74:ARG:HG3	2.04	0.57
2:K:69:GLU:HG2	1:O:77:ARG:HH22	1.69	0.57
1:A:38:LYS:HD3	1:A:39:GLN:HE22	1.69	0.57
1:E:132:VAL:HG11	1:E:217:VAL:HB	1.85	0.57
1:E:295:SER:HB2	1:E:296:LEU:HD23	1.87	0.57
1:O:253:GLU:H	1:O:253:GLU:CD	2.06	0.57
2:K:69:GLU:CD	1:O:77:ARG:HH22	2.06	0.57
1:Q:181:ASP:OD2	1:Q:195:ARG:NH1	2.37	0.57
1:C:333:LYS:NZ	1:C:333:LYS:HB2	2.20	0.57
1:D:10:ARG:HB2	3:D:401:NAD:O1N	2.04	0.57
1:B:277:PRO:HB2	1:D:194:ARG:HE	1.70	0.57
1:D:133:ASN:ND2	1:D:217:VAL:HA	2.19	0.57
1:D:319:GLN:NE2	1:D:319:GLN:HA	2.20	0.57
1:E:265:LYS:HB2	1:E:266:GLU:OE1	2.05	0.57
1:G:-1:ALA:HB3	1:G:26:ASP:HB2	1.86	0.57
1:G:281:VAL:HG11	1:H:48:SER:HA	1.85	0.57
1:G:294:SER:C	1:G:296:LEU:H	2.08	0.57
1:O:202:ASN:ND2	1:Q:281:VAL:HG12	2.20	0.57
1:A:122(A):LYS:HD3	1:A:123:GLY:N	2.19	0.57
1:B:204:VAL:HA	1:D:279:VAL:HG12	1.86	0.57
1:D:55:ALA:O	1:D:57:VAL:HG23	2.03	0.57
1:G:153:CYS:O	1:G:156:PRO:HD2	2.05	0.57
1:C:77:ARG:O	1:C:79:PRO:HD3	2.05	0.57
1:E:106:GLY:O	1:E:109:ILE:HG12	2.04	0.57
1:F:221:LEU:HA	1:F:224:LYS:HD2	1.86	0.57
2:M:76:TYR:N	2:M:76:TYR:HD1	2.02	0.57
1:B:185:LEU:HD21	1:C:178:TYR:CE1	2.36	0.57
1:B:280:SER:HA	1:B:310:TRP:CZ3	2.40	0.57
1:F:29:ALA:HA	1:F:72:GLN:O	2.04	0.57
1:H:178:TYR:CE2	1:H:200:ALA:HB2	2.40	0.57
1:D:62:THR:HG21	1:H:74:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:60:LEU:HD21	2:N:64:CYS:SG	2.44	0.57
1:B:280:SER:HB3	1:D:203:ILE:HB	1.87	0.57
1:O:126:PRO:HB2	1:O:144:ILE:HG22	1.86	0.57
1:F:172:MET:HE1	1:F:211:ALA:HB2	1.85	0.57
1:F:282:ASP:OD2	1:H:197:ARG:NH1	2.34	0.57
1:G:37:VAL:HG13	1:G:73:VAL:HB	1.87	0.57
1:Q:281:VAL:O	1:Q:284:ARG:HG3	2.04	0.57
1:D:139:HIS:CD2	1:D:333:LYS:HB2	2.40	0.56
1:D:144:ILE:HD12	1:D:144:ILE:C	2.25	0.56
1:B:171:THR:HG21	1:D:306:LYS:HE3	1.87	0.56
1:D:15:PHE:CD1	1:D:322:VAL:HG22	2.40	0.56
1:D:1:LEU:HD22	1:D:329:ALA:HA	1.87	0.56
1:E:70:ILE:HD13	1:E:70:ILE:N	2.15	0.56
1:D:117:ILE:CG2	1:D:144:ILE:HD11	2.15	0.56
1:B:28:ILE:HD11	1:B:89:ILE:HD12	1.87	0.56
1:E:63:ALA:HB2	1:E:72:GLN:HA	1.85	0.56
1:A:32:ASP:OD1	3:A:401:NAD:H1B	2.05	0.56
1:C:87:LEU:HB2	1:C:89:ILE:CD1	2.35	0.56
1:D:79:PRO:HA	1:D:82:LEU:CD1	2.35	0.56
1:H:3:VAL:HG13	1:H:27:ILE:HA	1.87	0.56
2:N:63:TYR:CE1	2:N:67:ASN:ND2	2.73	0.56
1:E:1:LEU:HD21	1:E:332:TRP:CE3	2.39	0.56
1:E:312:ASP:O	1:E:314:GLU:N	2.38	0.56
1:F:251:PHE:CE2	1:F:253:GLU:HB3	2.40	0.56
1:F:298:MET:HE2	1:F:306:LYS:HD3	1.87	0.56
1:G:131:GLY:N	1:G:134:ALA:HB2	2.17	0.56
1:G:213:ALA:HA	1:G:216:LEU:HD12	1.87	0.56
1:H:149:CYS:HA	1:H:317:TYR:HD1	1.69	0.56
1:Q:115:LYS:HG3	1:Q:142:PRO:O	2.05	0.56
1:C:271:LEU:HD12	1:C:272:ASP:N	2.20	0.56
1:C:84:TRP:CE3	1:C:84:TRP:HA	2.40	0.56
1:O:206:THR:HG23	1:O:229:ALA:HB3	1.86	0.56
1:O:323:ASP:O	1:O:327:ILE:HD13	2.05	0.56
1:A:74:VAL:HG23	1:A:75:SER:N	2.19	0.56
1:E:165:PHE:HD1	1:E:248:LYS:HD3	1.69	0.56
1:E:279:VAL:HG12	1:G:205:PRO:CD	2.36	0.56
1:G:130:VAL:HG23	1:G:320:ARG:HD3	1.86	0.56
1:H:18(A):TRP:HE1	1:H:23:SER:HB3	1.71	0.56
1:A:109:ILE:C	1:A:111:ALA:H	2.08	0.56
1:A:139:HIS:HB3	1:A:333:LYS:NZ	2.20	0.56
1:D:87:LEU:HD12	1:D:89:ILE:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:LYS:O	1:F:223:GLY:C	2.44	0.56
1:H:192:ASP:O	1:H:196:ALA:HB2	2.06	0.56
1:Q:260:ARG:HG2	1:Q:273:VAL:HG21	1.87	0.56
1:C:183:ARG:HG3	1:C:196:ALA:HA	1.87	0.56
1:C:289:SER:OG	1:C:320:ARG:HD2	2.05	0.56
1:E:226:ASN:HB3	1:G:300:MET:SD	2.46	0.56
1:F:126:PRO:CG	1:F:144:ILE:HG22	2.33	0.56
1:F:267:LEU:HB3	1:F:270:ILE:HB	1.88	0.56
1:H:130:VAL:HB	1:H:320:ARG:HD3	1.87	0.56
1:A:183:ARG:HE	1:A:187:ALA:HB3	1.70	0.56
1:B:279:VAL:HG11	1:D:204:VAL:HG13	1.87	0.56
1:E:18:CYS:HB3	1:E:319:GLN:OE1	2.05	0.56
1:F:144:ILE:C	1:F:144:ILE:HD12	2.27	0.56
1:H:162:ASP:O	1:H:166:GLY:N	2.38	0.56
1:D:7:GLY:HA3	1:D:96:THR:CG2	2.33	0.56
1:E:109:ILE:CA	1:E:113:ALA:HB3	2.35	0.56
1:E:3:VAL:HG22	1:E:91:ILE:CG2	2.36	0.56
1:F:296:LEU:HD22	1:H:228:ILE:HG21	1.88	0.56
1:H:266:GLU:HG2	1:H:267:LEU:HG	1.88	0.56
1:D:87:LEU:HD22	1:H:86:GLU:HB3	1.88	0.56
2:L:72:GLU:HG2	5:L:104:HOH:O	2.06	0.56
1:O:16:LEU:O	1:O:16:LEU:HD23	2.06	0.56
1:A:143:ILE:HD12	1:A:143:ILE:N	2.20	0.55
1:B:202:ASN:HD21	1:D:281:VAL:HG12	1.69	0.55
1:F:177:SER:HB3	1:F:234:THR:O	2.06	0.55
1:C:74:VAL:HG12	1:C:75:SER:H	1.71	0.55
1:F:92:VAL:O	1:F:116:VAL:HA	2.07	0.55
1:H:1:LEU:HD11	1:H:90:ASP:CB	2.32	0.55
2:K:74:ARG:C	1:O:181:ASP:OD1	2.45	0.55
1:A:28:ILE:HG22	1:A:69:LYS:NZ	2.21	0.55
1:B:162:ASP:HB2	1:B:167:ILE:HD12	1.88	0.55
1:D:215:ALA:CB	1:D:222:LYS:HA	2.35	0.55
1:F:7:GLY:O	1:F:9:GLY:N	2.37	0.55
1:G:251:PHE:CA	1:G:299:VAL:HG21	2.37	0.55
2:L:73:CYS:C	5:L:101:HOH:O	2.45	0.55
1:E:194:ARG:NH1	1:E:205:PRO:HB2	2.16	0.55
1:E:281:VAL:HG11	1:F:48:SER:OG	2.07	0.55
1:H:90:ASP:O	1:H:114:LYS:HB2	2.06	0.55
1:C:173:THR:HG23	1:C:228:ILE:HD11	1.89	0.55
1:C:251:PHE:CZ	1:C:254:GLU:HB2	2.41	0.55
1:D:168:ILE:HG12	1:D:246:VAL:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:67:ASN:O	2:N:73:CYS:SG	2.64	0.55
1:A:206:THR:HG21	1:A:231:ARG:HG2	1.87	0.55
1:B:281:VAL:CG1	1:D:202:ASN:HD21	2.20	0.55
1:D:15:PHE:CE1	1:D:322:VAL:HG22	2.42	0.55
1:D:3:VAL:O	1:D:27:ILE:HA	2.06	0.55
1:D:331:ASN:O	1:D:331:ASN:OD1	2.25	0.55
1:E:108:HIS:O	1:E:111:ALA:HB3	2.06	0.55
1:B:149:CYS:SG	2:J:78:ASN:CG	2.84	0.55
1:O:187:ALA:O	1:O:196:ALA:HB1	2.06	0.55
1:Q:14:ASN:ND2	1:Q:314:GLU:HB3	2.22	0.55
1:B:186:ASP:HB2	1:C:10:ARG:NH1	2.21	0.55
1:D:109:ILE:HA	1:D:113:ALA:O	2.07	0.55
1:D:154:LEU:HD21	1:D:172:MET:HG3	1.89	0.55
1:E:282:ASP:OD1	1:F:46:TYR:HB3	2.06	0.55
1:G:154:LEU:CD1	1:G:240:VAL:HG11	2.37	0.55
1:E:171:THR:CG2	1:G:306:LYS:HE3	2.36	0.55
1:F:167:ILE:HG21	1:F:221:LEU:CD1	2.36	0.55
1:F:270:ILE:HG23	1:F:289:SER:HB2	1.88	0.55
1:G:271:LEU:HD12	1:G:290:THR:O	2.06	0.55
1:H:72:GLN:N	1:H:72:GLN:NE2	2.55	0.55
1:H:188:SER:O	2:N:72:GLU:HB3	2.06	0.55
1:O:170:GLY:HA3	1:O:244:VAL:HG12	1.89	0.55
1:A:16:LEU:HD23	1:A:16:LEU:O	2.07	0.55
1:B:162:ASP:O	1:B:166:GLY:HA2	2.06	0.55
1:D:210:ALA:HA	1:D:213:ALA:HB3	1.89	0.55
1:F:202:ASN:CB	1:H:280:SER:OG	2.55	0.55
1:E:235:PRO:HB3	1:H:201:LEU:HD11	1.88	0.55
1:A:173:THR:HG23	1:A:228:ILE:CD1	2.37	0.55
1:B:172:MET:HG2	1:B:173:THR:N	2.22	0.55
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.89	0.55
1:C:70:ILE:HD13	1:C:70:ILE:C	2.26	0.55
1:E:299:VAL:HG13	1:E:304:MET:O	2.07	0.55
1:C:190:HIS:CB	1:C:196:ALA:HB2	2.37	0.54
1:D:191:ARG:NH1	2:I:61:GLU:HG2	2.22	0.54
1:D:332:TRP:HB3	5:D:519:HOH:O	2.08	0.54
1:F:14:ASN:HD22	1:F:314:GLU:HG2	1.70	0.54
1:F:222:LYS:O	1:F:222:LYS:HG3	2.07	0.54
1:F:298:MET:CE	1:F:306:LYS:HD3	2.36	0.54
1:G:193:LEU:H	1:G:193:LEU:HD22	1.72	0.54
2:M:57:SER:OG	2:M:60:LEU:HB3	2.06	0.54
1:O:28:ILE:HD11	1:O:89:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ALA:HB2	1:A:89:ILE:HD12	1.89	0.54
1:D:78:ASN:ND2	1:D:80:SER:HB2	2.15	0.54
1:Q:263:ALA:HB2	1:Q:271:LEU:HD23	1.88	0.54
1:E:79:PRO:HA	1:E:82:LEU:CD1	2.38	0.54
1:E:87:LEU:HB3	1:E:89:ILE:CD1	2.36	0.54
1:O:263:ALA:HB2	1:O:271:LEU:HD23	1.89	0.54
1:C:203:ILE:HG23	1:C:232:VAL:HG12	1.89	0.54
1:D:319:GLN:HE21	1:D:319:GLN:CA	2.21	0.54
1:E:181:ASP:HB2	4:E:402:SO4:O4	2.08	0.54
1:G:28:ILE:HD11	1:G:89:ILE:HD13	1.88	0.54
2:L:63:TYR:CZ	2:L:73:CYS:SG	3.01	0.54
1:A:293:ASP:CB	1:A:296:LEU:HD12	2.38	0.54
1:C:301:GLY:O	1:C:302:ASP:HB2	2.07	0.54
1:D:154:LEU:CD2	1:D:172:MET:HG3	2.38	0.54
1:D:157:PHE:CE1	1:D:242:LEU:HD23	2.43	0.54
1:F:107:LYS:HA	1:F:110:GLU:HG2	1.88	0.54
1:F:245:GLN:NE2	1:H:245:GLN:NE2	2.46	0.54
1:H:24:PRO:HB2	1:H:329:ALA:HB1	1.90	0.54
1:D:18:CYS:HB2	1:D:322:VAL:HG21	1.90	0.54
1:F:174:THR:HA	1:F:240:VAL:HA	1.88	0.54
1:H:218:LEU:HB3	1:H:221:LEU:HD23	1.89	0.54
1:O:233:PRO:HB2	1:Q:233:PRO:HB2	1.89	0.54
1:C:183:ARG:HH21	1:C:187:ALA:CB	2.20	0.54
1:C:214:VAL:CG1	1:C:218:LEU:HD12	2.38	0.54
1:E:176:HIS:ND1	1:E:231:ARG:NH1	2.56	0.54
1:E:178:TYR:HA	1:E:182:GLN:OE1	2.08	0.54
1:E:218:LEU:O	1:E:220:ASN:N	2.40	0.54
1:F:161:LEU:HB3	1:F:167:ILE:HD11	1.90	0.54
1:F:317:TYR:O	1:F:321:VAL:HG23	2.07	0.54
1:G:211:ALA:HB1	1:G:226:ASN:CA	2.32	0.54
1:B:255:VAL:O	1:B:258:ALA:HB3	2.08	0.54
1:D:198:ALA:HB1	1:D:201:LEU:HD21	1.88	0.54
1:D:327:ILE:O	1:D:331:ASN:HB3	2.08	0.54
1:E:133:ASN:HA	1:E:135:ASP:OD1	2.07	0.54
1:E:240:VAL:O	1:E:308:ILE:HA	2.08	0.54
1:G:162:ASP:O	1:G:166:GLY:N	2.36	0.54
1:O:139:HIS:HB3	1:O:333:LYS:NZ	2.22	0.54
1:O:17:ARG:NH1	1:O:53:PHE:HB2	2.22	0.54
1:C:14:ASN:HD22	1:C:14:ASN:N	2.06	0.54
1:A:39:GLN:HG2	1:D:188:SER:HB2	1.88	0.54
1:D:319:GLN:HE21	1:D:319:GLN:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:PHE:HB2	1:F:259:PHE:CE1	2.43	0.54
1:G:131:GLY:H	1:G:134:ALA:CB	2.17	0.54
1:G:232:VAL:O	1:G:234:THR:N	2.40	0.54
1:H:149:CYS:HA	1:H:317:TYR:CD1	2.43	0.54
1:B:202:ASN:ND2	1:D:281:VAL:HB	2.22	0.54
1:B:169:LYS:CD	1:D:301:GLY:HA3	2.38	0.54
1:D:323:ASP:C	1:D:325:ALA:N	2.61	0.54
1:A:188:SER:HB2	1:D:39:GLN:HE22	1.73	0.54
1:F:66:VAL:O	1:F:69:LYS:HG2	2.08	0.54
1:G:300:MET:CE	1:G:301:GLY:H	2.21	0.54
1:G:300:MET:HE3	1:G:301:GLY:H	1.72	0.54
2:L:63:TYR:CE2	2:L:72:GLU:HG3	2.43	0.54
1:C:330:ASN:ND2	1:C:330:ASN:N	2.54	0.53
1:D:1:LEU:HD23	1:D:91:ILE:CD1	2.38	0.53
1:E:133:ASN:N	1:E:133:ASN:ND2	2.56	0.53
1:E:269:GLY:HA2	1:E:288:PHE:CE1	2.44	0.53
1:F:139:HIS:HB2	1:F:331:ASN:OD1	2.08	0.53
1:G:226:ASN:ND2	1:G:227:GLY:H	2.06	0.53
1:H:81:LEU:O	1:H:82:LEU:C	2.46	0.53
2:L:60:LEU:HD22	2:L:63:TYR:CD2	2.43	0.53
1:B:0:LYS:HE2	1:B:25:LEU:O	2.09	0.53
1:C:29:ALA:HA	1:C:71:ILE:HG23	1.89	0.53
1:F:130:VAL:HG11	1:F:323:ASP:HB2	1.90	0.53
1:F:281:VAL:HG13	1:F:282:ASP:N	2.23	0.53
1:G:130:VAL:HA	1:G:134:ALA:CB	2.38	0.53
1:H:269:GLY:O	1:H:270:ILE:HD13	2.08	0.53
1:H:292:ILE:HD13	1:H:309:ALA:HB2	1.90	0.53
2:L:63:TYR:CE2	2:L:73:CYS:SG	3.01	0.53
1:O:84:TRP:CE3	1:O:84:TRP:HA	2.44	0.53
1:Q:129:VAL:H	1:Q:133:ASN:ND2	2.06	0.53
1:C:84:TRP:HE3	1:C:84:TRP:HA	1.73	0.53
1:D:167:ILE:HD12	1:D:221:LEU:HD11	1.91	0.53
1:E:182:GLN:HE22	1:E:231:ARG:HB3	1.74	0.53
1:E:3:VAL:HB	1:E:27:ILE:HD13	1.90	0.53
1:F:191:ARG:HG3	5:F:503:HOH:O	2.08	0.53
1:H:16:LEU:O	1:H:16:LEU:HD23	2.08	0.53
1:O:226:ASN:HB2	1:Q:300:MET:CE	2.38	0.53
1:E:20:ARG:HH22	1:E:322:VAL:HB	1.73	0.53
1:F:202:ASN:HB3	1:H:281:VAL:HG23	1.89	0.53
1:F:210:ALA:O	1:F:214:VAL:HG23	2.08	0.53
1:H:177:SER:HB3	1:H:235:PRO:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:ARG:NH1	1:H:195:ARG:HB2	2.23	0.53
2:K:69:GLU:HG2	1:O:77:ARG:NH2	2.23	0.53
1:Q:110:GLU:O	1:Q:112:GLY:N	2.42	0.53
1:Q:109:ILE:HA	1:Q:113:ALA:O	2.09	0.53
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.09	0.53
1:C:79:PRO:HB3	1:C:108:HIS:CE1	2.44	0.53
1:D:133:ASN:HD21	1:D:217:VAL:HA	1.73	0.53
1:F:21:LYS:H	1:F:21:LYS:CE	2.22	0.53
1:H:236:ASN:O	1:H:237:VAL:HB	2.08	0.53
1:A:256:ASN:O	1:A:260:ARG:HG3	2.08	0.53
1:C:173:THR:HG23	1:C:228:ILE:CD1	2.38	0.53
1:D:116:VAL:HG12	1:D:117:ILE:N	2.23	0.53
1:E:171:THR:HG23	1:G:306:LYS:HE3	1.91	0.53
1:E:280:SER:HB3	1:G:202:ASN:HB2	1.91	0.53
1:G:205:PRO:HB3	1:G:230:LEU:CD2	2.38	0.53
1:A:28:ILE:O	1:A:28:ILE:HG12	2.07	0.53
1:B:226:ASN:HD22	1:D:298:MET:CE	2.22	0.53
1:D:137:TYR:CZ	1:D:328:VAL:HG22	2.44	0.53
1:E:-1:ALA:O	1:E:0:LYS:HB2	2.07	0.53
1:F:262:SER:HA	1:F:266:GLU:HG3	1.90	0.53
1:F:277:PRO:CG	1:H:193:LEU:HD12	2.39	0.53
1:F:26:ASP:OD2	1:F:28:ILE:HD11	2.09	0.53
1:F:289:SER:HG	1:F:320:ARG:HD2	1.74	0.53
1:G:129:VAL:N	1:G:133:ASN:HD21	2.01	0.53
1:G:154:LEU:O	1:G:155:ALA:C	2.47	0.53
1:Q:100:VAL:HA	1:Q:118:ILE:HD13	1.89	0.53
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.90	0.53
1:A:86:GLU:CD	1:A:86:GLU:H	2.12	0.53
1:F:20:ARG:HB3	1:F:23:SER:OG	2.08	0.53
1:H:13:ARG:O	1:H:17:ARG:HG3	2.09	0.53
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.74	0.53
1:B:266:GLU:O	1:B:267:LEU:HD23	2.09	0.53
1:B:2:LYS:HB3	1:B:28:ILE:HD13	1.91	0.53
1:C:18(A):TRP:CD2	1:C:27:ILE:HD13	2.44	0.53
1:C:87:LEU:HB2	1:C:89:ILE:HD11	1.90	0.53
1:E:169:LYS:NZ	1:E:245:GLN:OE1	2.42	0.53
1:E:279:VAL:HB	1:G:203:ILE:O	2.08	0.53
1:H:66:VAL:O	1:H:68:GLY:N	2.41	0.53
2:M:70:THR:HG22	2:M:71:ASN:N	2.23	0.53
1:C:126:PRO:HG2	1:C:141:GLU:CG	2.39	0.53
1:E:279:VAL:CG1	1:G:204:VAL:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:THR:OG1	1:G:251:PHE:N	2.41	0.53
1:H:4:ALA:HB2	1:H:89:ILE:HD12	1.91	0.53
1:O:172:MET:HE1	1:O:211:ALA:HB2	1.90	0.53
1:A:1:LEU:HD22	1:A:329:ALA:HB2	1.91	0.52
1:B:190:HIS:ND1	1:B:191:ARG:N	2.58	0.52
1:B:173:THR:O	1:B:241:ASP:HB3	2.08	0.52
1:C:318:SER:O	1:C:322:VAL:HG23	2.09	0.52
1:E:79:PRO:HA	1:E:82:LEU:HG	1.91	0.52
1:H:271:LEU:HD12	1:H:272:ASP:H	1.74	0.52
1:H:42:HIS:C	1:H:43:LEU:HD23	2.29	0.52
1:O:298:MET:HE3	1:Q:226:ASN:HD22	1.74	0.52
1:B:27:ILE:HD12	1:B:27:ILE:N	2.25	0.52
1:D:174:THR:HB	1:D:240:VAL:HG12	1.91	0.52
1:E:171:THR:HA	1:E:226:ASN:O	2.09	0.52
1:F:130:VAL:HG22	1:F:324:LEU:HB2	1.92	0.52
1:F:131:GLY:H	1:F:134:ALA:HB2	1.75	0.52
1:G:312:ASP:HB3	1:G:316:GLY:H	1.75	0.52
1:H:4:ALA:CB	1:H:89:ILE:HD12	2.39	0.52
1:O:263:ALA:O	1:O:268:LYS:HA	2.09	0.52
1:Q:250:THR:OG1	1:Q:251:PHE:N	2.41	0.52
1:A:172:MET:HG2	1:A:173:THR:N	2.24	0.52
1:A:28:ILE:H	1:A:28:ILE:HD13	1.74	0.52
1:E:235:PRO:CG	1:E:284:ARG:NH2	2.72	0.52
1:F:32:ASP:HA	3:F:401:NAD:H2A	1.91	0.52
1:G:303:ASP:HB2	5:G:532:HOH:O	2.10	0.52
1:H:123:GLY:O	1:H:125:ILE:N	2.42	0.52
2:K:77:ASP:OD1	2:K:78:ASN:N	2.43	0.52
1:Q:110:GLU:C	1:Q:112:GLY:H	2.12	0.52
1:A:293:ASP:HB3	1:A:296:LEU:HD12	1.92	0.52
1:D:195:ARG:NH1	2:I:76:TYR:O	2.43	0.52
1:E:246:VAL:HG22	1:E:303:ASP:O	2.08	0.52
1:E:320:ARG:HA	1:E:320:ARG:NE	2.25	0.52
1:F:156:PRO:CB	1:F:290:THR:HG21	2.37	0.52
1:H:85:LYS:HB2	1:H:112:GLY:HA3	1.91	0.52
2:J:58:ASP:N	2:J:59:PRO:CD	2.73	0.52
1:B:253:GLU:HG3	4:B:402:SO4:O3	2.09	0.52
1:C:36:GLY:O	1:C:40:ALA:HB2	2.08	0.52
1:E:100:VAL:O	1:E:122(A):LYS:HB2	2.09	0.52
1:E:155:ALA:HB3	1:E:156:PRO:HD3	1.92	0.52
1:E:80:SER:HB3	1:E:107:LYS:HE2	1.91	0.52
1:F:17:ARG:NH2	1:F:53:PHE:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:LEU:HD13	1:G:271:LEU:CB	2.40	0.52
1:G:304:MET:HG2	1:G:304:MET:O	2.09	0.52
1:H:106:GLY:HA2	1:H:143:ILE:HD11	1.91	0.52
1:H:148:SER:HB2	5:N:110:HOH:O	2.09	0.52
1:H:66:VAL:C	1:H:68:GLY:N	2.63	0.52
1:Q:306:LYS:NZ	5:Q:526:HOH:O	2.38	0.52
1:B:256:ASN:HD21	1:B:297:THR:HG1	1.55	0.52
1:B:115:LYS:HD2	1:B:332:TRP:CZ3	2.44	0.52
1:D:249:LYS:HD2	1:D:302:ASP:CB	2.37	0.52
1:E:175:THR:HB	1:E:239:VAL:CG1	2.39	0.52
1:E:270:ILE:O	1:E:270:ILE:HG22	2.09	0.52
1:G:133:ASN:N	1:G:133:ASN:ND2	2.58	0.52
1:G:139:HIS:CD2	1:G:333:LYS:H	2.26	0.52
1:G:210:ALA:O	1:G:213:ALA:HB3	2.09	0.52
1:G:256:ASN:HA	1:G:259:PHE:CD2	2.45	0.52
1:H:215:ALA:HB1	1:H:222:LYS:CA	2.34	0.52
1:H:72:GLN:N	1:H:72:GLN:HE21	2.03	0.52
2:K:70:THR:OG1	2:K:73:CYS:SG	2.68	0.52
1:A:29:ALA:N	1:A:71:ILE:HG13	2.24	0.52
1:A:86:GLU:CD	1:A:86:GLU:N	2.63	0.52
1:H:314:GLU:HG2	3:H:401:NAD:H72N	1.74	0.52
2:L:58:ASP:N	2:L:59:PRO:CD	2.72	0.52
1:O:39:GLN:N	1:O:39:GLN:NE2	2.55	0.52
1:E:16:LEU:HD23	1:E:16:LEU:O	2.09	0.52
1:E:65:SER:HA	1:E:70:ILE:HA	1.92	0.52
1:E:28:ILE:CA	1:E:71:ILE:HD12	2.39	0.52
1:F:168:ILE:HD11	1:F:247:SER:HB3	1.92	0.52
1:G:18(A):TRP:HD1	1:G:25:LEU:HD12	1.75	0.52
1:H:183:ARG:HB2	1:H:196:ALA:O	2.09	0.52
1:O:281:VAL:HB	1:Q:202:ASN:HD21	1.73	0.52
1:C:183:ARG:CG	1:C:196:ALA:HA	2.40	0.52
1:D:252:ALA:N	1:D:299:VAL:HG21	2.25	0.52
1:E:3:VAL:HG11	1:E:93:ILE:HD11	1.92	0.52
1:G:85:LYS:N	1:G:112:GLY:HA3	2.25	0.52
1:O:280:SER:HB3	1:Q:203:ILE:HB	1.92	0.52
1:A:172:MET:HG2	1:A:173:THR:H	1.75	0.52
1:B:152:ASN:ND2	1:B:320:ARG:HG3	2.25	0.52
1:C:98:VAL:HG23	1:C:99:PHE:CE2	2.45	0.52
1:E:183:ARG:HA	1:E:183:ARG:HH11	1.75	0.52
1:F:37:VAL:HG13	1:F:64:ILE:CG2	2.39	0.52
1:G:239:VAL:HB	1:G:310:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASP:OD2	1:A:195:ARG:NH1	2.43	0.51
1:A:70:ILE:HG22	1:A:71:ILE:N	2.25	0.51
1:C:266:GLU:HG2	1:C:267:LEU:N	2.25	0.51
1:E:194:ARG:HD3	1:E:205:PRO:HD2	1.91	0.51
1:E:19:GLY:O	1:E:20:ARG:O	2.28	0.51
1:E:195:ARG:NH2	1:E:231:ARG:HH21	2.08	0.51
1:F:248:LYS:HE3	5:F:524:HOH:O	2.09	0.51
1:G:330:ASN:C	1:G:331:ASN:HD22	2.14	0.51
1:Q:168:ILE:HD11	1:Q:247:SER:CB	2.39	0.51
1:B:16:LEU:HD23	1:B:16:LEU:O	2.09	0.51
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.45	0.51
1:E:133:ASN:H	1:E:133:ASN:HD22	1.55	0.51
1:E:289:SER:HB2	1:E:320:ARG:HH11	1.76	0.51
1:E:28:ILE:C	1:E:71:ILE:HG23	2.29	0.51
1:F:274:CYS:SG	1:F:275:ASP:N	2.84	0.51
1:F:300:MET:CE	1:H:169:LYS:HB2	2.40	0.51
1:A:30:ILE:HG12	1:A:71:ILE:HD11	1.92	0.51
1:B:234:THR:HG22	1:D:233:PRO:HG2	1.93	0.51
1:C:270:ILE:HD12	1:C:270:ILE:N	2.24	0.51
1:F:186:ASP:HA	1:F:196:ALA:O	2.10	0.51
1:F:190:HIS:ND1	1:F:192:ASP:N	2.56	0.51
1:F:61:GLU:HA	5:F:510:HOH:O	2.08	0.51
1:H:81:LEU:CD1	1:H:81:LEU:H	2.24	0.51
1:H:94:GLU:CD	1:H:99:PHE:HD2	2.14	0.51
1:B:133:ASN:HD22	1:B:133:ASN:H	1.58	0.51
1:D:320:ARG:HA	1:D:320:ARG:HE	1.74	0.51
1:E:166:GLY:O	1:E:246:VAL:HA	2.10	0.51
1:E:46:TYR:CD1	1:E:52:ILE:HG22	2.45	0.51
1:G:252:ALA:N	1:G:299:VAL:HG21	2.24	0.51
1:G:331:ASN:N	1:G:331:ASN:HD22	2.07	0.51
2:N:62:GLU:HG2	5:N:104:HOH:O	2.10	0.51
1:C:0:LYS:HB3	1:C:0:LYS:NZ	2.26	0.51
1:B:226:ASN:HB3	1:D:298:MET:CE	2.40	0.51
1:F:117:ILE:CB	1:F:144:ILE:HD11	2.41	0.51
1:F:228:ILE:HD13	1:F:228:ILE:H	1.75	0.51
1:G:294:SER:O	1:G:297:THR:HG22	2.11	0.51
1:H:85:LYS:O	1:H:87:LEU:N	2.37	0.51
1:O:31:ASN:HB2	1:O:74:VAL:HG22	1.92	0.51
1:Q:3:VAL:HG21	1:Q:25:LEU:HB3	1.91	0.51
1:A:228:ILE:C	1:A:228:ILE:HD12	2.31	0.51
1:B:292:ILE:HD12	1:B:307:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HA	1:B:320:ARG:NE	2.26	0.51
1:G:167:ILE:HG23	1:G:244:VAL:HB	1.93	0.51
1:E:205:PRO:HG3	1:G:310:TRP:HZ2	1.76	0.51
1:H:148:SER:OG	1:H:210:ALA:HB2	2.11	0.51
1:Q:171:THR:O	1:Q:242:LEU:HD12	2.10	0.51
1:A:128:TYR:CZ	1:A:137:TYR:HA	2.45	0.51
1:D:182:GLN:HE22	1:D:231:ARG:HB3	1.76	0.51
1:E:320:ARG:HA	1:E:320:ARG:HE	1.76	0.51
1:O:298:MET:HE1	1:Q:226:ASN:HB3	1.93	0.51
1:C:3:VAL:HG22	1:C:91:ILE:HG23	1.92	0.51
1:C:46:TYR:O	1:C:47:ASP:HB2	2.10	0.51
1:D:8:PHE:O	1:D:13:ARG:HG3	2.11	0.51
1:D:10:ARG:O	1:D:14:ASN:HB2	2.10	0.51
1:D:130:VAL:HG21	1:D:320:ARG:O	2.11	0.51
1:E:78:ASN:OD1	1:E:80:SER:HB3	2.10	0.51
1:G:294:SER:O	1:G:296:LEU:N	2.44	0.51
2:M:71:ASN:HA	2:M:74:ARG:NH1	2.26	0.51
1:E:120:ALA:O	1:E:145:SER:OG	2.29	0.51
1:E:131:GLY:HA3	1:E:270:ILE:HG21	1.93	0.51
1:G:6:ASN:ND2	1:G:31:ASN:HD22	2.09	0.51
1:H:25:LEU:HD21	1:H:325:ALA:HB1	1.93	0.51
1:B:87:LEU:HB2	1:B:89:ILE:CD1	2.41	0.51
1:E:109:ILE:HG23	1:E:116:VAL:HG23	1.92	0.51
1:E:5:ILE:HD13	1:E:5:ILE:C	2.30	0.51
1:F:3:VAL:HG12	1:F:4:ALA:N	2.25	0.51
1:G:251:PHE:HA	1:G:299:VAL:HG21	1.91	0.51
1:H:137:TYR:OH	1:H:328:VAL:HG13	2.11	0.51
1:F:226:ASN:ND2	1:H:298:MET:SD	2.83	0.51
2:N:73:CYS:O	2:N:74:ARG:C	2.49	0.51
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.76	0.51
1:Q:154:LEU:HA	1:Q:157:PHE:CE2	2.45	0.51
1:B:109:ILE:HA	1:B:113:ALA:O	2.11	0.50
1:B:134:ALA:HB1	1:B:327:ILE:HD13	1.93	0.50
1:D:265:LYS:HB2	1:D:266:GLU:OE1	2.11	0.50
1:D:20:ARG:HE	1:D:319:GLN:HE22	1.59	0.50
1:E:208:THR:HA	4:E:403:SO4:O1	2.11	0.50
1:F:172:MET:SD	1:F:172:MET:O	2.69	0.50
1:F:191:ARG:HG2	1:F:191:ARG:HH11	1.76	0.50
1:F:31:ASN:HA	1:F:74:VAL:O	2.12	0.50
1:G:208:THR:HG23	1:G:208:THR:O	2.10	0.50
1:H:157:PHE:HB2	1:H:259:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:LEU:C	1:O:16:LEU:HD23	2.30	0.50
1:A:101:ASP:CG	1:A:103:GLU:HB3	2.32	0.50
1:A:215:ALA:CB	1:A:222:LYS:HA	2.41	0.50
1:D:320:ARG:HA	1:D:320:ARG:NE	2.27	0.50
1:E:157:PHE:CE1	1:E:242:LEU:HD23	2.46	0.50
1:E:324:LEU:O	1:E:328:VAL:HG23	2.11	0.50
1:F:154:LEU:HD11	1:F:242:LEU:HD12	1.92	0.50
1:F:246:VAL:O	1:F:303:ASP:HB2	2.10	0.50
1:F:0:LYS:HZ3	1:F:24:PRO:HG3	1.76	0.50
1:G:184:LEU:O	1:G:185:LEU:HD23	2.10	0.50
1:E:280:SER:CB	1:G:203:ILE:H	2.23	0.50
1:D:86:GLU:HB3	1:H:28:ILE:HD11	1.94	0.50
1:O:169:LYS:HE2	1:Q:301:GLY:HA3	1.93	0.50
1:O:28:ILE:HD11	1:O:89:ILE:CD1	2.41	0.50
1:A:281:VAL:CB	1:C:202:ASN:HD21	2.24	0.50
1:F:139:HIS:CD2	1:F:333:LYS:HD2	2.47	0.50
1:F:325:ALA:O	1:F:328:VAL:HB	2.12	0.50
1:G:176:HIS:O	1:G:231:ARG:HA	2.11	0.50
1:H:108:HIS:HD2	1:H:116:VAL:HG11	1.76	0.50
1:H:44:LEU:O	1:H:53:PHE:HB2	2.10	0.50
1:O:301:GLY:HA3	1:Q:169:LYS:HD3	1.92	0.50
1:O:84:TRP:HE3	1:O:84:TRP:HA	1.75	0.50
1:A:82:LEU:HD13	1:A:84:TRP:CE2	2.46	0.50
1:A:98:VAL:HG23	1:A:99:PHE:N	2.27	0.50
1:C:250:THR:OG1	1:C:251:PHE:N	2.44	0.50
1:C:89:ILE:H	1:C:89:ILE:CD1	2.21	0.50
1:C:46:TYR:CE2	1:D:278:LEU:HD21	2.46	0.50
1:E:135:ASP:C	1:E:137:TYR:H	2.14	0.50
1:E:241:ASP:HA	1:E:308:ILE:HD13	1.92	0.50
1:E:281:VAL:HG21	1:F:48:SER:HA	1.93	0.50
1:G:179:THR:C	1:G:181:ASP:N	2.64	0.50
1:G:20:ARG:HH11	1:G:20:ARG:HG3	1.76	0.50
1:G:177:SER:OG	1:G:234:THR:HG22	2.11	0.50
1:H:162:ASP:HA	1:H:167:ILE:HG13	1.92	0.50
1:H:29:ALA:HA	1:H:71:ILE:HG23	1.94	0.50
1:H:242:LEU:O	1:H:306:LYS:HA	2.11	0.50
1:Q:170:GLY:HA3	1:Q:244:VAL:HG12	1.93	0.50
1:B:83:PRO:HG2	1:B:87:LEU:CD1	2.41	0.50
1:D:4:ALA:HB2	1:D:89:ILE:HG12	1.93	0.50
1:D:64:ILE:HG23	1:D:73:VAL:CG2	2.41	0.50
1:G:132:VAL:HG12	1:G:133:ASN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:GLN:HA	1:H:195:ARG:O	2.12	0.50
1:H:31:ASN:OD1	1:H:75:SER:HA	2.12	0.50
1:H:83:PRO:HB2	1:H:86:GLU:CG	2.41	0.50
1:Q:206:THR:HG22	1:Q:229:ALA:HB3	1.93	0.50
1:D:146:ASN:HD22	1:D:321:VAL:HG23	1.76	0.50
1:E:170:GLY:HA3	1:E:244:VAL:HG12	1.92	0.50
1:E:198:ALA:HB3	1:E:201:LEU:HD11	1.92	0.50
1:E:157:PHE:CE1	1:E:307:VAL:HB	2.46	0.50
1:F:202:ASN:HB2	1:H:280:SER:OG	2.12	0.50
1:F:32:ASP:O	1:F:75:SER:HB2	2.12	0.50
1:G:1:LEU:HD13	1:G:329:ALA:HB1	1.94	0.50
1:Q:28:ILE:C	1:Q:28:ILE:HD12	2.31	0.50
1:A:139:HIS:CE1	1:A:333:LYS:H	2.29	0.50
1:D:162:ASP:O	1:D:166:GLY:HA2	2.12	0.50
1:E:174:THR:O	1:E:174:THR:HG23	2.11	0.50
1:F:284:ARG:HA	1:F:312:ASP:OD2	2.11	0.50
1:H:183:ARG:O	1:H:198:ALA:HA	2.11	0.50
1:H:195:ARG:HG2	1:H:195:ARG:O	2.11	0.50
1:O:266:GLU:HG2	1:O:267:LEU:HG	1.94	0.50
1:A:146:ASN:ND2	1:A:321:VAL:HG22	2.27	0.50
1:A:37:VAL:CG2	1:A:63:ALA:N	2.75	0.50
1:D:288:PHE:N	1:D:288:PHE:CD1	2.80	0.50
1:E:114:LYS:HD2	1:E:332:TRP:HZ2	1.76	0.50
1:E:-1:ALA:N	5:E:514:HOH:O	2.43	0.50
1:E:85:LYS:HB2	1:E:112:GLY:HA3	1.93	0.50
1:F:5:ILE:CB	1:F:30:ILE:HG23	2.34	0.50
1:F:89:ILE:O	1:F:113:ALA:HA	2.12	0.50
1:G:173:THR:HG23	1:G:228:ILE:CD1	2.42	0.50
1:H:317:TYR:O	1:H:320:ARG:HB2	2.11	0.50
1:O:281:VAL:CG2	1:Q:202:ASN:HD21	2.24	0.50
1:D:178:TYR:HA	1:D:231:ARG:HD2	1.93	0.50
1:D:62:THR:CG2	1:H:74:VAL:HG22	2.42	0.50
1:E:176:HIS:O	1:E:231:ARG:HA	2.12	0.50
1:E:330:ASN:HB3	5:E:540:HOH:O	2.11	0.50
1:E:9:GLY:HA3	3:E:401:NAD:O5B	2.12	0.50
1:F:31:ASN:ND2	5:F:502:HOH:O	2.44	0.50
2:L:60:LEU:HD22	2:L:63:TYR:HD2	1.77	0.50
1:A:266:GLU:HG2	1:A:267:LEU:N	2.26	0.49
1:B:134:ALA:HB1	1:B:327:ILE:CD1	2.42	0.49
1:B:279:VAL:HG21	1:D:197:ARG:HG3	1.93	0.49
1:F:165:PHE:CE1	1:F:250:THR:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ASP:CB	1:F:67:ASP:H	2.23	0.49
1:G:165:PHE:O	1:G:246:VAL:HB	2.11	0.49
1:G:84:TRP:CE3	1:G:89:ILE:HG13	2.47	0.49
1:H:156:PRO:HB2	1:H:290:THR:HG21	1.94	0.49
1:H:314:GLU:HG2	3:H:401:NAD:N7N	2.27	0.49
1:E:183:ARG:NH2	2:N:74:ARG:HH22	2.10	0.49
1:O:281:VAL:H	1:Q:202:ASN:ND2	2.06	0.49
1:Q:194:ARG:HD3	1:Q:205:PRO:O	2.12	0.49
1:D:118:ILE:HG22	1:D:118:ILE:O	2.10	0.49
1:F:23:SER:O	1:F:25:LEU:N	2.41	0.49
1:H:20:ARG:HG3	1:H:20:ARG:HH11	1.77	0.49
1:H:221:LEU:N	1:H:221:LEU:HD22	2.27	0.49
1:F:300:MET:HG2	1:H:226:ASN:OD1	2.13	0.49
2:K:58:ASP:CG	2:K:61:GLU:HG3	2.32	0.49
1:E:146:ASN:HD22	1:E:324:LEU:HD22	1.77	0.49
