



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:44 AM UTC

PDB ID : 1FDV / pdb_00001fdv
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

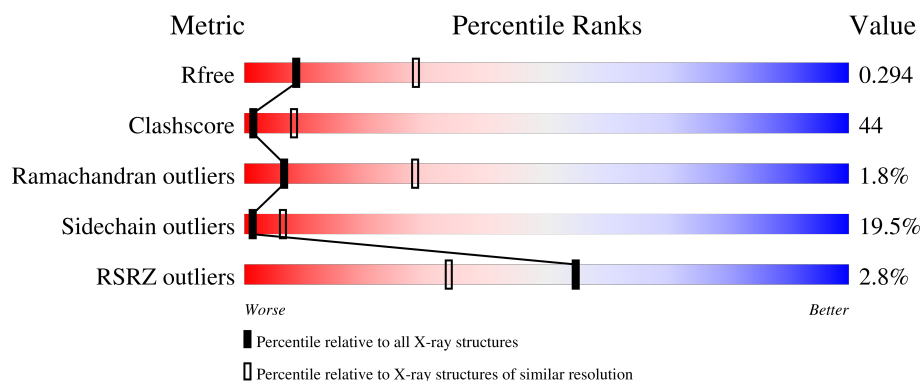
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of 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	327	2% 21% 39% 23% 5% 13%
1	B	327	% 22% 41% 18% • 16%
1	C	327	4% 19% 39% 22% 7% 13%
1	D	327	2% 19% 37% 24% • 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

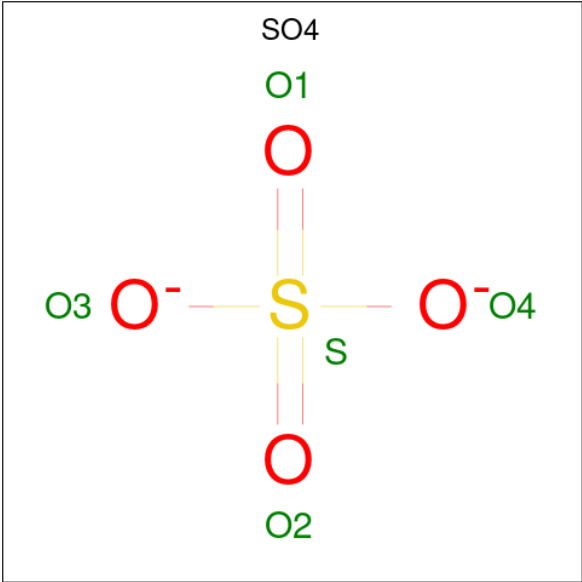
- Molecule 1 is a protein called 17-BETA-HYDROXYSTEROID DEHYDROGENASE.

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:

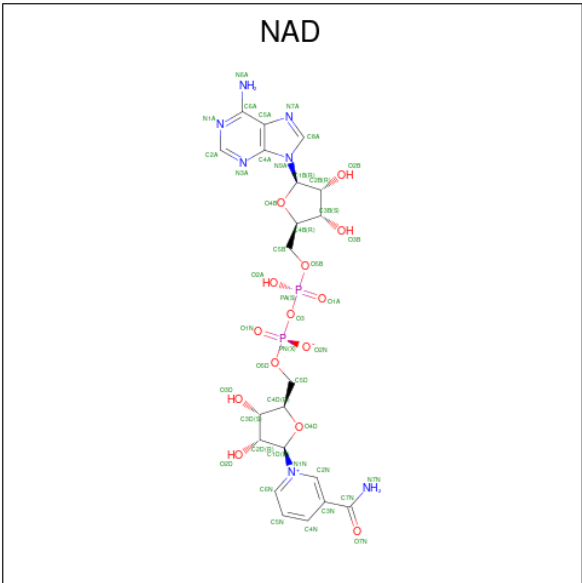
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	HIS	engineered mutation	UNP P14061
A	301	ARG	ALA	conflict	UNP P14061
B	221	LEU	HIS	engineered mutation	UNP P14061
B	301	ARG	ALA	conflict	UNP P14061
C	221	LEU	HIS	engineered mutation	UNP P14061
C	301	ARG	ALA	conflict	UNP P14061
D	221	LEU	HIS	engineered mutation	UNP P14061
D	301	ARG	ALA	conflict	UNP P14061

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: 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		

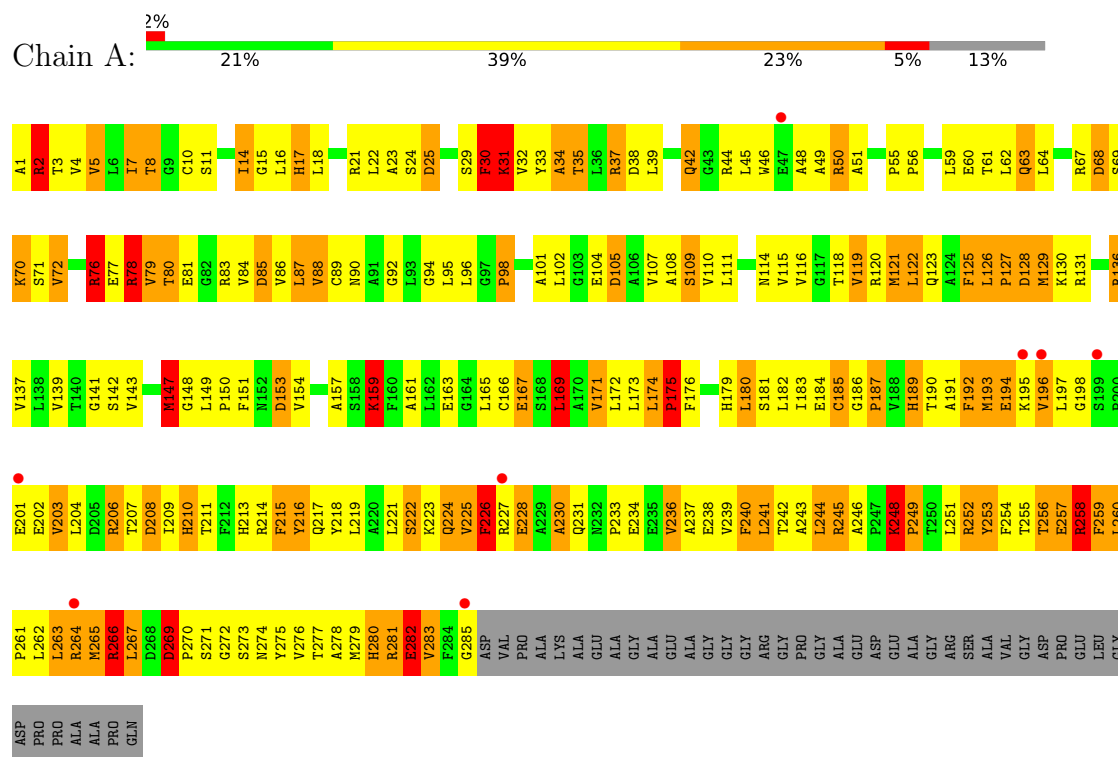
- Molecule 4 is water.

