



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:23 PM GMT

PDB ID : 1FDV  
Title : HUMAN 17-BETA-HYDROXYSTEROID-DEHYDROGENASE TYPE 1  
MUTANT H221L COMPLEXED WITH NAD+  
Authors : Mazza, C.; Breton, R.; Housset, D.; Fontecilla-Camps, J.-C.  
Deposited on : 1998-01-15  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

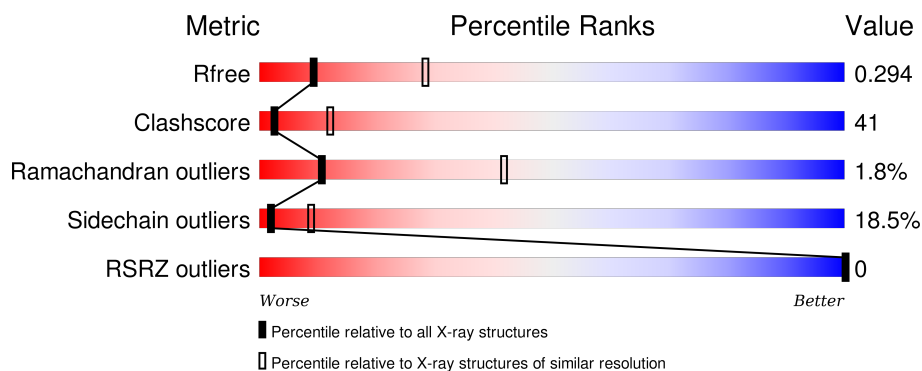
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>29%</div> <div>42%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>
1	B	327	<div> <div>30%</div> <div>40%</div> <div>13%</div> <div>•</div> <div>16%</div> </div>
1	C	327	<div> <div>25%</div> <div>46%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>
1	D	327	<div> <div>28%</div> <div>40%</div> <div>14%</div> <div>•</div> <div>16%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAD	A	361	X	-	-	-
3	NAD	B	364	X	-	-	X
3	NAD	D	362	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8812 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.

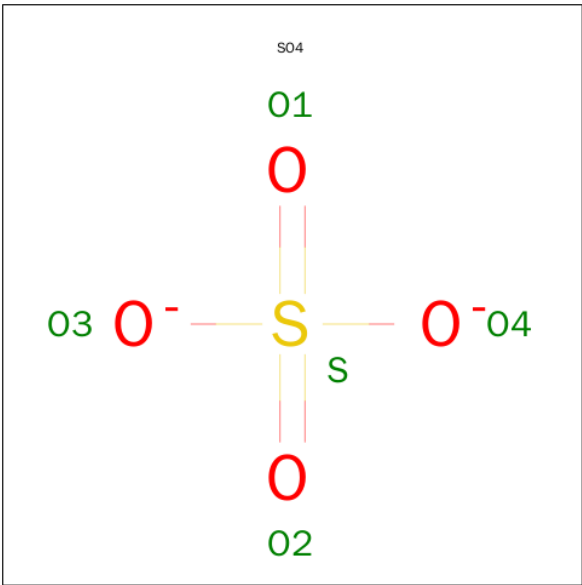
- Molecule 1 is a protein called 17-BETA-HYDROXYSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2179	1384	384	399	12			
1	B	275	Total	C	N	O	S	0	0	0
			2104	1334	373	386	11			
1	C	285	Total	C	N	O	S	0	0	0
			2179	1384	384	399	12			
1	D	275	Total	C	N	O	S	0	0	0
			2104	1334	373	386	11			

There are 8 discrepancies between the modelled and reference sequences:

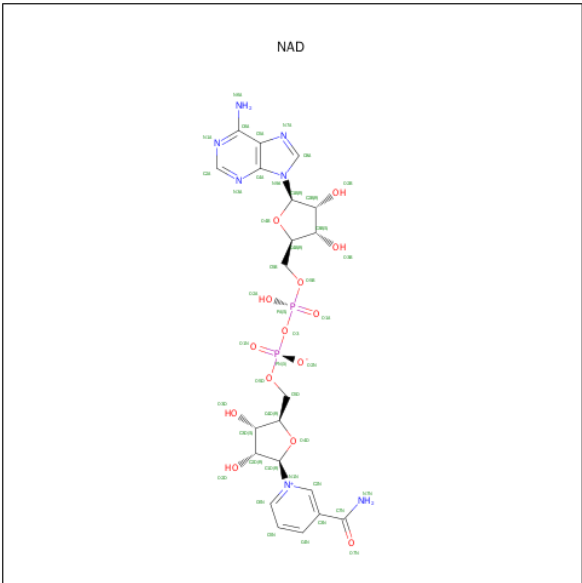
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	HIS	ENGINEERED	UNP P14061
A	301	ARG	ALA	CONFLICT	UNP P14061
B	221	LEU	HIS	ENGINEERED	UNP P14061
B	301	ARG	ALA	CONFLICT	UNP P14061
C	221	LEU	HIS	ENGINEERED	UNP P14061
C	301	ARG	ALA	CONFLICT	UNP P14061
D	221	LEU	HIS	ENGINEERED	UNP P14061
D	301	ARG	ALA	CONFLICT	UNP P14061

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

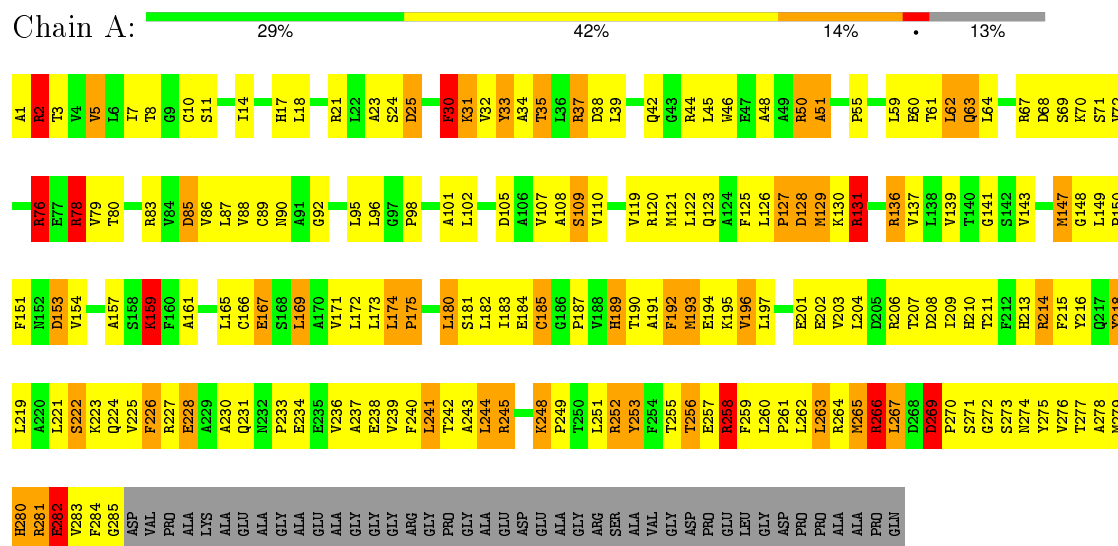
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	11	Total	O	0	0
			11	11		
4	C	18	Total	O	0	0
			18	18		
4	D	13	Total	O	0	0
			13	13		

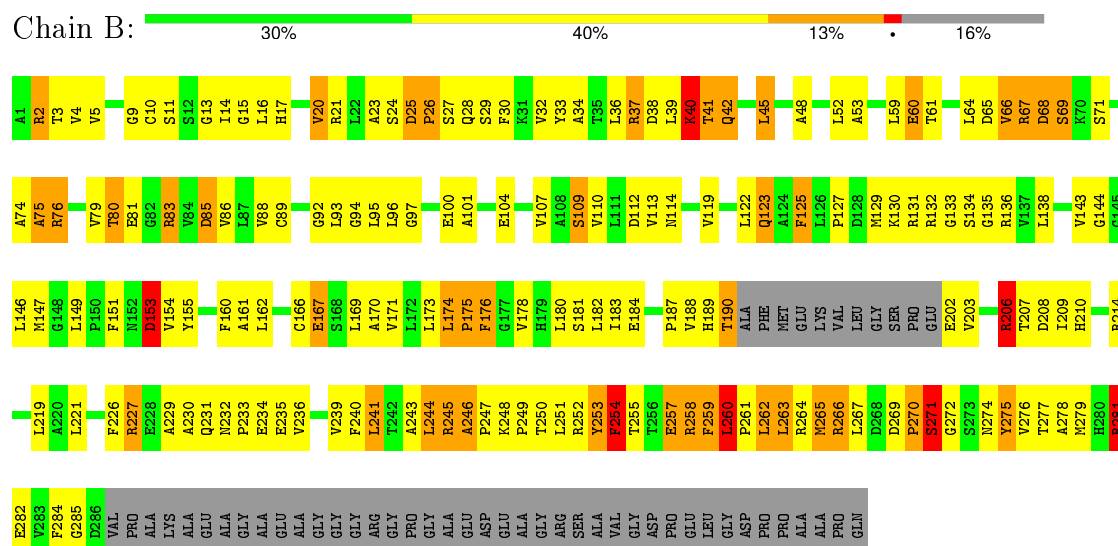
### 3 Residue-property plots

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

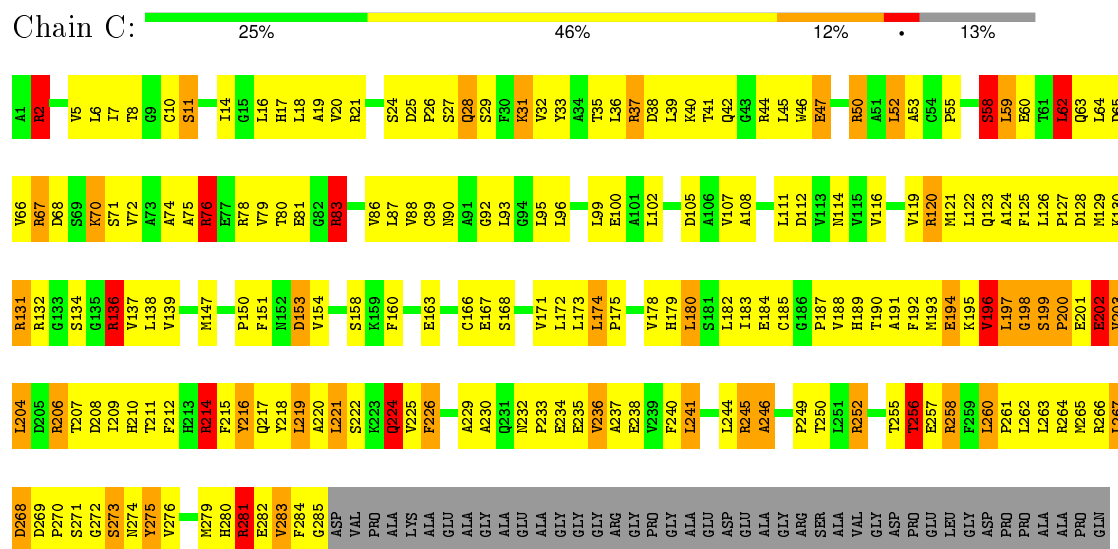
#### • Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE



#### • Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE



#### • Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.12Å 79.11Å 120.47Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.0 (10.00-3.10) 85.2 (10.00-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.36 (at 2.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.219 , 0.295 0.218 , 0.294	Depositor DCC
$R_{free}$ test set	1618 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 58.3	EDS
Estimated twinning fraction	0.001 for l,k,-h 0.018 for h,-k,-l 0.117 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 36231 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.87	0/2219	1.99	55/3010 (1.8%)
1	B	0.88	1/2141 (0.0%)	1.98	52/2904 (1.8%)
1	C	0.90	1/2219 (0.0%)	2.02	57/3010 (1.9%)
1	D	0.85	0/2141	1.92	56/2904 (1.9%)
All	All	0.88	2/8720 (0.0%)	1.98	220/11828 (1.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	GLU	CD-OE2	5.27	1.31	1.25
1	C	58	SER	CA-CB	5.04	1.60	1.52