1:E:176:HIS:CE1	1:E:231:ARG:NH1	2.81	0.49
1:F:109:ILE:C	1:F:111:ALA:H	2.15	0.49
1:F:260:ARG:HA	1:F:263:ALA:HB3	1.93	0.49
1:E:197:ARG:NH1	1:G:282:ASP:OD2	2.46	0.49
1:H:176:HIS:CE1	1:H:238:SER:HG	2.30	0.49
1:H:11:ILE:HD11	3:H:401:NAD:C3N	2.42	0.49
1:H:84:TRP:HB3	1:H:89:ILE:HG21	1.94	0.49
1:Q:61:GLU:HG3	5:Q:561:HOH:O	2.13	0.49
1:B:162:ASP:OD1	1:B:167:ILE:N	2.46	0.49
1:B:284:ARG:O	1:B:285:CYS:HB2	2.11	0.49
1:A:282:ASP:HA	1:B:52:ILE:HD11	1.92	0.49
1:C:236:ASN:HD21	1:C:312:ASP:CG	2.16	0.49
1:C:281:VAL:C	1:C:283:PHE:H	2.14	0.49
1:D:109:ILE:HG22	1:D:113:ALA:O	2.12	0.49
1:D:168:ILE:O	1:D:224:LYS:HD3	2.13	0.49
1:E:94:GLU:OE2	1:E:99:PHE:HB2	2.13	0.49
1:F:173:THR:HG23	1:F:228:ILE:HD11	1.94	0.49
1:G:256:ASN:ND2	1:G:256:ASN:H	2.10	0.49
1:O:218:LEU:HB3	1:O:221:LEU:HD23	1.95	0.49
1:O:31:ASN:HA	1:O:74:VAL:O	2.13	0.49
1:Q:127:THR:N	4:Q:404:SO4:O3	2.45	0.49
1:A:281:VAL:HB	1:C:202:ASN:HD21	1.77	0.49
1:C:197:ARG:HH11	1:C:197:ARG:HG3	1.76	0.49
1:C:214:VAL:O	1:C:218:LEU:HB2	2.12	0.49
1:E:85:LYS:N	1:E:112:GLY:HA3	2.27	0.49
1:G:28:ILE:N	1:G:28:ILE:HD13	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:THR:HG21	1:O:77:ARG:HE	1.77	0.49
1:O:202:ASN:ND2	1:Q:281:VAL:H	2.11	0.49
1:A:171:THR:CG2	1:C:306:LYS:HZ3	2.25	0.49
1:A:293:ASP:CG	1:A:296:LEU:HD12	2.32	0.49
1:C:157:PHE:HB2	1:C:259:PHE:CE1	2.48	0.49
1:D:16:LEU:HD23	1:D:16:LEU:C	2.33	0.49
1:E:157:PHE:HB2	1:E:259:PHE:CZ	2.48	0.49
2:I:69:GLU:OE2	2:I:69:GLU:N	2.40	0.49
1:Q:204:VAL:HB	1:Q:231:ARG:HB2	1.95	0.49
1:A:183:ARG:NE	1:A:187:ALA:HB3	2.28	0.49
1:B:53:PHE:CE2	1:B:55:ALA:HB3	2.48	0.49
1:C:133:ASN:C	1:C:135:ASP:N	2.66	0.49
1:B:279:VAL:HG22	1:D:197:ARG:HG3	1.95	0.49
1:D:83:PRO:HB3	1:H:72:GLN:OE1	2.12	0.49
1:E:132:VAL:HG11	1:E:217:VAL:CG2	2.43	0.49
1:E:38:LYS:HB2	1:E:39:GLN:HE22	1.77	0.49
1:F:128:TYR:HA	1:F:133:ASN:HD21	1.77	0.49
1:H:154:LEU:O	1:H:158:VAL:HG23	2.13	0.49
1:F:300:MET:HG2	1:H:226:ASN:HD21	1.77	0.49
1:Q:157:PHE:HB2	1:Q:259:PHE:CE1	2.47	0.49
1:B:117:ILE:C	1:B:117:ILE:HD13	2.32	0.49
1:C:271:LEU:HA	1:C:290:THR:O	2.13	0.49
1:D:124:ASP:O	1:D:125:ILE:CB	2.61	0.49
1:B:194:ARG:NH2	1:D:277:PRO:HA	2.27	0.49
1:H:96:THR:OG1	1:H:98:VAL:HG22	2.11	0.49
1:A:109:ILE:HA	1:A:113:ALA:O	2.13	0.49
1:B:102:ARG:HG2	1:B:102:ARG:NH1	2.28	0.49
1:B:192:ASP:OD1	1:B:194:ARG:HB2	2.12	0.49
1:D:142:PRO:O	1:D:143:ILE:HD12	2.13	0.49
1:E:118:ILE:HD12	1:E:118:ILE:H	1.77	0.49
1:E:1:LEU:HD22	1:E:329:ALA:HA	1.94	0.49
1:E:204:VAL:HA	1:E:205:PRO:HD3	1.70	0.49
1:F:211:ALA:HB1	1:F:226:ASN:HA	1.95	0.49
2:K:71:ASN:HB3	1:O:183:ARG:CZ	2.43	0.49
1:O:194:ARG:HD2	1:O:205:PRO:O	2.12	0.49
1:A:130:VAL:HG23	5:A:503:HOH:O	2.12	0.49
1:A:192:ASP:HA	5:A:509:HOH:O	2.11	0.49
1:B:292:ILE:HD12	1:B:307:VAL:CG1	2.43	0.49
1:D:11:ILE:HD11	3:D:401:NAD:C2N	2.42	0.49
1:E:175:THR:HB	1:E:239:VAL:HG12	1.95	0.49
1:G:18(A):TRP:CH2	1:G:69:LYS:HE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:ASN:HB2	1:G:74:VAL:HG22	1.95	0.49
2:J:58:ASP:HA	2:J:61:GLU:HG3	1.94	0.49
2:M:58:ASP:H	2:M:59:PRO:CD	2.26	0.49
1:Q:98:VAL:HG23	1:Q:99:PHE:CE2	2.48	0.49
1:B:39:GLN:OE1	1:C:188:SER:HB2	2.13	0.48
1:B:226:ASN:HB3	1:D:298:MET:HE1	1.93	0.48
1:E:154:LEU:HD11	1:E:172:MET:HG3	1.95	0.48
1:E:38:LYS:HB2	1:E:39:GLN:NE2	2.27	0.48
1:E:63:ALA:HB1	1:E:72:GLN:HA	1.94	0.48
1:F:178:TYR:HD1	1:F:178:TYR:O	1.96	0.48
1:F:260:ARG:HB3	1:F:264:GLU:OE2	2.13	0.48
2:K:69:GLU:HB3	1:O:98:VAL:CG1	2.33	0.48
1:O:26:ASP:O	1:O:28:ILE:HG23	2.12	0.48
1:B:177:SER:CB	1:B:234:THR:O	2.61	0.48
1:C:74:VAL:HG12	1:C:75:SER:N	2.28	0.48
1:D:203:ILE:HG12	1:D:232:VAL:HG12	1.95	0.48
1:D:215:ALA:HB3	5:D:539:HOH:O	2.13	0.48
1:D:232:VAL:O	1:D:234:THR:N	2.44	0.48
1:D:169:LYS:NZ	1:D:245:GLN:NE2	2.61	0.48
1:F:114:LYS:N	1:F:114:LYS:CD	2.74	0.48
1:F:56:ASP:HB2	1:F:67:ASP:CA	2.43	0.48
1:H:64:ILE:HG13	1:H:64:ILE:O	2.13	0.48
1:H:8:PHE:CE1	1:H:16:LEU:HD12	2.49	0.48
1:O:17:ARG:HD2	1:O:53:PHE:CE1	2.48	0.48
1:O:58:LYS:C	1:O:58:LYS:HD3	2.34	0.48
1:Q:251:PHE:CZ	1:Q:254:GLU:HB2	2.48	0.48
1:A:13:ARG:NE	1:A:43:LEU:HB3	2.29	0.48
1:C:258:ALA:HA	1:C:261:ASP:OD2	2.13	0.48
1:D:172:MET:CG	1:D:173:THR:N	2.77	0.48
1:E:315:TRP:O	1:E:318:SER:HB2	2.13	0.48
1:F:238:SER:HB2	1:F:311:TYR:CZ	2.48	0.48
1:F:52:ILE:HD12	1:F:52:ILE:N	2.28	0.48
1:G:18(A):TRP:CD1	1:G:25:LEU:HD12	2.48	0.48
1:F:235:PRO:HB3	1:G:201:LEU:HD11	1.94	0.48
1:G:293:ASP:HB3	1:G:296:LEU:CD1	2.39	0.48
1:H:86:GLU:CD	1:H:86:GLU:N	2.64	0.48
1:O:27:ILE:CD1	1:O:27:ILE:N	2.76	0.48
1:A:101:ASP:O	1:A:102:ARG:C	2.52	0.48
1:B:4:ALA:HA	1:B:29:ALA:O	2.13	0.48
1:C:213:ALA:O	1:C:216:LEU:HB2	2.14	0.48
1:D:245:GLN:HG2	1:D:303:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ASN:O	1:H:298:MET:HE3	2.13	0.48
1:F:9:GLY:HA3	3:F:401:NAD:O5B	2.13	0.48
1:H:79:PRO:HG3	1:H:99:PHE:CZ	2.49	0.48
1:Q:115:LYS:HE2	1:Q:141:GLU:O	2.14	0.48
1:Q:132:VAL:HG21	1:Q:155:ALA:HB1	1.95	0.48
1:B:149:CYS:SG	2:J:78:ASN:ND2	2.86	0.48
1:B:36:GLY:HA3	1:B:38:LYS:HE3	1.95	0.48
1:D:231:ARG:HH21	2:I:78:ASN:C	2.17	0.48
1:E:78:ASN:OD1	1:E:107:LYS:HE2	2.13	0.48
1:H:20:ARG:NH1	1:H:20:ARG:HG3	2.28	0.48
2:N:62:GLU:O	2:N:65:LYS:HB3	2.13	0.48
1:Q:242:LEU:HD12	1:Q:243:VAL:H	1.78	0.48
1:C:146:ASN:O	1:C:147:ALA:HB3	2.13	0.48
1:D:143:ILE:O	1:D:143:ILE:HG22	2.13	0.48
1:G:197:ARG:HG3	1:G:197:ARG:HH11	1.79	0.48
1:O:176:HIS:HB3	1:O:231:ARG:HD3	1.96	0.48
1:Q:28:ILE:HD12	1:Q:29:ALA:HB2	1.96	0.48
1:B:195:ARG:HH12	2:J:76:TYR:H	1.62	0.48
1:B:251:PHE:CE2	1:B:253:GLU:HB2	2.49	0.48
1:B:307:VAL:HG12	1:B:308:ILE:N	2.28	0.48
1:B:52:ILE:N	1:B:52:ILE:HD12	2.29	0.48
1:C:126:PRO:HD2	1:C:143:ILE:O	2.14	0.48
1:C:27:ILE:CG2	1:C:71:ILE:HD13	2.43	0.48
1:D:21:LYS:O	1:D:22:ASP:HB2	2.13	0.48
1:F:52:ILE:CD1	1:F:52:ILE:H	2.27	0.48
1:G:20:ARG:NH1	1:G:20:ARG:HG3	2.29	0.48
1:H:164:LYS:H	1:H:164:LYS:CD	2.26	0.48
1:H:81:LEU:HD12	1:H:81:LEU:N	2.29	0.48
1:A:87:LEU:HB2	1:A:89:ILE:HG12	1.96	0.48
1:B:27:ILE:CD1	1:B:27:ILE:N	2.77	0.48
1:E:10:ARG:HB2	3:E:401:NAD:O1N	2.13	0.48
1:F:306:LYS:NZ	1:H:173:THR:OG1	2.28	0.48
2:I:71:ASN:HA	2:I:74:ARG:NH2	2.28	0.48
1:O:298:MET:HE3	1:Q:226:ASN:ND2	2.29	0.48
1:Q:37:VAL:HG22	1:Q:73:VAL:HB	1.96	0.48
1:A:139:HIS:CD2	1:A:333:LYS:HE2	2.48	0.48
1:A:202:ASN:O	1:A:233:PRO:HD3	2.13	0.48
1:B:220:ASN:HD22	1:B:220:ASN:C	2.17	0.48
1:C:91:ILE:HD11	1:C:93:ILE:CD1	2.43	0.48
1:D:117:ILE:HA	1:D:144:ILE:HG13	1.96	0.48
1:D:260:ARG:O	1:D:263:ALA:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:PHE:HE2	1:F:253:GLU:HB3	1.79	0.48
1:G:181:ASP:OD2	2:M:75:THR:HA	2.14	0.48
1:H:11:ILE:HD11	3:H:401:NAD:H71N	1.79	0.48
1:H:288:PHE:C	1:H:290:THR:N	2.67	0.48
1:Q:16:LEU:O	1:Q:16:LEU:HD12	2.14	0.48
1:O:281:VAL:CB	1:Q:202:ASN:HD21	2.27	0.48
1:Q:31:ASN:OD1	1:Q:74:VAL:HG22	2.14	0.48
1:A:78:ASN:HD22	1:A:81:LEU:CD1	2.26	0.48
1:B:14:ASN:OD1	1:B:50:LEU:HD11	2.14	0.48
1:E:281:VAL:O	1:E:281:VAL:HG22	2.14	0.48
1:H:42:HIS:O	1:H:43:LEU:HD23	2.14	0.48
1:O:18(A):TRP:CE2	1:O:27:ILE:HD13	2.48	0.48
1:A:194:ARG:HD3	1:C:278:LEU:O	2.14	0.47
1:C:29:ALA:HA	1:C:71:ILE:CG2	2.43	0.47
1:D:122:GLY:HA3	1:D:125:ILE:HG21	1.95	0.47
1:E:22:ASP:HA	5:E:514:HOH:O	2.14	0.47
1:F:85:LYS:HE2	1:F:112:GLY:HA2	1.94	0.47
1:G:162:ASP:HA	1:G:167:ILE:HG12	1.96	0.47
1:G:252:ALA:HB1	1:G:297:THR:HG23	1.94	0.47
2:N:60:LEU:HD11	2:N:72:GLU:HB2	1.96	0.47
1:D:270:ILE:HD12	1:D:270:ILE:N	2.29	0.47
1:E:172:MET:HA	1:E:241:ASP:O	2.14	0.47
1:E:279:VAL:HG12	1:G:204:VAL:HA	1.95	0.47
1:G:133:ASN:H	1:G:133:ASN:ND2	2.12	0.47
1:G:1:ALA:CB	1:G:26:ASP:HB2	2.43	0.47
1:G:271:LEU:CD1	1:G:290:THR:O	2.61	0.47
1:H:84:TRP:CG	1:H:89:ILE:HG21	2.49	0.47
1:A:142:PRO:C	1:A:143:ILE:HD12	2.34	0.47
1:C:48:SER:HA	1:D:281:VAL:HG11	1.96	0.47
1:D:62:THR:CB	1:H:74:VAL:HG22	2.45	0.47
1:E:274:CYS:SG	1:E:276:GLU:HB2	2.54	0.47
1:E:5:ILE:O	1:E:5:ILE:HG23	2.13	0.47
1:G:166:GLY:O	1:G:246:VAL:HA	2.13	0.47
1:H:133:ASN:OD1	1:H:217:VAL:HG12	2.14	0.47
1:C:9:GLY:O	1:C:13:ARG:HG3	2.14	0.47
1:A:280:SER:HG	1:C:203:ILE:H	1.60	0.47
1:E:158:VAL:HG11	1:E:225:LEU:HD11	1.95	0.47
1:F:38:LYS:CE	1:G:193:LEU:HD21	2.44	0.47
1:F:300:MET:HE3	1:H:169:LYS:HD2	1.96	0.47
1:F:279:VAL:HG11	1:H:204:VAL:HG22	1.95	0.47
1:E:193:LEU:HD21	1:H:39:GLN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ASP:HB3	1:H:51:GLY:H	1.79	0.47
2:M:75:THR:C	2:M:76:TYR:HD1	2.18	0.47
2:L:71:ASN:HB2	1:Q:183:ARG:CZ	2.45	0.47
1:A:156:PRO:HB2	1:A:290:THR:CG2	2.41	0.47
1:A:17:ARG:CZ	1:A:53:PHE:HB2	2.44	0.47
1:B:68:GLY:O	1:B:70:ILE:HD12	2.14	0.47
1:D:231:ARG:HH11	1:D:231:ARG:HG3	1.79	0.47
1:B:171:THR:CG2	1:D:306:LYS:HE3	2.44	0.47
1:D:11:ILE:HD11	3:D:401:NAD:N1N	2.29	0.47
1:E:151:THR:HG23	1:E:214:VAL:HG22	1.97	0.47
1:E:218:LEU:C	1:E:220:ASN:H	2.18	0.47
1:F:222:LYS:O	1:F:224:LYS:N	2.47	0.47
1:F:303:ASP:OD1	1:H:169:LYS:NZ	2.48	0.47
1:G:186:ASP:HA	1:G:196:ALA:O	2.14	0.47
1:G:271:LEU:CD1	1:G:292:ILE:HD13	2.29	0.47
1:H:119:THR:O	1:H:120:ALA:HB2	2.14	0.47
2:N:60:LEU:HD23	2:N:60:LEU:C	2.33	0.47
1:O:85:LYS:HB3	1:O:86:GLU:OE1	2.15	0.47
1:B:252:ALA:O	1:B:255:VAL:N	2.47	0.47
1:C:126:PRO:HG2	1:C:141:GLU:HG3	1.96	0.47
1:C:280:SER:HA	1:C:310:TRP:CZ3	2.49	0.47
1:C:324:LEU:O	1:C:328:VAL:HG23	2.15	0.47
1:D:192:ASP:OD2	1:D:195:ARG:HG3	2.14	0.47
1:F:287:ASP:OD1	1:F:319:GLN:NE2	2.37	0.47
1:F:315:TRP:O	1:F:319:GLN:HG2	2.15	0.47
1:F:66:VAL:O	1:F:67:ASP:HB2	2.14	0.47
1:G:123:GLY:O	1:G:125:ILE:N	2.45	0.47
1:H:164:LYS:N	1:H:164:LYS:CD	2.74	0.47
2:K:73:CYS:O	2:K:74:ARG:C	2.52	0.47
1:H:181:ASP:OD1	2:N:76:TYR:CG	2.68	0.47
1:O:320:ARG:NE	1:O:320:ARG:HA	2.29	0.47
1:A:78:ASN:HD22	1:A:81:LEU:HD11	1.80	0.47
1:B:149:CYS:HG	2:J:78:ASN:CG	2.16	0.47
1:C:64:ILE:HG23	1:C:73:VAL:HG21	1.97	0.47
1:D:288:PHE:C	1:D:290:THR:H	2.17	0.47
1:D:57:VAL:O	1:D:57:VAL:HG12	2.14	0.47
1:G:221:LEU:HD21	1:G:225:LEU:CD1	2.44	0.47
1:G:96:THR:OG1	1:G:98:VAL:HG22	2.15	0.47
1:B:326:ASP:O	1:B:330:ASN:OD1	2.33	0.47
1:E:138:SER:C	1:E:140:ASP:H	2.18	0.47
1:E:161:LEU:HD13	1:E:244:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:GLU:OE2	1:E:276:GLU:HA	2.15	0.47
1:F:225:LEU:O	1:F:226:ASN:HB2	2.14	0.47
1:G:208:THR:C	1:G:210:ALA:H	2.18	0.47
1:H:250:THR:OG1	1:H:251:PHE:N	2.47	0.47
1:H:84:TRP:CE3	1:H:89:ILE:HG13	2.49	0.47
2:K:76:TYR:H	1:O:181:ASP:CG	2.17	0.47
1:A:76:ASN:HD22	1:A:76:ASN:C	2.16	0.47
1:C:177:SER:CB	1:C:234:THR:O	2.59	0.47
1:D:105:ALA:O	1:D:108:HIS:HB2	2.15	0.47
1:D:130:VAL:HB	1:D:320:ARG:HD3	1.97	0.47
1:E:80:SER:HB2	1:E:107:LYS:CG	2.45	0.47
1:E:272:ASP:HB2	1:E:288:PHE:CG	2.50	0.47
1:E:10:ARG:N	3:E:401:NAD:O2A	2.44	0.47
1:H:1:LEU:CD1	1:H:90:ASP:CB	2.92	0.47
1:O:281:VAL:CG2	1:Q:202:ASN:ND2	2.75	0.47
1:Q:168:ILE:CD1	1:Q:247:SER:HB3	2.43	0.47
1:Q:289:SER:C	1:Q:290:THR:HG22	2.35	0.47
1:A:62:THR:O	1:A:62:THR:HG23	2.15	0.47
1:C:84:TRP:HB3	1:C:113:ALA:H	1.79	0.47
1:F:109:ILE:H	1:F:109:ILE:HD12	1.79	0.47
1:F:236:ASN:O	1:F:237:VAL:HB	2.14	0.47
1:F:55:ALA:HB1	1:F:67:ASP:OD1	2.15	0.47
1:H:78:ASN:CG	1:H:81:LEU:HD13	2.35	0.47
1:O:172:MET:HE3	1:O:211:ALA:HB2	1.97	0.47
1:A:255:VAL:HG12	1:A:259:PHE:CE2	2.50	0.47
1:B:128:TYR:HE1	1:B:136:ALA:HB3	1.80	0.47
1:C:183:ARG:HH21	1:C:187:ALA:HB1	1.79	0.47
1:C:194:ARG:O	1:C:197:ARG:HG2	2.15	0.47
1:D:271:LEU:C	1:D:271:LEU:HD23	2.36	0.47
1:H:88:GLY:O	1:H:89:ILE:C	2.53	0.47
1:D:150:THR:H	2:I:78:ASN:ND2	2.13	0.47
1:O:79:PRO:HB2	1:O:107:LYS:HB2	1.96	0.47
1:B:236:ASN:C	1:B:237:VAL:HG23	2.35	0.46
1:B:251:PHE:CZ	1:B:254:GLU:HB2	2.50	0.46
1:C:191:ARG:HB2	1:C:191:ARG:HH11	1.80	0.46
1:E:250:THR:HA	1:E:254:GLU:OE1	2.15	0.46
1:E:37:VAL:O	1:E:41:SER:HB2	2.14	0.46
1:F:149:CYS:HB3	3:F:401:NAD:C5N	2.40	0.46
1:F:205:PRO:HA	1:F:230:LEU:HD23	1.97	0.46
1:F:277:PRO:HA	1:H:194:ARG:NE	2.30	0.46
1:O:115:LYS:HG3	1:O:142:PRO:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:137:TYR:HE2	5:Q:527:HOH:O	1.98	0.46
1:A:279:VAL:CG1	1:C:204:VAL:HG22	2.44	0.46
1:A:28:ILE:N	1:A:28:ILE:HD13	2.31	0.46
1:B:168:ILE:HD11	1:B:247:SER:OG	2.14	0.46
1:B:307:VAL:CG1	1:B:308:ILE:N	2.79	0.46
1:B:45:LYS:NZ	1:B:55:ALA:O	2.48	0.46
1:C:146:ASN:HB3	1:C:317:TYR:OH	2.15	0.46
1:C:208:THR:HG22	1:C:228:ILE:HA	1.97	0.46
1:D:169:LYS:NZ	1:D:245:GLN:HE22	2.12	0.46
1:E:2:LYS:O	1:E:90:ASP:HB2	2.15	0.46
1:E:58:LYS:HG3	5:E:503:HOH:O	2.14	0.46
1:F:126:PRO:HG2	1:F:144:ILE:HA	1.97	0.46
1:G:38:LYS:HG3	1:G:39:GLN:N	2.30	0.46
1:G:37:VAL:HG13	1:G:73:VAL:CG1	2.45	0.46
1:G:79:PRO:O	1:G:111:ALA:HB2	2.15	0.46
1:A:0:LYS:H3	1:A:0:LYS:CE	2.25	0.46
1:A:200:ALA:C	1:A:201:LEU:HG	2.36	0.46
1:A:272:ASP:O	1:A:291:THR:HA	2.16	0.46
1:D:106:GLY:C	1:D:108:HIS:N	2.68	0.46
1:D:154:LEU:HD22	1:D:172:MET:HE2	1.97	0.46
1:F:0:LYS:HZ2	1:F:24:PRO:HG3	1.78	0.46
1:F:13:ARG:HH11	1:F:13:ARG:HG3	1.79	0.46
1:F:256:ASN:HD21	1:F:297:THR:CB	2.28	0.46
1:F:27:ILE:N	1:F:27:ILE:CD1	2.78	0.46
1:F:243:VAL:HG22	1:F:306:LYS:HG3	1.96	0.46
1:H:139:HIS:HE1	1:H:332:TRP:CE3	2.34	0.46
1:H:266:GLU:HG2	1:H:267:LEU:N	2.29	0.46
1:A:176:HIS:HB3	1:A:231:ARG:HD3	1.98	0.46
1:E:-1:ALA:HB1	1:E:26:ASP:HB2	1.96	0.46
1:F:166:GLY:O	1:F:246:VAL:HA	2.15	0.46
1:O:183:ARG:HG2	1:O:196:ALA:HA	1.98	0.46
1:B:277:PRO:CB	1:D:194:ARG:HE	2.28	0.46
1:E:236:ASN:CG	1:E:237:VAL:H	2.19	0.46
1:E:279:VAL:HG11	1:G:204:VAL:HG13	1.96	0.46
1:G:194:ARG:HD3	1:G:205:PRO:O	2.15	0.46
1:C:0:LYS:HG2	1:C:0:LYS:O	2.16	0.46
1:D:204:VAL:HA	1:D:205:PRO:HD3	1.74	0.46
1:E:139:HIS:CG	1:E:139:HIS:O	2.68	0.46
1:E:138:SER:O	1:E:140:ASP:N	2.49	0.46
1:E:279:VAL:HG11	1:G:204:VAL:CG2	2.34	0.46
1:E:5:ILE:HG22	1:E:29:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:VAL:O	1:G:130:VAL:C	2.54	0.46
1:H:32:ASP:O	1:H:75:SER:HB2	2.15	0.46
2:N:58:ASP:N	2:N:59:PRO:CD	2.78	0.46
1:Q:43:LEU:HA	1:Q:43:LEU:HD23	1.71	0.46
1:A:171:THR:HG23	1:C:306:LYS:HZ3	1.81	0.46
1:A:2:LYS:HB3	1:A:28:ILE:HD11	1.98	0.46
1:A:277:PRO:O	1:C:194:ARG:HG2	2.15	0.46
1:D:146:ASN:ND2	1:D:321:VAL:CG2	2.78	0.46
1:E:85:LYS:HB2	1:E:112:GLY:CA	2.44	0.46
1:G:162:ASP:C	1:G:164:LYS:H	2.19	0.46
1:H:142:PRO:HG2	1:H:143:ILE:H	1.81	0.46
1:H:232:VAL:O	1:H:234:THR:N	2.41	0.46
1:H:81:LEU:H	1:H:81:LEU:HD12	1.80	0.46
2:I:71:ASN:HA	2:I:74:ARG:CZ	2.44	0.46
1:G:181:ASP:CG	2:M:76:TYR:H	2.18	0.46
1:O:126:PRO:CG	1:O:141:GLU:HG2	2.44	0.46
1:C:187:ALA:O	1:C:196:ALA:HB1	2.16	0.46
1:C:18(B):HIS:C	1:C:20:ARG:H	2.19	0.46
1:C:4:ALA:HB2	1:C:89:ILE:HG12	1.98	0.46
1:D:102:ARG:O	1:D:106:GLY:N	2.41	0.46
1:D:139:HIS:HE1	1:D:332:TRP:CD2	2.34	0.46
1:D:162:ASP:HA	1:D:167:ILE:H	1.81	0.46
1:E:114:LYS:HB2	1:E:332:TRP:HH2	1.81	0.46
1:F:109:ILE:N	1:F:109:ILE:HD12	2.30	0.46
1:H:76:ASN:HB3	1:H:82:LEU:HD23	1.98	0.46
1:H:79:PRO:CG	1:H:99:PHE:HZ	2.26	0.46
2:I:67:ASN:HB3	2:I:70:THR:HG23	1.98	0.46
2:M:71:ASN:OD1	2:M:74:ARG:NH2	2.46	0.46
1:O:171:THR:O	1:O:242:LEU:HD12	2.16	0.46
1:Q:26:ASP:OD1	1:Q:69:LYS:HE2	2.16	0.46
1:A:301:GLY:O	1:A:302:ASP:HB2	2.16	0.46
1:C:271:LEU:HD12	1:C:290:THR:O	2.16	0.46
1:D:133:ASN:ND2	1:D:217:VAL:CA	2.79	0.46
1:D:181:ASP:OD1	1:D:195:ARG:HD3	2.16	0.46
1:D:210:ALA:O	1:D:214:VAL:HG23	2.15	0.46
1:E:221:LEU:HD22	1:E:221:LEU:N	2.30	0.46
1:H:23:SER:C	1:H:25:LEU:H	2.19	0.46
1:H:260:ARG:HG3	1:H:260:ARG:HH11	1.80	0.46
1:H:94:GLU:OE1	1:H:99:PHE:HD2	1.97	0.46
1:O:129:VAL:N	1:O:133:ASN:HD21	2.08	0.46
1:O:179:THR:C	1:O:181:ASP:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:OG1	1:A:251:PHE:N	2.49	0.46
1:B:260:ARG:O	1:B:263:ALA:HB3	2.16	0.46
1:B:281:VAL:CB	1:D:202:ASN:HD21	2.28	0.46
1:C:322:VAL:O	1:C:325:ALA:HB3	2.15	0.46
1:C:333:LYS:HB2	1:C:333:LYS:HZ2	1.80	0.46
1:D:195:ARG:NE	5:D:502:HOH:O	2.48	0.46
1:D:139:HIS:HD2	1:D:333:LYS:HD2	1.81	0.46
1:E:129:VAL:H	1:E:133:ASN:HD21	1.62	0.46
1:E:183:ARG:HG2	1:E:196:ALA:HA	1.97	0.46
1:F:133:ASN:HD22	1:F:133:ASN:H	1.64	0.46
1:F:220:ASN:C	1:F:221:LEU:HD22	2.36	0.46
1:F:64:ILE:HD13	1:F:66:VAL:HG23	1.99	0.46
1:G:211:ALA:CB	1:G:226:ASN:HA	2.38	0.46
1:G:273:VAL:HG13	1:G:292:ILE:O	2.16	0.46
1:H:101:ASP:OD1	1:H:103:GLU:HB3	2.16	0.46
1:H:183:ARG:HG3	1:H:187:ALA:HB3	1.98	0.46
1:H:301:GLY:O	1:H:302:ASP:HB2	2.16	0.46
1:H:55:ALA:O	1:H:56:ASP:CB	2.63	0.46
2:N:70:THR:HG22	2:N:72:GLU:OE2	2.16	0.46
1:B:149:CYS:HB3	3:B:401:NAD:H4N	1.97	0.45
1:C:281:VAL:O	1:C:283:PHE:N	2.49	0.45
1:D:285:CYS:HA	1:D:315:TRP:CD1	2.51	0.45
1:E:119:THR:HG22	1:E:321:VAL:CG1	2.42	0.45
1:E:200:ALA:O	1:E:233:PRO:HB3	2.15	0.45
1:H:85:LYS:CB	1:H:112:GLY:HA3	2.45	0.45
2:L:72:GLU:HB3	1:Q:188:SER:O	2.16	0.45
1:A:146:ASN:HD22	1:A:321:VAL:HG22	1.80	0.45
1:D:94:GLU:OE1	1:D:99:PHE:HD2	1.99	0.45
1:E:168:ILE:HD12	1:E:245:GLN:HG2	1.98	0.45
1:E:270:ILE:O	1:E:270:ILE:CG2	2.65	0.45
1:F:221:LEU:HD22	1:F:221:LEU:N	2.31	0.45
1:G:243:VAL:CG2	1:G:306:LYS:HE2	2.46	0.45
1:A:139:HIS:CD2	1:A:333:LYS:HB3	2.51	0.45
1:A:206:THR:HG23	1:A:229:ALA:HB3	1.97	0.45
1:A:133:ASN:OD1	1:A:217:VAL:HG12	2.17	0.45
1:C:91:ILE:HD11	1:C:93:ILE:HD12	1.98	0.45
1:D:28:ILE:HD13	1:D:28:ILE:H	1.80	0.45
1:E:109:ILE:HG13	1:E:110:GLU:N	2.31	0.45
1:E:177:SER:OG	1:E:237:VAL:O	2.32	0.45
1:E:257:ALA:HA	1:E:260:ARG:HH11	1.82	0.45
1:E:37:VAL:HG23	1:E:38:LYS:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:MET:CB	1:H:226:ASN:HD21	2.29	0.45
1:H:211:ALA:CB	1:H:226:ASN:HA	2.46	0.45
1:O:17:ARG:HD2	1:O:53:PHE:CD1	2.51	0.45
1:Q:175:THR:HB	1:Q:239:VAL:HG12	1.98	0.45
1:B:184:LEU:O	1:B:185:LEU:HD23	2.16	0.45
1:B:232:VAL:O	1:B:234:THR:N	2.40	0.45
1:E:96:THR:HB	1:E:98:VAL:HG22	1.98	0.45
1:F:0:LYS:HD2	1:F:24:PRO:CA	2.46	0.45
1:F:133:ASN:CG	1:F:217:VAL:HG12	2.36	0.45
1:F:206:THR:HG22	1:F:229:ALA:HB3	1.97	0.45
1:H:125:ILE:HD12	1:H:143:ILE:HG22	1.98	0.45
1:F:169:LYS:NZ	1:H:303:ASP:OD1	2.49	0.45
2:I:63:TYR:CE2	2:I:70:THR:HG21	2.52	0.45
1:O:115:LYS:NZ	1:O:137:TYR:OH	2.37	0.45
1:O:255:VAL:O	1:O:258:ALA:HB3	2.16	0.45
1:Q:93:ILE:HG22	1:Q:93:ILE:O	2.16	0.45
1:A:29:ALA:O	1:A:30:ILE:HD13	2.17	0.45
1:B:162:ASP:HA	1:B:167:ILE:H	1.81	0.45
1:B:183:ARG:HG2	1:B:196:ALA:HA	1.99	0.45
1:B:294:SER:C	1:B:296:LEU:H	2.20	0.45
1:D:133:ASN:O	1:D:133:ASN:OD1	2.34	0.45
1:D:21:LYS:H	1:D:21:LYS:HG2	1.60	0.45
1:D:323:ASP:O	1:D:325:ALA:N	2.49	0.45
1:F:285:CYS:O	1:F:315:TRP:CD1	2.69	0.45
1:G:152:ASN:O	1:G:156:PRO:HG2	2.17	0.45
1:H:211:ALA:HB1	1:H:226:ASN:HA	1.98	0.45
2:I:74:ARG:HB2	2:I:74:ARG:HH21	1.80	0.45
2:L:57:SER:HB2	2:L:59:PRO:HD3	1.98	0.45
1:A:215:ALA:HB2	1:A:222:LYS:HA	1.98	0.45
1:B:28:ILE:HD11	1:B:89:ILE:CD1	2.47	0.45
1:D:172:MET:HG2	1:D:173:THR:N	2.31	0.45
1:D:32:ASP:OD1	3:D:401:NAD:H1B	2.16	0.45
1:D:38:LYS:C	1:D:40:ALA:H	2.19	0.45
1:E:10:ARG:HH21	1:E:314:GLU:CD	2.20	0.45
1:F:260:ARG:O	1:F:264:GLU:OE2	2.35	0.45
1:G:173:THR:OG1	1:G:228:ILE:HD11	2.17	0.45
1:G:187:ALA:O	1:G:196:ALA:HB1	2.17	0.45
1:H:32:ASP:HA	3:H:401:NAD:N3A	2.32	0.45
1:D:62:THR:HG22	1:H:62:THR:CG2	2.47	0.45
1:D:62:THR:HB	1:H:74:VAL:HG22	1.97	0.45
2:J:73:CYS:O	2:J:74:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:69:GLU:CD	1:O:77:ARG:NH2	2.68	0.45
1:B:281:VAL:HG12	1:D:202:ASN:ND2	2.28	0.45
1:C:91:ILE:HA	1:C:115:LYS:O	2.17	0.45
1:D:162:ASP:HB2	1:D:167:ILE:HD12	1.99	0.45
1:D:165:PHE:HA	1:D:248:LYS:HB3	1.98	0.45
1:D:260:ARG:NH2	4:D:402:SO4:O3	2.48	0.45
1:E:-1:ALA:CB	1:E:26:ASP:HB2	2.46	0.45
1:F:119:THR:O	1:F:120:ALA:HB2	2.17	0.45
1:F:144:ILE:C	1:F:144:ILE:CD1	2.85	0.45
1:F:272:ASP:OD1	1:F:273:VAL:N	2.49	0.45
1:H:163:GLN:CB	1:H:164:LYS:HD2	2.47	0.45
1:H:79:PRO:O	1:H:80:SER:C	2.55	0.45
2:L:59:PRO:C	2:L:61:GLU:H	2.20	0.45
1:A:37:VAL:HG21	1:A:63:ALA:N	2.24	0.45
1:B:152:ASN:HD22	1:B:320:ARG:HG3	1.81	0.45
1:D:218:LEU:HB3	1:D:221:LEU:HD23	1.97	0.45
1:E:114:LYS:HB2	1:E:332:TRP:CH2	2.52	0.45
1:E:90:ASP:O	1:E:114:LYS:HB2	2.16	0.45
1:H:330:ASN:N	1:H:330:ASN:HD22	2.15	0.45
1:B:162:ASP:HA	1:B:167:ILE:HG13	1.99	0.45
1:D:195:ARG:NH1	2:I:75:THR:HG23	2.32	0.45
1:D:54:ASP:O	1:D:55:ALA:CB	2.63	0.45
1:E:151:THR:HG23	1:E:214:VAL:CG2	2.47	0.45
1:E:217:VAL:O	1:E:218:LEU:HD23	2.16	0.45
1:E:178:TYR:CE1	1:E:235:PRO:HA	2.52	0.45
1:E:267:LEU:CD1	1:E:271:LEU:HD13	2.44	0.45
1:E:28:ILE:HA	1:E:71:ILE:CD1	2.40	0.45
1:F:10:ARG:NH1	1:G:186:ASP:HB2	2.32	0.45
1:F:98:VAL:HG23	1:F:99:PHE:CD2	2.52	0.45
1:G:162:ASP:O	1:G:164:LYS:N	2.49	0.45
1:G:16:LEU:C	1:G:16:LEU:HD23	2.37	0.45
1:H:163:GLN:HB3	1:H:164:LYS:HD2	1.99	0.45
1:H:307:VAL:C	1:H:308:ILE:HD13	2.37	0.45
1:H:79:PRO:HG2	1:H:99:PHE:CE1	2.52	0.45
2:K:74:ARG:HA	5:K:115:HOH:O	2.16	0.45
2:K:76:TYR:CD2	2:K:76:TYR:N	2.83	0.45
2:K:78:ASN:HB3	1:O:150:THR:OG1	2.17	0.45
1:O:98:VAL:HG23	1:O:99:PHE:CD2	2.52	0.45
1:Q:32:ASP:O	1:Q:34:GLY:N	2.50	0.45
1:A:281:VAL:HG11	1:B:48:SER:HA	1.99	0.45
1:B:20:ARG:NH1	1:B:20:ARG:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG23	1:B:311:TYR:CE1	2.52	0.45
1:E:108:HIS:HB2	1:E:116:VAL:HG21	1.97	0.45
1:E:153:CYS:O	1:E:156:PRO:HD2	2.17	0.45
1:E:46:TYR:HD1	1:E:52:ILE:HG22	1.82	0.45
1:F:294:SER:C	1:F:296:LEU:H	2.20	0.45
1:G:262:SER:C	1:G:267:LEU:HB2	2.37	0.45
2:L:55:ASP:OD2	2:L:55:ASP:N	2.49	0.45
1:O:194:ARG:CZ	1:Q:277:PRO:HA	2.47	0.45
1:O:224:LYS:O	1:O:225:LEU:HD23	2.17	0.45
1:D:141:GLU:OE1	1:D:141:GLU:HA	2.17	0.44
1:D:169:LYS:HZ1	1:D:245:GLN:HE22	1.64	0.44
1:F:138:SER:O	1:F:141:GLU:OE1	2.35	0.44
1:G:179:THR:O	1:G:181:ASP:N	2.50	0.44
1:H:179:THR:O	1:H:181:ASP:N	2.50	0.44
1:F:277:PRO:HG2	1:H:193:LEU:HD12	1.99	0.44
1:H:168:ILE:HG21	1:H:245:GLN:OE1	2.17	0.44
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.99	0.44
1:B:197:ARG:NH1	1:B:197:ARG:HG3	2.32	0.44
1:B:30:ILE:HG22	1:B:31:ASN:N	2.31	0.44
1:C:18(A):TRP:CE2	1:C:27:ILE:HD13	2.51	0.44
1:C:191:ARG:HG3	1:C:192:ASP:N	2.31	0.44
1:D:106:GLY:O	1:D:108:HIS:N	2.50	0.44
1:F:161:LEU:O	1:F:165:PHE:HB2	2.17	0.44
1:G:167:ILE:HD12	1:G:244:VAL:HG21	1.99	0.44
1:O:251:PHE:CE2	1:O:253:GLU:HB2	2.51	0.44
1:A:193:LEU:HG	5:A:509:HOH:O	2.18	0.44
1:A:37:VAL:HG13	1:A:64:ILE:CG2	2.46	0.44
1:D:151:THR:OG1	1:D:210:ALA:HA	2.18	0.44
1:E:118:ILE:HD12	1:E:118:ILE:N	2.32	0.44
1:E:5:ILE:HD13	1:E:6:ASN:N	2.33	0.44
1:F:132:VAL:HG11	1:F:218:LEU:HG	1.99	0.44
1:F:16:LEU:CD2	1:F:44:LEU:HD21	2.48	0.44
1:G:221:LEU:O	1:G:221:LEU:HG	2.17	0.44
1:O:70:ILE:HD12	1:O:70:ILE:N	2.33	0.44
1:A:16:LEU:HD23	1:A:16:LEU:C	2.38	0.44
1:B:73:VAL:O	1:B:73:VAL:HG12	2.16	0.44
1:E:172:MET:HA	1:E:242:LEU:HA	1.99	0.44
1:E:243:VAL:HG21	1:G:171:THR:HG21	1.99	0.44
1:E:161:LEU:HD21	1:E:305:VAL:HG11	1.98	0.44
1:G:98:VAL:HG23	1:G:99:PHE:CD2	2.51	0.44
1:H:9:GLY:N	3:H:401:NAD:H4B	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:4:ALA:HB2	1:Q:89:ILE:CG1	2.40	0.44
1:D:109:ILE:HG13	1:D:110:GLU:N	2.32	0.44
1:D:17:ARG:NH1	1:D:53:PHE:HB2	2.33	0.44
1:D:214:VAL:HB	1:D:225:LEU:HD12	1.99	0.44
1:D:79:PRO:HG3	1:D:99:PHE:CE2	2.52	0.44
1:E:79:PRO:HB3	1:E:108:HIS:ND1	2.33	0.44
1:E:179:THR:O	1:E:181:ASP:N	2.50	0.44
1:H:167:ILE:HD12	1:H:221:LEU:HD11	1.99	0.44
1:H:224:LYS:O	1:H:225:LEU:HD23	2.18	0.44
1:H:153:CYS:HA	1:H:289:SER:O	2.17	0.44
2:L:57:SER:C	2:L:59:PRO:HD3	2.37	0.44
1:Q:284:ARG:O	1:Q:285:CYS:HB2	2.18	0.44
1:Q:98:VAL:HG23	1:Q:99:PHE:CD2	2.53	0.44
1:A:226:ASN:ND2	1:C:300:MET:HB2	2.32	0.44
1:D:215:ALA:HB1	1:D:222:LYS:HD2	2.00	0.44
1:D:71:ILE:O	1:D:72:GLN:C	2.56	0.44
1:E:115:LYS:HD3	1:E:328:VAL:CG1	2.48	0.44
1:E:125:ILE:HG23	1:E:143:ILE:O	2.16	0.44
1:H:44:LEU:HB3	1:H:57:VAL:HG11	1.98	0.44
1:B:52:ILE:CD1	1:B:52:ILE:N	2.80	0.44
1:C:167:ILE:HG23	1:C:244:VAL:HB	2.00	0.44
1:C:174:THR:HA	1:C:240:VAL:HA	2.00	0.44
1:C:281:VAL:O	1:C:284:ARG:HG2	2.16	0.44
1:D:201:LEU:HD23	1:D:201:LEU:N	2.33	0.44
1:D:204:VAL:HB	1:D:231:ARG:HB2	1.99	0.44