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		

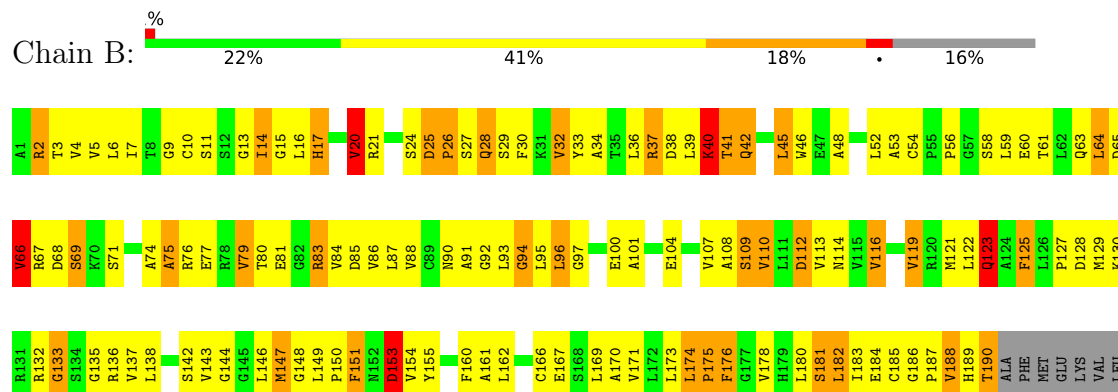
3 Residue-property plots

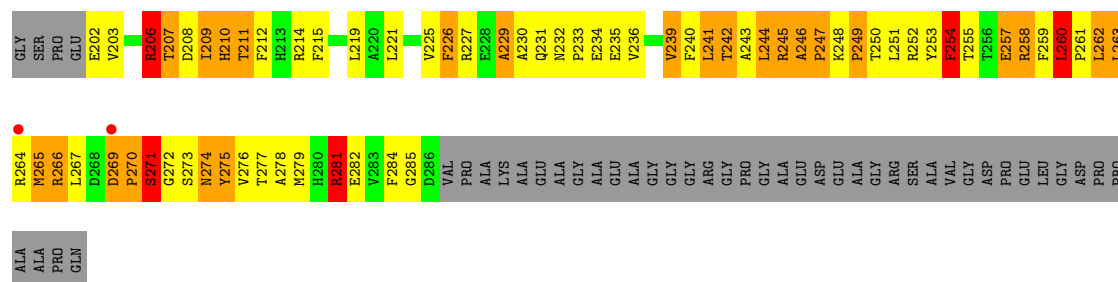
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 17-BETA-HYDROXYSTEROID DEHYDROGENASE

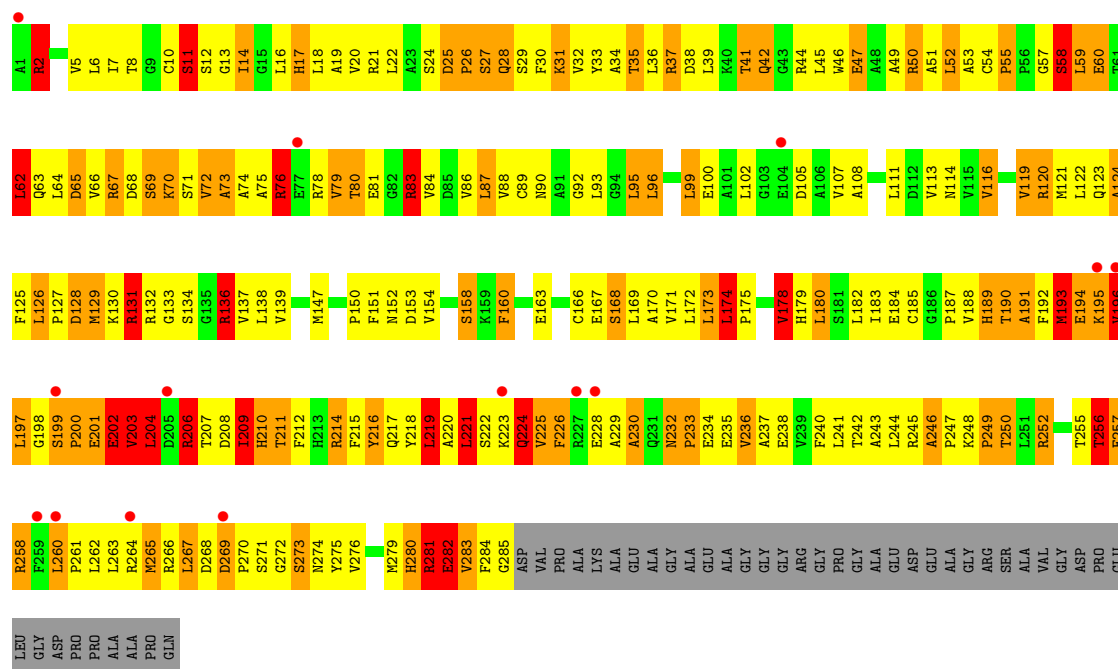
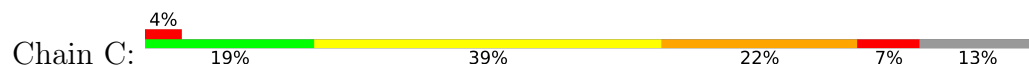


• Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE

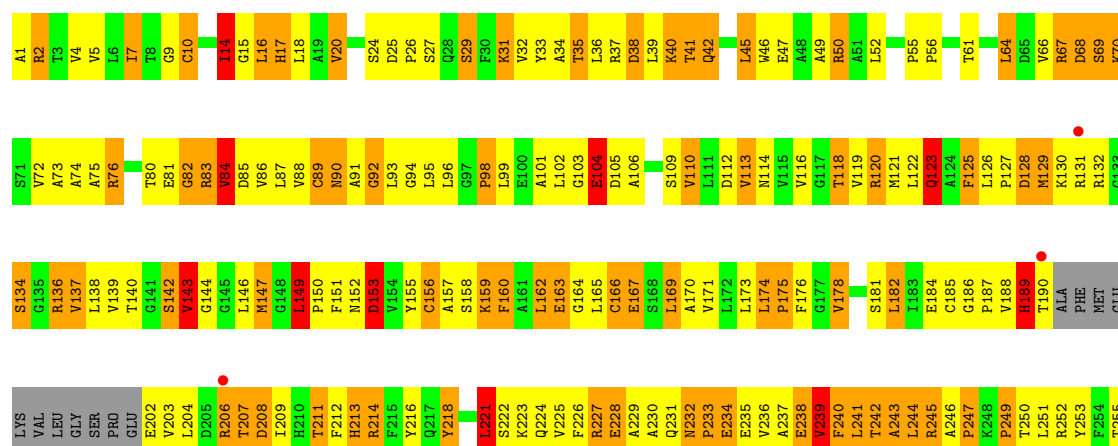
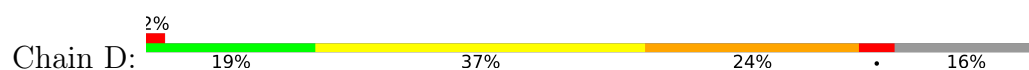