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	ARG	NE-CZ-NH2	-18.13	111.23	120.30
1	B	2	ARG	NE-CZ-NH2	-17.50	111.55	120.30
1	C	136	ARG	NE-CZ-NH2	-17.47	111.57	120.30
1	C	2	ARG	NE-CZ-NH1	16.72	128.66	120.30
1	B	2	ARG	NE-CZ-NH1	16.30	128.45	120.30
1	A	78	ARG	NE-CZ-NH1	16.23	128.41	120.30
1	A	37	ARG	NE-CZ-NH2	-15.91	112.35	120.30
1	D	2	ARG	NE-CZ-NH2	-15.71	112.45	120.30
1	D	136	ARG	NE-CZ-NH2	-15.45	112.57	120.30
1	B	83	ARG	NE-CZ-NH1	14.90	127.75	120.30
1	C	2	ARG	CD-NE-CZ	14.37	143.72	123.60
1	B	37	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	A	76	ARG	NE-CZ-NH2	-14.26	113.17	120.30
1	C	67	ARG	CD-NE-CZ	14.09	143.32	123.60
1	C	120	ARG	NE-CZ-NH2	-13.89	113.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	C	37	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	B	2	ARG	CD-NE-CZ	13.23	142.12	123.60
1	A	252	ARG	NE-CZ-NH2	-13.21	113.70	120.30
1	A	76	ARG	NE-CZ-NH1	12.92	126.76	120.30
1	A	78	ARG	CD-NE-CZ	12.65	141.30	123.60
1	C	120	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	C	2	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	D	214	ARG	CD-NE-CZ	12.15	140.61	123.60
1	C	83	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	A	136	ARG	NE-CZ-NH1	-12.11	114.25	120.30
1	B	264	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	A	78	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	B	214	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	B	25	ASP	CB-CG-OD1	-11.24	108.18	118.30
1	A	25	ASP	CB-CG-OD1	-11.20	108.22	118.30
1	A	37	ARG	NE-CZ-NH1	11.09	125.85	120.30
1	C	78	ARG	NE-CZ-NH2	10.92	125.76	120.30
1	D	266	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	B	67	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	C	252	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	A	136	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	B	281	ARG	CA-CB-CG	10.64	136.82	113.40
1	B	281	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	A	136	ARG	NH1-CZ-NH2	10.36	130.79	119.40
1	D	214	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	B	83	ARG	CD-NE-CZ	10.17	137.84	123.60
1	B	214	ARG	CD-NE-CZ	10.14	137.79	123.60
1	B	258	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	C	136	ARG	NE-CZ-NH1	9.89	125.24	120.30
1	C	44	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	C	206	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	C	120	ARG	CD-NE-CZ	9.43	136.80	123.60
1	A	50	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	D	136	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	C	67	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	76	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	214	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	D	37	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	B	281	ARG	CD-NE-CZ	8.82	135.95	123.60
1	C	76	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	A	258	ARG	N-CA-CB	8.56	126.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ARG	CG-CD-NE	8.36	129.36	111.80
1	B	37	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	D	89	CYS	CA-CB-SG	-8.27	99.12	114.00
1	C	281	ARG	CD-NE-CZ	8.24	135.13	123.60
1	D	21	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	282	GLU	N-CA-CB	8.15	125.28	110.60
1	C	199	SER	CB-CA-C	8.14	125.58	110.10
1	D	227	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	C	245	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	D	214	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	B	227	ARG	N-CA-CB	7.86	124.75	110.60
1	A	37	ARG	CD-NE-CZ	7.84	134.58	123.60
1	A	192	PHE	CB-CA-C	7.81	126.02	110.40
1	A	253	TYR	CB-CG-CD2	7.71	125.62	121.00
1	C	76	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	265	MET	CA-CB-CG	-7.62	100.34	113.30
1	D	37	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	85	ASP	CB-CG-OD1	-7.54	111.52	118.30
1	C	281	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	A	253	TYR	CB-CG-CD1	-7.46	116.53	121.00
1	D	76	ARG	CD-NE-CZ	7.41	133.97	123.60
1	B	258	ARG	CD-NE-CZ	7.34	133.88	123.60
1	C	258	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	A	76	ARG	CD-NE-CZ	7.29	133.80	123.60
1	A	214	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	A	245	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	A	33	TYR	CB-CG-CD1	7.16	125.29	121.00
1	C	153	ASP	CB-CG-OD2	6.99	124.59	118.30
1	D	40	LYS	CA-CB-CG	6.99	128.77	113.40
1	D	164	GLY	O-C-N	6.95	133.82	122.70
1	C	44	ARG	NH1-CZ-NH2	-6.91	111.80	119.40
1	C	196	VAL	C-N-CA	6.90	138.95	121.70
1	D	104	GLU	OE1-CD-OE2	-6.90	115.02	123.30
1	A	196	VAL	N-CA-C	6.85	129.50	111.00
1	C	204	LEU	CA-CB-CG	6.85	131.06	115.30
1	B	75	ALA	N-CA-CB	6.84	119.68	110.10
1	C	206	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	D	50	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	A	197	LEU	CB-CA-C	-6.65	97.57	110.20
1	B	206	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	120	ARG	CD-NE-CZ	6.60	132.84	123.60
1	A	283	VAL	CA-CB-CG2	-6.60	101.01	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	D	281	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	51	ALA	CB-CA-C	6.48	119.83	110.10
1	A	120	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	245	ARG	CD-NE-CZ	6.47	132.66	123.60
1	D	29	SER	N-CA-CB	-6.45	100.82	110.50
1	D	260	LEU	CB-CA-C	6.45	122.45	110.20
1	D	227	ARG	CG-CD-NE	-6.41	98.34	111.80
1	A	228	GLU	OE1-CD-OE2	6.32	130.89	123.30
1	B	125	PHE	N-CA-C	6.30	128.01	111.00
1	C	58	SER	CB-CA-C	-6.28	98.17	110.10
1	C	194	GLU	CB-CA-C	6.27	122.94	110.40
1	C	192	PHE	N-CA-CB	-6.27	99.31	110.60
1	D	167	GLU	OE1-CD-OE2	6.26	130.82	123.30
1	C	275	TYR	CB-CG-CD1	-6.25	117.25	121.00
1	A	131	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	C	37	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	202	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	B	83	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	C	62	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	245	ARG	CD-NE-CZ	6.08	132.11	123.60
1	C	216	TYR	CB-CA-C	6.06	122.51	110.40
1	C	214	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	D	78	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	D	250	THR	CA-CB-CG2	-6.02	103.97	112.40
1	A	25	ASP	OD1-CG-OD2	6.00	134.71	123.30
1	C	38	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	B	266	ARG	CD-NE-CZ	-6.00	115.20	123.60
1	A	280	HIS	CA-CB-CG	-5.95	103.48	113.60
1	D	211	THR	CA-CB-CG2	-5.95	104.07	112.40
1	B	253	TYR	CB-CG-CD2	5.95	124.57	121.00
1	A	85	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	78	ARG	CB-CA-C	5.83	122.06	110.40
1	D	282	GLU	C-N-CA	5.82	136.26	121.70
1	B	210	HIS	CA-CB-CG	-5.81	103.72	113.60
1	A	108	ALA	CA-C-N	5.81	129.98	117.20
1	C	78	ARG	CG-CD-NE	5.80	123.99	111.80
1	D	123	GLN	CA-CB-CG	5.80	126.17	113.40
1	D	21	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	183	ILE	CB-CA-C	-5.77	100.05	111.60
1	B	190	THR	N-CA-CB	5.76	121.24	110.30
1	A	63	GLN	CG-CD-OE1	5.72	133.05	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	258	ARG	CD-NE-CZ	5.69	131.56	123.60
1	D	247	PRO	N-CA-CB	5.67	110.11	103.30
1	D	76	ARG	NH1-CZ-NH2	5.67	125.63	119.40
1	D	108	ALA	CB-CA-C	5.67	118.60	110.10
1	D	2	ARG	NH1-CZ-NH2	5.66	125.62	119.40
1	D	76	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	78	ARG	CA-CB-CG	5.64	125.81	113.40
1	C	224	GLN	CB-CA-C	5.64	121.68	110.40
1	B	270	PRO	N-CA-CB	5.62	110.05	103.30
1	B	167	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	B	246	ALA	N-CA-CB	5.61	117.95	110.10
1	B	125	PHE	CA-C-N	5.57	129.46	117.20
1	D	2	ARG	CA-CB-CG	5.57	125.65	113.40
1	B	40	LYS	CA-CB-CG	5.55	125.61	113.40
1	C	44	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	D	83	ARG	C-N-CA	5.52	135.50	121.70
1	D	208	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	B	153	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	B	245	ARG	CB-CA-C	5.50	121.41	110.40
1	A	62	LEU	CA-CB-CG	5.48	127.90	115.30
1	D	33	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	D	67	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	89	CYS	CA-CB-SG	-5.45	104.20	114.00
1	B	231	GLN	CA-CB-CG	5.44	125.36	113.40
1	A	48	ALA	O-C-N	5.44	131.40	122.70
1	D	153	ASP	CA-CB-CG	-5.43	101.45	113.40
1	C	50	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	C	112	ASP	CB-CG-OD1	-5.43	113.42	118.30
1	C	256	THR	N-CA-C	-5.43	96.34	111.00
1	B	68	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	B	206	ARG	CD-NE-CZ	5.41	131.18	123.60
1	D	116	VAL	C-N-CA	5.41	133.67	122.30
1	A	159	LYS	CB-CA-C	5.41	121.22	110.40
1	D	93	LEU	CB-CA-C	-5.41	99.92	110.20
1	B	160	PHE	CA-CB-CG	5.39	126.84	113.90
1	D	50	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	D	265	MET	CA-CB-CG	-5.34	104.21	113.30
1	C	268	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	D	275	TYR	CB-CG-CD2	5.32	124.19	121.00
1	A	270	PRO	N-CA-CB	5.32	109.68	103.30
1	A	185	CYS	CA-CB-SG	5.31	123.56	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	ARG	CD-NE-CZ	-5.30	116.18	123.60
1	B	175	PRO	N-CA-CB	5.29	109.64	103.30
1	C	28	GLN	CB-CA-C	5.29	120.97	110.40
1	D	237	ALA	O-C-N	-5.27	114.26	122.70
1	A	153	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	C	93	LEU	CA-C-O	-5.26	109.06	120.10
1	C	200	PRO	O-C-N	5.25	131.09	122.70
1	B	271	SER	O-C-N	-5.24	114.30	123.20
1	B	60	GLU	OE1-CD-OE2	5.23	129.58	123.30
1	C	93	LEU	CB-CA-C	-5.22	100.28	110.20
1	C	47	GLU	N-CA-CB	-5.22	101.21	110.60
1	C	197	LEU	N-CA-CB	5.21	120.82	110.40
1	C	112	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	254	PHE	N-CA-CB	5.20	119.96	110.60
1	A	269	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	31	LYS	CB-CA-C	5.18	120.76	110.40
1	C	246	ALA	CB-CA-C	-5.17	102.34	110.10
1	B	23	ALA	CB-CA-C	5.16	117.84	110.10
1	B	26	PRO	N-CA-CB	5.15	109.48	103.30
1	A	10	CYS	CA-C-N	5.12	128.48	117.20
1	A	128	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	B	275	TYR	CB-CA-C	-5.12	100.16	110.40
1	A	23	ALA	N-CA-CB	5.11	117.25	110.10
1	B	85	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	D	176	PHE	CA-C-N	5.11	126.41	116.20
1	D	281	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	211	THR	CA-CB-OG1	5.10	119.70	109.00
1	A	30	PHE	CB-CA-C	-5.09	100.22	110.40
1	C	112	ASP	OD1-CG-OD2	5.09	132.96	123.30
1	B	260	LEU	N-CA-CB	5.08	120.56	110.40
1	D	227	ARG	CB-CA-C	-5.06	100.28	110.40
1	D	232	ASN	CB-CA-C	-5.06	100.29	110.40
1	D	275	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	266	ARG	CA-C-O	5.03	130.66	120.10
1	B	127	PRO	N-CA-CB	5.03	109.33	103.30
1	D	166	CYS	CB-CA-C	5.03	120.45	110.40
1	D	153	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2179	0	2225	200	0
1	B	2104	0	2145	162	0
1	C	2179	0	2225	213	0
1	D	2104	0	2145	186	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	44	0	25	6	0
3	B	44	0	26	10	0
3	C	44	0	24	5	0
3	D	44	0	26	13	0
4	A	8	0	0	0	0
4	B	11	0	0	3	0
4	C	18	0	0	3	0
4	D	13	0	0	0	0
All	All	8812	0	8841	714	0

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 41.