1:E:39:GLN:NE2	1:E:39:GLN:N	2.65	0.44
1:F:178:TYR:CD1	1:F:178:TYR:C	2.91	0.44
1:G:101:ASP:O	1:G:104:GLY:N	2.50	0.44
1:H:135:ASP:C	1:H:137:TYR:H	2.20	0.44
1:H:99:PHE:HB3	1:H:105:ALA:HB2	1.98	0.44
2:N:68:PRO:O	2:N:73:CYS:HB2	2.16	0.44
2:K:74:ARG:O	1:O:181:ASP:OD1	2.35	0.44
1:O:86:GLU:H	1:O:86:GLU:CD	2.18	0.44
1:A:28:ILE:C	1:A:71:ILE:HG13	2.38	0.44
1:B:114:LYS:HB2	1:B:114:LYS:HZ2	1.83	0.44
1:C:87:LEU:HD12	1:C:89:ILE:HD11	2.00	0.44
1:D:293:ASP:HB3	1:D:296:LEU:HD12	2.00	0.44
1:D:249:LYS:CD	1:D:302:ASP:HB3	2.41	0.44
1:D:39:GLN:O	1:D:43:LEU:HD12	2.18	0.44
1:D:75:SER:HB3	1:H:61:GLU:HB2	2.00	0.44
1:E:194:ARG:HE	1:G:277:PRO:C	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:VAL:CG2	1:E:240:VAL:N	2.80	0.44
1:E:280:SER:HB3	1:G:202:ASN:CB	2.48	0.44
1:F:27:ILE:C	1:F:28:ILE:HD12	2.38	0.44
1:Q:287:ASP:OD1	1:Q:315:TRP:NE1	2.42	0.44
1:A:172:MET:HE1	1:A:210:ALA:HB3	2.00	0.44
1:A:300:MET:HG3	1:C:169:LYS:HB2	1.99	0.44
1:B:220:ASN:C	1:B:222:LYS:H	2.20	0.44
1:B:50:LEU:HA	1:B:284:ARG:NH2	2.33	0.44
1:C:16:LEU:HD23	1:C:18(A):TRP:HE3	1.81	0.44
1:D:191:ARG:HA	2:I:60:LEU:HD23	1.99	0.44
1:D:250:THR:O	1:D:302:ASP:O	2.35	0.44
1:E:132:VAL:HG11	1:E:217:VAL:CB	2.48	0.44
1:E:194:ARG:HH12	1:G:296:LEU:HD21	1.83	0.44
1:E:129:VAL:HG21	1:E:217:VAL:HG11	2.00	0.44
1:E:58:LYS:HB3	1:E:58:LYS:HZ3	1.83	0.44
1:F:62:THR:O	1:F:63:ALA:HB2	2.17	0.44
1:E:300:MET:O	1:G:169:LYS:HE2	2.17	0.44
2:L:59:PRO:C	2:L:61:GLU:N	2.71	0.44
1:O:89:ILE:O	1:O:113:ALA:HA	2.18	0.44
1:B:91:ILE:HD11	1:B:117:ILE:HG21	2.00	0.43
1:B:129:VAL:H	1:B:133:ASN:HD21	1.66	0.43
1:C:206:THR:HG22	1:C:229:ALA:HB3	2.01	0.43
1:E:214:VAL:HG12	1:E:214:VAL:O	2.17	0.43
1:H:211:ALA:HB1	1:H:226:ASN:CA	2.48	0.43
1:H:191:ARG:CD	2:N:73:CYS:HA	2.48	0.43
1:C:21:LYS:O	1:C:21:LYS:HG2	2.18	0.43
1:F:1:LEU:HD22	1:F:329:ALA:HB1	2.00	0.43
1:F:167:ILE:HG21	1:F:221:LEU:HD11	2.00	0.43
1:G:162:ASP:HB2	1:G:167:ILE:HG12	2.00	0.43
1:G:173:THR:HG23	1:G:228:ILE:HD12	2.00	0.43
1:G:280:SER:O	1:G:282:ASP:N	2.51	0.43
1:A:109:ILE:CD1	1:A:116:VAL:HG23	2.48	0.43
1:A:200:ALA:O	1:A:201:LEU:HG	2.18	0.43
1:C:228:ILE:HD13	1:C:228:ILE:N	2.33	0.43
1:D:116:VAL:HG12	1:D:117:ILE:H	1.82	0.43
1:E:183:ARG:HH22	2:N:74:ARG:NH1	2.15	0.43
1:E:18:CYS:SG	1:E:319:GLN:OE1	2.76	0.43
1:F:105:ALA:HB1	1:F:143:ILE:HD12	2.00	0.43
1:G:262:SER:HA	1:G:266:GLU:OE2	2.18	0.43
1:E:204:VAL:HG22	1:G:279:VAL:CG1	2.49	0.43
1:G:37:VAL:HG13	1:G:73:VAL:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:ARG:HG2	1:H:53:PHE:HE1	1.81	0.43
1:Q:1:LEU:HD12	1:Q:1:LEU:HA	1.87	0.43
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.83	0.43
1:D:211:ALA:CB	1:D:226:ASN:HA	2.48	0.43
1:D:307:VAL:C	1:D:308:ILE:HD12	2.38	0.43
1:F:1:LEU:N	1:F:1:LEU:CD1	2.81	0.43
1:G:154:LEU:HD21	1:G:172:MET:HG3	1.99	0.43
1:G:158:VAL:HG11	1:G:221:LEU:HD22	1.98	0.43
1:G:176:HIS:HA	1:G:238:SER:OG	2.18	0.43
1:G:267:LEU:HD23	1:G:267:LEU:HA	1.82	0.43
1:F:193:LEU:HD21	1:G:39:GLN:HG2	2.00	0.43
1:G:57:VAL:HA	1:G:65:SER:O	2.18	0.43
1:H:204:VAL:HB	1:H:231:ARG:HB2	2.00	0.43
1:H:3:VAL:HG22	1:H:4:ALA:N	2.33	0.43
1:H:79:PRO:HG3	1:H:99:PHE:HZ	1.83	0.43
1:A:109:ILE:C	1:A:111:ALA:N	2.72	0.43
1:A:125:ILE:CG2	1:A:143:ILE:HG22	2.47	0.43
1:A:149:CYS:HB3	3:A:401:NAD:H4N	2.00	0.43
1:B:195:ARG:NH1	2:J:76:TYR:H	2.16	0.43
1:B:194:ARG:HD2	1:B:205:PRO:HD2	2.00	0.43
1:B:84:TRP:CE3	1:B:84:TRP:HA	2.53	0.43
1:C:177:SER:OG	1:C:237:VAL:O	2.28	0.43
1:D:23:SER:OG	1:D:24:PRO:HD2	2.18	0.43
1:E:153:CYS:O	1:E:290:THR:CG2	2.66	0.43
1:E:20:ARG:HH12	1:E:322:VAL:HG12	1.82	0.43
1:E:161:LEU:HD13	1:E:244:VAL:CG2	2.49	0.43
1:F:91:ILE:HD11	1:F:117:ILE:HD12	2.00	0.43
1:F:128:TYR:HA	1:F:133:ASN:ND2	2.34	0.43
1:F:206:THR:CG2	1:F:229:ALA:HB3	2.48	0.43
2:I:76:TYR:CD1	2:I:76:TYR:N	2.85	0.43
1:Q:110:GLU:C	1:Q:112:GLY:N	2.71	0.43
1:Q:159:LYS:O	1:Q:163:GLN:HG3	2.17	0.43
1:Q:191:ARG:HG3	1:Q:191:ARG:NH1	2.32	0.43
1:Q:211:ALA:HB1	1:Q:226:ASN:HA	2.01	0.43
1:A:184:LEU:HG	1:A:185:LEU:CD1	2.43	0.43
1:B:8:PHE:CE1	1:B:16:LEU:HD12	2.53	0.43
1:D:191:ARG:HH22	2:I:61:GLU:HB3	1.82	0.43
1:F:107:LYS:HA	1:F:110:GLU:CG	2.49	0.43
1:F:232:VAL:HG11	1:H:232:VAL:HG11	2.00	0.43
1:H:17:ARG:HD3	1:H:50:LEU:CD1	2.49	0.43
1:F:226:ASN:HB3	1:H:300:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:ILE:HD12	1:O:27:ILE:N	2.33	0.43
1:A:124:ASP:HB3	4:A:406:SO4:O2	2.18	0.43
1:B:198:ALA:CB	1:B:201:LEU:HD12	2.48	0.43
1:B:31:ASN:HB2	1:B:74:VAL:HG22	2.00	0.43
1:B:50:LEU:HD23	1:B:284:ARG:HH22	1.83	0.43
1:A:281:VAL:HG12	1:C:202:ASN:HD21	1.83	0.43
1:E:167:ILE:HG23	1:E:244:VAL:HB	2.00	0.43
1:E:239:VAL:HG23	1:E:309:ALA:O	2.18	0.43
1:E:30:ILE:HG13	1:E:71:ILE:CG2	2.48	0.43
1:E:39:GLN:H	1:E:39:GLN:NE2	2.16	0.43
1:E:4:ALA:HB3	1:E:92:VAL:HG22	1.99	0.43
1:E:96:THR:CB	1:E:98:VAL:HG22	2.49	0.43
1:H:29:ALA:C	1:H:30:ILE:HG13	2.38	0.43
1:H:328:VAL:O	1:H:332:TRP:HB2	2.19	0.43
1:H:69:LYS:HE2	1:H:70:ILE:HD13	1.99	0.43
2:M:70:THR:HG22	2:M:71:ASN:H	1.82	0.43
1:D:153:CYS:HA	1:D:289:SER:O	2.18	0.43
1:D:266:GLU:HG2	1:D:267:LEU:HG	2.01	0.43
1:E:169:LYS:HB2	1:E:169:LYS:HE2	1.73	0.43
1:E:37:VAL:O	1:E:41:SER:CB	2.67	0.43
1:F:152:ASN:ND2	1:F:317:TYR:CE1	2.87	0.43
1:F:159:LYS:O	1:F:163:GLN:HG3	2.19	0.43
1:F:190:HIS:CB	1:F:196:ALA:HB2	2.44	0.43
1:F:78:ASN:OD1	1:F:80:SER:HB2	2.19	0.43
1:G:132:VAL:C	1:G:134:ALA:H	2.22	0.43
1:G:160:VAL:O	1:G:164:LYS:HB3	2.19	0.43
1:E:300:MET:CB	1:G:169:LYS:HD3	2.49	0.43
1:G:182:GLN:HB3	1:G:199:ALA:HB2	2.01	0.43
1:G:214:VAL:CG1	1:G:218:LEU:HD12	2.49	0.43
1:G:146:ASN:OD1	1:G:324:LEU:HD22	2.19	0.43
1:E:193:LEU:HD22	1:H:42:HIS:HB3	2.00	0.43
1:H:8:PHE:CE2	1:H:13:ARG:HG2	2.53	0.43
1:O:15:PHE:O	1:O:18:CYS:HB2	2.19	0.43
1:Q:139:HIS:C	1:Q:141:GLU:H	2.20	0.43
1:A:129:VAL:N	1:A:133:ASN:HD21	2.12	0.43
1:A:82:LEU:C	1:A:84:TRP:H	2.22	0.43
1:B:284:ARG:HG2	1:B:284:ARG:HH11	1.83	0.43
1:C:239:VAL:CG2	1:C:308:ILE:HG23	2.49	0.43
1:C:54:ASP:O	1:C:55:ALA:HB2	2.19	0.43
1:D:206:THR:HG21	1:D:231:ARG:NH1	2.34	0.43
1:D:240:VAL:HG13	1:D:311:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:SER:O	1:D:267:LEU:HB2	2.19	0.43
1:E:242:LEU:CD1	1:E:244:VAL:HG13	2.45	0.43
1:E:15:PHE:CE2	1:E:93:ILE:HD13	2.54	0.43
1:F:228:ILE:HG12	1:F:229:ALA:N	2.33	0.43
1:G:174:THR:HG22	1:G:229:ALA:HA	2.01	0.43
1:G:327:ILE:CD1	1:G:327:ILE:N	2.82	0.43
1:H:161:LEU:O	1:H:165:PHE:HB2	2.19	0.43
1:H:29:ALA:HA	1:H:71:ILE:CG2	2.49	0.43
1:O:253:GLU:CD	1:O:253:GLU:N	2.72	0.43
1:A:0:LYS:H1	1:A:0:LYS:HG3	1.67	0.43
1:A:188:SER:HB2	1:D:39:GLN:NE2	2.33	0.43
1:B:202:ASN:O	1:B:233:PRO:HD3	2.19	0.43
1:A:306:LYS:HD2	1:C:171:THR:OG1	2.18	0.43
1:C:317:TYR:O	1:C:320:ARG:HB2	2.19	0.43
1:E:293:ASP:OD1	1:E:296:LEU:HG	2.19	0.43
1:E:45:LYS:O	1:E:52:ILE:HA	2.19	0.43
1:G:162:ASP:CB	1:G:167:ILE:HG12	2.49	0.43
1:G:319:GLN:OE1	1:G:319:GLN:HA	2.18	0.43
1:H:190:HIS:HA	2:N:72:GLU:O	2.19	0.43
1:Q:125:ILE:HA	1:Q:126:PRO:HD3	1.97	0.43
1:Q:261:ASP:O	1:Q:265:LYS:HG3	2.19	0.43
1:A:139:HIS:CE1	1:A:332:TRP:HA	2.54	0.42
1:A:173:THR:HG23	1:A:228:ILE:HD12	2.01	0.42
1:C:1:LEU:CD2	1:C:329:ALA:HA	2.48	0.42
1:E:299:VAL:HG13	1:E:304:MET:C	2.39	0.42
1:F:133:ASN:ND2	1:F:133:ASN:N	2.66	0.42
1:F:152:ASN:HD21	1:F:317:TYR:HE1	1.67	0.42
1:F:250:THR:OG1	1:F:251:PHE:N	2.51	0.42
1:G:125:ILE:HA	1:G:126:PRO:HD3	1.88	0.42
1:H:39:GLN:O	1:H:43:LEU:HG	2.18	0.42
1:B:197:ARG:HH11	1:B:197:ARG:HG3	1.83	0.42
1:B:129:VAL:HG23	1:B:217:VAL:HG11	2.00	0.42
1:B:262:SER:O	1:B:265:LYS:N	2.50	0.42
1:C:263:ALA:O	1:C:268:LYS:HA	2.18	0.42
1:C:281:VAL:C	1:C:283:PHE:N	2.73	0.42
1:E:239:VAL:CG2	1:E:240:VAL:H	2.28	0.42
1:H:82:LEU:HD13	1:H:84:TRP:CZ2	2.53	0.42
2:M:60:LEU:O	2:M:63:TYR:N	2.52	0.42
1:A:139:HIS:CB	1:A:333:LYS:HE2	2.48	0.42
1:C:132:VAL:HG21	1:C:155:ALA:HB1	2.01	0.42
1:A:193:LEU:HD12	1:C:277:PRO:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH2	1:C:282:ASP:OD1	2.44	0.42
1:C:313:ASN:HB2	3:C:401:NAD:O7N	2.18	0.42
1:D:119:THR:O	1:D:120:ALA:HB2	2.19	0.42
1:D:191:ARG:HH12	2:I:61:GLU:HG2	1.83	0.42
1:E:208:THR:HB	1:E:229:ALA:HB2	2.02	0.42
1:F:239:VAL:HG13	1:F:239:VAL:O	2.18	0.42
1:F:173:THR:O	1:F:241:ASP:HB3	2.19	0.42
1:F:60:SER:O	1:F:63:ALA:HB3	2.19	0.42
1:H:3:VAL:O	1:H:28:ILE:HG22	2.18	0.42
1:O:125:ILE:HA	1:O:126:PRO:HD3	1.93	0.42
1:O:251:PHE:O	1:O:254:GLU:HB3	2.19	0.42
1:O:298:MET:CE	1:Q:226:ASN:ND2	2.82	0.42
1:A:9:GLY:O	1:A:13:ARG:HG3	2.20	0.42
1:A:226:ASN:C	1:A:226:ASN:OD1	2.58	0.42
1:A:279:VAL:HG22	1:C:197:ARG:HH12	1.84	0.42
1:B:177:SER:HB3	1:B:234:THR:O	2.20	0.42
1:C:218:LEU:HB3	1:C:221:LEU:HD23	2.02	0.42
1:C:266:GLU:HG2	1:C:267:LEU:H	1.84	0.42
1:D:144:ILE:CD1	1:D:145:SER:N	2.81	0.42
1:D:172:MET:HG2	1:D:173:THR:H	1.84	0.42
1:D:190:HIS:C	2:I:60:LEU:HD21	2.39	0.42
1:D:31:ASN:OD1	1:D:74:VAL:HG23	2.19	0.42
1:C:253:GLU:HG2	1:E:103:GLU:HG3	2.01	0.42
1:E:278:LEU:HD21	1:F:46:TYR:CE2	2.53	0.42
1:F:85:LYS:N	1:F:112:GLY:HA3	2.35	0.42
1:F:134:ALA:C	1:F:136:ALA:H	2.21	0.42
1:F:142:PRO:O	1:F:143:ILE:HD13	2.19	0.42
1:F:222:LYS:NZ	1:F:224:LYS:HE2	2.35	0.42
1:F:280:SER:OG	1:H:202:ASN:CB	2.67	0.42
1:F:34:GLY:HA2	2:M:60:LEU:HB2	2.00	0.42
1:G:154:LEU:HD12	1:G:240:VAL:HG11	2.01	0.42
1:G:252:ALA:O	1:G:255:VAL:HB	2.19	0.42
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.85	0.42
1:H:10:ARG:HB2	3:H:401:NAD:O2N	2.20	0.42
1:H:114:LYS:O	1:H:115:LYS:HG3	2.20	0.42
1:F:202:ASN:ND2	1:H:281:VAL:CG2	2.74	0.42
1:H:32:ASP:O	1:H:75:SER:CB	2.68	0.42
1:B:114:LYS:NZ	1:B:114:LYS:HB2	2.35	0.42
1:C:116:VAL:HG12	1:C:117:ILE:N	2.34	0.42
1:C:9:GLY:HA3	3:C:401:NAD:O5B	2.20	0.42
1:D:181:ASP:OD1	1:D:195:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ILE:HA	1:E:126:PRO:HD3	1.90	0.42
1:F:285:CYS:HA	1:F:315:TRP:CG	2.55	0.42
1:F:63:ALA:HB2	1:F:72:GLN:OE1	2.19	0.42
1:H:90:ASP:HA	1:H:114:LYS:HD2	2.02	0.42
1:H:250:THR:CB	1:H:254:GLU:OE1	2.68	0.42
1:H:79:PRO:O	1:H:82:LEU:HG	2.19	0.42
1:H:8:PHE:CZ	1:H:16:LEU:HD12	2.54	0.42
1:Q:164:LYS:O	1:Q:248:LYS:HD3	2.19	0.42
1:B:234:THR:CG2	1:D:233:PRO:HG2	2.49	0.42
1:C:115:LYS:NZ	1:C:115:LYS:HB2	2.35	0.42
1:B:296:LEU:CD2	1:D:228:ILE:HG21	2.44	0.42
1:D:319:GLN:NE2	1:D:319:GLN:CA	2.81	0.42
1:E:194:ARG:HE	1:G:277:PRO:CB	2.32	0.42
1:F:32:ASP:HA	3:F:401:NAD:C2A	2.50	0.42
1:G:152:ASN:O	1:G:289:SER:HB3	2.20	0.42
1:G:256:ASN:HB3	1:G:260:ARG:HH12	1.84	0.42
1:G:327:ILE:HD12	1:G:327:ILE:N	2.34	0.42
1:H:108:HIS:HB2	1:H:116:VAL:HG21	2.02	0.42
1:H:23:SER:O	1:H:25:LEU:N	2.42	0.42
1:H:280:SER:O	1:H:281:VAL:C	2.58	0.42
1:H:5:ILE:HB	1:H:30:ILE:HG23	2.02	0.42
1:A:324:LEU:O	1:A:327:ILE:HB	2.20	0.42
1:A:39:GLN:CD	1:A:39:GLN:H	2.23	0.42
1:D:155:ALA:H	1:D:156:PRO:CD	2.32	0.42
1:E:137:TYR:CZ	1:E:139:HIS:HA	2.54	0.42
1:E:179:THR:C	1:E:181:ASP:N	2.73	0.42
1:E:62:THR:O	1:E:63:ALA:HB2	2.19	0.42
1:F:31:ASN:HB2	1:F:74:VAL:HG13	2.02	0.42
1:G:171:THR:HG22	1:G:243:VAL:HB	2.00	0.42
3:H:401:NAD:O1A	2:N:76:TYR:OH	2.37	0.42
1:H:41:SER:CB	1:H:59:PRO:HG3	2.50	0.42
1:H:41:SER:HA	1:H:57:VAL:HG12	2.00	0.42
1:O:274:CYS:SG	1:O:278:LEU:HD12	2.60	0.42
1:O:298:MET:HE1	1:Q:226:ASN:CB	2.49	0.42
1:A:5:ILE:HD11	1:A:27:ILE:HD12	2.01	0.42
1:B:253:GLU:H	1:B:253:GLU:CD	2.23	0.42
1:B:84:TRP:HA	1:B:84:TRP:HE3	1.84	0.42
1:C:262:SER:C	1:C:264:GLU:H	2.22	0.42
1:D:183:ARG:HG3	1:D:187:ALA:HB3	2.01	0.42
1:D:316:GLY:O	1:D:319:GLN:HB2	2.19	0.42
1:E:285:CYS:HA	1:E:315:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:ASN:CB	1:G:260:ARG:NH1	2.83	0.42
1:H:150:THR:HG22	1:H:172:MET:HE2	2.01	0.42
1:H:213:ALA:O	1:H:216:LEU:HD13	2.19	0.42
1:H:63:ALA:CB	1:H:72:GLN:HA	2.49	0.42
1:H:3:VAL:HB	1:H:91:ILE:HG22	2.00	0.42
1:O:202:ASN:HD21	1:Q:281:VAL:CB	2.32	0.42
1:O:15:PHE:HA	1:O:318:SER:HB3	2.02	0.42
1:Q:129:VAL:N	1:Q:133:ASN:HD21	2.16	0.42
1:Q:33:THR:HG22	1:Q:77:ARG:HG2	2.01	0.42
1:A:173:THR:HG23	1:A:228:ILE:HD11	2.02	0.42
1:A:185:LEU:O	1:A:187:ALA:N	2.53	0.42
1:B:57:VAL:O	1:B:58:LYS:HB3	2.19	0.42
1:B:70:ILE:HD12	1:B:70:ILE:H	1.81	0.42
1:D:162:ASP:CA	1:D:167:ILE:HG13	2.48	0.42
1:B:202:ASN:ND2	1:D:281:VAL:HG12	2.33	0.42
1:D:78:ASN:HA	1:D:79:PRO:HD3	1.81	0.42
1:D:84:TRP:CE3	1:D:84:TRP:HA	2.55	0.42
1:F:178:TYR:CD1	1:F:178:TYR:O	2.73	0.42
1:F:301:GLY:O	1:F:302:ASP:HB2	2.18	0.42
1:F:56:ASP:HB2	1:F:67:ASP:HA	2.01	0.42
1:G:256:ASN:HB3	1:G:260:ARG:NH1	2.35	0.42
1:H:32:ASP:HA	3:H:401:NAD:C2A	2.50	0.42
1:Q:79:PRO:HB2	1:Q:107:LYS:HB2	2.01	0.42
1:A:1:LEU:HD21	1:A:332:TRP:CE3	2.55	0.42
1:B:271:LEU:HD22	1:B:290:THR:HG23	2.02	0.42
1:C:27:ILE:HG21	1:C:71:ILE:HD13	2.02	0.42
1:D:157:PHE:O	1:D:161:LEU:HG	2.20	0.42
1:D:280:SER:HB3	1:D:310:TRP:HZ3	1.84	0.42
1:E:139:HIS:HB3	5:E:531:HOH:O	2.19	0.42
1:G:18(A):TRP:HH2	1:G:69:LYS:HE2	1.84	0.42
1:F:300:MET:HE1	1:H:169:LYS:HB2	2.02	0.42
1:H:25:LEU:HD12	1:H:25:LEU:N	2.35	0.42
2:N:70:THR:HG22	2:N:72:GLU:HG2	2.02	0.42
1:Q:18(A):TRP:CD2	1:Q:27:ILE:HG12	2.55	0.42
1:A:301:GLY:O	1:A:302:ASP:CB	2.67	0.41
1:A:60:SER:O	1:A:63:ALA:HB3	2.20	0.41
1:C:218:LEU:O	1:C:221:LEU:HB2	2.20	0.41
1:C:24:PRO:HD2	1:C:25:LEU:HG	2.01	0.41
1:C:27:ILE:O	1:C:71:ILE:HG12	2.20	0.41
1:D:1:LEU:HD23	1:D:91:ILE:HD12	2.01	0.41
1:D:255:VAL:HG11	1:D:305:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:PRO:HD2	1:E:143:ILE:O	2.20	0.41
1:E:280:SER:O	1:E:282:ASP:N	2.53	0.41
1:F:227:GLY:HA2	1:H:298:MET:HE3	2.02	0.41
1:H:141:GLU:OE1	1:H:141:GLU:HA	2.20	0.41
1:H:250:THR:OG1	1:H:254:GLU:OE1	2.38	0.41
1:H:315:TRP:CD1	1:H:315:TRP:C	2.93	0.41
1:H:52:ILE:HD12	1:H:52:ILE:N	2.34	0.41
1:O:172:MET:O	1:O:227:GLY:HA2	2.20	0.41
1:O:76:ASN:HD21	1:O:81:LEU:HB2	1.85	0.41
1:Q:32:ASP:OD2	3:Q:401:NAD:H1B	2.20	0.41
1:B:163:GLN:C	1:B:163:GLN:CD	2.78	0.41
1:C:84:TRP:CE3	1:C:84:TRP:CA	3.02	0.41
1:E:101:ASP:OD2	1:E:103:GLU:HB3	2.20	0.41
1:E:236:ASN:CG	1:E:237:VAL:N	2.74	0.41
1:E:284:ARG:O	1:E:285:CYS:HB2	2.20	0.41
1:F:277:PRO:HG3	1:H:193:LEU:HD12	2.00	0.41
1:H:15:PHE:HE1	1:H:321:VAL:HG12	1.85	0.41
1:D:62:THR:HG21	1:H:74:VAL:HA	2.02	0.41
2:N:70:THR:CG2	2:N:72:GLU:HG2	2.50	0.41
1:O:157:PHE:HD2	1:O:290:THR:HG21	1.85	0.41
1:Q:154:LEU:HD12	1:Q:157:PHE:CZ	2.55	0.41
1:A:300:MET:HE3	1:C:226:ASN:HD22	1.79	0.41
1:C:253:GLU:HG3	4:C:404:SO4:O2	2.20	0.41
1:D:125:ILE:HD11	1:D:143:ILE:CG2	2.50	0.41
1:D:133:ASN:C	1:D:135:ASP:N	2.73	0.41
1:D:261:ASP:C	1:D:263:ALA:N	2.73	0.41
1:D:252:ALA:HA	1:D:299:VAL:HG23	2.01	0.41
1:E:109:ILE:N	1:E:113:ALA:HB3	2.35	0.41
1:E:146:ASN:HB3	1:E:317:TYR:OH	2.20	0.41
1:E:198:ALA:CB	1:E:201:LEU:HD11	2.50	0.41
1:F:101:ASP:O	1:F:102:ARG:C	2.59	0.41
1:F:138:SER:OG	1:F:140:ASP:OD1	2.36	0.41
1:F:164:LYS:O	1:F:165:PHE:CG	2.74	0.41
1:F:85:LYS:HB2	1:F:85:LYS:HE3	1.72	0.41
1:G:236:ASN:O	1:G:237:VAL:HB	2.20	0.41
1:H:32:ASP:O	1:H:75:SER:OG	2.38	0.41
1:H:45:LYS:HG3	1:H:45:LYS:O	2.20	0.41
1:Q:172:MET:CE	1:Q:211:ALA:HB2	2.50	0.41
1:A:5:ILE:HD11	1:A:27:ILE:CD1	2.50	0.41
1:B:139:HIS:CB	1:B:333:LYS:HG3	2.47	0.41
1:D:191:ARG:CZ	2:I:61:GLU:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ARG:O	1:D:285:CYS:HB2	2.21	0.41
1:E:15:PHE:CD1	1:E:322:VAL:HG22	2.54	0.41
1:E:204:VAL:HG22	1:G:279:VAL:HG11	2.02	0.41
1:E:76:ASN:HB3	1:E:82:LEU:CD2	2.51	0.41
1:F:165:PHE:HE1	1:F:250:THR:HB	1.84	0.41
1:F:254:GLU:O	1:F:257:ALA:HB3	2.18	0.41
1:G:84:TRP:CE3	1:G:84:TRP:HA	2.56	0.41
1:H:152:ASN:O	1:H:289:SER:HB3	2.19	0.41
1:H:17:ARG:NE	1:H:53:PHE:CD1	2.87	0.41
1:H:269:GLY:HA2	1:H:288:PHE:CE2	2.44	0.41
1:H:41:SER:HA	1:H:57:VAL:CG1	2.50	0.41
1:O:96:THR:OG1	1:O:98:VAL:HG22	2.20	0.41
1:Q:176:HIS:HA	1:Q:238:SER:OG	2.21	0.41
1:A:104:GLY:O	1:A:106:GLY:N	2.53	0.41
1:B:318:SER:O	1:B:322:VAL:HG23	2.19	0.41
1:C:266:GLU:C	1:C:268:LYS:H	2.22	0.41
1:C:47:ASP:C	1:C:49:THR:H	2.24	0.41
1:D:84:TRP:HA	1:D:84:TRP:HE3	1.84	0.41
1:F:170:GLY:HA3	1:F:244:VAL:HG12	2.03	0.41
1:F:3:VAL:CG1	1:F:4:ALA:N	2.83	0.41
1:G:109:ILE:CD1	1:G:116:VAL:HG23	2.50	0.41
1:G:214:VAL:HG12	1:G:218:LEU:HD12	2.02	0.41
1:H:108:HIS:C	1:H:110:GLU:N	2.74	0.41
1:H:57:VAL:O	1:H:57:VAL:HG12	2.20	0.41
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.55	0.41
1:Q:211:ALA:CB	1:Q:226:ASN:HA	2.50	0.41
1:B:120:ALA:O	1:B:145:SER:OG	2.35	0.41
1:B:8:PHE:CZ	1:B:16:LEU:HD12	2.56	0.41
1:D:29:ALA:HA	1:D:72:GLN:O	2.21	0.41
1:E:327:ILE:C	1:E:329:ALA:N	2.73	0.41
1:F:139:HIS:HD2	1:F:333:LYS:HD2	1.83	0.41
1:F:197:ARG:HH21	1:G:48:SER:N	2.19	0.41
1:G:313:ASN:HB2	3:G:401:NAD:O7N	2.19	0.41
1:H:173:THR:O	1:H:241:ASP:HB3	2.20	0.41
2:I:67:ASN:HB3	2:I:70:THR:CG2	2.50	0.41
1:B:195:ARG:CZ	2:J:75:THR:HG23	2.50	0.41
1:O:284:ARG:O	1:O:285:CYS:HB2	2.19	0.41
1:O:298:MET:CE	1:Q:226:ASN:HB3	2.50	0.41
1:A:68:GLY:O	1:A:69:LYS:C	2.58	0.41
1:A:31:ASN:OD1	1:A:74:VAL:HG23	2.20	0.41
1:D:252:ALA:HA	1:D:299:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:TYR:HD1	1:F:178:TYR:C	2.23	0.41
1:F:222:LYS:O	1:F:224:LYS:HG3	2.21	0.41
1:F:38:LYS:HE3	1:G:193:LEU:HD21	2.02	0.41
1:G:278:LEU:HD22	1:H:46:TYR:CD1	2.56	0.41
1:H:129:VAL:H	1:H:133:ASN:HD21	1.68	0.41
1:H:294:SER:C	1:H:296:LEU:H	2.23	0.41
1:H:293:ASP:CB	1:H:296:LEU:HD12	2.43	0.41
1:H:59:PRO:HA	1:H:64:ILE:HG22	2.03	0.41
1:H:63:ALA:HA	1:H:73:VAL:HG23	2.03	0.41
1:A:70:ILE:CG2	1:A:71:ILE:N	2.83	0.41
1:B:109:ILE:HG23	1:B:113:ALA:O	2.21	0.41
1:B:182:GLN:OE1	1:B:231:ARG:NH1	2.54	0.41
1:C:117:ILE:HD11	1:C:328:VAL:HG21	2.02	0.41
1:C:69:LYS:HE2	5:C:521:HOH:O	2.20	0.41
1:D:105:ALA:CB	1:D:118:ILE:HD11	2.50	0.41
1:E:116:VAL:HB	1:E:143:ILE:CD1	2.50	0.41
1:E:13:ARG:HG3	1:E:13:ARG:HH11	1.85	0.41
1:E:193:LEU:HD13	1:H:42:HIS:CG	2.56	0.41
1:Q:333:LYS:HA	1:Q:333:LYS:HD3	1.77	0.41
1:Q:37:VAL:CG2	1:Q:73:VAL:HB	2.50	0.41
1:B:221:LEU:H	1:B:221:LEU:CD2	2.34	0.41
1:B:252:ALA:O	1:B:254:GLU:N	2.53	0.41
1:D:151:THR:C	1:D:153:CYS:H	2.25	0.41
1:D:296:LEU:HD12	1:D:308:ILE:CG2	2.51	0.41
1:E:255:VAL:HG21	1:E:299:VAL:HG21	2.03	0.41
1:E:54:ASP:O	1:E:55:ALA:HB2	2.21	0.41
1:F:132:VAL:C	1:F:134:ALA:H	2.24	0.41
1:G:25:LEU:H	1:G:25:LEU:HG	1.62	0.41
1:G:284:ARG:O	1:G:285:CYS:HB2	2.21	0.41
1:D:62:THR:HG1	1:H:74:VAL:HG13	1.76	0.41
1:H:190:HIS:HA	2:N:72:GLU:CA	2.51	0.41
1:B:156:PRO:HB2	1:B:290:THR:HG21	2.03	0.41
1:C:320:ARG:HG2	1:C:320:ARG:NH1	2.36	0.41
1:E:119:THR:HB	1:E:317:TYR:HE2	1.86	0.41
1:E:65:SER:CB	1:E:70:ILE:HG22	2.51	0.41
1:F:133:ASN:ND2	1:F:133:ASN:H	2.19	0.41
1:F:210:ALA:CA	1:F:213:ALA:HB3	2.48	0.41
1:F:64:ILE:HD12	1:F:64:ILE:C	2.40	0.41
1:G:168:ILE:O	1:G:224:LYS:HD3	2.21	0.41
1:D:191:ARG:NH2	2:I:61:GLU:HG2	2.36	0.41
1:Q:85:LYS:HB2	1:Q:112:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:234:THR:HG21	1:Q:203:ILE:HG13	2.02	0.41
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.55	0.41
1:A:101:ASP:OD2	1:A:103:GLU:HB3	2.20	0.41
1:A:125:ILE:HG22	1:A:144:ILE:HA	2.01	0.41
1:B:162:ASP:CA	1:B:167:ILE:HG13	2.51	0.41
1:C:262:SER:C	1:C:264:GLU:N	2.74	0.41
1:D:121:PRO:HG3	1:D:148:SER:HB3	2.02	0.41
1:A:43:LEU:HD11	1:D:187:ALA:O	2.21	0.41
1:E:6:ASN:ND2	1:E:108:HIS:CE1	2.89	0.41
1:E:66:VAL:C	1:E:68:GLY:H	2.25	0.41
1:F:37:VAL:HA	1:F:73:VAL:HG11	2.03	0.41
1:H:157:PHE:HE1	1:H:242:LEU:HD23	1.85	0.41
1:H:229:ALA:O	1:H:230:LEU:HD23	2.20	0.41
1:H:3:VAL:CG2	1:H:4:ALA:N	2.84	0.41
1:H:50:LEU:HD21	5:H:503:HOH:O	2.20	0.41
1:O:236:ASN:O	1:O:237:VAL:HB	2.20	0.41
1:O:154:LEU:CD2	1:O:240:VAL:HG11	2.45	0.41
1:Q:79:PRO:HB2	1:Q:107:LYS:CB	2.51	0.41
1:A:37:VAL:HG23	1:A:62:THR:HA	2.02	0.40
1:B:92:VAL:O	1:B:117:ILE:HG22	2.21	0.40
1:A:281:VAL:CG1	1:C:202:ASN:HD21	2.33	0.40
1:C:27:ILE:O	1:C:27:ILE:HG22	2.21	0.40
1:C:84:TRP:HB3	1:C:113:ALA:N	2.36	0.40
1:D:174:THR:O	1:D:174:THR:HG23	2.22	0.40
1:D:210:ALA:CA	1:D:213:ALA:HB3	2.51	0.40
1:D:27:ILE:C	1:D:27:ILE:HD13	2.41	0.40
1:D:28:ILE:N	1:D:28:ILE:HD13	2.37	0.40
1:E:161:LEU:O	1:E:162:ASP:C	2.60	0.40
1:E:317:TYR:O	1:E:321:VAL:HG23	2.21	0.40
1:F:228:ILE:H	1:F:228:ILE:CD1	2.34	0.40
1:F:23:SER:C	1:F:25:LEU:N	2.72	0.40
1:G:138:SER:OG	1:G:140:ASP:OD2	2.39	0.40
1:G:158:VAL:CG1	1:G:221:LEU:HD22	2.51	0.40
1:Q:179:THR:C	1:Q:181:ASP:H	2.25	0.40
1:Q:205:PRO:HA	1:Q:229:ALA:O	2.21	0.40
1:Q:84:TRP:CE3	1:Q:84:TRP:HA	2.56	0.40
1:B:25:LEU:HD11	1:B:325:ALA:HB3	2.03	0.40
1:B:32:ASP:OD2	1:B:32:ASP:N	2.55	0.40
1:C:183:ARG:HG2	1:C:195:ARG:O	2.21	0.40
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.87	0.40
1:G:239:VAL:HG23	1:G:309:ALA:C	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:VAL:HB	1:H:91:ILE:CG2	2.51	0.40
1:H:80:SER:O	1:H:111:ALA:HB2	2.20	0.40
1:H:84:TRP:HE3	1:H:89:ILE:HG13	1.85	0.40
1:A:202:ASN:ND2	1:C:279:VAL:CG2	2.84	0.40
1:A:206:THR:CG2	1:A:231:ARG:HG2	2.50	0.40
1:A:300:MET:HB2	1:C:226:ASN:HD22	1.80	0.40
1:A:76:ASN:OD1	1:A:81:LEU:HB2	2.21	0.40
1:D:106:GLY:C	1:D:108:HIS:H	2.23	0.40
1:D:157:PHE:HE1	1:D:242:LEU:HD23	1.85	0.40
1:D:153:CYS:HB2	1:D:289:SER:O	2.21	0.40
1:E:316:GLY:C	1:E:318:SER:N	2.72	0.40
1:E:91:ILE:HA	1:E:115:LYS:O	2.21	0.40
1:F:162:ASP:CA	1:F:167:ILE:HD13	2.51	0.40
1:F:183:ARG:HG3	1:F:196:ALA:HA	2.03	0.40
1:G:256:ASN:OD1	1:G:297:THR:HG21	2.20	0.40
1:H:11:ILE:HD11	3:H:401:NAD:N7N	2.36	0.40
1:H:133:ASN:HD22	1:H:133:ASN:C	2.23	0.40
1:H:70:ILE:H	1:H:70:ILE:HD13	1.87	0.40
1:D:191:ARG:HH22	2:I:61:GLU:CB	2.35	0.40
1:Q:242:LEU:O	1:Q:306:LYS:HA	2.21	0.40
1:A:198:ALA:HB1	1:A:201:LEU:HD12	2.01	0.40
1:A:236:ASN:O	1:A:237:VAL:HB	2.21	0.40
1:B:173:THR:HA	1:B:228:ILE:O	2.22	0.40
1:B:3:VAL:HG12	1:B:4:ALA:N	2.36	0.40
1:E:183:ARG:NH1	1:E:183:ARG:HA	2.36	0.40
1:G:255:VAL:HG12	1:G:259:PHE:CE2	2.57	0.40
1:G:137:TYR:CE2	1:G:328:VAL:HA	2.57	0.40
1:H:102:ARG:NH2	1:H:124:ASP:HB3	2.31	0.40
1:H:126:PRO:O	1:H:144:ILE:HB	2.21	0.40
1:H:243:VAL:HG22	1:H:306:LYS:HE3	2.02	0.40
1:O:176:HIS:O	1:O:231:ARG:HA	2.21	0.40
1:O:98:VAL:CG2	1:O:99:PHE:CE2	3.03	0.40
1:A:3:VAL:HG12	1:A:4:ALA:N	2.36	0.40
1:A:56:ASP:O	1:A:66:VAL:HA	2.21	0.40
1:B:100:VAL:HA	1:B:118:ILE:HD13	2.03	0.40
1:B:154:LEU:HD12	1:B:154:LEU:N	2.36	0.40
1:B:251:PHE:CE1	1:B:254:GLU:HB2	2.57	0.40
1:B:38:LYS:N	1:B:38:LYS:HD2	2.37	0.40
1:D:173:THR:HA	1:D:228:ILE:O	2.21	0.40
1:E:10:ARG:HB2	3:E:401:NAD:PN	2.61	0.40
1:E:165:PHE:CD1	1:E:248:LYS:HD3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:ALA:HB1	1:F:151:THR:HB	2.04	0.40
1:G:183:ARG:CZ	1:G:187:ALA:HB3	2.51	0.40
1:G:197:ARG:O	1:G:199:ALA:N	2.55	0.40
1:G:173:THR:OG1	1:G:228:ILE:CD1	2.70	0.40
1:G:74:VAL:HG23	1:G:75:SER:N	2.37	0.40
1:H:73:VAL:O	1:H:73:VAL:CG1	2.62	0.40
2:M:60:LEU:O	2:M:61:GLU:C	2.60	0.40
1:O:69:LYS:NZ	5:O:540:HOH:O	2.37	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)
5:Q:541:HOH:O	5:Q:541:HOH:O[2_665]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/337 (99%)	272 (81%)	54 (16%)	8 (2%)	6	15
1	B	334/337 (99%)	267 (80%)	55 (16%)	12 (4%)	3	7
1	C	334/337 (99%)	281 (84%)	44 (13%)	9 (3%)	5	12
1	D	334/337 (99%)	247 (74%)	63 (19%)	24 (7%)	1	1
1	E	334/337 (99%)	248 (74%)	58 (17%)	28 (8%)	1	1
1	F	334/337 (99%)	250 (75%)	64 (19%)	20 (6%)	1	2
1	G	335/337 (99%)	270 (81%)	47 (14%)	18 (5%)	2	3
1	H	333/337 (99%)	250 (75%)	51 (15%)	32 (10%)	0	0
1	O	335/337 (99%)	303 (90%)	29 (9%)	3 (1%)	17	40
1	Q	334/337 (99%)	294 (88%)	32 (10%)	8 (2%)	6	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	20/82 (24%)	19 (95%)	1 (5%)	0	100	100
2	J	19/82 (23%)	15 (79%)	3 (16%)	1 (5%)	2	3
2	K	19/82 (23%)	16 (84%)	1 (5%)	2 (10%)	0	0
2	L	17/82 (21%)	12 (71%)	4 (24%)	1 (6%)	1	2
2	M	20/82 (24%)	16 (80%)	3 (15%)	1 (5%)	2	4
2	N	17/82 (21%)	9 (53%)	7 (41%)	1 (6%)	1	2
All	All	3453/3862 (89%)	2769 (80%)	516 (15%)	168 (5%)	2	4