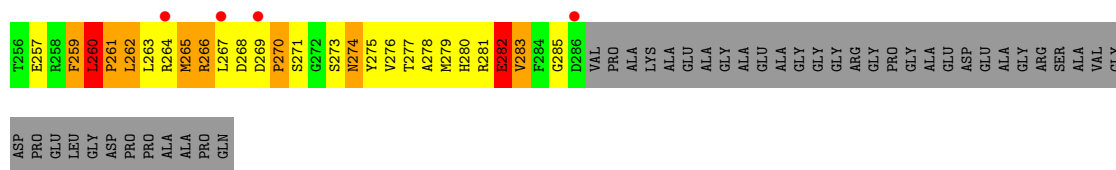


• Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE



• 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, α , β , γ	115.12Å 79.11Å 120.47Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.0 (10.00-3.10) 82.6 (10.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1805 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.001 for l,k,-h 0.018 for h,-k,-l 0.117 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8812	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	2/2219 (0.1%)	2.45	150/3010 (5.0%)
1	B	1.10	0/2141	2.39	125/2904 (4.3%)
1	C	1.14	1/2219 (0.0%)	2.48	157/3010 (5.2%)
1	D	1.10	1/2141 (0.0%)	2.40	133/2904 (4.6%)
All	All	1.11	4/8720 (0.0%)	2.43	565/11828 (4.8%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	ARG	N-CA	-5.30	1.39	1.46
1	D	94	GLY	N-CA	5.26	1.49	1.44
1	A	31	LYS	CA-CB	-5.13	1.45	1.53
1	C	190	THR	C-O	5.13	1.30	1.24