All (714) 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:A:258:ARG:HB2	1:A:258:ARG:HH11	1.08	1.10
1:A:267:LEU:HB3	1:B:267:LEU:HB3	1.36	1.02
1:C:64:LEU:HD21	1:C:72:VAL:HG22	1.43	1.00
1:D:92:GLY:H	3:D:362:NAD:H3D	1.22	0.97
1:A:267:LEU:HA	1:B:267:LEU:HD22	1.44	0.96
1:A:31:LYS:HE3	1:A:60:GLU:HG3	1.47	0.95
3:D:362:NAD:N7N	3:D:362:NAD:O2N	1.99	0.95
1:D:42:GLN:NE2	1:D:46:TRP:HE1	1.66	0.92
1:D:92:GLY:N	3:D:362:NAD:H3D	1.83	0.92
1:A:42:GLN:HE21	1:A:46:TRP:HE1	1.18	0.92
1:B:2:ARG:NH1	1:B:83:ARG:HH12	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG21	1:A:244:LEU:HD11	1.51	0.91
1:C:2:ARG:HA	1:C:2:ARG:HE	1.38	0.88
1:A:89:CYS:HB2	1:A:139:VAL:HG22	1.54	0.88
1:B:187:PRO:HB3	1:B:226:PHE:CD1	2.09	0.86
1:B:92:GLY:HA3	3:B:364:NAD:H3D	1.57	0.85
1:C:174:LEU:HB3	1:C:175:PRO:CD	2.07	0.85
1:D:189:HIS:CE1	1:D:230:ALA:HB3	2.12	0.85
1:A:5:VAL:HG13	1:A:86:VAL:HB	1.61	0.83
1:A:42:GLN:NE2	1:A:46:TRP:HE1	1.76	0.83
1:B:37:ARG:HH21	3:B:364:NAD:H2B	1.42	0.83
1:C:131:ARG:CZ	1:D:208:ASP:HB3	2.09	0.83
1:C:16:LEU:HG	1:C:45:LEU:HD23	1.59	0.83
1:C:136:ARG:HH11	1:C:136:ARG:HG2	1.43	0.82
1:B:174:LEU:HB3	1:B:175:PRO:CD	2.10	0.80
1:D:279:MET:O	1:D:279:MET:HE3	1.82	0.80
1:C:214:ARG:HG3	1:C:284:PHE:CE1	2.17	0.79
1:D:14:ILE:HD12	1:D:236:VAL:HG11	1.64	0.79
1:B:147:MET:HG3	1:B:275:TYR:OH	1.81	0.79
3:A:361:NAD:H52N	3:A:361:NAD:H52A	1.63	0.79
1:A:258:ARG:HB2	1:A:258:ARG:NH1	1.93	0.78
1:A:45:LEU:HD11	1:A:59:LEU:HD21	1.64	0.78
1:D:241:LEU:HD23	1:D:245:ARG:HD3	1.65	0.78
1:B:260:LEU:N	1:B:261:PRO:HD2	2.00	0.77
1:A:1:ALA:O	1:A:2:ARG:HD2	1.84	0.77
1:B:66:VAL:HG22	3:B:364:NAD:N6A	1.99	0.77
1:C:100:GLU:HA	1:D:123:GLN:HG2	1.64	0.77
1:A:267:LEU:HB3	1:B:267:LEU:CB	2.12	0.77
1:D:89:CYS:HB2	1:D:139:VAL:HG22	1.67	0.77
1:D:279:MET:HE2	1:D:283:VAL:HG23	1.67	0.77
1:D:16:LEU:HG	1:D:45:LEU:HD23	1.67	0.76
1:A:67:ARG:NH1	1:A:109:SER:HB3	2.01	0.76
1:B:20:VAL:HG23	1:B:52:LEU:HD22	1.68	0.75
1:D:238:GLU:HA	1:D:238:GLU:OE1	1.86	0.75
1:A:123:GLN:HG2	1:B:100:GLU:HA	1.67	0.75
1:C:2:ARG:CZ	1:C:83:ARG:HH22	2.00	0.75
1:C:279:MET:HE1	1:C:282:GLU:HB3	1.68	0.75
1:A:185:CYS:HB2	3:A:361:NAD:H5N	1.69	0.74
1:D:136:ARG:NH2	1:D:246:ALA:O	2.16	0.73
1:B:76:ARG:HG3	1:B:125:PHE:CZ	2.23	0.73
1:D:20:VAL:HG23	1:D:52:LEU:HD22	1.71	0.73
1:D:244:LEU:HD12	1:D:244:LEU:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HA	1:D:102:LEU:HD12	1.69	0.72
1:C:266:ARG:HB3	1:C:267:LEU:HD23	1.72	0.72
1:B:86:VAL:HG21	1:B:244:LEU:HD21	1.70	0.72
1:A:280:HIS:CG	1:B:174:LEU:HD23	2.25	0.72
1:B:2:ARG:HH11	1:B:83:ARG:HH12	1.37	0.72
1:A:92:GLY:HA3	3:A:361:NAD:H3D	1.72	0.72
1:A:266:ARG:HB3	1:A:267:LEU:HD23	1.72	0.71
1:B:174:LEU:HB3	1:B:175:PRO:HD3	1.70	0.71
1:B:265:MET:HG3	1:B:266:ARG:N	2.04	0.71
1:C:189:HIS:CE1	1:C:230:ALA:HB3	2.25	0.71
1:D:9:GLY:HA2	3:D:362:NAD:H1B	1.72	0.71
1:A:122:LEU:HD21	1:A:137:VAL:HG11	1.73	0.71
1:C:174:LEU:HB3	1:C:175:PRO:HD2	1.74	0.70
1:D:35:THR:CG2	1:D:64:LEU:HB3	2.22	0.70
1:A:157:ALA:HB1	1:B:161:ALA:HB1	1.71	0.70
1:A:2:ARG:HE	1:A:83:ARG:HH22	1.40	0.70
1:D:66:VAL:HG22	3:D:362:NAD:N6A	2.07	0.70
1:C:267:LEU:HD13	1:D:267:LEU:HA	1.72	0.70
1:B:281:ARG:HH11	1:B:281:ARG:HG2	1.57	0.70
1:D:146:LEU:HD13	1:D:263:LEU:HD11	1.72	0.70
1:C:89:CYS:HB2	1:C:139:VAL:HG22	1.72	0.70
1:A:203:VAL:O	1:A:207:THR:HG22	1.93	0.69
1:C:99:LEU:HD12	1:C:102:LEU:HD12	1.75	0.69
1:A:257:GLU:HG2	1:A:260:LEU:HD22	1.74	0.69
1:D:279:MET:CE	1:D:283:VAL:HG23	2.23	0.69
1:B:92:GLY:CA	3:B:364:NAD:H3D	2.21	0.69
1:A:107:VAL:HG13	1:A:154:VAL:HG11	1.75	0.69
1:D:241:LEU:CD2	1:D:245:ARG:HD3	2.23	0.68
1:A:169:LEU:HD23	1:B:153:ASP:OD2	1.94	0.68
1:C:8:THR:O	1:C:90:ASN:HB3	1.94	0.68
1:B:76:ARG:HG3	1:B:125:PHE:CE2	2.28	0.68
1:B:67:ARG:NH1	1:B:109:SER:OG	2.27	0.68
1:C:221:LEU:CD1	1:C:283:VAL:HG22	2.24	0.68
1:C:86:VAL:HG21	1:C:244:LEU:HD11	1.75	0.68
3:B:364:NAD:O2N	3:B:364:NAD:H2N	1.94	0.68
1:C:45:LEU:HD11	1:C:59:LEU:HD11	1.75	0.68
1:D:20:VAL:HG23	1:D:52:LEU:CD2	2.24	0.68
1:A:21:ARG:NH2	1:A:241:LEU:HD11	2.09	0.67
1:C:131:ARG:NH2	1:D:208:ASP:HB3	2.09	0.67
1:C:221:LEU:HD12	1:C:283:VAL:HG22	1.77	0.67
1:C:131:ARG:NH2	4:C:502:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HD23	1:C:267:LEU:N	2.09	0.67
1:B:20:VAL:CG2	1:B:52:LEU:HD22	2.24	0.67
1:D:147:MET:CE	1:D:262:LEU:HG	2.25	0.67
1:A:267:LEU:CA	1:B:267:LEU:HD22	2.22	0.67
1:C:122:LEU:O	1:C:126:LEU:HB2	1.95	0.67
3:C:363:NAD:H51A	3:C:363:NAD:H52N	1.77	0.67
1:A:8:THR:HG22	1:A:64:LEU:HD13	1.76	0.67
1:C:2:ARG:HH22	1:C:81:GLU:HG2	1.60	0.66
1:A:234:GLU:O	1:A:237:ALA:HB3	1.95	0.66
1:C:120:ARG:NE	1:D:104:GLU:OE2	2.25	0.66
1:B:34:ALA:O	1:B:61:THR:HA	1.95	0.66
1:A:267:LEU:CB	1:B:267:LEU:HB3	2.18	0.66
1:C:71:SER:O	1:C:74:ALA:HB3	1.96	0.66
1:D:147:MET:HE3	1:D:262:LEU:HG	1.76	0.66
1:B:95:LEU:HB2	1:B:110:VAL:HG21	1.78	0.66
1:B:246:ALA:O	1:B:249:PRO:HG3	1.95	0.66
1:A:242:THR:HA	1:A:245:ARG:HE	1.61	0.66
1:A:280:HIS:CE1	1:B:175:PRO:HD3	2.31	0.66
1:D:35:THR:HG21	1:D:64:LEU:HD13	1.77	0.66
1:A:7:ILE:HG12	1:A:88:VAL:HB	1.78	0.66
1:D:130:LYS:HG2	1:D:176:PHE:CD2	2.31	0.65
1:C:272:GLY:O	1:C:276:VAL:HG23	1.94	0.65
1:A:267:LEU:N	1:A:267:LEU:HD23	2.11	0.65
1:B:187:PRO:HG2	1:B:229:ALA:HB3	1.78	0.65
1:A:210:HIS:O	1:A:213:HIS:HB3	1.96	0.65
1:C:55:PRO:O	1:C:58:SER:HB2	1.96	0.65
1:A:196:VAL:HG12	1:A:196:VAL:O	1.96	0.65
1:C:188:VAL:HG12	1:C:190:THR:HG23	1.78	0.65
1:A:38:ASP:HA	1:A:63:GLN:NE2	2.12	0.65
1:B:274:ASN:HD22	1:B:274:ASN:N	1.93	0.65
1:A:266:ARG:HH11	1:A:266:ARG:HG2	1.62	0.64
1:D:266:ARG:HH11	1:D:266:ARG:HG2	1.60	0.64
1:C:139:VAL:HG12	1:C:182:LEU:HD23	1.78	0.64
1:C:261:PRO:HG2	1:C:262:LEU:H	1.62	0.64
1:A:267:LEU:O	1:B:267:LEU:HD13	1.98	0.64
1:A:34:ALA:O	1:A:61:THR:HA	1.98	0.64
1:B:66:VAL:HG22	3:B:364:NAD:H62A	1.62	0.64
1:B:232:ASN:N	1:B:235:GLU:OE2	2.27	0.63
1:D:126:LEU:N	1:D:127:PRO:CD	2.61	0.63
1:A:267:LEU:HD13	1:B:267:LEU:HA	1.81	0.63
1:A:218:TYR:O	1:A:222:SER:OG	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:HD12	1:B:236:VAL:HB	1.79	0.63
1:A:263:LEU:O	1:A:267:LEU:HG	1.99	0.62
1:C:68:ASP:HB3	1:C:71:SER:HB2	1.81	0.62
1:A:266:ARG:HG2	1:A:267:LEU:HD23	1.80	0.62
1:D:35:THR:HG21	1:D:64:LEU:HB3	1.79	0.62
1:A:167:GLU:O	1:A:171:VAL:HG23	1.99	0.62
1:C:238:GLU:HA	1:C:241:LEU:CD1	2.29	0.62
1:C:86:VAL:CG2	1:C:244:LEU:HD11	2.30	0.62
1:C:260:LEU:O	1:C:263:LEU:HB3	2.00	0.62
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.65	0.62
1:C:197:LEU:O	1:C:198:GLY:O	2.18	0.61
1:A:256:THR:OG1	1:A:258:ARG:NH1	2.33	0.61
1:D:187:PRO:HB3	1:D:226:PHE:CD2	2.35	0.61
1:A:266:ARG:CG	1:A:267:LEU:HD23	2.30	0.61
1:D:42:GLN:NE2	1:D:46:TRP:NE1	2.46	0.61
1:D:27:SER:OG	1:D:29:SER:OG	2.18	0.61
1:C:2:ARG:HA	1:C:2:ARG:NE	2.07	0.61
1:D:126:LEU:N	1:D:127:PRO:HD2	2.15	0.61
1:D:7:ILE:HG12	1:D:88:VAL:HB	1.81	0.60
1:C:267:LEU:HD23	1:C:267:LEU:H	1.66	0.60
1:D:173:LEU:HD13	1:D:178:VAL:HB	1.81	0.60
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.66	0.60
1:B:180:LEU:HD23	1:B:181:SER:N	2.16	0.60
1:A:68:ASP:HB3	1:A:71:SER:HB3	1.82	0.60
1:A:241:LEU:O	1:A:245:ARG:HG3	2.02	0.60
1:C:87:LEU:HB3	1:C:137:VAL:HG22	1.83	0.60
1:A:174:LEU:HB3	1:A:175:PRO:CD	2.32	0.60
1:C:150:PRO:HG3	1:D:171:VAL:HG11	1.84	0.60
1:B:147:MET:HE1	1:B:262:LEU:HD23	1.84	0.60
1:D:99:LEU:HA	1:D:102:LEU:CD1	2.32	0.60
1:B:39:LEU:O	1:B:42:GLN:HG2	2.02	0.60
1:B:37:ARG:HH21	3:B:364:NAD:C2B	2.13	0.59
1:B:182:LEU:HD12	1:B:182:LEU:N	2.15	0.59
1:B:2:ARG:CZ	1:B:83:ARG:HH22	2.14	0.59
1:A:266:ARG:CG	1:A:266:ARG:HH11	2.16	0.59
1:C:67:ARG:HD2	4:C:525:HOH:O	2.01	0.59
1:D:31:LYS:HE2	1:D:33:TYR:CE1	2.36	0.59
1:B:203:VAL:O	1:B:207:THR:HG22	2.02	0.59
1:D:38:ASP:O	1:D:41:THR:HG23	2.02	0.59
1:D:92:GLY:HA3	3:D:362:NAD:O2D	2.02	0.59
1:A:46:TRP:O	1:A:50:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:CG1	1:A:196:VAL:O	2.50	0.59