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ASP
1	B	221	LEU
1	D	22	ASP
1	D	199	ALA
1	D	210	ALA
1	E	0	LYS
1	E	20	ARG
1	E	177	SER
1	E	186	ASP
1	E	199	ALA
1	E	237	VAL
1	E	302	ASP
1	E	313	ASN
1	F	130	VAL
1	G	130	VAL
1	G	132	VAL
1	G	198	ALA
1	H	56	ASP
1	H	89	ILE
1	H	124	ASP
1	H	130	VAL
1	H	199	ALA
1	Q	33	THR
1	B	166	GLY
1	B	233	PRO
1	B	237	VAL
1	B	263	ALA
1	C	134	ALA
1	C	186	ASP

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Mol	Chain	Res	Type
1	C	237	VAL
1	D	55	ALA
1	D	72	GLN
1	D	130	VAL
1	D	180	GLY
1	D	200	ALA
1	D	313	ASN
1	E	33	THR
1	E	43	LEU
1	E	55	ALA
1	E	61	GLU
1	E	63	ALA
1	E	94	GLU
1	E	139	HIS
1	E	200	ALA
1	E	219	PRO
1	E	252	ALA
1	E	280	SER
1	F	8	PHE
1	F	132	VAL
1	F	135	ASP
1	F	248	LYS
1	F	331	ASN
1	G	135	ASP
1	G	154	LEU
1	G	163	GLN
1	G	166	GLY
1	G	233	PRO
1	G	281	VAL
1	G	295	SER
1	H	10	ARG
1	H	61	GLU
1	H	105	ALA
1	H	133	ASN
1	H	139	HIS
1	H	180	GLY
1	H	200	ALA
1	H	237	VAL
2	K	74	ARG
2	N	74	ARG
1	O	237	VAL
1	Q	1	LEU