All (565) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	ARG	CD-NE-CZ	13.80	143.72	124.40
1	A	196	VAL	N-CA-C	13.75	129.50	113.42
1	C	67	ARG	CD-NE-CZ	13.52	143.32	124.40
1	B	160	PHE	CA-CB-CG	13.04	126.84	113.80
1	B	2	ARG	CD-NE-CZ	12.66	142.12	124.40
1	D	116	VAL	CA-C-N	12.33	133.67	119.98
1	D	116	VAL	C-N-CA	12.33	133.67	119.98
1	A	78	ARG	CD-NE-CZ	12.07	141.30	124.40
1	D	164	GLY	O-C-N	11.81	133.82	122.13
1	B	125	PHE	N-CA-C	11.80	128.01	113.50
1	D	214	ARG	CD-NE-CZ	11.58	140.61	124.40
1	B	281	ARG	CA-CB-CG	11.36	136.82	114.10
1	D	153	ASP	CA-CB-CG	-11.15	101.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	PHE	CA-CB-CG	10.99	124.79	113.80
1	A	226	PHE	CA-CB-CG	-10.97	102.83	113.80
1	A	29	SER	N-CA-C	10.69	122.69	111.14
1	A	63	GLN	OE1-CD-NE2	-10.36	112.24	122.60
1	C	93	LEU	CA-C-O	-10.35	109.06	121.06
1	A	280	HIS	CA-CB-CG	-10.32	103.48	113.80
1	A	282	GLU	N-CA-CB	10.31	125.28	110.12
1	B	227	ARG	N-CA-CB	10.17	124.75	110.01
1	B	210	HIS	CA-CB-CG	-10.08	103.72	113.80
1	C	183	ILE	CB-CA-C	-10.00	100.05	112.45
1	A	116	VAL	CA-C-N	9.95	131.02	119.98
1	A	116	VAL	C-N-CA	9.95	131.02	119.98
1	A	192	PHE	N-CA-C	-9.76	98.89	112.45
1	B	83	ARG	CD-NE-CZ	9.60	137.84	124.40
1	B	214	ARG	CD-NE-CZ	9.56	137.79	124.40
1	C	256	THR	CA-C-O	-9.39	111.41	121.45
1	B	6	LEU	CA-C-O	-9.37	110.27	120.30
1	A	246	ALA	CA-C-N	9.27	129.01	119.64
1	A	246	ALA	C-N-CA	9.27	129.01	119.64
1	D	32	VAL	CA-C-O	9.21	130.38	120.53
1	D	282	GLU	CA-C-N	9.21	136.26	121.34
1	D	282	GLU	C-N-CA	9.21	136.26	121.34
1	A	258	ARG	N-CA-CB	9.19	126.02	110.49
1	A	197	LEU	N-CA-C	9.16	123.66	108.73
1	D	32	VAL	N-CA-C	9.15	121.06	107.80
1	A	230	ALA	CA-C-O	-9.13	111.87	121.55
1	D	160	PHE	CA-CB-CG	9.05	122.85	113.80
1	C	232	ASN	CA-C-O	9.04	130.45	120.05
1	D	90	ASN	CA-CB-CG	8.97	121.57	112.60
1	D	221	LEU	CA-C-O	8.94	130.46	120.90
1	C	120	ARG	CD-NE-CZ	8.86	136.80	124.40
1	D	76	ARG	NE-CZ-NH2	-8.85	111.23	119.20
1	A	136	ARG	NH1-CZ-NH2	8.84	130.79	119.30
1	B	32	VAL	N-CA-C	8.72	120.28	107.37
1	A	48	ALA	O-C-N	8.71	131.40	122.08
1	D	174	LEU	CA-C-N	8.58	128.31	119.56
1	D	174	LEU	C-N-CA	8.58	128.31	119.56
1	B	17	HIS	CA-CB-CG	-8.55	105.25	113.80
1	B	2	ARG	NE-CZ-NH2	-8.50	111.55	119.20
1	C	136	ARG	NE-CZ-NH2	-8.48	111.57	119.20
1	D	227	ARG	CA-C-O	-8.48	110.52	120.10
1	C	256	THR	N-CA-C	-8.47	96.34	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	ALA	CA-C-O	-8.46	111.88	121.19
1	A	142	SER	CA-C-O	-8.46	111.59	120.89
1	A	192	PHE	CB-CA-C	8.42	126.02	110.11
1	B	247	PRO	N-CA-C	-8.38	102.16	113.40
1	B	25	ASP	CA-CB-CG	-8.32	104.28	112.60
1	C	80	THR	N-CA-C	8.31	121.38	111.33
1	C	42	GLN	N-CA-C	8.26	123.19	113.20
1	D	269	ASP	CA-C-N	8.26	127.98	119.56
1	D	269	ASP	C-N-CA	8.26	127.98	119.56
1	B	249	PRO	N-CA-CB	8.25	108.76	103.23
1	B	281	ARG	CD-NE-CZ	8.25	135.95	124.40
1	C	12	SER	CA-C-O	-8.22	112.51	121.31
1	B	269	ASP	CA-C-N	8.22	129.01	119.47
1	B	269	ASP	C-N-CA	8.22	129.01	119.47
1	C	25	ASP	CA-CB-CG	-8.19	104.41	112.60
1	B	254	PHE	CA-CB-CG	8.14	121.94	113.80
1	D	189	HIS	CA-CB-CG	-8.14	105.66	113.80
1	A	254	PHE	CA-CB-CG	-8.11	105.69	113.80
1	A	14	ILE	N-CA-CB	8.02	119.41	110.51
1	B	20	VAL	N-CA-C	8.01	118.11	110.42
1	A	2	ARG	CG-CD-NE	7.89	129.36	112.00
1	C	199	SER	CB-CA-C	7.82	125.58	110.17
1	A	77	GLU	CA-C-O	7.80	128.94	119.97
1	A	197	LEU	CB-CA-C	-7.79	97.57	110.19
1	A	128	ASP	CA-CB-CG	7.79	120.39	112.60
1	C	281	ARG	CD-NE-CZ	7.67	135.13	124.40
1	C	173	LEU	N-CA-C	7.66	121.89	112.54
1	A	206	ARG	N-CA-C	7.64	121.69	112.38
1	C	11	SER	CA-C-O	-7.64	112.46	120.55
1	C	196	VAL	CA-C-N	7.63	138.95	121.87
1	C	196	VAL	C-N-CA	7.63	138.95	121.87
1	A	37	ARG	NE-CZ-NH2	-7.62	112.35	119.20
1	A	185	CYS	CA-C-O	-7.59	112.53	121.11
1	A	10	CYS	N-CA-C	7.56	122.53	111.87
1	C	189	HIS	CA-CB-CG	-7.55	106.25	113.80
1	D	83	ARG	CA-C-N	7.52	135.50	121.97
1	D	83	ARG	C-N-CA	7.52	135.50	121.97
1	D	2	ARG	NE-CZ-NH2	-7.50	112.45	119.20
1	D	164	GLY	CA-C-O	-7.50	113.33	121.05
1	A	37	ARG	CA-C-N	-7.48	112.24	122.86
1	A	37	ARG	C-N-CA	-7.48	112.24	122.86
1	A	125	PHE	CA-CB-CG	7.41	121.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	ALA	O-C-N	-7.41	114.26	122.12
1	D	136	ARG	NE-CZ-NH2	-7.36	112.57	119.20
1	C	192	PHE	N-CA-CB	-7.35	99.31	110.12
1	D	259	PHE	CA-CB-CG	-7.33	106.47	113.80
1	D	40	LYS	CA-CB-CG	7.33	128.77	114.10
1	D	134	SER	CA-C-O	7.30	129.04	120.43