1:A:14:ILE:HD12	1:A:236:VAL:HG11	1.84	0.59
1:B:254:PHE:CE2	1:B:260:LEU:HD11	2.37	0.59
1:C:136:ARG:NH1	1:C:136:ARG:HG2	2.14	0.59
1:B:272:GLY:O	1:B:276:VAL:HG23	2.03	0.59
1:C:50:ARG:HG3	1:C:50:ARG:HH11	1.67	0.58
1:A:8:THR:O	1:A:90:ASN:HB3	2.04	0.58
1:C:5:VAL:HG22	1:C:86:VAL:HB	1.84	0.58
1:D:139:VAL:O	1:D:182:LEU:HA	2.03	0.58
1:D:268:ASP:O	1:D:270:PRO:HD3	2.03	0.58
1:B:249:PRO:HA	1:B:253:TYR:OH	2.03	0.58
1:B:262:LEU:HD12	1:B:265:MET:HG2	1.86	0.58
1:D:139:VAL:HG11	1:D:162:LEU:HD21	1.86	0.58
1:B:21:ARG:NH1	1:B:21:ARG:O	2.37	0.58
1:D:274:ASN:N	1:D:274:ASN:HD22	2.01	0.58
1:C:96:LEU:HD21	1:C:219:LEU:HD21	1.86	0.58
1:C:96:LEU:HD11	1:C:218:TYR:HE2	1.66	0.58
1:A:266:ARG:CB	1:A:267:LEU:HD23	2.33	0.58
1:A:45:LEU:CD1	1:A:59:LEU:HD21	2.31	0.58
1:B:34:ALA:HB2	1:B:59:LEU:HD11	1.84	0.58
1:D:68:ASP:O	1:D:72:VAL:HG23	2.03	0.58
1:C:129:MET:O	1:C:130:LYS:C	2.43	0.58
1:D:136:ARG:HH12	1:D:249:PRO:HG3	1.69	0.58
1:C:76:ARG:HB3	1:C:76:ARG:HH11	1.69	0.58
1:A:98:PRO:HG2	1:A:203:VAL:HG13	1.86	0.57
1:A:211:THR:OG1	1:B:130:LYS:HE2	2.04	0.57
1:B:247:PRO:O	1:B:249:PRO:HD3	2.03	0.57
1:B:260:LEU:CD1	1:B:263:LEU:HD12	2.34	0.57
1:A:190:THR:O	1:A:191:ALA:HB3	2.04	0.57
1:C:2:ARG:NH2	1:C:83:ARG:HH22	2.02	0.57
1:C:189:HIS:NE2	1:C:230:ALA:HB3	2.20	0.57
1:A:130:LYS:HE3	1:A:173:LEU:HD23	1.85	0.57
1:A:274:ASN:HD22	1:A:274:ASN:N	2.02	0.57
1:B:166:CYS:HB3	1:B:180:LEU:HD22	1.87	0.57
1:B:176:PHE:CD1	1:B:176:PHE:N	2.73	0.57
1:B:260:LEU:HD11	1:B:263:LEU:HD12	1.87	0.56
1:B:260:LEU:N	1:B:261:PRO:CD	2.67	0.56
1:C:95:LEU:HD12	1:C:197:LEU:HD12	1.86	0.56
1:A:119:VAL:HG22	1:A:165:LEU:HD22	1.87	0.56
1:C:173:LEU:HD13	1:C:178:VAL:HG12	1.86	0.56
1:A:258:ARG:CB	1:A:258:ARG:HH11	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:O	1:A:275:TYR:OH	2.23	0.56
1:D:110:VAL:HG13	1:D:114:ASN:HD22	1.70	0.56
1:C:32:VAL:O	1:C:59:LEU:HA	2.06	0.56
1:D:89:CYS:SG	1:D:118:THR:HG23	2.46	0.56
1:C:150:PRO:HG3	1:D:171:VAL:CG1	2.36	0.56
1:A:69:SER:HB3	1:B:104:GLU:OE2	2.04	0.56
1:D:203:VAL:HG13	1:D:207:THR:HG21	1.86	0.56
1:D:20:VAL:CG2	1:D:52:LEU:HD22	2.35	0.56
1:C:232:ASN:HB3	1:C:234:GLU:OE1	2.06	0.56
1:D:224:GLN:O	1:D:228:GLU:HG3	2.05	0.56
1:A:272:GLY:O	1:A:276:VAL:HG23	2.05	0.56
1:A:107:VAL:HG13	1:A:154:VAL:CG1	2.35	0.56
1:A:68:ASP:O	1:A:72:VAL:HG23	2.06	0.56
1:B:74:ALA:O	1:B:75:ALA:C	2.42	0.56
1:D:83:ARG:HH11	1:D:83:ARG:HG2	1.71	0.56
1:D:279:MET:CE	1:D:282:GLU:HB3	2.36	0.55
1:D:87:LEU:HD22	1:D:125:PHE:HB2	1.89	0.55
1:D:149:LEU:HB2	1:D:156:CYS:SG	2.46	0.55
1:C:194:GLU:O	1:C:196:VAL:N	2.38	0.55
1:A:260:LEU:N	1:A:261:PRO:HD2	2.21	0.55
1:A:136:ARG:HH12	1:A:249:PRO:HG3	1.70	0.55
1:D:257:GLU:HG2	1:D:260:LEU:HD22	1.89	0.55
1:A:148:GLY:HA3	1:B:167:GLU:HG2	1.88	0.55
1:B:173:LEU:O	1:B:174:LEU:C	2.45	0.55
1:D:83:ARG:HD2	1:D:85:ASP:OD1	2.06	0.55
1:A:131:ARG:CZ	1:B:208:ASP:HB3	2.37	0.55
1:A:261:PRO:HG2	1:A:262:LEU:H	1.71	0.55
1:D:232:ASN:HB2	1:D:235:GLU:HG3	1.89	0.55
1:C:14:ILE:HD12	1:C:236:VAL:HG11	1.86	0.55
1:B:284:PHE:O	1:B:285:GLY:C	2.45	0.55
1:A:256:THR:OG1	1:A:258:ARG:HB2	2.06	0.55
1:B:188:VAL:N	3:B:364:NAD:O7N	2.40	0.55
1:A:216:TYR:CD2	1:C:200:PRO:HB2	2.42	0.55
1:C:252:ARG:HB2	1:D:271:SER:HA	1.88	0.55
1:C:16:LEU:HG	1:C:45:LEU:CD2	2.32	0.55
1:D:129:MET:HB3	1:D:134:SER:O	2.07	0.55
1:B:52:LEU:O	1:B:53:ALA:HB3	2.07	0.55
1:D:66:VAL:HG22	3:D:362:NAD:C6A	2.36	0.55
1:A:241:LEU:O	1:A:244:LEU:HB3	2.07	0.55
1:D:266:ARG:NH1	1:D:266:ARG:HG2	2.19	0.55
1:C:252:ARG:HG3	1:C:252:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:HD12	1:B:97:GLY:N	2.22	0.55
1:D:67:ARG:HB3	1:D:112:ASP:OD2	2.06	0.55
1:C:27:SER:O	1:C:28:GLN:C	2.43	0.55
1:D:103:GLY:O	1:D:106:ALA:N	2.40	0.55
1:B:13:GLY:O	1:B:17:HIS:HD2	1.90	0.54
1:B:10:CYS:HA	1:B:15:GLY:HA3	1.90	0.54
1:B:189:HIS:NE2	1:B:230:ALA:HB3	2.22	0.54
1:C:203:VAL:HG11	1:C:216:TYR:OH	2.07	0.54
1:A:192:PHE:HB2	3:A:361:NAD:O3	2.07	0.54
1:C:42:GLN:NE2	1:C:46:TRP:HE1	2.04	0.54
1:B:4:VAL:N	1:B:85:ASP:OD2	2.31	0.54
1:D:24:SER:OG	1:D:52:LEU:HD23	2.06	0.54
1:B:3:THR:HB	1:B:30:PHE:CD1	2.42	0.54
1:A:167:GLU:HB2	1:A:251:LEU:HD21	1.90	0.54
1:C:207:THR:OG1	1:C:208:ASP:N	2.41	0.54
1:D:105:ASP:O	1:D:106:ALA:C	2.46	0.54
1:B:170:ALA:CB	1:B:251:LEU:HD13	2.38	0.54
1:A:256:THR:HG1	1:A:258:ARG:H	1.55	0.54
1:A:5:VAL:HA	1:A:86:VAL:O	2.08	0.54
1:D:184:GLU:O	1:D:255:THR:HG23	2.06	0.54
1:C:280:HIS:CG	1:D:174:LEU:HD23	2.43	0.54
1:D:2:ARG:HA	1:D:83:ARG:HH21	1.73	0.53
1:C:151:PHE:CE2	1:C:215:PHE:HA	2.43	0.53
1:A:267:LEU:HD22	1:B:267:LEU:HD22	1.89	0.53
1:C:64:LEU:CD2	1:C:72:VAL:HG22	2.27	0.53
1:D:35:THR:HG23	1:D:64:LEU:HB3	1.89	0.53
1:C:271:SER:HB2	1:D:250:THR:HB	1.89	0.53
1:C:224:GLN:O	1:C:225:VAL:C	2.46	0.53
1:A:76:ARG:HB3	1:A:76:ARG:HH11	1.72	0.53
1:D:126:LEU:CD2	1:D:178:VAL:HG11	2.38	0.53
1:B:119:VAL:O	1:B:123:GLN:HG3	2.09	0.53
1:D:279:MET:HE1	1:D:282:GLU:HB3	1.90	0.53
1:C:147:MET:HB2	1:C:275:TYR:OH	2.08	0.53
1:D:162:LEU:HD23	1:D:166:CYS:HG	1.73	0.53
1:A:166:CYS:SG	1:A:180:LEU:HD21	2.48	0.53
1:C:111:LEU:O	1:C:116:VAL:HG23	2.09	0.53
1:D:9:GLY:O	1:D:15:GLY:HA3	2.09	0.53
1:C:120:ARG:HA	1:C:123:GLN:HE21	1.72	0.53
1:C:74:ALA:O	1:C:75:ALA:C	2.47	0.53
1:A:266:ARG:HG2	1:A:267:LEU:CD2	2.39	0.53
1:D:31:LYS:NZ	1:D:81:GLU:OE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PRO:HB3	1:B:226:PHE:CE1	2.42	0.53
1:A:216:TYR:HA	1:A:219:LEU:HB2	1.91	0.53
1:D:169:LEU:O	1:D:170:ALA:C	2.48	0.53
1:D:110:VAL:HG13	1:D:114:ASN:ND2	2.24	0.53
1:D:126:LEU:HD22	1:D:173:LEU:HD11	1.91	0.53
1:C:111:LEU:HD23	1:C:158:SER:HB3	1.90	0.53
1:B:93:LEU:HG	1:B:113:VAL:HG11	1.90	0.53
1:C:131:ARG:NH1	1:D:208:ASP:HB3	2.23	0.52
1:C:267:LEU:CD2	1:C:267:LEU:N	2.72	0.52
1:B:21:ARG:HH12	1:B:25:ASP:HA	1.74	0.52
1:A:78:ARG:HH11	1:A:78:ARG:HA	1.75	0.52
1:C:105:ASP:O	1:C:108:ALA:HB3	2.09	0.52
1:A:67:ARG:HH12	1:A:109:SER:HB3	1.73	0.52
1:C:66:VAL:O	1:C:120:ARG:HD2	2.09	0.52
1:A:267:LEU:CB	1:B:267:LEU:HD22	2.39	0.52
1:C:238:GLU:HA	1:C:241:LEU:HD13	1.91	0.52
1:C:199:SER:O	1:C:200:PRO:C	2.47	0.52
1:A:141:GLY:HA3	1:A:184:GLU:OE1	2.09	0.52
1:C:76:ARG:HH11	1:C:76:ARG:CB	2.21	0.52
1:D:34:ALA:O	1:D:61:THR:HA	2.09	0.52
1:A:17:HIS:CD2	1:A:233:PRO:HB2	2.44	0.52
1:C:263:LEU:C	1:C:263:LEU:HD13	2.29	0.52
1:A:173:LEU:O	1:A:174:LEU:C	2.48	0.52
1:C:86:VAL:HG13	1:C:136:ARG:HB3	1.92	0.52
1:D:162:LEU:HD23	1:D:166:CYS:SG	2.49	0.52
1:C:197:LEU:HD23	1:C:198:GLY:N	2.25	0.52
1:A:231:GLN:HE22	1:A:255:THR:HB	1.75	0.52
1:D:241:LEU:HD22	1:D:245:ARG:NH1	2.25	0.52
1:A:231:GLN:HE22	1:A:255:THR:CB	2.23	0.52
1:C:266:ARG:NH2	1:D:167:GLU:OE2	2.41	0.52
1:B:274:ASN:N	1:B:274:ASN:ND2	2.57	0.52
1:D:122:LEU:HD21	1:D:137:VAL:HG11	1.92	0.52
1:C:174:LEU:HB3	1:C:175:PRO:HD3	1.90	0.51
1:C:120:ARG:NH2	1:D:104:GLU:OE2	2.43	0.51
1:D:203:VAL:HG13	1:D:207:THR:CG2	2.40	0.51
1:C:237:ALA:O	1:C:241:LEU:HD12	2.11	0.51
1:C:52:LEU:O	1:C:53:ALA:HB3	2.10	0.51
1:D:66:VAL:HG22	3:D:362:NAD:H62A	1.73	0.51
1:C:126:LEU:N	1:C:127:PRO:CD	2.72	0.51
1:B:3:THR:HB	1:B:30:PHE:HD1	1.76	0.51
1:A:263:LEU:O	1:A:263:LEU:HD22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:HA	1:C:244:LEU:HB3	1.92	0.51
1:A:281:ARG:O	1:A:285:GLY:N	2.43	0.51
1:A:207:THR:OG1	1:A:208:ASP:N	2.44	0.51
1:D:174:LEU:HB3	1:D:175:PRO:CD	2.40	0.51
1:D:142:SER:HB2	3:D:362:NAD:C5N	2.40	0.51
1:D:263:LEU:O	1:D:266:ARG:N	2.44	0.51
1:B:24:SER:O	1:B:25:ASP:C	2.49	0.51
1:A:5:VAL:HG13	1:A:86:VAL:CB	2.36	0.51
1:B:5:VAL:HA	1:B:86:VAL:O	2.11	0.51
1:B:239:VAL:HG21	1:B:255:THR:HA	1.92	0.51
1:B:147:MET:CE	1:B:262:LEU:HD23	2.41	0.51
1:A:42:GLN:NE2	1:A:46:TRP:NE1	2.51	0.51
1:C:95:LEU:HD23	1:C:154:VAL:HB	1.93	0.51
1:A:33:TYR:CE2	1:A:79:VAL:HG13	2.45	0.51
1:A:96:LEU:HD11	1:A:218:TYR:CE1	2.46	0.51