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Mol	Chain	Res	Type
1	Q	111	ALA
1	Q	124	ASP
1	A	105	ALA
1	B	253	GLU
1	C	47	ASP
1	C	166	GLY
1	C	198	ALA
1	C	282	ASP
1	D	80	SER
1	D	146	ASN
1	D	155	ALA
1	D	193	LEU
1	D	237	VAL
1	D	289	SER
1	E	111	ALA
1	E	136	ALA
1	E	281	VAL
1	F	69	LYS
1	F	156	PRO
1	F	165	PHE
1	F	226	ASN
1	F	257	ALA
1	G	102	ARG
1	G	191	ARG
1	G	211	ALA
1	G	223	GLY
1	H	55	ALA
1	H	136	ALA
1	H	233	PRO
2	K	59	PRO
1	O	186	ASP
1	Q	237	VAL
1	A	110	GLU
1	A	237	VAL
1	B	193	LEU
1	B	198	ALA
1	B	223	GLY
1	D	125	ILE
1	E	142	PRO
1	E	317	TYR
1	F	62	THR
1	F	186	ASP

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Mol	Chain	Res	Type
1	F	223	GLY
1	F	252	ALA
1	F	253	GLU
1	F	258	ALA
1	G	237	VAL
1	H	52	ILE
1	H	86	GLU
1	H	142	PRO
1	H	146	ASN
1	H	178	TYR
2	J	74	ARG
1	Q	136	ALA
1	A	69	LYS
1	B	220	ASN
1	D	2	LYS
1	D	8	PHE
1	D	255	VAL
1	D	302	ASP
1	E	18(A)	TRP
1	E	28	ILE
1	E	233	PRO
1	F	237	VAL
1	G	155	ALA
1	G	226	ASN
1	H	67	ASP
1	H	87	LEU
1	H	147	ALA
1	H	163	GLN
1	H	211	ALA
1	H	282	ASP
1	A	38	LYS
1	A	83	PRO
1	A	233	PRO
1	B	94	GLU
1	C	233	PRO
1	D	54	ASP
1	D	233	PRO
1	E	56	ASP
1	F	24	PRO
1	H	79	PRO
1	H	82	LEU
1	Q	233	PRO

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Mol	Chain	Res	Type
1	Q	302	ASP
1	D	168	ILE
1	G	180	GLY
1	H	126	PRO
1	H	132	VAL
1	O	166	GLY
1	D	9	GLY
2	L	58	ASP
1	B	219	PRO
1	F	233	PRO
2	M	58	ASP
1	C	27	ILE
1	H	235	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/279 (100%)	260 (93%)	19 (7%)	16	36
1	B	279/279 (100%)	259 (93%)	20 (7%)	14	34
1	C	279/279 (100%)	255 (91%)	24 (9%)	10	24
1	D	279/279 (100%)	255 (91%)	24 (9%)	10	24
1	E	278/279 (100%)	255 (92%)	23 (8%)	11	25
1	F	279/279 (100%)	259 (93%)	20 (7%)	14	34
1	G	279/279 (100%)	261 (94%)	18 (6%)	17	38
1	H	278/279 (100%)	265 (95%)	13 (5%)	26	54
1	O	279/279 (100%)	260 (93%)	19 (7%)	16	36
1	Q	279/279 (100%)	266 (95%)	13 (5%)	26	54
2	I	22/65 (34%)	19 (86%)	3 (14%)	3	8
2	J	21/65 (32%)	21 (100%)	0	100	100
2	K	21/65 (32%)	19 (90%)	2 (10%)	8	20
2	L	18/65 (28%)	10 (56%)	8 (44%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	22/65 (34%)	22 (100%)	0	100	100
2	N	19/65 (29%)	19 (100%)	0	100	100
All	All	2911/3180 (92%)	2705 (93%)	206 (7%)	14	34

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	LYS
1	A	2	LYS
1	A	8	PHE
1	A	27	ILE
1	A	28	ILE
1	A	33	THR
1	A	69	LYS
1	A	74	VAL
1	A	76	ASN
1	A	84	TRP
1	A	133	ASN
1	A	164	LYS
1	A	171	THR
1	A	207	SER
1	A	239	VAL
1	A	240	VAL
1	A	245	GLN
1	A	280	SER
1	A	290	THR
1	B	38	LYS
1	B	84	TRP
1	B	91	ILE
1	B	94	GLU
1	B	103	GLU
1	B	117	ILE
1	B	133	ASN
1	B	135	ASP
1	B	152	ASN
1	B	157	PHE
1	B	163	GLN
1	B	172	MET
1	B	175	THR
1	B	178	TYR
1	B	191	ARG

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Mol	Chain	Res	Type
1	B	220	ASN
1	B	271	LEU
1	B	279	VAL
1	B	290	THR
1	B	311	TYR
1	C	14	ASN
1	C	16	LEU
1	C	21	LYS
1	C	25	LEU
1	C	61	GLU
1	C	65	SER
1	C	70	ILE
1	C	76	ASN
1	C	84	TRP
1	C	91	ILE
1	C	94	GLU
1	C	133	ASN
1	C	141	GLU
1	C	152	ASN
1	C	169	LYS
1	C	171	THR
1	C	203	ILE
1	C	208	THR
1	C	228	ILE
1	C	266	GLU
1	C	290	THR
1	C	295	SER
1	C	313	ASN
1	C	330	ASN
1	D	8	PHE
1	D	21	LYS
1	D	27	ILE
1	D	28	ILE
1	D	39	GLN
1	D	58	LYS
1	D	62	THR
1	D	67	ASP
1	D	84	TRP
1	D	87	LEU
1	D	124	ASP
1	D	152	ASN
1	D	169	LYS

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Mol	Chain	Res	Type
1	D	172	MET
1	D	178	TYR
1	D	191	ARG
1	D	201	LEU
1	D	202	ASN
1	D	220	ASN
1	D	228	ILE
1	D	234	THR
1	D	238	SER
1	D	245	GLN
1	D	261	ASP
1	E	5	ILE
1	E	28	ILE
1	E	37	VAL
1	E	38	LYS
1	E	56	ASP
1	E	58	LYS
1	E	61	GLU
1	E	67	ASP
1	E	70	ILE
1	E	84	TRP
1	E	87	LEU
1	E	133	ASN
1	E	144	ILE
1	E	163	GLN
1	E	172	MET
1	E	173	THR
1	E	178	TYR
1	E	179	THR
1	E	226	ASN
1	E	251	PHE
1	E	256	ASN
1	E	296	LEU
1	E	300	MET
1	F	1	LEU
1	F	8	PHE
1	F	14	ASN
1	F	18	CYS
1	F	21	LYS
1	F	84	TRP
1	F	94	GLU
1	F	122(A)	LYS

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Mol	Chain	Res	Type
1	F	124	ASP
1	F	127	THR
1	F	133	ASN
1	F	141	GLU
1	F	164	LYS
1	F	172	MET
1	F	178	TYR
1	F	228	ILE
1	F	274	CYS
1	F	290	THR
1	F	300	MET
1	F	302	ASP
1	G	23	SER
1	G	25	LEU
1	G	28	ILE
1	G	72	GLN
1	G	85	LYS
1	G	87	LEU
1	G	130	VAL
1	G	133	ASN
1	G	148	SER
1	G	169	LYS
1	G	205	PRO
1	G	242	LEU
1	G	253	GLU
1	G	256	ASN
1	G	264	GLU
1	G	291	THR
1	G	311	TYR
1	G	313	ASN
1	H	56	ASP
1	H	58	LYS
1	H	70	ILE
1	H	72	GLN
1	H	76	ASN
1	H	91	ILE
1	H	133	ASN
1	H	144	ILE
1	H	164	LYS
1	H	178	TYR
1	H	201	LEU
1	H	206	THR

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Mol	Chain	Res	Type
1	H	295	SER
2	I	58	ASP
2	I	74	ARG
2	I	77	ASP
2	K	67	ASN
2	K	69	GLU
2	L	55	ASP
2	L	58	ASP
2	L	61	GLU
2	L	62	GLU
2	L	63	TYR
2	L	65	LYS
2	L	70	THR
2	L	71	ASN
1	O	14	ASN
1	O	27	ILE
1	O	39	GLN
1	O	56	ASP
1	O	58	LYS
1	O	61	GLU
1	O	62	THR
1	O	74	VAL
1	O	75	SER
1	O	84	TRP
1	O	91	ILE
1	O	103	GLU
1	O	133	ASN
1	O	135	ASP
1	O	154	LEU
1	O	191	ARG
1	O	247	SER
1	O	265	LYS
1	O	268	LYS
1	Q	16	LEU
1	Q	74	VAL
1	Q	76	ASN
1	Q	84	TRP
1	Q	103	GLU
1	Q	124	ASP
1	Q	133	ASN
1	Q	140	ASP
1	Q	141	GLU

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Mol	Chain	Res	Type
1	Q	164	LYS
1	Q	290	THR
1	Q	323	ASP
1	Q	331	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	78	ASN
1	A	133	ASN
1	A	146	ASN
1	A	152	ASN
1	A	163	GLN
1	A	202	ASN
1	A	256	ASN
1	A	330	ASN
1	B	133	ASN
1	B	146	ASN
1	B	152	ASN
1	B	202	ASN
1	B	220	ASN
1	B	256	ASN
1	B	330	ASN
1	C	14	ASN
1	C	133	ASN
1	C	152	ASN
1	C	163	GLN
1	C	202	ASN
1	C	226	ASN
1	C	256	ASN
1	C	330	ASN
1	D	39	GLN
1	D	42	HIS
1	D	78	ASN
1	D	133	ASN
1	D	146	ASN
1	D	152	ASN
1	D	202	ASN
1	D	245	GLN
1	D	256	ASN
1	D	319	GLN

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Mol	Chain	Res	Type
1	D	330	ASN
1	D	331	ASN
1	E	39	GLN
1	E	76	ASN
1	E	133	ASN
1	E	146	ASN
1	E	152	ASN
1	E	330	ASN
1	F	14	ASN
1	F	18(B)	HIS
1	F	42	HIS
1	F	133	ASN
1	F	139	HIS
1	F	152	ASN
1	F	163	GLN
1	F	202	ASN
1	F	226	ASN
1	F	256	ASN
1	F	330	ASN
1	G	6	ASN
1	G	72	GLN
1	G	133	ASN
1	G	152	ASN
1	G	202	ASN
1	G	226	ASN
1	G	330	ASN
1	G	331	ASN
1	H	39	GLN
1	H	72	GLN
1	H	133	ASN
1	H	139	HIS
1	H	152	ASN
1	H	202	ASN
1	H	226	ASN
1	H	245	GLN
1	H	256	ASN
1	H	330	ASN
2	I	78	ASN
2	J	78	ASN
2	K	78	ASN
2	M	78	ASN
1	O	6	ASN

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Mol	Chain	Res	Type
1	O	39	GLN
1	O	72	GLN
1	O	133	ASN
1	O	152	ASN
1	O	202	ASN
1	O	256	ASN
1	Q	76	ASN
1	Q	133	ASN
1	Q	146	ASN
1	Q	152	ASN
1	Q	163	GLN
1	Q	202	ASN
1	Q	226	ASN
1	Q	256	ASN
1	Q	330	ASN
1	Q	331	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

38 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
4	SO4	B	402	-	4,4,4	0.25	0	6,6,6	0.15	0
3	NAD	H	401	-	42,48,48	1.54	7 (16%)	50,73,73	1.98	13 (26%)
4	SO4	E	403	-	4,4,4	0.21	0	6,6,6	0.08	0
4	SO4	E	404	-	4,4,4	0.29	0	6,6,6	0.10	0
4	SO4	Q	405	-	4,4,4	0.32	0	6,6,6	0.13	0
4	SO4	C	406	-	4,4,4	0.25	0	6,6,6	0.21	0
4	SO4	A	402	-	4,4,4	0.26	0	6,6,6	0.18	0
4	SO4	E	402	-	4,4,4	0.23	0	6,6,6	0.05	0
4	SO4	A	404	-	4,4,4	0.27	0	6,6,6	0.18	0
4	SO4	A	408	-	4,4,4	0.24	0	6,6,6	0.05	0
4	SO4	F	402	-	4,4,4	0.22	0	6,6,6	0.18	0
4	SO4	Q	402	-	4,4,4	0.31	0	6,6,6	0.13	0
4	SO4	H	402	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	A	407	-	4,4,4	0.22	0	6,6,6	0.12	0
4	SO4	Q	404	-	4,4,4	0.34	0	6,6,6	0.13	0
4	SO4	A	406	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	O	402	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	A	405	-	4,4,4	0.32	0	6,6,6	0.08	0
4	SO4	D	402	-	4,4,4	0.26	0	6,6,6	0.15	0
3	NAD	E	401	-	42,48,48	1.49	7 (16%)	50,73,73	1.99	13 (26%)
4	SO4	F	403	-	4,4,4	0.22	0	6,6,6	0.12	0
3	NAD	O	401	-	42,48,48	1.45	7 (16%)	50,73,73	1.90	13 (26%)
3	NAD	B	401	-	42,48,48	1.65	8 (19%)	50,73,73	1.93	13 (26%)
3	NAD	Q	401	-	42,48,48	1.70	8 (19%)	50,73,73	1.86	12 (24%)
3	NAD	F	401	-	42,48,48	1.69	8 (19%)	50,73,73	1.98	13 (26%)
4	SO4	B	403	-	4,4,4	0.28	0	6,6,6	0.16	0
4	SO4	O	403	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	C	405	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	C	402	-	4,4,4	0.28	0	6,6,6	0.12	0
3	NAD	A	401	-	42,48,48	1.52	10 (23%)	50,73,73	1.93	13 (26%)
3	NAD	C	401	-	42,48,48	1.67	8 (19%)	50,73,73	1.92	13 (26%)
4	SO4	C	404	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	A	403	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	C	403	-	4,4,4	0.28	0	6,6,6	0.17	0
4	SO4	G	402	-	4,4,4	0.22	0	6,6,6	0.11	0
3	NAD	D	401	-	42,48,48	1.49	9 (21%)	50,73,73	2.03	13 (26%)
3	NAD	G	401	-	42,48,48	1.66	8 (19%)	50,73,73	1.93	13 (26%)
4	SO4	Q	403	-	4,4,4	0.21	0	6,6,6	0.06	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
3	NAD	C	401	-	-	4/26/62/62	0/5/5/5
3	NAD	E	401	-	-	16/26/62/62	0/5/5/5
3	NAD	H	401	-	-	10/26/62/62	0/5/5/5
3	NAD	G	401	-	-	11/26/62/62	0/5/5/5
3	NAD	O	401	-	-	5/26/62/62	0/5/5/5
3	NAD	B	401	-	-	9/26/62/62	0/5/5/5
3	NAD	Q	401	-	-	9/26/62/62	0/5/5/5
3	NAD	D	401	-	-	16/26/62/62	0/5/5/5
3	NAD	F	401	-	-	7/26/62/62	0/5/5/5
3	NAD	A	401	-	-	9/26/62/62	0/5/5/5

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	NAD	C3N-C7N	5.91	1.59	1.50
3	Q	401	NAD	C3N-C7N	5.57	1.59	1.50
3	B	401	NAD	C3N-C7N	5.46	1.58	1.50
3	G	401	NAD	C3N-C7N	4.88	1.57	1.50
3	C	401	NAD	C3N-C7N	4.74	1.57	1.50
3	C	401	NAD	C6N-N1N	4.08	1.45	1.35
3	H	401	NAD	C3N-C7N	4.07	1.56	1.50
3	C	401	NAD	C2N-N1N	3.93	1.39	1.35
3	F	401	NAD	C2N-N1N	3.90	1.39	1.35
3	H	401	NAD	C6N-N1N	3.87	1.44	1.35
3	O	401	NAD	C6N-N1N	3.86	1.44	1.35
3	A	401	NAD	C6N-N1N	3.81	1.44	1.35
3	D	401	NAD	C6N-N1N	3.79	1.44	1.35
3	B	401	NAD	C6N-N1N	3.76	1.44	1.35
3	G	401	NAD	C6N-N1N	3.68	1.44	1.35
3	Q	401	NAD	C6N-N1N	3.68	1.44	1.35
3	D	401	NAD	C4A-N3A	3.63	1.40	1.35
3	E	401	NAD	C6N-N1N	3.59	1.44	1.35
3	E	401	NAD	C3N-C7N	3.56	1.55	1.50
3	Q	401	NAD	C4N-C3N	3.52	1.45	1.39
3	C	401	NAD	C4N-C3N	3.50	1.45	1.39
3	A	401	NAD	C3N-C7N	3.50	1.55	1.50
3	G	401	NAD	C2N-N1N	3.43	1.39	1.35
3	H	401	NAD	C2N-N1N	3.40	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	NAD	C6N-N1N	3.38	1.43	1.35
3	E	401	NAD	C2N-N1N	3.27	1.38	1.35
3	B	401	NAD	C4N-C3N	3.26	1.44	1.39
3	G	401	NAD	C4N-C3N	3.24	1.44	1.39
3	G	401	NAD	O4B-C1B	3.20	1.45	1.41
3	O	401	NAD	C3N-C7N	3.09	1.55	1.50
3	Q	401	NAD	O4B-C1B	3.06	1.45	1.41
3	Q	401	NAD	C2N-N1N	3.02	1.38	1.35
3	C	401	NAD	O4B-C1B	3.01	1.45	1.41
3	A	401	NAD	C2N-N1N	3.01	1.38	1.35
3	H	401	NAD	C4N-C3N	2.89	1.44	1.39
3	B	401	NAD	C2N-N1N	2.89	1.38	1.35
3	D	401	NAD	C3N-C7N	2.87	1.54	1.50
3	E	401	NAD	C4A-N3A	2.84	1.39	1.35
3	F	401	NAD	C4N-C3N	2.81	1.44	1.39
3	H	401	NAD	O4B-C1B	2.78	1.45	1.41
3	O	401	NAD	C2N-N1N	2.75	1.38	1.35
3	A	401	NAD	C4N-C3N	2.73	1.44	1.39
3	O	401	NAD	C4N-C3N	2.73	1.44	1.39
3	F	401	NAD	C2B-C1B	-2.68	1.49	1.53
3	E	401	NAD	C4N-C3N	2.67	1.43	1.39
3	A	401	NAD	C4A-N3A	2.67	1.39	1.35
3	B	401	NAD	O4B-C1B	2.63	1.44	1.41
3	G	401	NAD	C4A-N3A	2.63	1.39	1.35
3	H	401	NAD	C4A-N3A	2.62	1.39	1.35
3	Q	401	NAD	C2A-N3A	2.52	1.36	1.32
3	D	401	NAD	C4N-C3N	2.49	1.43	1.39
3	D	401	NAD	C2A-N3A	2.42	1.36	1.32
3	F	401	NAD	O4B-C1B	2.38	1.44	1.41
3	A	401	NAD	C2A-N3A	2.37	1.35	1.32
3	G	401	NAD	O5B-C5B	2.37	1.53	1.44
3	B	401	NAD	O5B-C5B	2.35	1.53	1.44
3	D	401	NAD	O4B-C1B	2.33	1.44	1.41
3	D	401	NAD	C2N-N1N	2.27	1.37	1.35
3	F	401	NAD	C4A-N3A	2.25	1.38	1.35
3	E	401	NAD	O5B-C5B	2.21	1.53	1.44
3	A	401	NAD	O3D-C3D	2.21	1.48	1.43
3	O	401	NAD	C3D-C4D	2.19	1.58	1.53
3	Q	401	NAD	O5B-C5B	2.19	1.53	1.44
3	D	401	NAD	C2A-N1A	2.15	1.37	1.33
3	B	401	NAD	C2A-N3A	2.14	1.35	1.32
3	G	401	NAD	O3D-C3D	2.14	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	C4A-N3A	2.14	1.38	1.35
3	Q	401	NAD	O3D-C3D	2.11	1.47	1.43
3	O	401	NAD	O4B-C1B	2.11	1.44	1.41
3	A	401	NAD	O4B-C1B	2.09	1.44	1.41
3	C	401	NAD	C5N-C4N	2.08	1.43	1.38
3	C	401	NAD	O3D-C3D	2.05	1.47	1.43
3	F	401	NAD	O5B-C5B	2.04	1.52	1.44
3	A	401	NAD	C5N-C4N	2.04	1.43	1.38
3	C	401	NAD	O5B-C5B	2.03	1.52	1.44
3	A	401	NAD	O5B-C5B	2.03	1.52	1.44
3	E	401	NAD	C2A-N1A	2.03	1.37	1.33
3	O	401	NAD	C2A-N1A	2.02	1.37	1.33
3	D	401	NAD	O5B-C5B	2.01	1.52	1.44
3	H	401	NAD	O5B-C5B	2.00	1.52	1.44