1	C	57	GLY	CA-C-N	7.29	131.40	120.31
1	C	57	GLY	C-N-CA	7.29	131.40	120.31
1	C	78	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	D	29	SER	N-CA-CB	-7.29	100.82	110.88
1	A	283	VAL	N-CA-C	7.29	118.94	111.00
1	D	125	PHE	N-CA-C	7.29	123.19	113.72
1	C	269	ASP	CA-C-N	7.28	126.81	119.24
1	C	269	ASP	C-N-CA	7.28	126.81	119.24
1	A	37	ARG	CD-NE-CZ	7.27	134.58	124.40
1	A	136	ARG	NE-CZ-NH1	-7.25	114.25	121.50
1	C	96	LEU	O-C-N	-7.25	114.86	123.27
1	A	240	PHE	CA-CB-CG	-7.24	106.56	113.80
1	C	194	GLU	CB-CA-C	7.21	122.94	110.68
1	D	17	HIS	CA-CB-CG	-7.18	106.62	113.80
1	C	2	ARG	NE-CZ-NH1	7.16	128.66	121.50
1	C	196	VAL	CA-C-O	7.15	129.72	120.78
1	B	42	GLN	N-CA-C	7.15	120.87	112.72
1	D	14	ILE	N-CA-C	-7.14	103.56	110.42
1	B	136	ARG	CA-C-O	-7.14	112.64	120.43
1	C	60	GLU	CA-C-O	-7.10	112.08	120.60
1	A	266	ARG	CA-C-O	7.10	130.66	120.51
1	C	116	VAL	CA-C-N	7.07	127.98	119.99
1	C	116	VAL	C-N-CA	7.07	127.98	119.99
1	C	246	ALA	CA-C-N	7.04	126.87	119.05
1	C	246	ALA	C-N-CA	7.04	126.87	119.05
1	A	17	HIS	CA-CB-CG	-7.03	106.77	113.80
1	B	229	ALA	N-CA-C	7.03	119.97	111.40
1	B	227	ARG	CA-C-O	-7.03	113.44	120.82
1	B	206	ARG	N-CA-C	7.00	121.67	113.20
1	D	83	ARG	N-CA-C	-7.00	99.87	109.95
1	A	282	GLU	CA-C-O	-6.98	113.15	120.55
1	A	248	LYS	CA-C-N	6.97	126.73	119.76
1	A	248	LYS	C-N-CA	6.97	126.73	119.76
1	B	2	ARG	NE-CZ-NH1	6.95	128.45	121.50
1	D	82	GLY	CA-C-O	6.93	126.47	119.27
1	B	90	ASN	O-C-N	-6.92	114.73	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	A	42	GLN	N-CA-C	6.90	121.70	113.28
1	A	265	MET	CA-CB-CG	-6.88	100.34	114.10
1	A	208	ASP	CA-CB-CG	6.85	119.45	112.60
1	C	49	ALA	N-CA-C	-6.84	103.75	111.07
1	D	76	ARG	CD-NE-CZ	6.84	133.97	124.40
1	C	72	VAL	N-CA-C	6.83	116.95	110.53
1	C	183	ILE	N-CA-CB	6.82	118.99	111.89
1	B	25	ASP	CA-C-N	6.81	126.95	119.87
1	B	25	ASP	C-N-CA	6.81	126.95	119.87
1	B	258	ARG	CD-NE-CZ	6.77	133.88	124.40
1	B	275	TYR	CB-CA-C	-6.77	100.16	110.92
1	C	224	GLN	CB-CA-C	6.77	121.68	110.92
1	A	85	ASP	CA-C-O	6.76	128.10	121.00
1	C	13	GLY	N-CA-C	6.74	123.22	111.50
1	D	211	THR	CA-CB-OG1	6.74	119.70	109.60
1	D	249	PRO	N-CA-CB	6.74	109.21	103.35
1	A	108	ALA	CA-C-O	-6.72	113.30	120.42
1	B	37	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	A	76	ARG	CD-NE-CZ	6.71	133.80	124.40
1	A	76	ARG	NE-CZ-NH2	-6.70	113.17	119.20
1	C	192	PHE	N-CA-C	-6.69	103.99	111.28
1	C	26	PRO	CA-C-N	6.67	131.28	120.60
1	C	26	PRO	C-N-CA	6.67	131.28	120.60
1	B	188	VAL	CA-C-O	-6.67	113.17	120.43
1	A	98	PRO	CA-C-O	-6.65	114.29	121.27
1	D	89	CYS	CA-CB-SG	-6.64	99.12	114.40
1	A	55	PRO	CA-C-N	6.64	127.03	119.93
1	A	55	PRO	C-N-CA	6.64	127.03	119.93
1	B	150	PRO	N-CA-CB	6.63	109.12	103.35
1	D	243	ALA	CA-C-O	6.63	128.36	121.07
1	A	225	VAL	CB-CA-C	-6.62	103.22	111.70
1	C	191	ALA	CA-C-O	6.62	127.96	119.16
1	D	104	GLU	CB-CG-CD	6.61	123.84	112.60
1	C	119	VAL	N-CA-CB	6.61	117.85	110.51
1	A	269	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	217	GLN	N-CA-C	-6.59	104.02	111.14
1	A	159	LYS	CB-CA-C	6.59	121.22	110.88
1	A	215	PHE	O-C-N	-6.58	115.29	122.07
1	A	105	ASP	CA-C-N	6.58	129.63	120.29
1	A	105	ASP	C-N-CA	6.58	129.63	120.29
1	C	152	ASN	OD1-CG-ND2	6.57	129.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	ARG	CD-NE-CZ	-6.57	115.20	124.40
1	D	149	LEU	CB-CA-C	-6.57	101.42	110.16
1	D	169	LEU	O-C-N	-6.56	115.31	122.07
1	D	56	PRO	N-CA-CB	6.54	109.16	103.27
1	D	31	LYS	CB-CA-C	6.52	120.76	110.19
1	D	240	PHE	CA-C-N	6.51	129.33	120.54
1	D	240	PHE	C-N-CA	6.51	129.33	120.54
1	C	58	SER	CB-CA-C	-6.51	98.17	110.67
1	B	133	GLY	O-C-N	6.51	129.18	122.54
1	C	128	ASP	CA-CB-CG	6.50	119.10	112.60
1	C	281	ARG	N-CA-C	-6.50	104.28	111.36
1	C	120	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	A	269	ASP	CA-C-N	6.49	126.42	119.28
1	A	269	ASP	C-N-CA	6.49	126.42	119.28
1	C	41	THR	N-CA-C	6.49	120.81	113.02
1	D	251	LEU	CA-C-O	6.49	127.43	119.97
1	C	95	LEU	CA-C-N	6.49	132.15	123.00
1	C	95	LEU	C-N-CA	6.49	132.15	123.00
1	B	75	ALA	N-CA-CB	6.49	119.68	109.82
1	B	226	PHE	O-C-N	6.48	129.03	122.03
1	B	64	LEU	CA-C-O	-6.47	113.80	121.11
1	B	26	PRO	N-CA-CB	6.46	109.48	103.41
1	C	233	PRO	CA-C-N	6.45	129.25	120.54
1	C	233	PRO	C-N-CA	6.45	129.25	120.54
1	C	168	SER	N-CA-C	-6.45	104.17	111.14
1	B	227	ARG	N-CA-C	-6.43	104.19	111.07
1	C	17	HIS	N-CA-C	6.43	117.95	111.07
1	C	216	TYR	CB-CA-C	6.42	122.51	110.63
1	A	249	PRO	N-CA-C	6.41	121.25	111.19