1:A:7:ILE:HG23	1:A:88:VAL:HB	1.93	0.51
1:D:66:VAL:O	1:D:120:ARG:HD2	2.11	0.50
1:C:138:LEU:HD13	1:C:240:PHE:HD1	1.76	0.50
1:C:68:ASP:CG	1:C:71:SER:H	2.15	0.50
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.75	0.50
1:D:165:LEU:HD12	1:D:165:LEU:O	2.09	0.50
1:D:92:GLY:HA2	1:D:114:ASN:OD1	2.11	0.50
1:C:200:PRO:HA	1:C:203:VAL:HG12	1.92	0.50
1:C:261:PRO:O	1:C:262:LEU:C	2.49	0.50
1:C:232:ASN:O	1:C:233:PRO:C	2.50	0.50
1:B:27:SER:OG	1:B:29:SER:OG	2.29	0.50
1:C:132:ARG:HG2	1:C:134:SER:OG	2.11	0.50
1:B:187:PRO:HG2	1:B:229:ALA:CB	2.40	0.50
1:C:16:LEU:HD11	1:C:45:LEU:HA	1.93	0.50
1:C:282:GLU:HA	1:C:282:GLU:OE1	2.09	0.50
1:A:252:ARG:HG3	1:A:252:ARG:NH1	2.26	0.50
1:B:38:ASP:O	1:B:41:THR:HG23	2.11	0.50
1:D:260:LEU:N	1:D:261:PRO:HD2	2.25	0.50
1:B:38:ASP:HB3	1:B:41:THR:HG23	1.94	0.50
1:A:187:PRO:HB3	1:A:226:PHE:CE2	2.47	0.50
1:A:267:LEU:HD22	1:B:267:LEU:CD2	2.41	0.50
1:B:234:GLU:HG3	4:B:520:HOH:O	2.11	0.50
1:B:143:VAL:HG13	1:B:144:GLY:N	2.27	0.50
1:B:247:PRO:C	1:B:249:PRO:HD3	2.32	0.50
1:A:174:LEU:HB3	1:A:175:PRO:HD2	1.93	0.50
1:C:182:LEU:HB3	1:C:184:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:O	1:B:59:LEU:HD12	2.12	0.50
1:B:38:ASP:OD1	1:B:40:LYS:HG2	2.12	0.50
1:B:92:GLY:HA3	3:B:364:NAD:C3D	2.37	0.49
1:C:208:ASP:OD1	1:C:211:THR:OG1	2.30	0.49
1:C:187:PRO:HB3	1:C:226:PHE:CE1	2.47	0.49
1:A:183:ILE:HD13	1:A:253:TYR:HB2	1.94	0.49
1:A:35:THR:HG22	1:A:62:LEU:HD12	1.94	0.49
1:C:68:ASP:OD1	1:C:70:LYS:N	2.46	0.49
1:D:70:LYS:O	1:D:73:ALA:HB3	2.11	0.49
1:D:98:PRO:HG2	1:D:207:THR:HG21	1.94	0.49
1:D:155:TYR:CZ	1:D:159:LYS:HD2	2.47	0.49
1:C:204:LEU:HD23	1:C:212:PHE:CE2	2.48	0.49
1:C:8:THR:HG22	1:C:64:LEU:HD13	1.94	0.49
1:B:88:VAL:HG22	1:B:138:LEU:HB2	1.94	0.49
1:D:147:MET:HG3	1:D:275:TYR:OH	2.13	0.49
1:D:127:PRO:O	1:D:128:ASP:C	2.50	0.49
1:D:82:GLY:O	1:D:132:ARG:NH2	2.45	0.49
1:B:14:ILE:HD12	1:B:236:VAL:CB	2.43	0.49
1:D:17:HIS:CG	1:D:233:PRO:HB2	2.47	0.49
1:C:238:GLU:HA	1:C:241:LEU:HD12	1.95	0.49
1:D:203:VAL:HG12	1:D:212:PHE:CE2	2.48	0.49
1:B:184:GLU:OE2	1:B:252:ARG:HG2	2.13	0.49
1:A:86:VAL:CG2	1:A:244:LEU:HD11	2.34	0.49
1:C:281:ARG:HA	1:C:285:GLY:O	2.12	0.49
1:C:273:SER:O	1:C:274:ASN:C	2.49	0.49
1:A:95:LEU:HG	1:A:102:LEU:HD22	1.93	0.49
1:C:37:ARG:HB2	3:C:363:NAD:C2A	2.43	0.49
1:C:139:VAL:CG1	1:C:182:LEU:HD23	2.42	0.49
1:B:17:HIS:CD2	1:B:233:PRO:HB2	2.48	0.49
1:C:241:LEU:O	1:C:245:ARG:N	2.41	0.49
1:A:222:SER:O	1:A:225:VAL:HB	2.13	0.48
1:D:261:PRO:O	1:D:265:MET:N	2.35	0.48
1:C:236:VAL:HG22	1:C:255:THR:HG21	1.95	0.48
1:A:248:LYS:HD2	1:A:249:PRO:HD2	1.95	0.48
1:D:36:LEU:HD22	1:D:42:GLN:HB3	1.95	0.48
1:C:16:LEU:O	1:C:19:ALA:HB3	2.14	0.48
1:B:59:LEU:HG	1:B:60:GLU:N	2.29	0.48
1:D:126:LEU:CD2	1:D:173:LEU:HD11	2.43	0.48
1:A:101:ALA:CB	1:A:206:ARG:HB3	2.44	0.48
1:A:278:ALA:O	1:A:279:MET:C	2.52	0.48
1:C:202:GLU:OE2	1:C:206:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:LEU:O	1:D:263:LEU:C	2.50	0.48
1:B:129:MET:O	1:B:130:LYS:C	2.52	0.48
1:A:150:PRO:O	1:A:151:PHE:HB2	2.12	0.48
1:A:236:VAL:HG22	1:A:255:THR:HG21	1.95	0.48
1:A:187:PRO:O	1:A:230:ALA:HA	2.14	0.48
1:D:203:VAL:HG12	1:D:212:PHE:CD2	2.49	0.48
1:B:9:GLY:O	1:B:15:GLY:HA3	2.14	0.48
1:B:94:GLY:HA2	1:B:155:TYR:CD1	2.48	0.48
1:A:281:ARG:O	1:A:282:GLU:C	2.52	0.48
1:C:280:HIS:CE1	1:D:175:PRO:HD3	2.49	0.48
1:C:67:ARG:CD	4:C:525:HOH:O	2.60	0.48
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.29	0.48
1:A:141:GLY:O	3:A:361:NAD:H6N	2.14	0.48
1:C:260:LEU:N	1:C:261:PRO:HD2	2.29	0.48
1:C:11:SER:HA	1:C:36:LEU:CD2	2.44	0.48
1:C:7:ILE:HG23	1:C:88:VAL:CG1	2.44	0.48
1:B:13:GLY:H	1:B:190:THR:HG21	1.79	0.47
1:D:98:PRO:HG2	1:D:203:VAL:HG13	1.96	0.47
1:C:221:LEU:O	1:C:222:SER:C	2.53	0.47
1:D:143:VAL:HG21	1:D:259:PHE:CB	2.45	0.47
1:B:68:ASP:O	1:B:69:SER:C	2.52	0.47
1:D:190:THR:O	3:D:362:NAD:O2N	2.32	0.47
1:A:86:VAL:HA	1:A:136:ARG:O	2.15	0.47
1:A:68:ASP:HB3	1:A:71:SER:CB	2.44	0.47
1:C:42:GLN:HE22	1:C:46:TRP:HE1	1.62	0.47
1:B:68:ASP:O	1:B:71:SER:N	2.46	0.47
1:A:185:CYS:HA	1:A:255:THR:OG1	2.14	0.47
1:D:247:PRO:O	1:D:249:PRO:HD3	2.14	0.47
1:B:241:LEU:HD23	1:B:245:ARG:HD3	1.96	0.47
1:A:274:ASN:ND2	1:A:274:ASN:N	2.62	0.47
1:B:277:THR:O	1:B:278:ALA:C	2.53	0.47
1:C:89:CYS:N	1:C:138:LEU:O	2.43	0.47
1:A:165:LEU:O	1:A:169:LEU:HG	2.15	0.47
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.58	0.47
1:C:42:GLN:NE2	1:C:46:TRP:NE1	2.62	0.47
1:C:172:LEU:HD21	1:D:211:THR:HG23	1.96	0.47
1:A:266:ARG:HB3	1:A:267:LEU:H	1.50	0.47
1:A:267:LEU:HA	1:B:267:LEU:CD2	2.30	0.47
1:A:136:ARG:NH1	1:A:249:PRO:HG3	2.29	0.47
1:A:185:CYS:HB2	3:A:361:NAD:C5N	2.43	0.47
1:C:262:LEU:O	1:C:263:LEU:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ASP:OD2	1:D:132:ARG:NH2	2.47	0.47
1:D:38:ASP:O	1:D:40:LYS:N	2.47	0.47
1:C:217:GLN:O	1:C:220:ALA:HB3	2.15	0.47
1:A:273:SER:HB3	1:B:250:THR:HG22	1.97	0.47
1:C:122:LEU:HD21	1:C:137:VAL:HG11	1.97	0.47
1:D:83:ARG:NH1	1:D:83:ARG:HG2	2.29	0.47
1:C:211:THR:HG21	1:D:130:LYS:NZ	2.30	0.47
1:C:221:LEU:O	1:C:225:VAL:HG23	2.15	0.47
1:D:1:ALA:O	1:D:2:ARG:NH2	2.47	0.47
1:B:176:PHE:HD1	1:B:176:PHE:H	1.63	0.47
1:C:269:ASP:HA	1:C:270:PRO:HD2	1.64	0.47
1:B:48:ALA:O	1:B:52:LEU:N	2.47	0.46
1:C:266:ARG:HH21	1:D:167:GLU:CD	2.18	0.46
1:B:40:LYS:NZ	4:B:550:HOH:O	2.48	0.46
1:A:279:MET:HA	1:A:279:MET:CE	2.45	0.46
1:C:232:ASN:O	1:C:235:GLU:N	2.48	0.46
1:C:252:ARG:NH1	1:C:252:ARG:HG3	2.30	0.46
1:D:279:MET:HE2	1:D:283:VAL:CG2	2.40	0.46
1:C:185:CYS:HB2	3:C:363:NAD:C5N	2.46	0.46
1:A:165:LEU:O	1:A:165:LEU:HD12	2.16	0.46
1:D:143:VAL:HG21	1:D:259:PHE:HB2	1.97	0.46
1:C:250:THR:HG22	1:D:273:SER:HB3	1.98	0.46
1:A:267:LEU:H	1:A:267:LEU:HD23	1.79	0.46
1:A:122:LEU:HD21	1:A:137:VAL:CG1	2.41	0.46
1:A:122:LEU:O	1:A:126:LEU:HB2	2.16	0.46
1:C:25:ASP:OD1	1:C:27:SER:OG	2.34	0.46
1:A:95:LEU:HB2	1:A:110:VAL:HG21	1.96	0.46
1:D:221:LEU:O	1:D:225:VAL:HG23	2.15	0.46
1:C:167:GLU:O	1:C:171:VAL:HG23	2.16	0.46
1:A:248:LYS:HD2	1:A:248:LYS:HA	1.33	0.46
1:C:138:LEU:HD13	1:C:240:PHE:CD1	2.50	0.46
1:C:255:THR:OG1	1:C:256:THR:HG22	2.15	0.46
1:C:26:PRO:O	1:C:28:GLN:HG3	2.14	0.46
1:B:170:ALA:HB2	1:B:251:LEU:HD13	1.98	0.46
1:B:11:SER:O	1:B:16:LEU:HD12	2.15	0.46
1:C:65:ASP:OD1	1:C:67:ARG:HB2	2.16	0.46
1:A:240:PHE:O	1:A:244:LEU:HB2	2.16	0.46
1:C:173:LEU:O	1:C:174:LEU:C	2.54	0.46
1:B:166:CYS:HB3	1:B:180:LEU:CD2	2.46	0.46
1:C:179:HIS:HB3	1:C:249:PRO:HG2	1.96	0.46
1:A:236:VAL:O	1:A:237:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG21	1:A:215:PHE:CE2	2.51	0.46
1:C:188:VAL:CG1	1:C:190:THR:HG23	2.45	0.46
1:C:256:THR:OG1	1:C:258:ARG:HB2	2.15	0.46
1:C:166:CYS:SG	1:C:180:LEU:HD21	2.56	0.46
1:D:242:THR:O	1:D:243:ALA:C	2.52	0.46
1:C:2:ARG:NE	1:C:83:ARG:HH22	2.14	0.46
1:B:226:PHE:O	1:B:230:ALA:N	2.42	0.46
1:C:31:LYS:HE3	1:C:60:GLU:OE2	2.15	0.46
1:D:10:CYS:HA	1:D:15:GLY:HA3	1.97	0.45
1:D:279:MET:O	1:D:279:MET:HG3	2.16	0.45
1:D:187:PRO:HG2	1:D:229:ALA:CB	2.47	0.45
1:D:147:MET:HE1	1:D:262:LEU:HG	1.99	0.45
1:C:190:THR:O	1:C:191:ALA:HB3	2.16	0.45
1:D:173:LEU:O	1:D:174:LEU:C	2.54	0.45
1:A:159:LYS:HA	1:A:159:LYS:HD2	1.43	0.45
1:A:3:THR:O	1:A:30:PHE:HA	2.17	0.45
1:A:3:THR:HG23	1:A:85:ASP:HB3	1.99	0.45
1:A:265:MET:SD	1:A:275:TYR:HA	2.56	0.45
1:A:224:GLN:O	1:A:225:VAL:C	2.52	0.45
1:D:89:CYS:CB	1:D:139:VAL:HG22	2.42	0.45
1:A:7:ILE:HD13	1:A:18:LEU:HG	1.98	0.45
1:A:193:MET:HA	1:A:196:VAL:CG2	2.47	0.45
1:B:36:LEU:HD11	1:B:45:LEU:HD12	1.98	0.45
1:A:264:ARG:O	1:A:265:MET:C	2.54	0.45
1:D:245:ARG:HE	1:D:245:ARG:HB2	1.51	0.45
1:B:207:THR:OG1	1:B:208:ASP:N	2.49	0.45
1:A:44:ARG:NH2	2:A:401:SO4:S	2.89	0.45
1:D:236:VAL:O	1:D:239:VAL:N	2.47	0.45
1:A:96:LEU:HB3	1:A:196:VAL:HG12	1.97	0.45
1:D:86:VAL:HG12	1:D:88:VAL:HG23	1.99	0.45
1:A:215:PHE:CZ	1:A:219:LEU:HD11	2.52	0.45