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAD	C5N-C6N-N1N	-5.77	112.13	120.40
3	D	401	NAD	C5N-C6N-N1N	-5.72	112.19	120.40
3	O	401	NAD	C5N-C6N-N1N	-5.72	112.20	120.40
3	D	401	NAD	C6N-N1N-C2N	5.68	127.16	121.97
3	C	401	NAD	C5N-C6N-N1N	-5.62	112.34	120.40
3	B	401	NAD	C5N-C6N-N1N	-5.60	112.37	120.40
3	F	401	NAD	C5N-C6N-N1N	-5.60	112.38	120.40
3	E	401	NAD	C5N-C6N-N1N	-5.52	112.48	120.40
3	G	401	NAD	C5N-C6N-N1N	-5.45	112.59	120.40
3	H	401	NAD	C5N-C6N-N1N	-5.33	112.76	120.40
3	C	401	NAD	C6N-N1N-C2N	5.29	126.80	121.97
3	E	401	NAD	C6N-N1N-C2N	5.19	126.71	121.97
3	G	401	NAD	C6N-N1N-C2N	5.19	126.71	121.97
3	Q	401	NAD	C5N-C6N-N1N	-5.17	112.99	120.40
3	F	401	NAD	C6N-N1N-C2N	5.17	126.69	121.97
3	A	401	NAD	C6N-N1N-C2N	5.13	126.65	121.97
3	B	401	NAD	C6N-N1N-C2N	5.09	126.61	121.97
3	H	401	NAD	C6N-N1N-C2N	4.91	126.45	121.97
3	Q	401	NAD	C6N-N1N-C2N	4.65	126.21	121.97
3	O	401	NAD	C6N-N1N-C2N	4.61	126.17	121.97
3	F	401	NAD	C6N-C5N-C4N	4.46	125.92	119.44
3	A	401	NAD	C6N-C5N-C4N	4.08	125.38	119.44
3	H	401	NAD	C4N-C3N-C7N	-4.03	110.25	121.04
3	E	401	NAD	C4N-C3N-C7N	-4.01	110.31	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	NAD	C6N-C5N-C4N	4.00	125.26	119.44
3	E	401	NAD	C6N-C5N-C4N	3.99	125.24	119.44
3	G	401	NAD	C3N-C7N-N7N	3.99	122.54	117.75
3	B	401	NAD	C6N-C5N-C4N	3.99	125.24	119.44
3	D	401	NAD	C3N-C2N-N1N	-3.99	116.53	120.43
3	G	401	NAD	C6N-C5N-C4N	3.97	125.22	119.44
3	O	401	NAD	C6N-C5N-C4N	3.95	125.18	119.44
3	D	401	NAD	C4N-C3N-C7N	-3.95	110.47	121.04
3	Q	401	NAD	C6N-C5N-C4N	3.95	125.17	119.44
3	C	401	NAD	C6N-C5N-C4N	3.89	125.09	119.44
3	D	401	NAD	C6N-C5N-C4N	3.85	125.03	119.44
3	F	401	NAD	C4N-C3N-C7N	-3.68	111.18	121.04
3	G	401	NAD	C4N-C3N-C7N	-3.67	111.21	121.04
3	E	401	NAD	C3N-C7N-N7N	3.61	122.08	117.75
3	O	401	NAD	C3N-C7N-N7N	3.59	122.06	117.75
3	B	401	NAD	C3N-C7N-N7N	3.57	122.04	117.75
3	H	401	NAD	C3N-C2N-N1N	-3.55	116.96	120.43
3	H	401	NAD	C3N-C7N-N7N	3.54	122.00	117.75
3	O	401	NAD	C4N-C3N-C7N	-3.52	111.62	121.04
3	A	401	NAD	C4N-C3N-C7N	-3.51	111.66	121.04
3	F	401	NAD	C3N-C7N-N7N	3.45	121.89	117.75
3	B	401	NAD	C4N-C3N-C7N	-3.41	111.90	121.04
3	D	401	NAD	C2N-C3N-C4N	3.41	122.12	118.26
3	E	401	NAD	C3N-C2N-N1N	-3.40	117.11	120.43
3	Q	401	NAD	C4N-C3N-C7N	-3.35	112.06	121.04
3	C	401	NAD	O3D-C3D-C4D	-3.32	101.44	111.05
3	O	401	NAD	C5N-C4N-C3N	-3.31	116.43	120.34
3	C	401	NAD	C4N-C3N-C7N	-3.27	112.28	121.04
3	Q	401	NAD	C3N-C7N-N7N	3.20	121.59	117.75
3	G	401	NAD	C3N-C2N-N1N	-3.18	117.32	120.43
3	F	401	NAD	C3N-C2N-N1N	-3.18	117.32	120.43
3	O	401	NAD	C2N-C3N-C4N	3.17	121.85	118.26
3	D	401	NAD	C3N-C7N-N7N	3.15	121.53	117.75
3	B	401	NAD	C5A-C6A-N6A	3.12	125.09	120.35
3	C	401	NAD	C3N-C2N-N1N	-3.10	117.40	120.43
3	H	401	NAD	C2N-C3N-C4N	3.08	121.75	118.26
3	D	401	NAD	O3D-C3D-C4D	-3.07	102.18	111.05
3	A	401	NAD	C5N-C4N-C3N	-3.04	116.75	120.34
3	E	401	NAD	C2N-C3N-C4N	3.03	121.69	118.26
3	E	401	NAD	C5N-C4N-C3N	-3.03	116.76	120.34
3	B	401	NAD	C5N-C4N-C3N	-3.00	116.79	120.34
3	F	401	NAD	C2N-C3N-C7N	2.99	128.13	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	NAD	C5N-C4N-C3N	-2.97	116.83	120.34
3	H	401	NAD	C2N-C3N-C7N	2.94	128.00	119.46
3	E	401	NAD	C2N-C3N-C7N	2.94	128.00	119.46
3	Q	401	NAD	C5N-C4N-C3N	-2.94	116.87	120.34
3	A	401	NAD	C3N-C7N-N7N	2.90	121.23	117.75
3	G	401	NAD	C5N-C4N-C3N	-2.90	116.92	120.34
3	Q	401	NAD	C3D-C2D-C1D	2.88	105.32	100.98
3	D	401	NAD	C5N-C4N-C3N	-2.85	116.97	120.34
3	E	401	NAD	O7N-C7N-C3N	-2.85	116.22	119.63
3	C	401	NAD	C3N-C7N-N7N	2.84	121.16	117.75
3	A	401	NAD	C3N-C2N-N1N	-2.83	117.67	120.43
3	Q	401	NAD	C3N-C2N-N1N	-2.82	117.67	120.43
3	F	401	NAD	C5N-C4N-C3N	-2.82	117.01	120.34
3	F	401	NAD	C3D-C2D-C1D	2.80	105.19	100.98
3	A	401	NAD	C2N-C3N-C4N	2.80	121.43	118.26
3	G	401	NAD	C2N-C3N-C7N	2.78	127.53	119.46
3	C	401	NAD	C5A-C6A-N6A	2.75	124.54	120.35
3	F	401	NAD	C5A-C6A-N6A	2.74	124.52	120.35
3	D	401	NAD	C2N-C3N-C7N	2.74	127.41	119.46
3	D	401	NAD	O7N-C7N-C3N	-2.71	116.38	119.63
3	C	401	NAD	O4D-C1D-C2D	-2.70	102.98	106.93
3	O	401	NAD	C3D-C2D-C1D	2.69	105.02	100.98
3	H	401	NAD	C3D-C2D-C1D	2.66	104.99	100.98
3	E	401	NAD	O3D-C3D-C4D	-2.66	103.35	111.05
3	G	401	NAD	C2N-C3N-C4N	2.64	121.26	118.26
3	A	401	NAD	O3D-C3D-C4D	-2.64	103.42	111.05
3	B	401	NAD	C3D-C2D-C1D	2.63	104.94	100.98
3	A	401	NAD	C5A-C6A-N6A	2.62	124.34	120.35
3	B	401	NAD	C2N-C3N-C7N	2.61	127.03	119.46
3	H	401	NAD	C5A-C6A-N6A	2.61	124.31	120.35
3	A	401	NAD	C2N-C3N-C7N	2.57	126.91	119.46
3	B	401	NAD	C3N-C2N-N1N	-2.56	117.92	120.43
3	Q	401	NAD	C2N-C3N-C7N	2.55	126.86	119.46
3	C	401	NAD	C5N-C4N-C3N	-2.54	117.33	120.34
3	E	401	NAD	C1B-N9A-C4A	-2.51	122.23	126.64
3	Q	401	NAD	C2N-C3N-C4N	2.49	121.08	118.26
3	C	401	NAD	C2N-C3N-C7N	2.49	126.68	119.46
3	G	401	NAD	O3D-C3D-C4D	-2.48	103.88	111.05
3	B	401	NAD	C2N-C3N-C4N	2.48	121.07	118.26
3	F	401	NAD	O3D-C3D-C4D	-2.48	103.89	111.05
3	O	401	NAD	O5B-C5B-C4B	-2.47	100.48	108.99
3	G	401	NAD	C5A-C6A-N6A	2.46	124.10	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	NAD	O7N-C7N-C3N	-2.46	116.69	119.63
3	C	401	NAD	C2N-C3N-C4N	2.45	121.04	118.26
3	O	401	NAD	C2N-C3N-C7N	2.43	126.53	119.46
3	D	401	NAD	C5A-C6A-N6A	2.43	124.04	120.35
3	G	401	NAD	O7N-C7N-C3N	-2.39	116.77	119.63
3	O	401	NAD	O7N-C7N-C3N	-2.37	116.79	119.63
3	Q	401	NAD	O3D-C3D-C4D	-2.37	104.19	111.05
3	O	401	NAD	C3N-C2N-N1N	-2.31	118.17	120.43
3	E	401	NAD	C5A-C6A-N6A	2.30	123.84	120.35
3	A	401	NAD	O5B-C5B-C4B	-2.27	101.19	108.99
3	F	401	NAD	C1B-N9A-C4A	-2.26	122.67	126.64
3	H	401	NAD	O3D-C3D-C4D	-2.23	104.60	111.05
3	Q	401	NAD	C5A-C6A-N6A	2.23	123.74	120.35
3	B	401	NAD	O3D-C3D-C4D	-2.22	104.64	111.05
3	G	401	NAD	C3D-C2D-C1D	2.19	104.28	100.98
3	F	401	NAD	C2N-C3N-C4N	2.14	120.69	118.26
3	A	401	NAD	O7N-C7N-C3N	-2.13	117.08	119.63
3	C	401	NAD	O5B-C5B-C4B	-2.08	101.85	108.99
3	O	401	NAD	C5A-C6A-N6A	2.03	123.44	120.35
3	B	401	NAD	C1B-N9A-C4A	-2.01	123.11	126.64
3	D	401	NAD	PN-O3-PA	2.00	139.69	132.83

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	401	NAD	O4D-C1D-N1N-C2N
3	H	401	NAD	O4D-C1D-N1N-C6N
3	H	401	NAD	C2N-C3N-C7N-N7N
3	A	401	NAD	O4D-C1D-N1N-C2N
3	A	401	NAD	O4D-C1D-N1N-C6N
3	A	401	NAD	C2D-C1D-N1N-C2N
3	A	401	NAD	C2D-C1D-N1N-C6N
3	E	401	NAD	C5B-O5B-PA-O1A
3	E	401	NAD	O4D-C1D-N1N-C2N
3	E	401	NAD	O4D-C1D-N1N-C6N
3	E	401	NAD	C2D-C1D-N1N-C6N
3	E	401	NAD	C2N-C3N-C7N-O7N
3	E	401	NAD	C2N-C3N-C7N-N7N
3	O	401	NAD	O4D-C1D-N1N-C2N
3	O	401	NAD	O4D-C1D-N1N-C6N
3	O	401	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	O	401	NAD	C2D-C1D-N1N-C6N
3	B	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	O4D-C1D-N1N-C2N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	C2D-C1D-N1N-C6N
3	Q	401	NAD	O4D-C1D-N1N-C2N
3	Q	401	NAD	O4D-C1D-N1N-C6N
3	Q	401	NAD	C2D-C1D-N1N-C2N
3	Q	401	NAD	C2D-C1D-N1N-C6N
3	F	401	NAD	O4D-C1D-N1N-C2N
3	C	401	NAD	O4D-C1D-N1N-C2N
3	G	401	NAD	C5B-O5B-PA-O1A
3	G	401	NAD	O4B-C4B-C5B-O5B
3	G	401	NAD	O4D-C1D-N1N-C2N
3	G	401	NAD	O4D-C1D-N1N-C6N
3	G	401	NAD	C2D-C1D-N1N-C2N
3	G	401	NAD	C2D-C1D-N1N-C6N
3	D	401	NAD	C5B-O5B-PA-O1A
3	D	401	NAD	C5B-O5B-PA-O2A
3	D	401	NAD	PN-O3-PA-O5B
3	D	401	NAD	O4B-C4B-C5B-O5B
3	D	401	NAD	O4D-C1D-N1N-C2N
3	D	401	NAD	O4D-C1D-N1N-C6N
3	D	401	NAD	C2D-C1D-N1N-C2N
3	D	401	NAD	C2D-C1D-N1N-C6N
3	E	401	NAD	C4N-C3N-C7N-N7N
3	E	401	NAD	C4N-C3N-C7N-O7N
3	H	401	NAD	C4N-C3N-C7N-N7N
3	H	401	NAD	C4N-C3N-C7N-O7N
3	H	401	NAD	C2N-C3N-C7N-O7N
3	D	401	NAD	C2N-C3N-C7N-O7N
3	D	401	NAD	C2N-C3N-C7N-N7N
3	D	401	NAD	C4N-C3N-C7N-N7N
3	D	401	NAD	C4N-C3N-C7N-O7N
3	E	401	NAD	O4B-C4B-C5B-O5B
3	E	401	NAD	C3B-C4B-C5B-O5B
3	G	401	NAD	C3B-C4B-C5B-O5B
3	D	401	NAD	C3B-C4B-C5B-O5B
3	B	401	NAD	C3B-C4B-C5B-O5B
3	A	401	NAD	C4N-C3N-C7N-O7N
3	A	401	NAD	C4N-C3N-C7N-N7N

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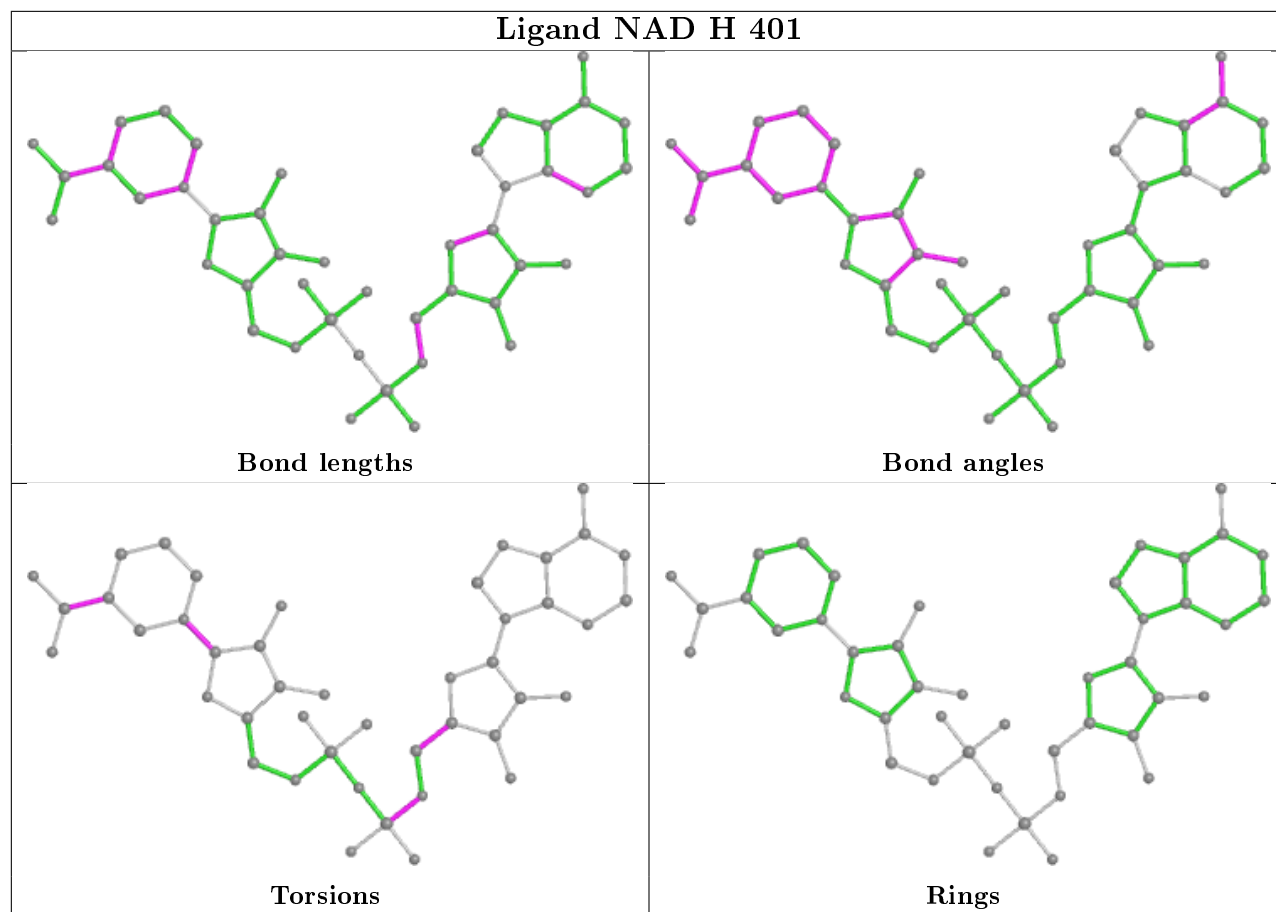
Mol	Chain	Res	Type	Atoms
3	A	401	NAD	C2N-C3N-C7N-O7N
3	A	401	NAD	C2N-C3N-C7N-N7N
3	F	401	NAD	PN-O3-PA-O5B
3	Q	401	NAD	O4B-C4B-C5B-O5B
3	E	401	NAD	C5B-O5B-PA-O3
3	B	401	NAD	C5B-O5B-PA-O3
3	Q	401	NAD	C5B-O5B-PA-O3
3	F	401	NAD	C5B-O5B-PA-O3
3	G	401	NAD	C5B-O5B-PA-O3
3	E	401	NAD	C5B-O5B-PA-O2A
3	B	401	NAD	C5B-O5B-PA-O1A
3	B	401	NAD	C5B-O5B-PA-O2A
3	Q	401	NAD	C5B-O5B-PA-O2A
3	F	401	NAD	C5B-O5B-PA-O2A
3	G	401	NAD	C5B-O5B-PA-O2A
3	O	401	NAD	O4B-C4B-C5B-O5B
3	F	401	NAD	PA-O3-PN-O2N
3	F	401	NAD	O4B-C4B-C5B-O5B
3	C	401	NAD	O4B-C4B-C5B-O5B
3	Q	401	NAD	PA-O3-PN-O2N
3	E	401	NAD	O4D-C4D-C5D-O5D
3	H	401	NAD	C5B-O5B-PA-O3
3	H	401	NAD	C2D-C1D-N1N-C6N
3	E	401	NAD	C2D-C1D-N1N-C2N
3	D	401	NAD	C5B-O5B-PA-O3
3	H	401	NAD	O4B-C4B-C5B-O5B
3	A	401	NAD	O4B-C4B-C5B-O5B
3	E	401	NAD	PA-O3-PN-O1N
3	Q	401	NAD	PA-O3-PN-O1N
3	C	401	NAD	PA-O3-PN-O1N
3	C	401	NAD	PA-O3-PN-O2N
3	G	401	NAD	PA-O3-PN-O1N
3	G	401	NAD	PA-O3-PN-O2N
3	D	401	NAD	PA-O3-PN-O1N
3	D	401	NAD	PA-O3-PN-O2N
3	H	401	NAD	C5B-O5B-PA-O2A
3	E	401	NAD	C3D-C4D-C5D-O5D
3	F	401	NAD	C4B-C5B-O5B-PA

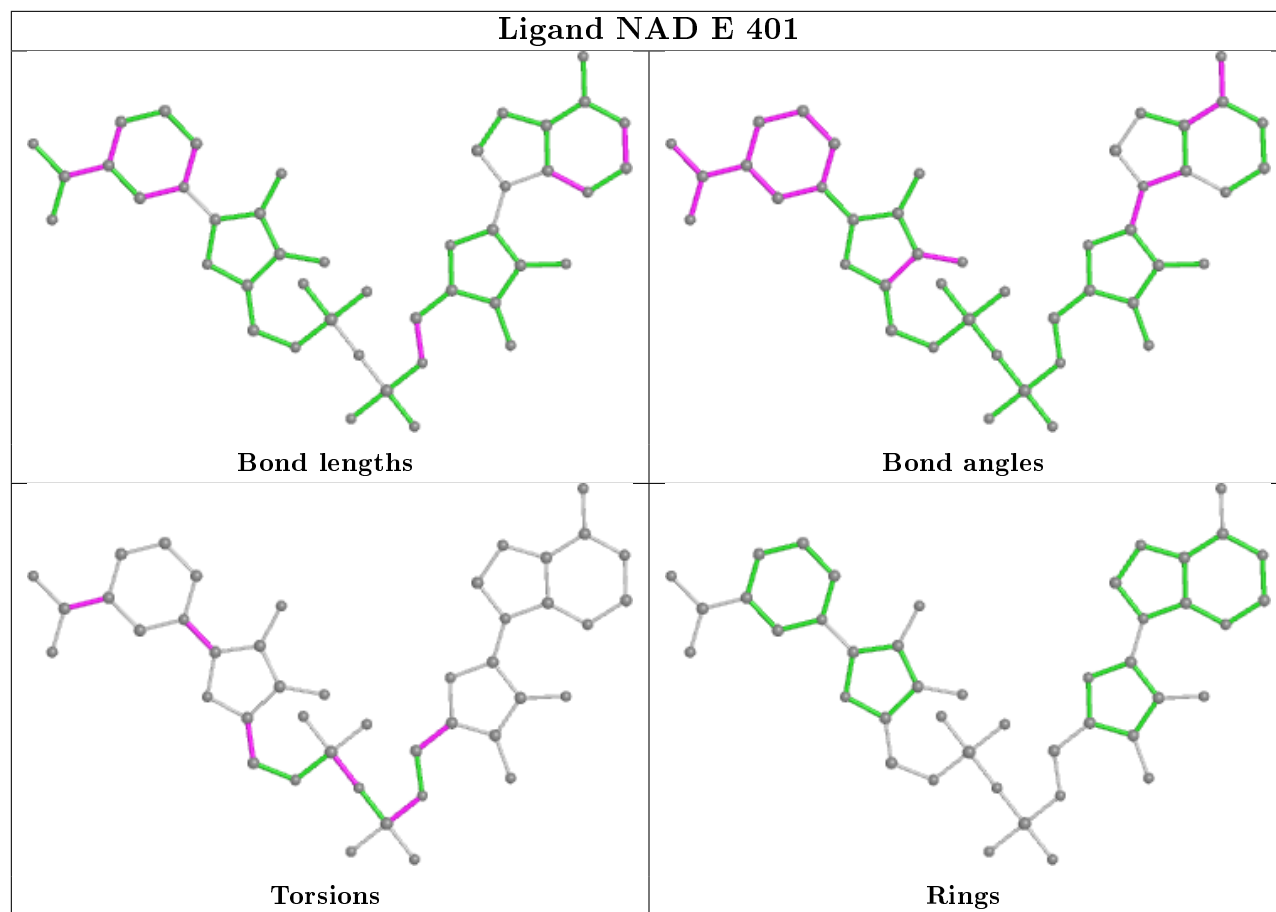
There are no ring outliers.

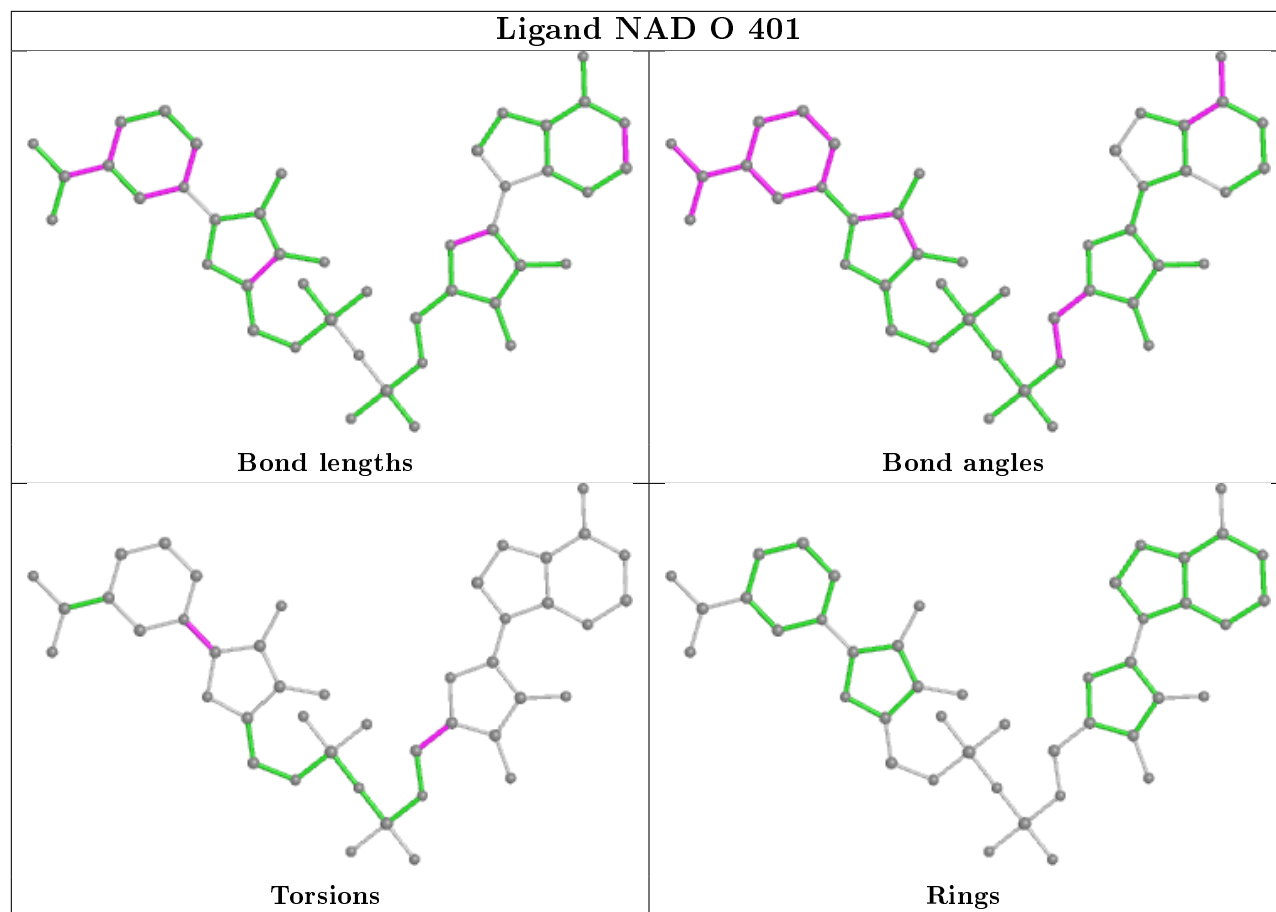
16 monomers are involved in 45 short contacts:

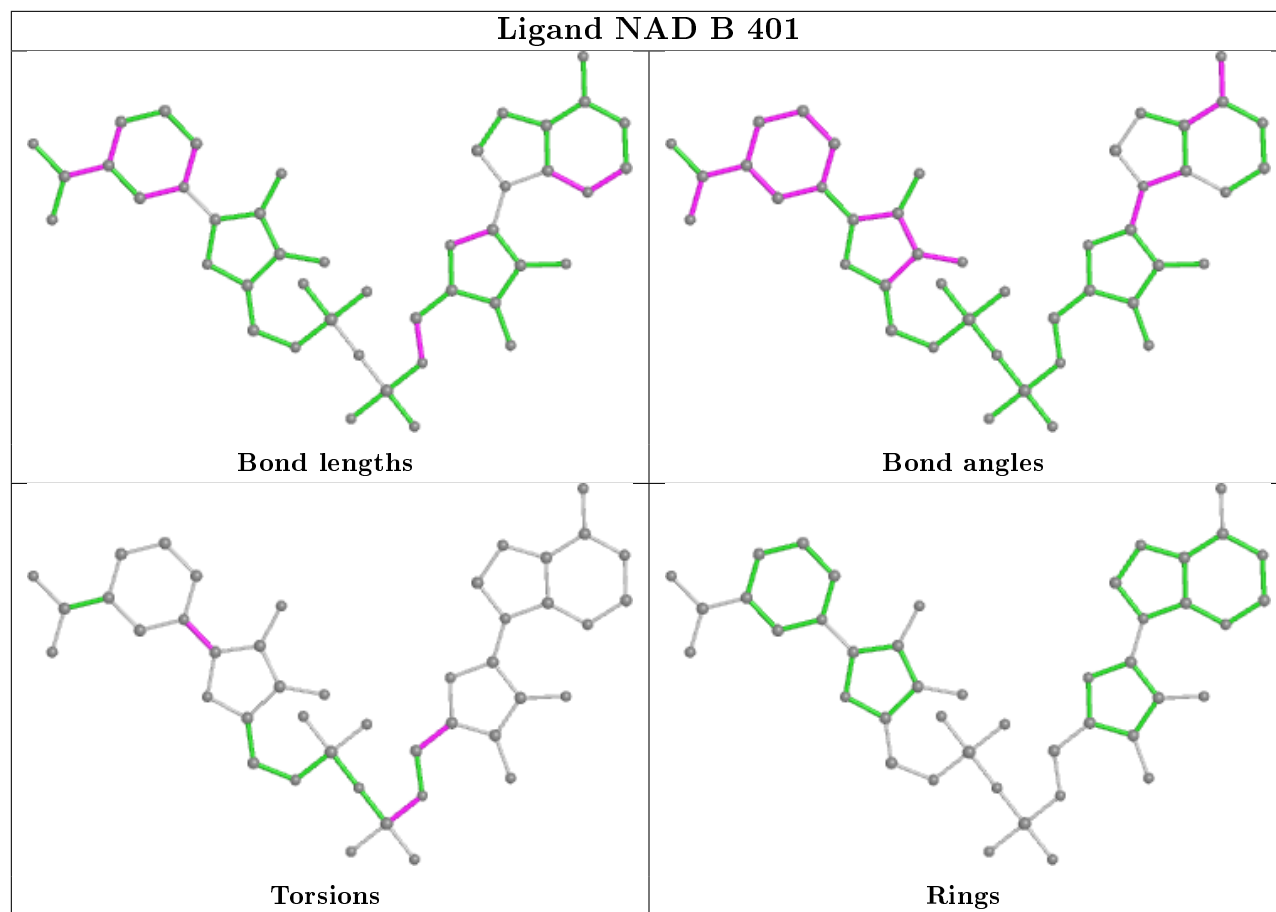
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	SO4	1	0
3	H	401	NAD	13	0
4	E	403	SO4	1	0
4	E	402	SO4	1	0
4	Q	404	SO4	1	0
4	A	406	SO4	1	0
4	D	402	SO4	1	0
3	E	401	NAD	5	0
3	B	401	NAD	1	0
3	Q	401	NAD	1	0
3	F	401	NAD	6	0
3	A	401	NAD	3	0
3	C	401	NAD	2	0
4	C	404	SO4	1	0
3	D	401	NAD	6	0
3	G	401	NAD	1	0

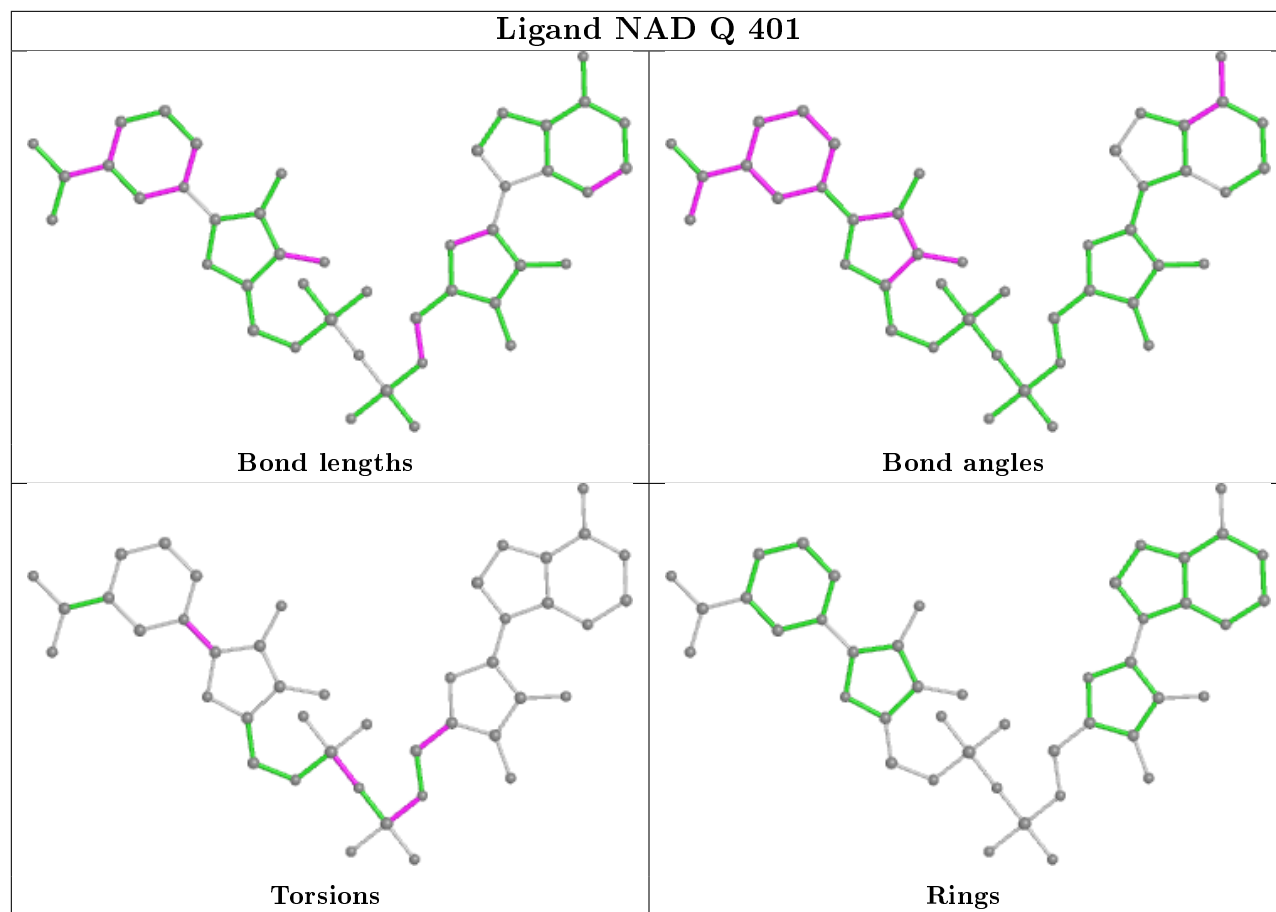
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

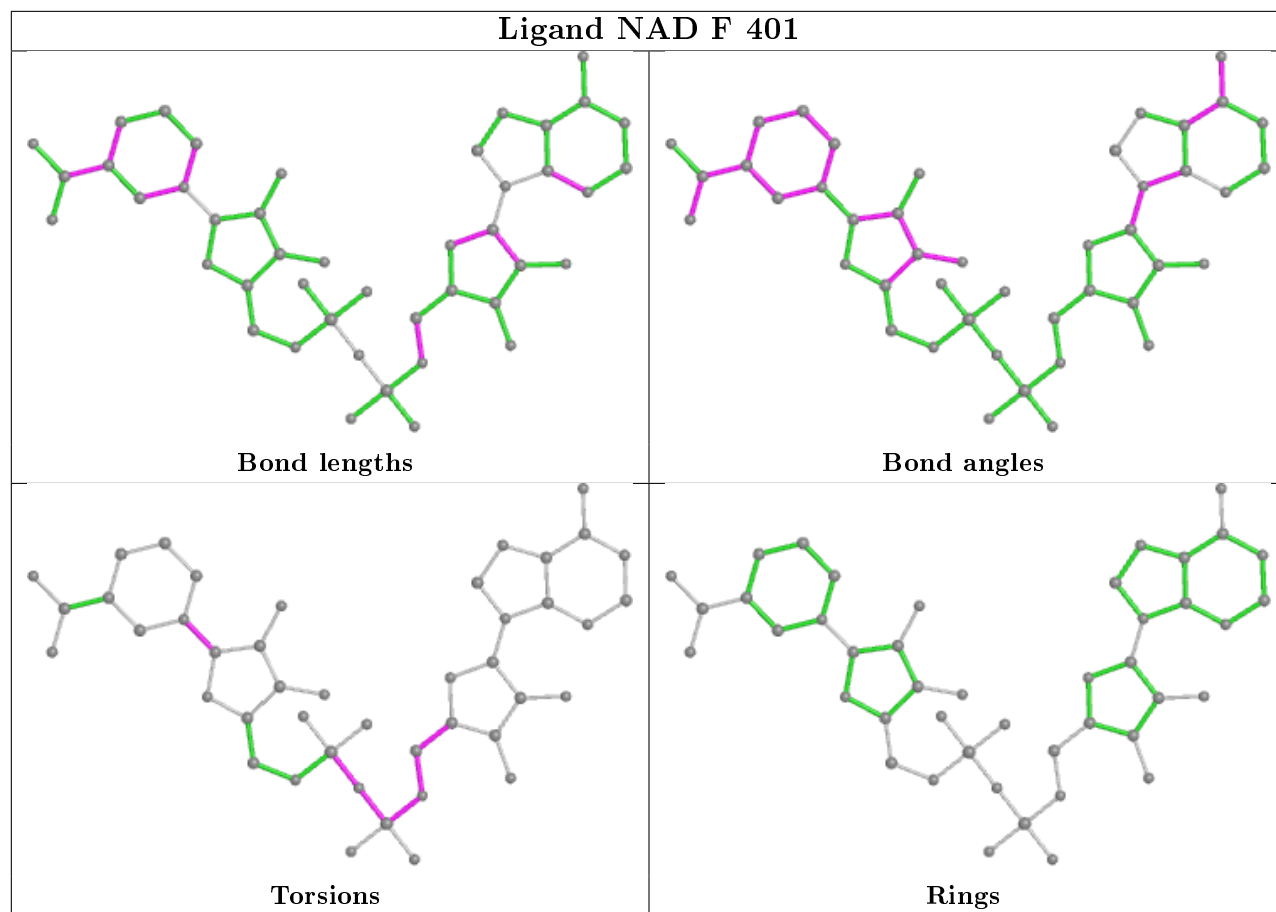


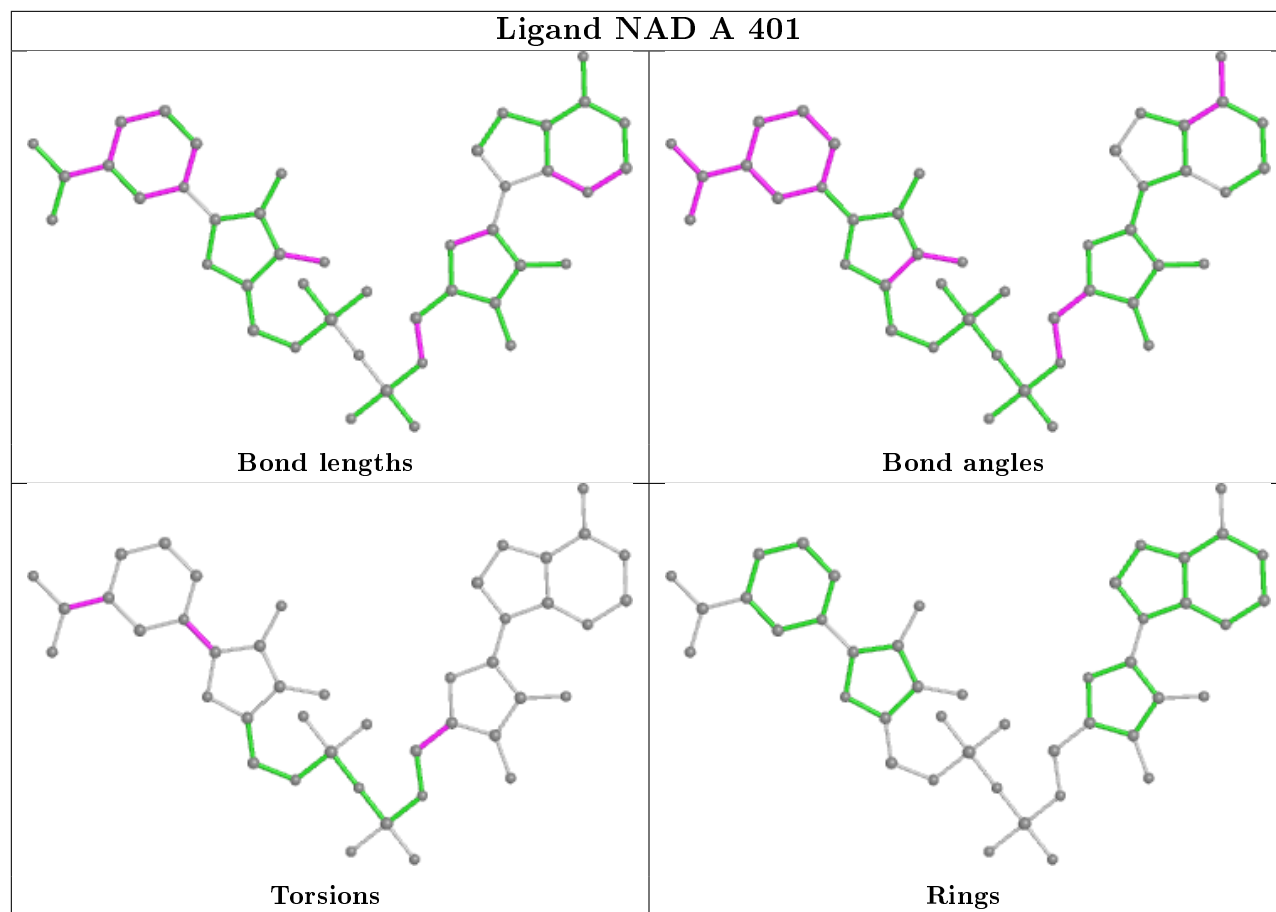


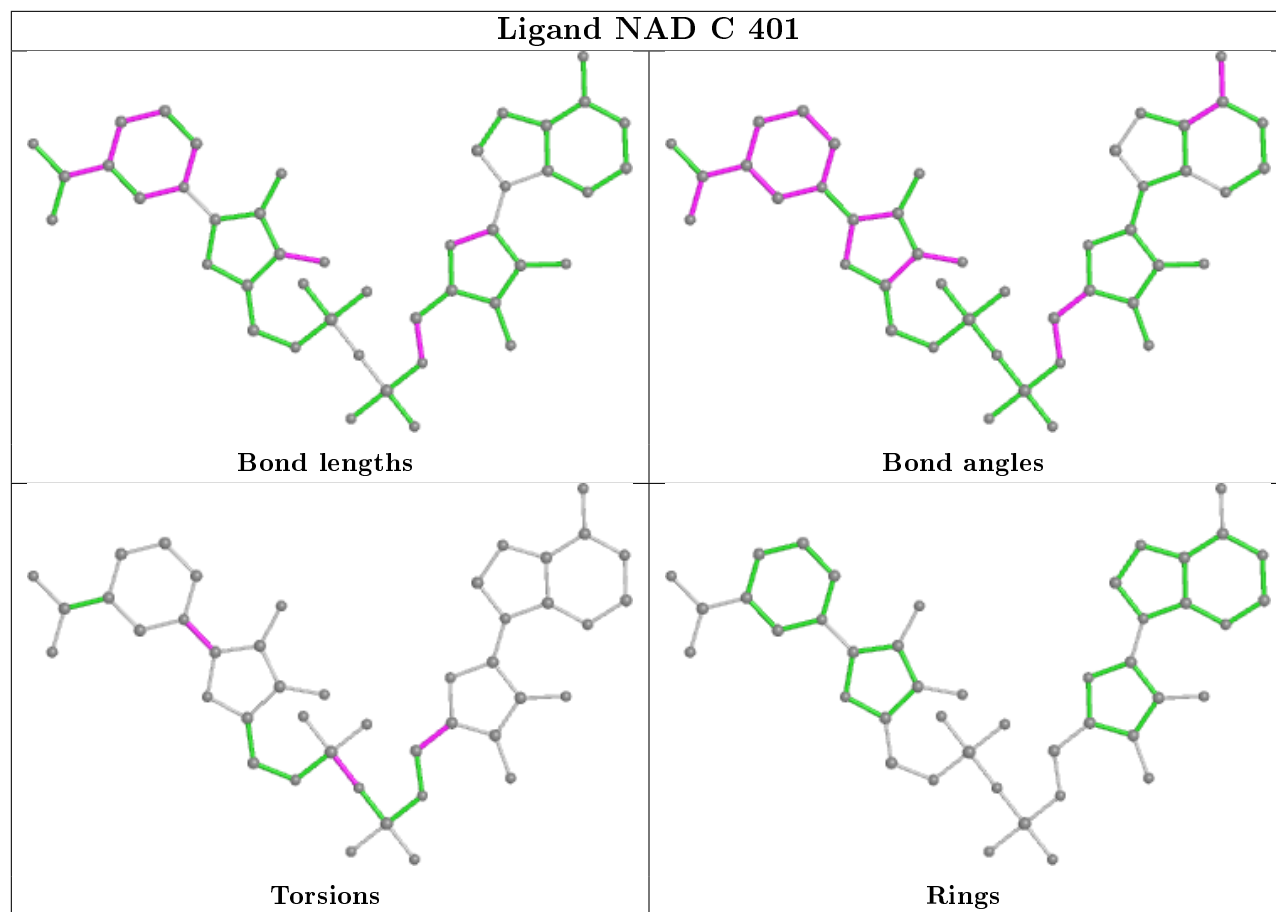


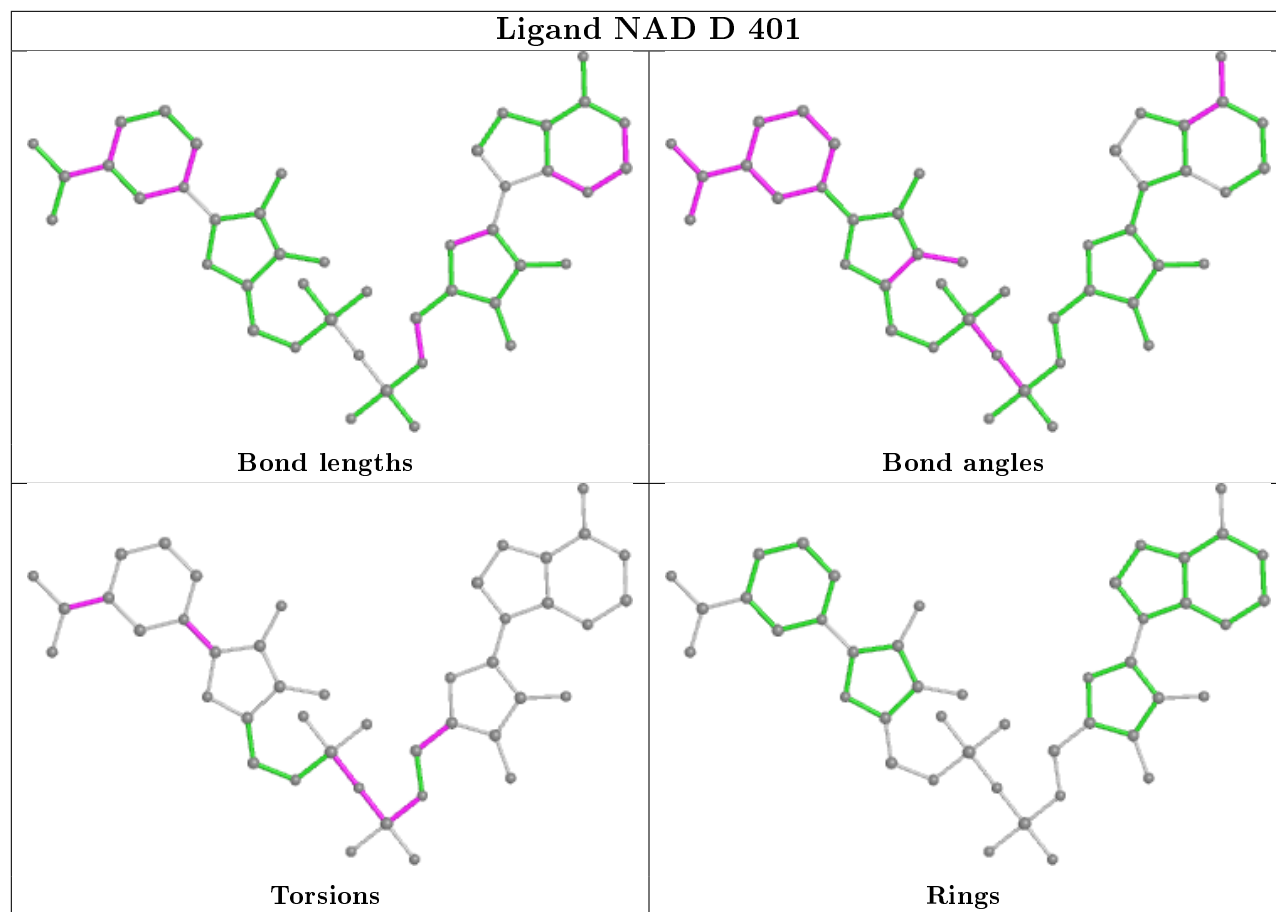


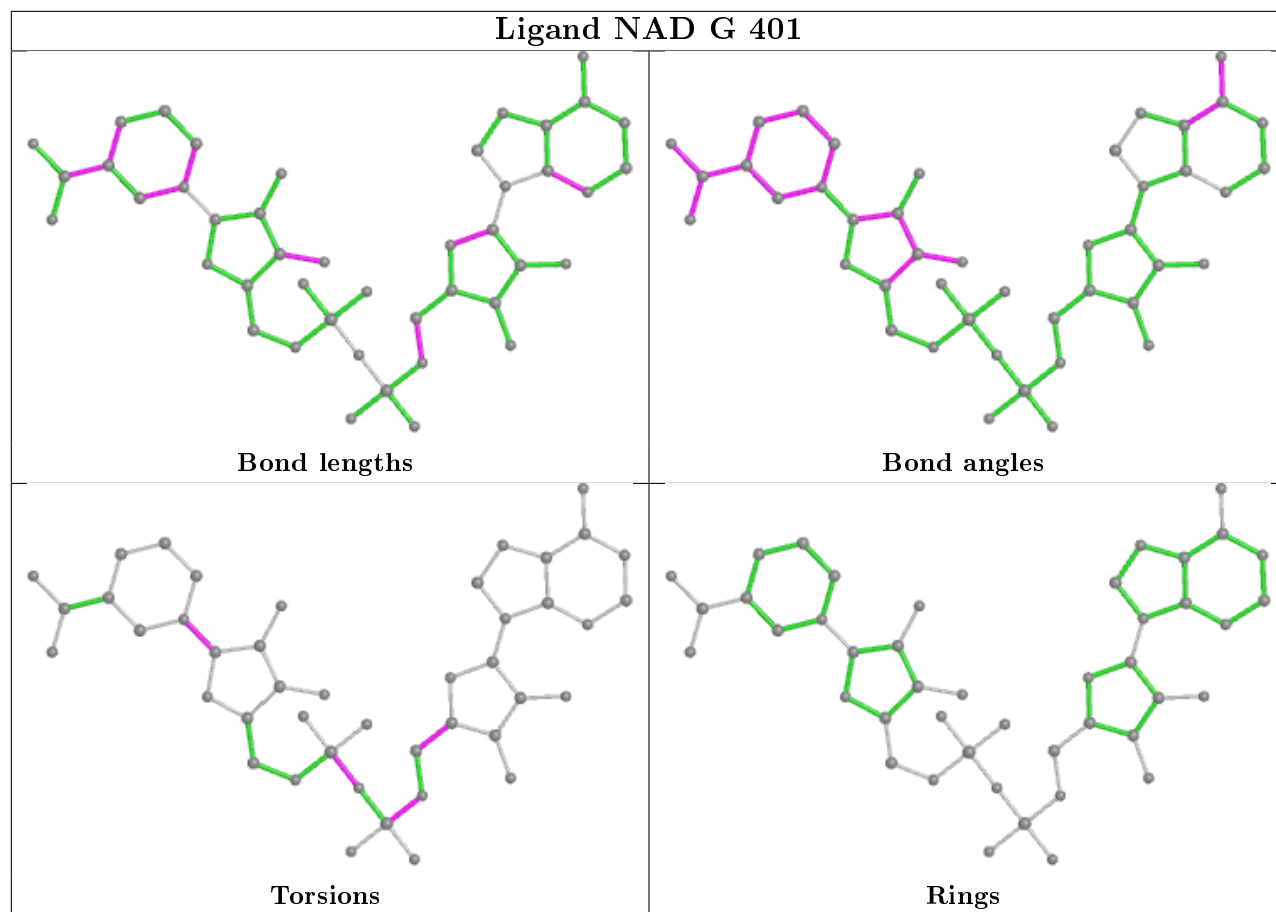












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/337 (99%)	0.24	4 (1%) 79 80	32, 50, 71, 80	0
1	B	336/337 (99%)	0.46	9 (2%) 54 55	37, 58, 81, 95	0
1	C	336/337 (99%)	0.53	14 (4%) 36 35	39, 57, 76, 95	0
1	D	336/337 (99%)	0.70	22 (6%) 18 17	50, 80, 97, 116	0
1	E	336/337 (99%)	1.73	120 (35%) 0 0	62, 87, 108, 113	0
1	F	336/337 (99%)	1.07	59 (17%) 1 1	46, 83, 102, 118	0
1	G	337/337 (100%)	0.70	23 (6%) 17 15	38, 66, 89, 98	0
1	H	335/337 (99%)	0.88	35 (10%) 6 4	51, 83, 109, 115	0
1	O	337/337 (100%)	0.31	0 100 100	17, 31, 47, 54	0
1	Q	336/337 (99%)	0.19	0 100 100	20, 37, 54, 74	0
2	I	22/82 (26%)	0.96	3 (13%) 3 2	76, 81, 88, 93	0
2	J	21/82 (25%)	0.69	2 (9%) 8 6	66, 75, 86, 91	0
2	K	21/82 (25%)	4.37	21 (100%) 0 0	9, 24, 31, 31	21 (100%)
2	L	19/82 (23%)	4.70	19 (100%) 0 0	38, 51, 70, 76	19 (100%)
2	M	22/82 (26%)	1.31	3 (13%) 3 2	64, 76, 98, 107	0
2	N	19/82 (23%)	2.24	8 (42%) 0 0	67, 81, 85, 86	19 (100%)
All	All	3485/3862 (90%)	0.74	342 (9%) 7 5	9, 64, 99, 118	59 (1%)

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	LEU	9.2
2	L	55	ASP	7.7
1	E	129	VAL	7.6
2	K	58	ASP	6.8
2	L	58	ASP	6.6