1	A	228	GLU	CA-C-N	-6.40	110.26	120.70
1	A	228	GLU	C-N-CA	-6.40	110.26	120.70
1	A	259	PHE	CA-CB-CG	6.39	120.19	113.80
1	C	250	THR	N-CA-CB	6.39	119.13	110.38
1	C	191	ALA	CA-C-N	6.37	128.82	120.28
1	C	191	ALA	C-N-CA	6.37	128.82	120.28
1	C	84	VAL	CA-C-O	-6.34	113.73	120.39
1	B	185	CYS	N-CA-C	6.34	119.87	109.85
1	C	37	ARG	NE-CZ-NH2	-6.33	113.50	119.20
1	C	38	ASP	CA-CB-CG	-6.33	106.27	112.60
1	C	124	ALA	CA-C-O	6.33	127.13	120.42
1	D	4	VAL	CB-CA-C	-6.33	104.40	111.23
1	D	42	GLN	N-CA-C	6.32	120.83	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	GLU	CA-C-O	-6.30	113.14	120.20
1	D	211	THR	N-CA-CB	6.30	119.38	110.12
1	A	78	ARG	CB-CA-C	6.29	122.06	110.11
1	C	211	THR	N-CA-C	-6.27	104.36	111.07
1	C	25	ASP	CA-C-N	6.27	127.68	119.84
1	C	25	ASP	C-N-CA	6.27	127.68	119.84
1	C	200	PRO	O-C-N	6.26	131.09	122.64
1	B	83	ARG	NE-CZ-NH1	6.25	127.75	121.50
1	C	203	VAL	CA-C-N	6.23	128.95	120.54
1	C	203	VAL	C-N-CA	6.23	128.95	120.54
1	D	260	LEU	CB-CA-C	6.23	122.45	110.17
1	A	76	ARG	N-CA-C	6.23	121.65	111.37
1	B	14	ILE	CA-C-O	-6.22	114.58	121.17
1	D	223	LYS	O-C-N	-6.21	115.53	122.12
1	C	265	MET	O-C-N	6.21	128.73	122.08
1	D	227	ARG	CG-CD-NE	-6.21	98.34	112.00
1	A	80	THR	N-CA-C	6.21	118.56	111.11
1	B	214	ARG	CA-C-O	6.20	127.33	120.63
1	C	79	VAL	CA-C-N	6.20	128.87	120.38
1	C	79	VAL	C-N-CA	6.20	128.87	120.38
1	A	171	VAL	CA-C-O	6.14	127.11	120.47
1	A	187	PRO	O-C-N	-6.14	115.95	123.01
1	A	176	PHE	CA-CB-CG	6.14	119.94	113.80
1	A	63	GLN	CG-CD-OE1	6.12	133.05	120.80
1	A	252	ARG	NE-CZ-NH2	-6.12	113.70	119.20
1	C	192	PHE	CA-CB-CG	-6.12	107.69	113.80
1	A	50	ARG	CA-C-O	6.11	126.90	120.42
1	D	98	PRO	CA-C-N	6.11	128.75	120.38
1	D	98	PRO	C-N-CA	6.11	128.75	120.38
1	A	163	GLU	CA-C-O	6.11	126.42	119.27
1	D	90	ASN	CA-C-O	-6.10	110.98	120.81
1	D	151	PHE	CA-C-N	6.10	132.44	121.15
1	D	151	PHE	C-N-CA	6.10	132.44	121.15
1	B	148	GLY	N-CA-C	6.10	118.49	111.36
1	B	175	PRO	N-CA-CB	6.09	109.64	103.25
1	B	245	ARG	CB-CA-C	6.09	121.41	109.72
1	D	55	PRO	CA-C-N	6.08	126.40	119.83
1	D	55	PRO	C-N-CA	6.08	126.40	119.83
1	B	153	ASP	CA-CB-CG	-6.08	106.52	112.60
1	B	215	PHE	CA-CB-CG	-6.06	107.74	113.80
1	D	143	VAL	CA-C-O	6.06	127.01	120.47
1	B	215	PHE	CA-C-O	-6.05	114.42	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	CYS	CB-CA-C	6.04	120.45	110.90
1	D	16	LEU	O-C-N	-6.04	115.26	122.15
1	D	38	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	75	ALA	N-CA-C	-6.04	103.66	111.02
1	D	89	CYS	CA-C-O	-6.04	114.60	121.66
1	D	123	GLN	CA-CB-CG	6.03	126.17	114.10
1	A	120	ARG	CD-NE-CZ	6.03	132.84	124.40
1	C	197	LEU	N-CA-CB	6.03	120.82	111.24
1	B	270	PRO	N-CA-CB	6.02	110.05	103.30
1	B	108	ALA	N-CA-C	6.02	118.63	111.71
1	C	28	GLN	CB-CA-C	6.01	120.97	111.95
1	D	260	LEU	CA-C-N	6.00	127.34	119.84
1	D	260	LEU	C-N-CA	6.00	127.34	119.84
1	C	206	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	B	90	ASN	N-CA-CB	-6.00	102.92	110.90
1	C	248	LYS	CB-CA-C	6.00	120.19	111.02
1	C	199	SER	N-CA-C	5.98	123.03	109.81
1	D	25	ASP	CA-C-N	5.98	125.66	119.56
1	D	25	ASP	C-N-CA	5.98	125.66	119.56
1	D	93	LEU	O-C-N	5.96	130.07	123.33
1	D	247	PRO	N-CA-CB	5.95	110.11	103.44
1	C	60	GLU	O-C-N	5.95	130.53	123.33
1	B	257	GLU	CB-CG-CD	5.93	122.69	112.60
1	D	98	PRO	CB-CA-C	5.92	118.02	111.56
1	B	116	VAL	CA-C-N	5.92	127.54	120.14
1	B	116	VAL	C-N-CA	5.92	127.54	120.14
1	D	274	ASN	CA-C-O	-5.91	114.11	121.02
1	A	4	VAL	N-CA-C	5.90	116.18	107.15
1	B	245	ARG	CD-NE-CZ	5.90	132.66	124.40
1	C	47	GLU	N-CA-CB	-5.90	101.21	110.06
1	A	147	MET	CA-C-N	5.90	126.33	120.31
1	A	147	MET	C-N-CA	5.90	126.33	120.31
1	D	247	PRO	CA-C-N	-5.89	115.50	123.46
1	D	247	PRO	C-N-CA	-5.89	115.50	123.46
1	C	252	ARG	N-CA-C	5.89	119.08	109.24
1	C	99	LEU	N-CA-C	5.88	118.44	111.33
1	C	258	ARG	CD-NE-CZ	-5.87	116.18	124.40
1	D	163	GLU	CA-C-O	5.87	126.95	120.90
1	D	163	GLU	CB-CG-CD	5.87	122.58	112.60
1	C	83	ARG	CA-C-N	-5.87	115.46	123.14
1	C	83	ARG	C-N-CA	-5.87	115.46	123.14
1	C	248	LYS	CA-C-N	5.86	126.06	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	248	LYS	C-N-CA	5.86	126.06	119.90
1	A	192	PHE	CA-C-N	5.86	131.40	121.14
1	A	192	PHE	C-N-CA	5.86	131.40	121.14
1	C	194	GLU	CA-C-O	-5.86	114.30	120.63
1	A	128	ASP	CA-C-O	-5.85	114.34	120.55
1	C	78	ARG	CA-CB-CG	5.85	125.81	114.10
1	C	87	LEU	CA-C-O	-5.85	114.45	120.54
1	C	131	ARG	O-C-N	-5.85	115.12	122.20