1:B:149:LEU:HD23	1:B:279:MET:CE	2.47	0.45
1:B:17:HIS:CG	1:B:233:PRO:HB2	2.52	0.45
1:C:219:LEU:O	1:C:220:ALA:C	2.55	0.45
1:D:281:ARG:HG2	1:D:281:ARG:NH1	2.32	0.45
1:D:110:VAL:O	1:D:114:ASN:HB2	2.17	0.45
1:C:280:HIS:CB	1:D:174:LEU:HD23	2.47	0.45
1:C:42:GLN:NE2	1:C:46:TRP:CD1	2.85	0.45
1:C:168:SER:CB	1:D:153:ASP:HA	2.47	0.45
1:C:100:GLU:OE2	1:D:130:LYS:NZ	2.48	0.44
1:A:271:SER:OG	1:A:273:SER:OG	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ASP:O	1:D:157:ALA:N	2.49	0.44
1:A:266:ARG:CG	1:A:266:ARG:NH1	2.78	0.44
1:D:185:CYS:HB2	3:D:362:NAD:H5N	1.99	0.44
1:D:231:GLN:NE2	1:D:255:THR:O	2.41	0.44
1:C:68:ASP:HB3	1:C:71:SER:CB	2.44	0.44
1:D:240:PHE:O	1:D:243:ALA:HB3	2.18	0.44
1:A:269:ASP:OD2	1:A:274:ASN:N	2.50	0.44
1:B:262:LEU:HA	1:B:262:LEU:HD12	1.81	0.44
1:C:95:LEU:HG	1:C:102:LEU:HD22	2.00	0.44
1:A:274:ASN:O	1:A:275:TYR:C	2.55	0.44
1:A:239:VAL:O	1:A:240:PHE:C	2.55	0.44
1:D:139:VAL:CG1	1:D:162:LEU:HD21	2.47	0.44
1:A:210:HIS:O	1:A:214:ARG:HG2	2.17	0.44
1:D:95:LEU:HD12	1:D:95:LEU:HA	1.74	0.44
1:A:262:LEU:O	1:A:263:LEU:C	2.56	0.44
1:C:263:LEU:HD13	1:C:263:LEU:O	2.18	0.44
1:A:192:PHE:O	1:A:196:VAL:HG23	2.17	0.44
1:B:259:PHE:O	1:B:263:LEU:HB2	2.17	0.44
1:D:16:LEU:O	1:D:20:VAL:HG13	2.18	0.44
1:D:67:ARG:HG2	1:D:113:VAL:HG22	2.00	0.44
1:C:173:LEU:HD13	1:C:178:VAL:CG1	2.47	0.44
1:C:174:LEU:CB	1:C:175:PRO:HD2	2.42	0.44
1:D:184:GLU:N	1:D:253:TYR:O	2.44	0.44
1:C:126:LEU:N	1:C:127:PRO:HD2	2.33	0.44
1:B:143:VAL:CG1	1:B:144:GLY:N	2.81	0.44
1:A:183:ILE:HG22	1:A:183:ILE:O	2.18	0.44
1:B:107:VAL:HG13	1:B:154:VAL:HG11	2.00	0.44
1:D:247:PRO:C	1:D:249:PRO:HD3	2.38	0.44
1:D:147:MET:HE3	1:D:275:TYR:HE2	1.82	0.44
1:D:260:LEU:HA	1:D:260:LEU:HD12	1.85	0.44
1:A:226:PHE:CD1	1:A:230:ALA:HB2	2.53	0.44
1:C:11:SER:HA	1:C:36:LEU:HD21	2.00	0.44
1:C:172:LEU:O	1:C:172:LEU:HD12	2.18	0.44
1:C:42:GLN:HE21	1:C:42:GLN:HB2	1.53	0.43
1:B:38:ASP:OD2	1:B:40:LYS:HG3	2.18	0.43
1:C:16:LEU:C	1:C:16:LEU:HD23	2.39	0.43
1:D:33:TYR:HE1	1:D:81:GLU:OE1	2.01	0.43
1:B:133:GLY:HA2	1:B:176:PHE:O	2.19	0.43
1:C:185:CYS:HB2	3:C:363:NAD:H5N	1.99	0.43
1:A:213:HIS:NE2	1:C:209:ILE:HD12	2.33	0.43
1:A:189:HIS:NE2	1:A:226:PHE:HD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLU:HA	1:C:182:LEU:HD11	2.00	0.43
1:C:199:SER:O	1:C:203:VAL:N	2.50	0.43
1:A:166:CYS:HB2	1:A:182:LEU:HD11	1.99	0.43
1:A:21:ARG:CZ	1:A:241:LEU:HD11	2.49	0.43
1:B:86:VAL:HG12	1:B:88:VAL:HG23	2.01	0.43
1:B:130:LYS:HG2	1:B:176:PHE:CD2	2.52	0.43
1:B:100:GLU:HG2	1:B:101:ALA:N	2.33	0.43
1:A:174:LEU:CB	1:A:175:PRO:CD	2.93	0.43
1:C:20:VAL:O	1:C:21:ARG:C	2.52	0.43
1:C:99:LEU:HD11	1:D:119:VAL:HG13	2.01	0.43
1:B:67:ARG:HG2	1:B:112:ASP:OD2	2.19	0.43
1:C:10:CYS:O	1:C:16:LEU:HB2	2.19	0.43
1:A:126:LEU:N	1:A:127:PRO:CD	2.82	0.43
1:C:107:VAL:HG13	1:C:154:VAL:HG11	2.01	0.43
1:C:25:ASP:HA	1:C:26:PRO:HD2	1.73	0.43
1:D:146:LEU:HD23	1:D:146:LEU:HA	1.83	0.43
1:A:17:HIS:O	1:A:18:LEU:C	2.57	0.43
1:D:152:ASN:O	1:D:156:CYS:HB2	2.19	0.43
1:A:76:ARG:HG3	1:A:125:PHE:CE1	2.54	0.43
1:B:33:TYR:CE1	1:B:79:VAL:HG13	2.54	0.43
1:D:2:ARG:HA	1:D:83:ARG:NH2	2.34	0.42
1:D:281:ARG:HG2	1:D:281:ARG:HH11	1.83	0.42
1:D:138:LEU:CD2	1:D:181:SER:HB2	2.48	0.42
1:A:279:MET:O	1:A:280:HIS:C	2.55	0.42
1:B:278:ALA:HA	1:B:281:ARG:CZ	2.48	0.42
1:A:149:LEU:HA	1:A:150:PRO:HD2	1.85	0.42
1:C:41:THR:O	1:C:41:THR:HG22	2.19	0.42
1:B:262:LEU:O	1:B:263:LEU:C	2.56	0.42
1:D:9:GLY:CA	3:D:362:NAD:H1B	2.46	0.42
1:A:221:LEU:O	1:A:225:VAL:HG23	2.20	0.42
1:A:251:LEU:HB3	1:B:271:SER:O	2.18	0.42
1:B:75:ALA:O	1:B:76:ARG:C	2.56	0.42
1:D:275:TYR:O	1:D:276:VAL:C	2.57	0.42
1:A:129:MET:O	1:A:130:LYS:C	2.57	0.42
1:D:202:GLU:O	1:D:206:ARG:N	2.32	0.42
1:C:92:GLY:HA3	3:C:363:NAD:H3D	2.01	0.42
1:A:46:TRP:CZ2	1:A:61:THR:HG23	2.54	0.42
1:B:101:ALA:HA	1:B:206:ARG:HB3	2.02	0.42
1:C:147:MET:CE	1:C:262:LEU:HD23	2.50	0.42
1:C:279:MET:CE	1:C:282:GLU:HB3	2.46	0.42
1:D:1:ALA:HB3	1:D:31:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASP:CG	1:B:26:PRO:HD2	2.40	0.42
1:C:2:ARG:O	1:C:83:ARG:NH2	2.52	0.42
1:C:21:ARG:HG2	1:C:241:LEU:HD11	2.01	0.42
1:B:96:LEU:HD21	1:B:219:LEU:HD21	2.02	0.42
1:C:18:LEU:HD23	1:C:88:VAL:HG11	2.01	0.42
1:D:252:ARG:HH11	1:D:252:ARG:HD2	1.66	0.42
1:C:99:LEU:HD12	1:C:102:LEU:CD1	2.46	0.42
1:B:66:VAL:HG22	3:B:364:NAD:C6A	2.49	0.42
1:B:174:LEU:HB3	1:B:175:PRO:HD2	1.93	0.42
1:A:221:LEU:C	1:A:221:LEU:HD13	2.39	0.42
1:B:244:LEU:HD12	1:B:244:LEU:O	2.20	0.42
1:D:7:ILE:O	1:D:35:THR:HB	2.20	0.42
1:A:161:ALA:HB2	1:B:161:ALA:HB2	2.01	0.42
1:B:80:THR:OG1	1:B:81:GLU:N	2.53	0.42
1:C:199:SER:O	1:C:202:GLU:N	2.53	0.42
1:B:153:ASP:N	1:B:153:ASP:OD1	2.53	0.42
1:D:83:ARG:HA	1:D:132:ARG:HH21	1.85	0.42
1:C:17:HIS:O	1:C:18:LEU:C	2.58	0.42
1:C:136:ARG:NH2	1:C:246:ALA:O	2.48	0.41
1:B:65:ASP:O	1:B:67:ARG:N	2.53	0.41
1:A:257:GLU:O	1:A:260:LEU:HB2	2.19	0.41
1:D:129:MET:O	1:D:130:LYS:C	2.58	0.41
1:D:132:ARG:HG2	1:D:132:ARG:NH1	2.34	0.41
1:C:50:ARG:HG3	1:C:50:ARG:NH1	2.35	0.41
1:D:90:ASN:HB2	1:D:140:THR:OG1	2.19	0.41
1:C:160:PHE:HB3	1:D:160:PHE:O	2.21	0.41
1:C:37:ARG:HA	1:C:64:LEU:O	2.21	0.41
1:D:52:LEU:HD12	1:D:52:LEU:HA	1.92	0.41
1:B:110:VAL:HG13	1:B:114:ASN:ND2	2.35	0.41
1:A:201:GLU:O	1:A:202:GLU:C	2.58	0.41
1:C:121:MET:O	1:C:124:ALA:N	2.52	0.41
1:B:240:PHE:O	1:B:243:ALA:HB3	2.20	0.41
1:A:256:THR:HG1	1:A:258:ARG:NH1	2.18	0.41
1:A:263:LEU:HD22	1:A:267:LEU:HD21	2.03	0.41
1:D:66:VAL:HG22	3:D:362:NAD:N1A	2.35	0.41
1:C:208:ASP:OD2	1:C:210:HIS:HB2	2.19	0.41
1:A:37:ARG:O	1:A:63:GLN:HG3	2.20	0.41
1:B:122:LEU:HD13	1:B:169:LEU:CD1	2.51	0.41
1:A:242:THR:O	1:A:243:ALA:C	2.59	0.41
1:A:18:LEU:HD12	1:A:18:LEU:O	2.21	0.41
1:C:261:PRO:HG2	1:C:262:LEU:N	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LEU:HA	1:C:262:LEU:HD12	1.70	0.41
1:C:76:ARG:HD2	1:C:125:PHE:CD2	2.55	0.41
1:D:155:TYR:CE1	1:D:159:LYS:HD2	2.56	0.41
1:C:131:ARG:HA	1:C:131:ARG:HD2	1.84	0.41
1:C:207:THR:HG23	1:C:208:ASP:O	2.20	0.41
1:C:264:ARG:O	1:C:265:MET:C	2.57	0.41
1:A:172:LEU:HD13	1:B:151:PHE:CZ	2.55	0.41
1:C:2:ARG:NH2	1:C:81:GLU:HG2	2.33	0.41
1:A:14:ILE:HD12	1:A:236:VAL:CG1	2.50	0.41
1:D:130:LYS:O	1:D:131:ARG:C	2.59	0.41
1:A:261:PRO:O	1:A:264:ARG:N	2.54	0.41
1:C:173:LEU:HD22	1:C:178:VAL:HG11	2.01	0.41
1:A:278:ALA:O	1:A:282:GLU:N	2.47	0.41
1:A:280:HIS:N	1:B:171:VAL:HG13	2.35	0.41
1:A:32:VAL:O	1:A:59:LEU:HA	2.20	0.41
1:A:252:ARG:NH1	1:A:252:ARG:CG	2.81	0.41
1:A:24:SER:O	1:A:25:ASP:C	2.59	0.41
1:B:263:LEU:HD22	1:B:267:LEU:HD11	2.02	0.41
1:C:64:LEU:HD23	1:C:65:ASP:N	2.36	0.41
1:A:50:ARG:O	1:A:51:ALA:C	2.58	0.41
1:A:244:LEU:HD12	1:A:244:LEU:O	2.21	0.41
1:B:189:HIS:O	1:B:190:THR:HB	2.20	0.41
1:C:163:GLU:CD	1:C:182:LEU:HD13	2.41	0.41
1:A:219:LEU:O	1:A:223:LYS:HD3	2.21	0.41
1:D:187:PRO:HG2	1:D:229:ALA:HB3	2.03	0.41
1:D:38:ASP:OD1	1:D:40:LYS:HE3	2.20	0.41
1:B:260:LEU:HD12	1:B:263:LEU:HB2	2.03	0.40
1:B:67:ARG:NH1	4:B:514:HOH:O	2.53	0.40
1:B:143:VAL:O	1:B:146:LEU:HB2	2.20	0.40
1:B:135:GLY:O	1:B:178:VAL:HG13	2.21	0.40
1:C:39:LEU:HG	1:C:63:GLN:HB2	2.02	0.40
1:C:35:THR:CG2	1:C:62:LEU:HD12	2.51	0.40
1:D:239:VAL:HG21	1:D:255:THR:HA	2.04	0.40
1:C:211:THR:OG1	1:D:130:LYS:HE2	2.21	0.40
1:C:202:GLU:O	1:C:203:VAL:C	2.60	0.40
1:C:119:VAL:HG12	1:C:123:GLN:NE2	2.37	0.40
1:C:260:LEU:HA	1:C:263:LEU:HB3	2.03	0.40
1:B:182:LEU:H	1:B:182:LEU:HD12	1.85	0.40
1:C:11:SER:CA	1:C:36:LEU:HD23	2.50	0.40
1:B:11:SER:HB3	1:B:36:LEU:HD23	2.03	0.40
1:B:269:ASP:HA	1:B:270:PRO:HD2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:CG2	1:A:147:MET:SD	3.10	0.40
1:C:33:TYR:CE2	1:C:79:VAL:HG22	2.56	0.40
1:A:257:GLU:CG	1:A:260:LEU:HD22	2.47	0.40
1:C:39:LEU:O	1:C:42:GLN:HG2	2.22	0.40
1:D:84:VAL:HG21	1:D:125:PHE:CE2	2.57	0.40
1:D:163:GLU:OE1	1:D:252:ARG:NE	2.45	0.40