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Mol	Chain	Res	Type	RSRZ
2	K	70	THR	6.5
2	K	64	CYS	6.4
1	E	229	ALA	6.3
1	E	64	ILE	6.0
1	E	44	LEU	5.9
2	N	70	THR	5.9
1	E	28	ILE	5.7
2	K	59	PRO	5.6
1	E	15	PHE	5.6
1	E	1	LEU	5.6
2	K	67	ASN	5.4
1	G	269	GLY	5.2
1	E	79	PRO	5.1
2	L	60	LEU	5.1
2	K	61	GLU	5.1
1	E	300	MET	5.1
2	L	59	PRO	5.1
2	K	73	CYS	5.0
2	L	63	TYR	5.0
2	L	64	CYS	5.0
2	L	56	GLY	4.9
2	K	66	ASP	4.9
2	M	57	SER	4.9
2	K	63	TYR	4.9
1	E	37	VAL	4.8
2	K	68	PRO	4.8
2	N	68	PRO	4.8
1	H	143	ILE	4.8
2	L	65	LYS	4.7
2	K	62	GLU	4.7
2	L	57	SER	4.7
1	D	95	GLY	4.7
1	E	29	ALA	4.6
1	E	-1	ALA	4.5
2	L	66	ASP	4.5
1	F	267	LEU	4.5
2	L	61	GLU	4.4
2	L	70	THR	4.4
1	E	116	VAL	4.4
2	K	60	LEU	4.4
1	H	57	VAL	4.4
1	E	212	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	333	LYS	4.4
1	E	55	ALA	4.4
2	L	73	CYS	4.3
1	E	143	ILE	4.3
1	E	328	VAL	4.3
1	H	89	ILE	4.3
2	L	71	ASN	4.3
1	E	118	ILE	4.2
1	H	225	LEU	4.2
1	E	100	VAL	4.2
2	L	62	GLU	4.2
1	C	332	TRP	4.1
1	E	98	VAL	4.1
1	E	53	PHE	4.1
1	E	187	ALA	4.1
1	E	114	LYS	4.0
1	E	157	PHE	4.0
1	E	158	VAL	4.0
2	K	76	TYR	3.9
1	E	258	ALA	3.9
1	G	305	VAL	3.8
1	E	171	THR	3.8
2	L	69	GLU	3.8
1	A	187	ALA	3.8
1	H	187	ALA	3.8
1	E	154	LEU	3.7
2	L	72	GLU	3.7
1	C	265	LYS	3.7
1	C	37	VAL	3.7
1	E	179	THR	3.6
1	E	21	LYS	3.6
2	L	67	ASN	3.6
1	E	324	LEU	3.6
1	E	292	ILE	3.6
1	F	315	TRP	3.6
1	E	310	TRP	3.6
1	G	274	CYS	3.5
2	K	69	GLU	3.5
1	H	84	TRP	3.5
2	N	60	LEU	3.5
2	M	78	ASN	3.5
2	K	78	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	57	VAL	3.4
1	E	273	VAL	3.4
1	G	244	VAL	3.4
1	F	278	LEU	3.4
1	H	227	GLY	3.4
1	F	218	LEU	3.4
1	F	87	LEU	3.4
1	D	329	ALA	3.4
1	F	43	LEU	3.4
1	H	119	THR	3.4
1	E	193	LEU	3.3
1	E	267	LEU	3.3
1	E	325	ALA	3.3
1	B	271	LEU	3.3
1	H	44	LEU	3.3
1	E	270	ILE	3.3
1	E	66	VAL	3.3
1	E	48	SER	3.2
1	D	128	TYR	3.2
1	F	296	LEU	3.2
1	E	7	GLY	3.2
1	G	130	VAL	3.2
1	G	254	GLU	3.2
1	D	332	TRP	3.2
2	N	69	GLU	3.2
1	F	237	VAL	3.2
1	H	228	ILE	3.2
1	E	204	VAL	3.2
1	E	109	ILE	3.2
1	E	322	VAL	3.2
1	F	322	VAL	3.2
2	L	68	PRO	3.2
1	E	228	ILE	3.1
2	N	59	PRO	3.1
1	F	299	VAL	3.1
2	K	65	LYS	3.1
1	F	268	LYS	3.1
1	E	24	PRO	3.1
1	E	317	TYR	3.1
1	G	-1	ALA	3.1
1	E	203	ILE	3.1
1	F	10	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	199	ALA	3.0
1	C	333	LYS	3.0
1	E	108	HIS	3.0
1	E	56	ASP	3.0
1	D	136	ALA	3.0
1	F	28	ILE	2.9
1	E	284	ARG	2.9
1	E	18(A)	TRP	2.9
2	K	77	ASP	2.9
1	F	5	ILE	2.9
1	F	259	PHE	2.9
1	G	273	VAL	2.9
1	H	128	TYR	2.9
2	K	72	GLU	2.9
1	H	157	PHE	2.8
1	C	88	GLY	2.8
1	F	332	TRP	2.8
1	G	160	VAL	2.8
1	H	24	PRO	2.8
1	G	225	LEU	2.8
1	D	137	TYR	2.8
1	F	56	ASP	2.8
1	E	50	LEU	2.8
1	F	252	ALA	2.8
1	E	138	SER	2.8
1	F	46	TYR	2.8
1	E	230	LEU	2.8
1	H	25	LEU	2.7
1	H	193	LEU	2.7
1	E	101	ASP	2.7
1	E	161	LEU	2.7
1	F	27	ILE	2.7
1	E	33	THR	2.7
1	F	164	LYS	2.7
1	D	53	PHE	2.7
1	F	128	TYR	2.7
1	E	206	THR	2.7
1	E	250	THR	2.7
1	F	153	CYS	2.7
1	E	74	VAL	2.7
1	E	81	LEU	2.7
1	E	84	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	84	TRP	2.7
1	F	167	ILE	2.7
1	F	286	SER	2.7
1	G	247	SER	2.7
1	F	330	ASN	2.6
1	F	288	PHE	2.6
1	C	91	ILE	2.6
1	H	28	ILE	2.6
1	F	312	ASP	2.6
1	E	211	ALA	2.6
1	E	259	PHE	2.6
1	F	261	ASP	2.6
1	E	78	ASN	2.6
2	N	61	GLU	2.6
1	C	84	TRP	2.6
1	F	311	TYR	2.6
1	E	183	ARG	2.6
1	D	119	THR	2.6
1	E	27	ILE	2.6
1	F	52	ILE	2.6
1	D	263	ALA	2.6
1	E	311	TYR	2.6
2	K	71	ASN	2.5
1	C	5	ILE	2.5
1	E	196	ALA	2.5
2	K	74	ARG	2.5
1	H	117	ILE	2.5
1	E	243	VAL	2.5
1	E	255	VAL	2.5
1	F	57	VAL	2.5
1	E	5	ILE	2.5
1	E	329	ALA	2.5
1	E	321	VAL	2.5
1	F	266	GLU	2.5
1	B	333	LYS	2.5
1	E	85	LYS	2.5
1	E	61	GLU	2.5
1	D	100	VAL	2.5
1	D	130	VAL	2.5
1	E	31	ASN	2.5
1	E	140	ASP	2.5
1	E	320	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	292	ILE	2.5
1	G	170	GLY	2.4
1	C	87	LEU	2.4
1	D	161	LEU	2.4
1	E	43	LEU	2.4
1	F	262	SER	2.4
1	E	127	THR	2.4
1	H	147	ALA	2.4
1	H	188	SER	2.4
1	E	59	PRO	2.4
1	D	267	LEU	2.4
1	H	332	TRP	2.4
1	C	25	LEU	2.4
1	D	89	ILE	2.4
1	F	273	VAL	2.4
1	E	283	PHE	2.4
1	F	111	ALA	2.4
1	A	89	ILE	2.4
1	C	322	VAL	2.4
1	E	278	LEU	2.4
1	E	14	ASN	2.4
1	F	89	ILE	2.4
1	H	191	ARG	2.4
1	E	298	MET	2.4
1	F	155	ALA	2.4
1	F	307	VAL	2.4
1	F	108	HIS	2.3
1	G	161	LEU	2.3
1	F	269	GLY	2.3
1	D	118	ILE	2.3
1	E	327	ILE	2.3
1	E	128	TYR	2.3
1	F	45	LYS	2.3
1	F	326	ASP	2.3
1	B	263	ALA	2.3
2	I	57	SER	2.3
2	K	75	THR	2.3
1	B	292	ILE	2.3
1	A	139	HIS	2.3
1	H	108	HIS	2.3
1	E	80	SER	2.3
1	E	76	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	83	PRO	2.3
1	H	185	LEU	2.3
1	C	89	ILE	2.3
1	H	116	VAL	2.3
1	C	36	GLY	2.3
1	H	315	TRP	2.3
1	E	96	THR	2.3
1	H	64	ILE	2.3
1	D	129	VAL	2.3
1	D	170	GLY	2.3
1	G	304	MET	2.3
1	E	314	GLU	2.3
1	E	182	GLN	2.2
1	B	161	LEU	2.2
1	D	184	LEU	2.2
1	G	216	LEU	2.2
1	G	128	TYR	2.2
1	E	275	ASP	2.2
1	F	112	GLY	2.2
1	H	144	ILE	2.2
1	G	201	LEU	2.2
2	J	60	LEU	2.2
1	E	30	ILE	2.2
1	F	70	ILE	2.2
1	F	146	ASN	2.2
1	G	221	LEU	2.2
1	H	42	HIS	2.2
1	E	99	PHE	2.2
1	H	63	ALA	2.2
1	E	144	ILE	2.2
1	D	28	ILE	2.2
1	E	245	GLN	2.2
1	E	231	ARG	2.2
1	B	240	VAL	2.2
1	E	89	ILE	2.2
1	E	117	ILE	2.2
1	E	246	VAL	2.2
1	F	130	VAL	2.2
1	E	92	VAL	2.1
1	B	139	HIS	2.1
2	M	60	LEU	2.1
1	E	67	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	241	ASP	2.1
2	I	77	ASP	2.1
1	F	300	MET	2.1
1	E	249	LYS	2.1
1	H	27	ILE	2.1
2	J	76	TYR	2.1
2	N	76	TYR	2.1
1	B	230	LEU	2.1
1	B	251	PHE	2.1
1	G	163	GLN	2.1
1	G	129	VAL	2.1
1	G	270	ILE	2.1
1	E	287	ASP	2.1
1	E	58	LYS	2.1
1	E	216	LEU	2.1
1	F	271	LEU	2.1
1	H	186	ASP	2.1
1	A	206	THR	2.1
1	F	0	LYS	2.1
1	E	82	LEU	2.1
1	E	106	GLY	2.1
1	F	14	ASN	2.1
1	D	154	LEU	2.1
1	E	39	GLN	2.1
1	E	77	ARG	2.1
1	F	82	LEU	2.1
1	H	218	LEU	2.1
1	D	117	ILE	2.1
1	F	270	ILE	2.1
1	E	46	TYR	2.1
2	N	66	ASP	2.1
1	F	255	VAL	2.0
1	D	325	ALA	2.0
1	H	113	ALA	2.0
1	E	318	SER	2.0
1	H	60	SER	2.0
1	C	50	LEU	2.0
2	I	60	LEU	2.0
1	G	268	LYS	2.0
1	F	242	LEU	2.0
1	E	12	GLY	2.0
1	E	151	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	8	PHE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

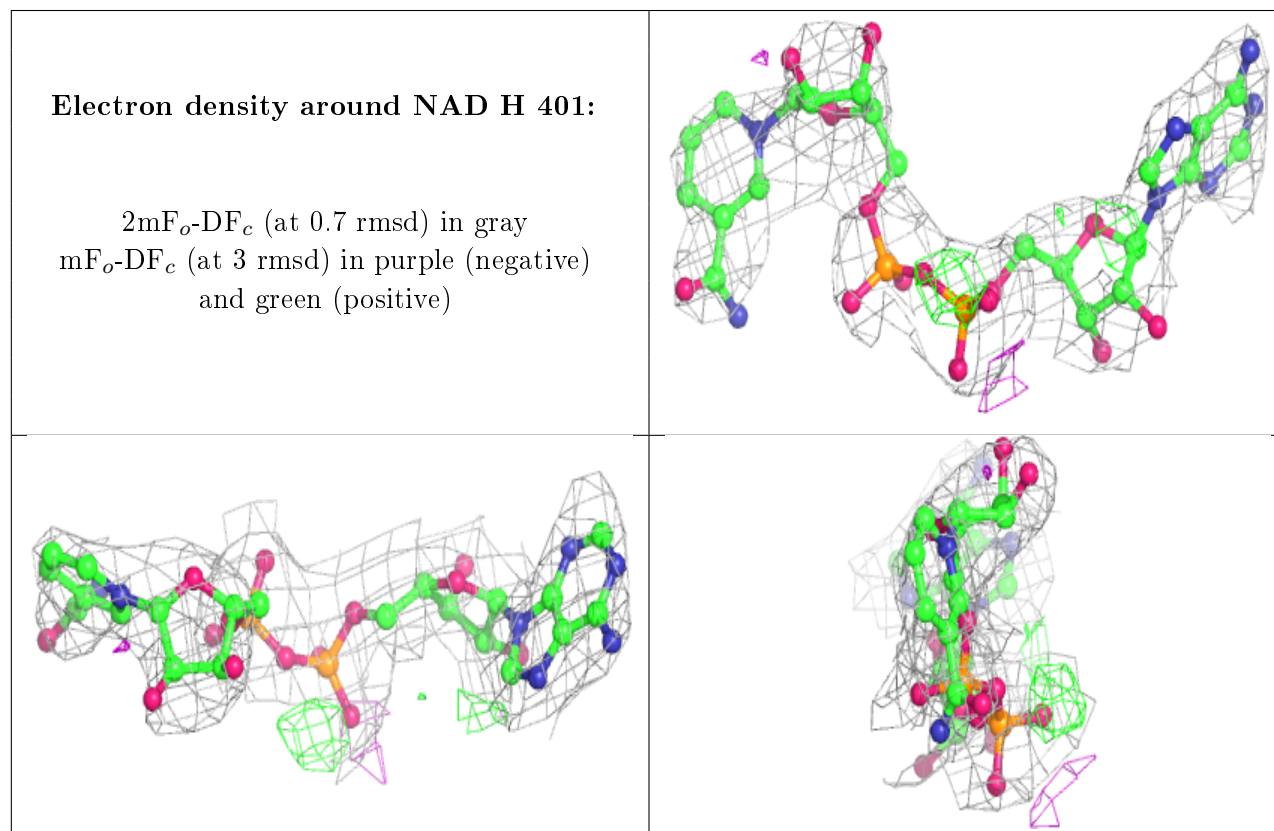
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	Q	404	5/5	0.79	0.33	50,51,52,52	5
4	SO4	D	402	5/5	0.80	0.25	44,45,46,47	5
4	SO4	B	403	5/5	0.80	0.48	61,62,63,64	5
4	SO4	G	402	5/5	0.80	0.33	54,54,55,55	5
4	SO4	E	403	5/5	0.84	0.20	58,58,59,60	5
4	SO4	A	408	5/5	0.85	0.24	69,70,70,71	5
4	SO4	Q	405	5/5	0.86	0.29	80,81,81,82	5
4	SO4	B	402	5/5	0.86	0.23	52,52,53,53	5
3	NAD	H	401	44/44	0.87	0.25	100,103,104,104	0
4	SO4	O	403	5/5	0.88	0.41	48,48,49,49	5
4	SO4	C	406	5/5	0.89	0.25	42,43,44,45	5
4	SO4	E	402	5/5	0.89	0.27	79,80,81,81	5
4	SO4	A	407	5/5	0.90	0.27	46,47,48,48	5
4	SO4	H	402	5/5	0.90	0.23	90,91,91,92	0
4	SO4	Q	403	5/5	0.90	0.25	50,50,50,52	5
4	SO4	E	404	5/5	0.91	0.11	72,72,73,74	5
4	SO4	C	404	5/5	0.91	0.22	69,69,70,70	5
4	SO4	C	405	5/5	0.92	0.21	68,69,70,70	5
4	SO4	F	403	5/5	0.92	0.16	78,79,79,80	5
4	SO4	O	402	5/5	0.92	0.29	38,38,40,41	5
3	NAD	D	401	44/44	0.92	0.24	70,76,81,81	0
3	NAD	E	401	44/44	0.92	0.25	87,90,92,94	0

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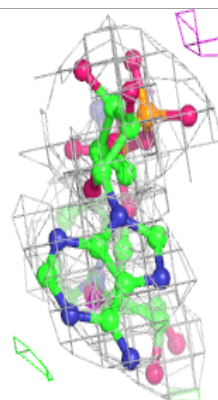
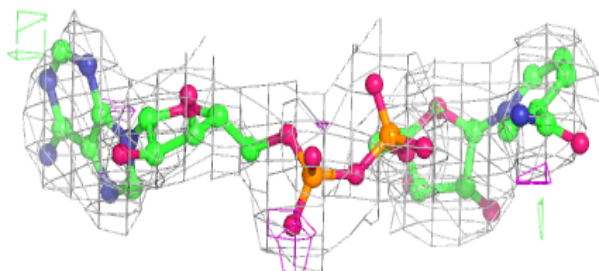
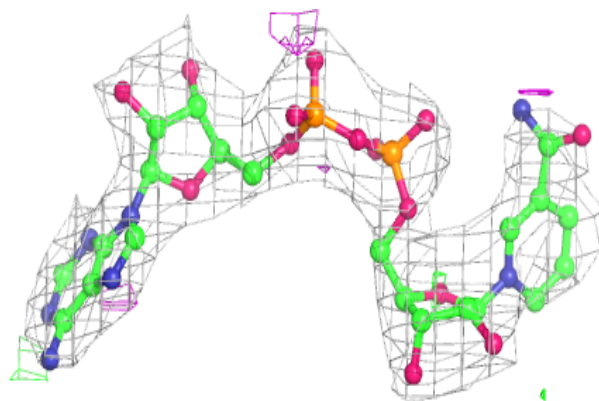
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAD	F	401	44/44	0.94	0.20	70,73,76,77	0
4	SO4	F	402	5/5	0.94	0.18	89,89,90,90	0
4	SO4	A	403	5/5	0.95	0.16	82,82,83,83	0
4	SO4	A	406	5/5	0.95	0.15	63,64,65,65	5
4	SO4	C	402	5/5	0.95	0.20	85,86,87,87	0
3	NAD	A	401	44/44	0.95	0.18	51,54,57,60	0
4	SO4	A	405	5/5	0.96	0.20	75,75,76,76	0
4	SO4	Q	402	5/5	0.96	0.20	80,80,80,81	0
3	NAD	B	401	44/44	0.96	0.20	52,57,59,60	0
3	NAD	C	401	44/44	0.96	0.18	50,55,58,60	0
3	NAD	Q	401	44/44	0.97	0.21	32,39,41,44	0
3	NAD	G	401	44/44	0.97	0.20	40,47,52,54	0
4	SO4	C	403	5/5	0.98	0.15	70,70,71,71	0
3	NAD	O	401	44/44	0.98	0.21	20,26,30,33	0
4	SO4	A	404	5/5	0.98	0.18	58,60,60,61	0
4	SO4	A	402	5/5	0.98	0.19	74,74,75,76	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.

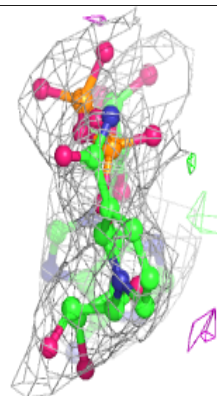
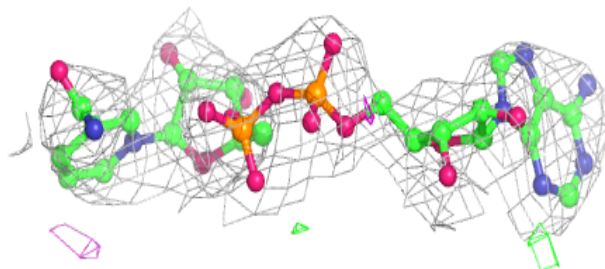
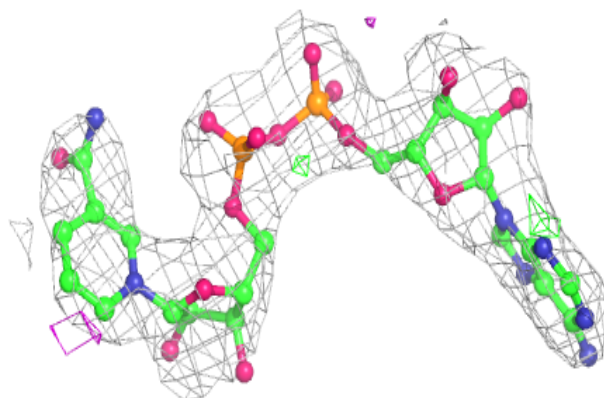


Electron density around NAD D 401:

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

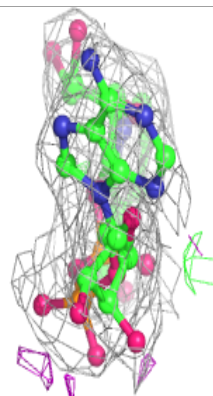
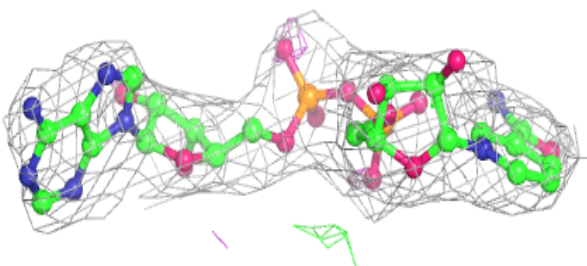
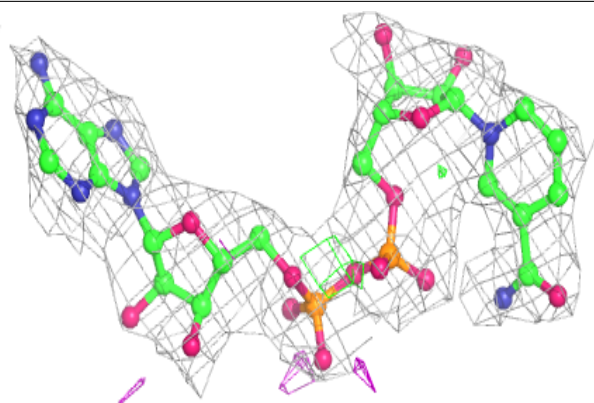
**Electron density around NAD E 401:**

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

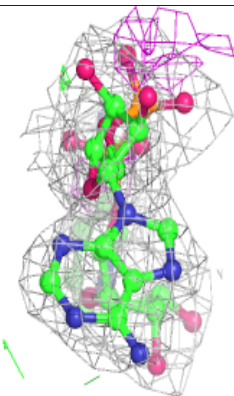
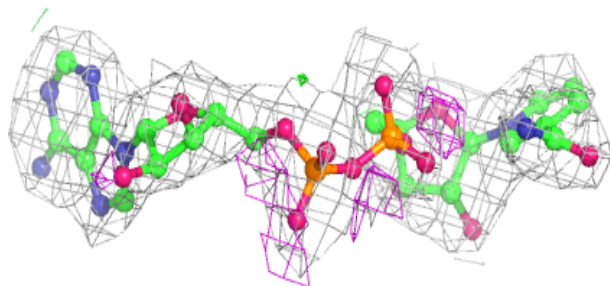
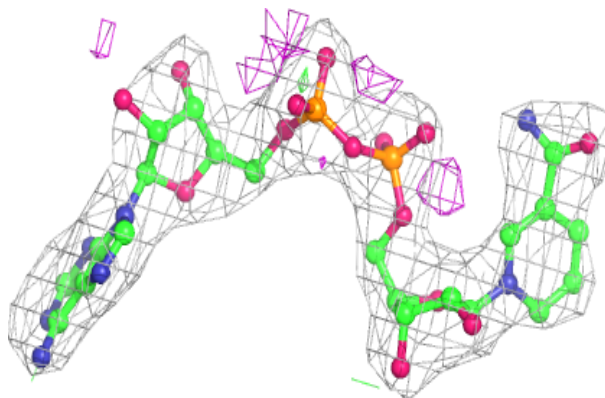


Electron density around NAD F 401:

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

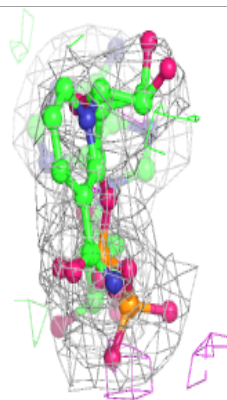
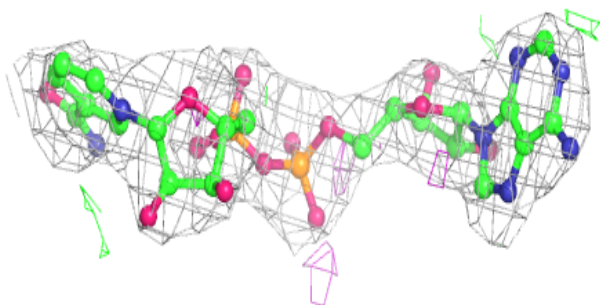
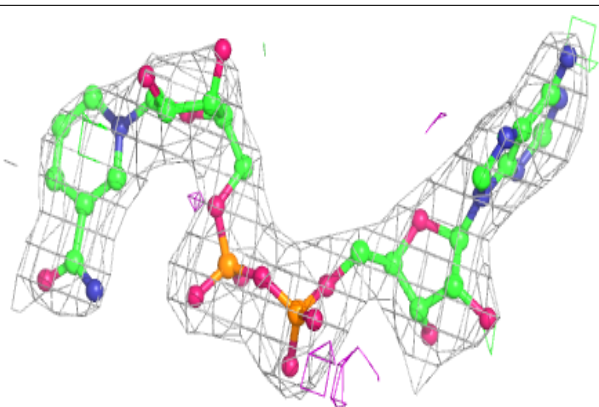
**Electron density around NAD A 401:**

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

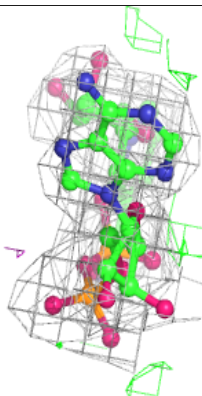
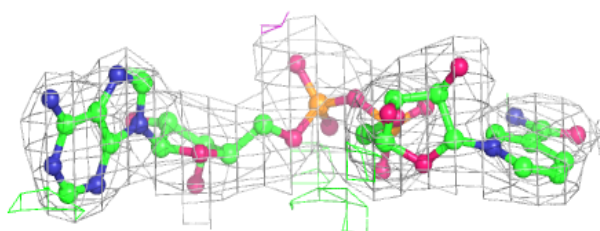
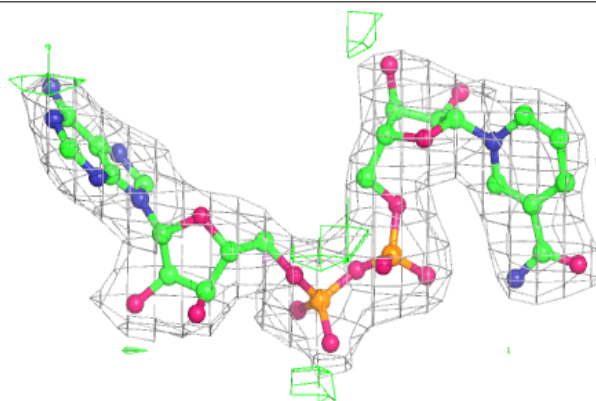


Electron density around NAD B 401:

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

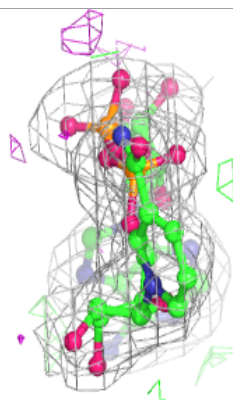
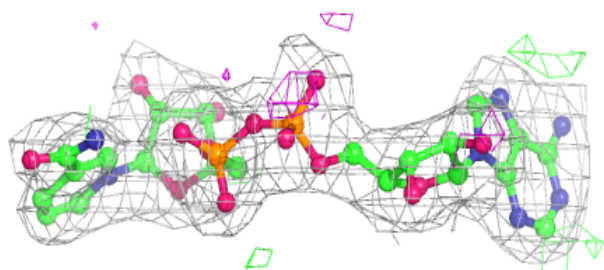
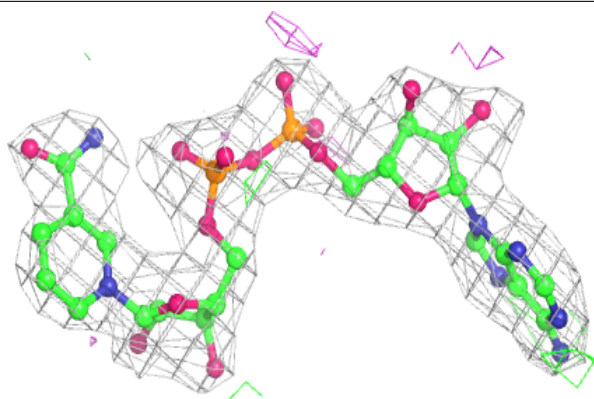
**Electron density around NAD C 401:**

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

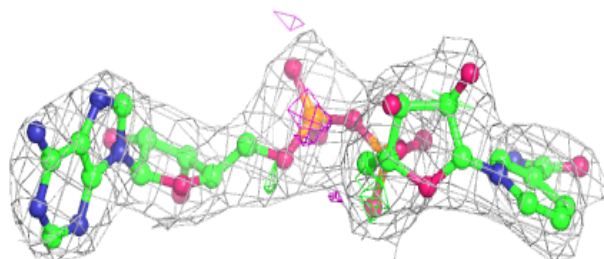
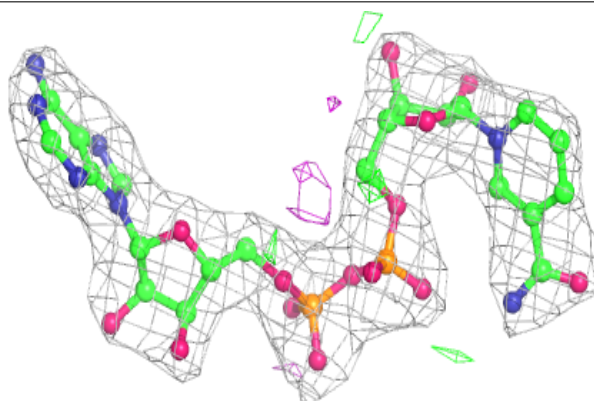


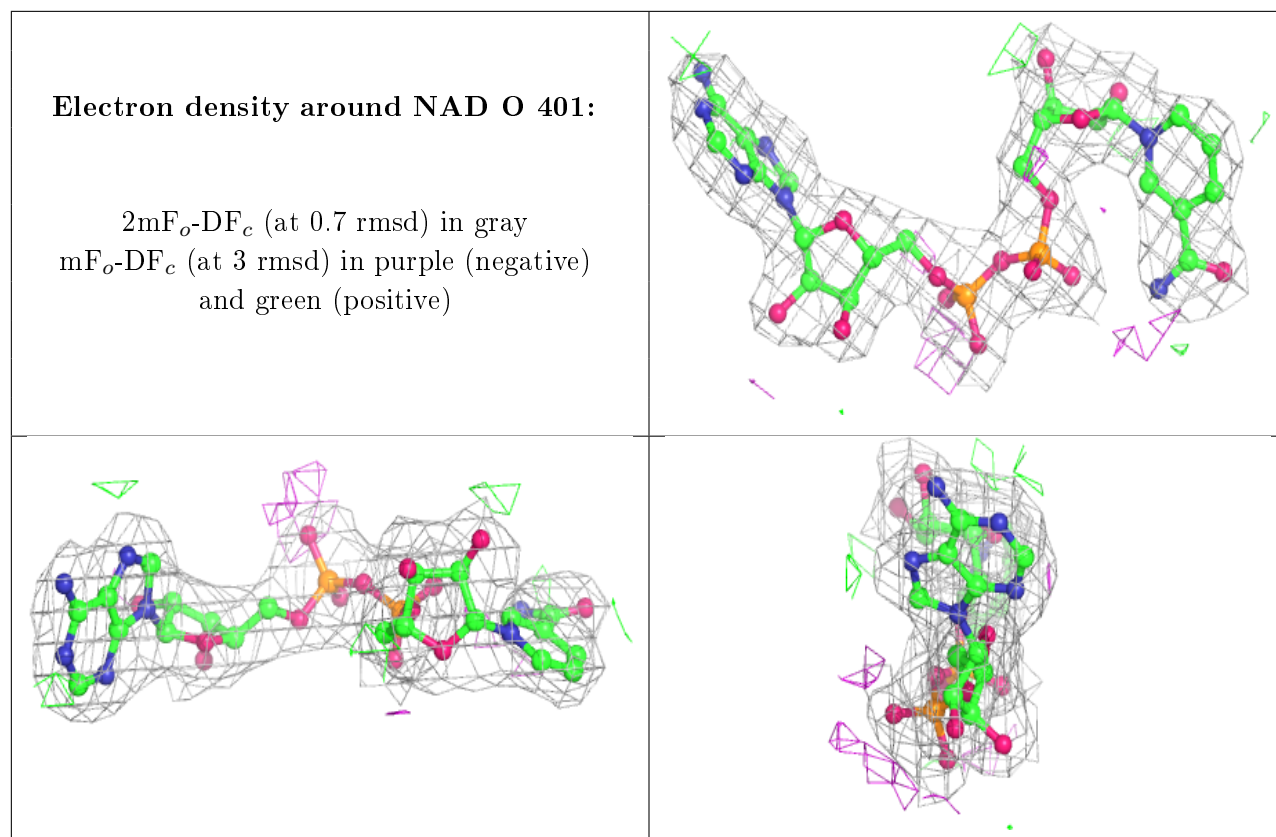
Electron density around NAD Q 401:

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

**Electron density around NAD G 401:**

$2mF_o-DF_c$ (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.