1	A	194	GLU	N-CA-C	-5.85	104.81	111.07
1	B	17	HIS	N-CA-C	5.85	118.41	111.33
1	C	22	LEU	CA-C-O	-5.84	114.64	121.07
1	C	204	LEU	CA-C-O	5.84	127.14	120.90
1	A	270	PRO	N-CA-CB	5.82	109.68	103.39
1	C	174	LEU	CA-C-N	5.81	127.11	119.84
1	C	174	LEU	C-N-CA	5.81	127.11	119.84
1	B	160	PHE	N-CA-C	-5.81	104.91	112.23
1	A	30	PHE	CB-CA-C	-5.81	100.22	109.80
1	D	274	ASN	CA-CB-CG	-5.80	106.80	112.60
1	C	2	ARG	CA-C-O	-5.79	112.22	120.51
1	B	127	PRO	N-CA-CB	5.79	109.33	103.25
1	C	50	ARG	N-CA-C	-5.79	104.16	111.11
1	D	69	SER	CA-C-O	-5.78	113.56	120.10
1	C	55	PRO	N-CA-C	-5.78	103.65	110.70
1	A	34	ALA	CA-C-N	-5.77	114.56	122.93
1	A	34	ALA	C-N-CA	-5.77	114.56	122.93
1	D	2	ARG	CA-CB-CG	5.77	125.65	114.10
1	B	110	VAL	CA-C-O	-5.77	114.95	120.95
1	C	44	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
1	B	40	LYS	CA-CB-CG	5.76	125.61	114.10
1	D	280	HIS	CA-C-N	5.76	128.46	120.63
1	D	280	HIS	C-N-CA	5.76	128.46	120.63
1	C	193	MET	CB-CA-C	-5.75	101.81	110.90
1	D	242	THR	N-CA-C	-5.75	104.70	110.97
1	A	94	GLY	CA-C-O	-5.75	114.13	122.52
1	C	47	GLU	CA-C-O	5.75	126.84	120.63
1	A	196	VAL	N-CA-CB	-5.74	104.42	112.35
1	D	150	PRO	N-CA-CB	5.74	108.42	103.31
1	C	73	ALA	N-CA-C	-5.74	104.22	111.11
1	D	270	PRO	N-CA-CB	5.73	109.21	103.48
1	B	190	THR	N-CA-CB	5.73	121.24	111.50
1	C	76	ARG	CA-C-N	5.73	128.53	120.28
1	C	76	ARG	C-N-CA	5.73	128.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	LEU	N-CA-CB	5.72	120.56	110.37
1	B	212	PHE	N-CA-C	5.72	117.98	111.11
1	C	211	THR	CB-CA-C	5.72	119.86	110.88
1	D	274	ASN	O-C-N	5.72	129.12	122.20
1	D	233	PRO	N-CA-C	-5.71	104.52	113.78
1	A	85	ASP	CA-CB-CG	-5.71	106.89	112.60
1	C	252	ARG	CA-C-O	5.70	127.21	120.66
1	B	116	VAL	O-C-N	-5.70	116.34	121.87
1	A	119	VAL	N-CA-CB	5.69	117.86	110.57
1	C	44	ARG	CA-C-O	-5.68	114.37	121.02
1	A	56	PRO	CB-CA-C	-5.68	104.42	111.64
1	C	191	ALA	O-C-N	-5.65	115.94	121.87
1	D	5	VAL	O-C-N	-5.65	117.38	123.14
1	D	17	HIS	N-CA-C	5.65	117.11	111.07
1	A	88	VAL	N-CA-C	5.64	116.53	107.73
1	C	96	LEU	N-CA-C	5.63	117.59	108.41
1	B	231	GLN	CA-CB-CG	5.63	125.36	114.10
1	D	26	PRO	N-CA-CB	5.63	109.11	103.48
1	D	84	VAL	N-CA-CB	5.63	120.52	111.23
1	A	258	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	169	LEU	N-CA-CB	5.61	119.54	110.40
1	B	211	THR	CA-C-N	5.60	128.10	120.54
1	B	211	THR	C-N-CA	5.60	128.10	120.54
1	B	90	ASN	CA-CB-CG	5.60	118.20	112.60
1	D	128	ASP	CB-CA-C	5.60	120.19	110.68
1	D	227	ARG	CB-CA-C	-5.59	100.28	110.63
1	A	10	CYS	CA-C-O	-5.59	113.78	120.65
1	D	186	GLY	N-CA-C	-5.59	100.94	112.34
1	D	234	GLU	N-CA-CB	5.58	118.32	110.12
1	B	58	SER	CA-C-O	-5.57	114.64	120.55
1	A	30	PHE	O-C-N	5.57	129.32	123.03
1	B	125	PHE	O-C-N	-5.56	115.04	122.49
1	C	2	ARG	NE-CZ-NH2	-5.56	114.20	119.20
1	C	280	HIS	CA-CB-CG	-5.55	108.25	113.80
1	A	179	HIS	CA-CB-CG	-5.53	108.28	113.80
1	A	283	VAL	CA-CB-CG2	-5.53	101.01	110.40
1	A	260	LEU	CA-C-N	5.52	126.74	119.84
1	A	260	LEU	C-N-CA	5.52	126.74	119.84
1	B	7	ILE	CB-CA-C	-5.52	102.28	110.33
1	D	232	ASN	OD1-CG-ND2	5.51	128.11	122.60
1	A	104	GLU	CA-C-N	5.51	127.67	120.28
1	A	104	GLU	C-N-CA	5.51	127.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	LEU	CA-C-O	-5.51	115.19	121.58
1	A	245	ARG	CD-NE-CZ	5.51	132.11	124.40
1	B	247	PRO	CA-C-N	-5.51	116.03	123.46
1	B	247	PRO	C-N-CA	-5.51	116.03	123.46
1	C	243	ALA	N-CA-C	-5.50	104.51	111.11
1	B	207	THR	CA-CB-OG1	-5.50	101.36	109.60
1	A	79	VAL	CA-C-N	5.49	127.95	120.54
1	A	79	VAL	C-N-CA	5.49	127.95	120.54
1	A	70	LYS	N-CA-C	-5.49	104.82	112.45
1	C	178	VAL	CA-C-O	-5.48	114.27	120.74
1	D	222	SER	CA-C-O	-5.47	115.08	120.82
1	A	111	LEU	N-CA-C	5.47	118.00	111.71
1	B	182	LEU	N-CA-CB	5.47	119.15	110.57
1	C	225	VAL	CB-CA-C	-5.47	102.32	111.29
1	B	207	THR	N-CA-C	5.46	117.27	109.14
1	C	30	PHE	CA-CB-CG	5.46	119.26	113.80
1	D	10	CYS	CA-C-O	-5.45	112.75	119.18
1	B	123	GLN	N-CA-CB	5.45	118.73	110.28
1	C	78	ARG	CG-CD-NE	5.45	123.99	112.00
1	B	119	VAL	CA-C-N	5.45	127.58	120.28
1	B	119	VAL	C-N-CA	5.45	127.58	120.28
1	C	282	GLU	CA-C-N	-5.44	115.93	122.35
1	C	282	GLU	C-N-CA	-5.44	115.93	122.35
1	D	232	ASN	CB-CA-C	-5.44	100.29	108.61
1	C	257	GLU	CA-C-O	5.44	125.90	119.48
1	C	41	THR	N-CA-CB	-5.43	102.59	110.47
1	D	38	ASP	O-C-N	-5.43	114.83	122.87
1	A	63	GLN	CB-CG-CD	5.43	121.83	112.60
1	C	242	THR	N-CA-C	-5.43	105.26	111.07
1	B	182	LEU	O-C-N	5.42	129.69	123.29