There are no symmetry-related clashes.

## 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	283/327 (86%)	246 (87%)	34 (12%)	3 (1%)	17	55
1	B	271/327 (83%)	244 (90%)	24 (9%)	3 (1%)	17	55
1	C	283/327 (86%)	235 (83%)	40 (14%)	8 (3%)	6	30
1	D	271/327 (83%)	239 (88%)	26 (10%)	6 (2%)	8	36
All	All	1108/1308 (85%)	964 (87%)	124 (11%)	20 (2%)	11	42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	ILE
1	C	196	VAL
1	C	198	GLY
1	D	209	ILE
1	C	229	ALA
1	C	153	ASP
1	D	104	GLU
1	D	189	HIS
1	A	39	LEU

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Mol	Chain	Res	Type
1	A	174	LEU
1	C	76	ARG
1	C	202	GLU
1	D	39	LEU
1	B	174	LEU
1	C	201	GLU
1	D	84	VAL
1	D	261	PRO
1	B	66	VAL
1	A	175	PRO
1	C	174	LEU

### 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	235/258 (91%)	183 (78%)	52 (22%)	1	5
1	B	227/258 (88%)	191 (84%)	36 (16%)	3	13
1	C	235/258 (91%)	195 (83%)	40 (17%)	2	11
1	D	227/258 (88%)	184 (81%)	43 (19%)	2	8
All	All	924/1032 (90%)	753 (82%)	171 (18%)	2	9

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	5	VAL
1	A	11	SER
1	A	30	PHE
1	A	31	LYS
1	A	35	THR
1	A	55	PRO
1	A	70	LYS
1	A	76	ARG
1	A	78	ARG

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Mol	Chain	Res	Type
1	A	80	THR
1	A	87	LEU
1	A	105	ASP
1	A	109	SER
1	A	121	MET
1	A	127	PRO
1	A	128	ASP
1	A	129	MET
1	A	131	ARG
1	A	147	MET
1	A	153	ASP
1	A	159	LYS
1	A	167	GLU
1	A	169	LEU
1	A	180	LEU
1	A	181	SER
1	A	189	HIS
1	A	193	MET
1	A	194	GLU
1	A	195	LYS
1	A	204	LEU
1	A	209	ILE
1	A	218	TYR
1	A	222	SER
1	A	226	PHE
1	A	227	ARG
1	A	228	GLU
1	A	238	GLU
1	A	241	LEU
1	A	244	LEU
1	A	248	LYS
1	A	256	THR
1	A	258	ARG
1	A	259	PHE
1	A	263	LEU
1	A	266	ARG
1	A	267	LEU
1	A	269	ASP
1	A	277	THR
1	A	281	ARG
1	A	282	GLU
1	A	284	PHE

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Mol	Chain	Res	Type
1	B	20	VAL
1	B	28	GLN
1	B	40	LYS
1	B	41	THR
1	B	42	GLN
1	B	45	LEU
1	B	64	LEU
1	B	69	SER
1	B	80	THR
1	B	109	SER
1	B	123	GLN
1	B	131	ARG
1	B	132	ARG
1	B	134	SER
1	B	153	ASP
1	B	162	LEU
1	B	176	PHE
1	B	183	ILE
1	B	202	GLU
1	B	206	ARG
1	B	221	LEU
1	B	227	ARG
1	B	241	LEU
1	B	244	LEU
1	B	248	LYS
1	B	254	PHE
1	B	257	GLU
1	B	258	ARG
1	B	259	PHE
1	B	260	LEU
1	B	262	LEU
1	B	263	LEU
1	B	265	MET
1	B	271	SER
1	B	281	ARG
1	B	282	GLU
1	C	2	ARG
1	C	6	LEU
1	C	11	SER
1	C	24	SER
1	C	29	SER
1	C	31	LYS

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Mol	Chain	Res	Type
1	C	40	LYS
1	C	47	GLU
1	C	52	LEU
1	C	58	SER
1	C	59	LEU
1	C	62	LEU
1	C	70	LYS
1	C	76	ARG
1	C	80	THR
1	C	83	ARG
1	C	114	ASN
1	C	128	ASP
1	C	131	ARG
1	C	136	ARG
1	C	180	LEU
1	C	193	MET
1	C	195	LYS
1	C	196	VAL
1	C	203	VAL
1	C	214	ARG
1	C	219	LEU
1	C	221	LEU
1	C	224	GLN
1	C	226	PHE
1	C	236	VAL
1	C	241	LEU
1	C	256	THR
1	C	257	GLU
1	C	260	LEU
1	C	267	LEU
1	C	268	ASP
1	C	273	SER
1	C	281	ARG
1	C	283	VAL
1	D	2	ARG
1	D	20	VAL
1	D	37	ARG
1	D	41	THR
1	D	45	LEU
1	D	47	GLU
1	D	50	ARG
1	D	67	ARG

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Mol	Chain	Res	Type
1	D	68	ASP
1	D	69	SER
1	D	70	LYS
1	D	80	THR
1	D	96	LEU
1	D	104	GLU
1	D	109	SER
1	D	110	VAL
1	D	118	THR
1	D	123	GLN
1	D	131	ARG
1	D	142	SER
1	D	143	VAL
1	D	153	ASP
1	D	162	LEU
1	D	182	LEU
1	D	188	VAL
1	D	204	LEU
1	D	207	THR
1	D	208	ASP
1	D	221	LEU
1	D	227	ARG
1	D	234	GLU
1	D	238	GLU
1	D	239	VAL
1	D	241	LEU
1	D	245	ARG
1	D	258	ARG
1	D	262	LEU
1	D	263	LEU
1	D	265	MET
1	D	266	ARG
1	D	268	ASP
1	D	277	THR
1	D	282	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	42	GLN
1	A	123	GLN

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Mol	Chain	Res	Type
1	A	152	ASN
1	A	231	GLN
1	A	274	ASN
1	A	280	HIS
1	B	17	HIS
1	B	42	GLN
1	B	224	GLN
1	B	231	GLN
1	B	274	ASN
1	C	17	HIS
1	C	42	GLN
1	C	123	GLN
1	C	224	GLN
1	C	231	GLN
1	C	280	HIS
1	D	42	GLN
1	D	123	GLN
1	D	189	HIS
1	D	274	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected



value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAD	A	361	-	38,48,48	1.27	5 (13%)	47,73,73	2.21	12 (25%)
2	SO4	A	401	-	4,4,4	0.82	0	6,6,6	0.46	0
3	NAD	B	364	-	38,48,48	1.21	2 (5%)	47,73,73	2.48	14 (29%)
2	SO4	B	400	-	4,4,4	0.88	0	6,6,6	0.20	0
3	NAD	C	363	-	38,48,48	1.42	6 (15%)	47,73,73	2.49	15 (31%)
2	SO4	C	403	-	4,4,4	0.94	0	6,6,6	0.20	0
3	NAD	D	362	-	38,48,48	1.27	3 (7%)	47,73,73	2.20	13 (27%)
2	SO4	D	402	-	4,4,4	0.92	0	6,6,6	0.44	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	A	361	-	1/1/11/11	0/22/62/62	0/5/5/5
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	NAD	B	364	-	1/1/11/11	0/22/62/62	0/5/5/5
2	SO4	B	400	-	-	0/0/0/0	0/0/0/0
3	NAD	C	363	-	-	0/22/62/62	0/5/5/5
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
3	NAD	D	362	-	-	0/22/62/62	0/5/5/5
2	SO4	D	402	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361	NAD	PN-O2N	-2.47	1.44	1.54
3	C	363	NAD	PA-O2A	-2.19	1.45	1.54
3	A	361	NAD	PA-O2A	-2.05	1.46	1.54
3	A	361	NAD	C5A-N7A	-2.02	1.32	1.39
3	C	363	NAD	PN-O2N	-2.01	1.46	1.54
3	C	363	NAD	C3N-C7N	2.06	1.53	1.50
3	B	364	NAD	C7N-N7N	2.13	1.37	1.33
3	D	362	NAD	C3N-C7N	2.30	1.54	1.50
3	D	362	NAD	C6N-N1N	2.40	1.41	1.35
3	C	363	NAD	C6N-N1N	2.59	1.42	1.35
3	A	361	NAD	C6N-N1N	2.71	1.42	1.35
3	C	363	NAD	O4B-C1B	3.71	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	363	NAD	O4D-C1D	3.81	1.46	1.41
3	A	361	NAD	O4D-C1D	4.21	1.46	1.41
3	B	364	NAD	O4D-C1D	4.45	1.46	1.41
3	D	362	NAD	O4D-C1D	5.14	1.47	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	364	NAD	N3A-C2A-N1A	-9.67	121.49	128.89
3	C	363	NAD	N3A-C2A-N1A	-8.28	122.56	128.89
3	D	362	NAD	N3A-C2A-N1A	-7.68	123.02	128.89
3	A	361	NAD	N3A-C2A-N1A	-7.23	123.36	128.89
3	C	363	NAD	C4B-O4B-C1B	-5.76	103.39	109.72
3	D	362	NAD	C3N-C7N-N7N	-4.74	112.63	117.82
3	C	363	NAD	C3N-C7N-N7N	-3.96	113.48	117.82
3	D	362	NAD	O2B-C2B-C3B	-3.69	99.83	111.83
3	B	364	NAD	O2B-C2B-C3B	-3.49	100.47	111.83
3	B	364	NAD	C3N-C7N-N7N	-3.15	114.37	117.82
3	B	364	NAD	C4D-O4D-C1D	-3.06	106.35	109.72
3	D	362	NAD	O3B-C3B-C2B	-3.02	102.02	111.83
3	D	362	NAD	O2D-C2D-C3D	-2.90	102.38	111.83
3	B	364	NAD	O7N-C7N-N7N	-2.79	118.66	122.59
3	C	363	NAD	C2B-C1B-N9A	-2.69	110.18	114.29
3	A	361	NAD	C3N-C7N-N7N	-2.62	114.95	117.82
3	B	364	NAD	O3B-C3B-C2B	-2.53	103.59	111.83
3	B	364	NAD	O3-PN-O5D	-2.52	96.24	102.94
3	D	362	NAD	C4D-O4D-C1D	-2.44	107.04	109.72
3	B	364	NAD	C4B-O4B-C1B	-2.32	107.17	109.72
3	A	361	NAD	O3-PN-O5D	-2.29	96.86	102.94
3	A	361	NAD	C4A-C5A-N7A	-2.26	107.40	109.48
3	A	361	NAD	O2B-C2B-C3B	-2.22	104.59	111.83
3	D	362	NAD	C1B-N9A-C4A	-2.21	123.61	126.94
3	C	363	NAD	C2D-C3D-C4D	-2.20	98.08	102.61
3	D	362	NAD	C2D-C3D-C4D	-2.15	98.20	102.61
3	A	361	NAD	C4B-O4B-C1B	-2.05	107.47	109.72
3	C	363	NAD	O5B-C5B-C4B	2.03	116.59	109.12
3	A	361	NAD	O2A-PA-O1A	2.06	123.70	112.53
3	D	362	NAD	O3-PA-O5B	2.08	108.46	102.94
3	C	363	NAD	O2A-PA-O1A	2.15	124.17	112.53
3	D	362	NAD	O2N-PN-O3	2.17	114.92	105.09
3	B	364	NAD	O5B-C5B-C4B	2.17	117.14	109.12
3	C	363	NAD	O2N-PN-O1N	2.22	124.57	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	364	NAD	PN-O3-PA	2.28	139.12	132.73
3	A	361	NAD	C1B-N9A-C4A	2.30	130.41	126.94
3	C	363	NAD	O4D-C4D-C5D	2.40	117.92	109.32
3	C	363	NAD	C5D-C4D-C3D	2.41	124.77	115.21
3	C	363	NAD	C5B-C4B-C3B	2.57	125.42	115.21
3	D	362	NAD	O4B-C1B-N9A	2.65	113.64	108.10
3	A	361	NAD	O2N-PN-O1N	2.65	126.89	112.53
3	B	364	NAD	O4D-C1D-N1N	2.99	111.41	108.13
3	A	361	NAD	C2B-C1B-N9A	3.03	118.92	114.29
3	A	361	NAD	O7N-C7N-C3N	3.13	123.00	119.59
3	C	363	NAD	O4B-C1B-N9A	3.81	116.06	108.10
3	B	364	NAD	C2B-C1B-N9A	4.30	120.86	114.29
3	D	362	NAD	PN-O3-PA	4.55	145.50	132.73
3	C	363	NAD	O5D-C5D-C4D	4.64	126.22	109.12
3	B	364	NAD	O4B-C1B-N9A	4.78	118.09	108.10
3	D	362	NAD	O7N-C7N-C3N	5.20	125.26	119.59
3	C	363	NAD	O7N-C7N-C3N	5.76	125.88	119.59
3	C	363	NAD	O4D-C1D-N1N	6.14	114.88	108.13
3	B	364	NAD	O7N-C7N-C3N	6.74	126.95	119.59
3	A	361	NAD	O4B-C1B-N9A	9.39	127.76	108.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	361	NAD	C1B
3	B	364	NAD	C1B

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	361	NAD	6	0
2	A	401	SO4	1	0
3	B	364	NAD	10	0
3	C	363	NAD	5	0
3	D	362	NAD	13	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	285/327 (87%)	-0.96	0 100 100	22, 22, 22, 22	16 (5%)
1	B	275/327 (84%)	-0.97	0 100 100	22, 22, 22, 22	8 (2%)
1	C	285/327 (87%)	-0.93	0 100 100	22, 22, 22, 22	16 (5%)
1	D	275/327 (84%)	-0.97	0 100 100	22, 22, 22, 22	10 (3%)
All	All	1120/1308 (85%)	-0.96	0 100 100	22, 22, 22, 22	50 (4%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	B	364	44/44	0.90	0.22	3.01	22,22,22,22	44
3	NAD	D	362	44/44	0.89	0.23	2.72	22,22,22,22	44

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	400	5/5	0.97	0.19	1.86	22,22,22,22	5
3	NAD	A	361	44/44	0.97	0.12	-0.25	22,22,22,22	0
3	NAD	C	363	44/44	0.97	0.11	-0.46	22,22,22,22	0
2	SO4	A	401	5/5	0.97	0.12	-0.71	22,22,22,22	5
2	SO4	D	402	5/5	0.95	0.17	-	22,22,22,22	5
2	SO4	C	403	5/5	0.97	0.11	-	22,22,22,22	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.