1	A	236	VAL	N-CA-C	-5.42	105.09	110.62
1	D	93	LEU	CA-C-N	-5.42	116.21	122.77
1	D	93	LEU	C-N-CA	-5.42	116.21	122.77
1	D	137	VAL	N-CA-C	-5.41	99.95	107.80
1	D	137	VAL	CA-C-O	-5.41	114.74	120.53
1	A	253	TYR	CA-C-O	-5.40	114.53	120.36
1	D	175	PRO	CB-CA-C	-5.40	104.19	111.85
1	B	79	VAL	CA-C-O	-5.39	115.98	121.70
1	A	203	VAL	N-CA-CB	5.39	120.12	111.23
1	A	153	ASP	CA-C-O	-5.38	115.15	121.07
1	D	89	CYS	CB-CA-C	-5.38	102.53	111.41
1	D	120	ARG	N-CA-C	5.38	117.57	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ALA	CA-C-O	5.37	124.78	119.51
1	C	202	GLU	CB-CG-CD	5.37	121.73	112.60
1	C	69	SER	CA-CB-OG	5.37	121.84	111.10
1	A	224	GLN	CB-CG-CD	5.36	121.72	112.60
1	C	35	THR	CB-CA-C	5.36	118.56	109.50
1	C	113	VAL	CB-CA-C	-5.36	104.95	111.87
1	D	228	GLU	CB-CG-CD	5.36	121.71	112.60
1	B	112	ASP	CA-CB-CG	-5.36	107.24	112.60
1	D	213	HIS	CA-C-O	5.36	126.22	120.70
1	A	48	ALA	CA-C-O	-5.35	115.18	121.07
1	D	18	LEU	O-C-N	5.35	128.25	122.15
1	B	181	SER	N-CA-C	5.35	117.22	108.55
1	B	133	GLY	N-CA-C	-5.34	103.47	114.16
1	B	128	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	91	ALA	N-CA-C	5.34	117.92	109.96
1	C	133	GLY	CA-C-N	5.34	130.96	122.74
1	C	133	GLY	C-N-CA	5.34	130.96	122.74
1	C	249	PRO	CA-C-O	-5.34	114.94	121.03
1	C	228	GLU	CA-C-O	-5.33	111.02	119.23
1	D	239	VAL	N-CA-CB	5.32	119.45	110.56
1	D	32	VAL	O-C-N	-5.32	116.88	123.10
1	B	212	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	186	GLY	N-CA-C	-5.31	101.51	112.34
1	A	175	PRO	N-CA-CB	5.31	108.82	103.25
1	C	210	HIS	CA-CB-CG	-5.30	108.50	113.80
1	B	54	CYS	CA-C-N	5.29	125.83	120.38
1	B	54	CYS	C-N-CA	5.29	125.83	120.38
1	C	247	PRO	CB-CA-C	-5.29	103.89	112.62
1	B	226	PHE	N-CA-C	-5.29	105.16	111.03
1	D	91	ALA	CA-C-O	5.28	128.06	120.51
1	C	129	MET	N-CA-C	-5.28	105.42	111.07
1	D	206	ARG	N-CA-C	5.28	118.98	112.54
1	D	7	ILE	CB-CA-C	-5.27	102.38	110.50
1	A	78	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	C	126	LEU	CA-C-N	5.26	126.42	119.84
1	C	126	LEU	C-N-CA	5.26	126.42	119.84
1	A	2	ARG	N-CA-C	5.26	120.18	113.18
1	D	156	CYS	O-C-N	-5.26	116.54	122.12
1	A	76	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	D	285	GLY	O-C-N	-5.25	117.78	122.77
1	A	282	GLU	CA-C-N	-5.25	112.15	120.55
1	A	282	GLU	C-N-CA	-5.25	112.15	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ARG	CB-CA-C	-5.25	101.09	109.75
1	B	254	PHE	N-CA-CB	5.25	119.96	110.83
1	B	225	VAL	N-CA-C	5.24	117.60	111.05
1	B	137	VAL	CA-C-N	-5.24	114.84	122.65
1	B	137	VAL	C-N-CA	-5.24	114.84	122.65
1	A	68	ASP	N-CA-C	5.24	117.21	107.99
1	A	245	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	A	258	ARG	CA-CB-CG	-5.24	103.63	114.10
1	C	219	LEU	O-C-N	-5.24	116.57	122.12
1	B	20	VAL	N-CA-CB	5.24	116.68	110.55
1	A	216	TYR	CA-CB-CG	-5.23	104.48	113.90
1	A	8	THR	N-CA-CB	5.23	118.71	110.23
1	A	179	HIS	CA-C-N	-5.22	115.35	122.93
1	A	179	HIS	C-N-CA	-5.22	115.35	122.93
1	B	151	PHE	CA-C-N	5.22	128.96	120.23
1	B	151	PHE	C-N-CA	5.22	128.96	120.23
1	A	48	ALA	N-CA-C	-5.22	104.65	111.02
1	D	227	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	C	65	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	203	VAL	CB-CA-C	-5.19	102.77	111.29
1	C	34	ALA	CA-C-N	-5.19	113.81	122.64
1	C	34	ALA	C-N-CA	-5.19	113.81	122.64
1	D	153	ASP	CB-CA-C	-5.19	102.67	110.92
1	D	247	PRO	N-CA-C	-5.19	106.45	113.40
1	A	264	ARG	CA-C-O	5.18	125.99	120.24
1	D	144	GLY	CA-C-O	5.18	125.31	119.09
1	A	49	ALA	CA-C-O	5.17	126.22	120.63
1	A	257	GLU	N-CA-C	-5.17	106.75	113.16
1	B	274	ASN	CA-CB-CG	-5.17	107.43	112.60
1	B	6	LEU	O-C-N	5.16	129.26	123.27
1	A	118	THR	N-CA-C	-5.16	105.73	112.23
1	A	248	LYS	CB-CA-C	5.16	118.04	110.87
1	B	186	GLY	N-CA-C	-5.16	101.82	112.34
1	D	218	TYR	N-CA-C	-5.16	105.57	111.14
1	C	158	SER	CA-C-N	-5.15	111.77	120.58
1	C	158	SER	C-N-CA	-5.15	111.77	120.58
1	B	142	SER	CA-C-O	5.15	127.46	121.44
1	D	283	VAL	N-CA-C	5.14	117.03	111.58
1	B	190	THR	CA-C-O	-5.14	112.07	120.80
1	A	84	VAL	CB-CA-C	5.13	116.84	110.73
1	C	190	THR	CA-CB-CG2	5.12	119.21	110.50
1	A	25	ASP	CA-CB-CG	-5.12	107.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	LEU	CA-C-O	5.12	125.89	120.10
1	C	84	VAL	N-CA-C	-5.12	100.94	108.11
1	D	129	MET	N-CA-CB	5.12	117.43	110.01
1	A	258	ARG	CD-NE-CZ	5.12	131.56	124.40
1	B	75	ALA	O-C-N	5.11	127.55	122.08
1	B	264	ARG	CB-CA-C	5.11	120.09	110.63
1	C	209	ILE	O-C-N	5.11	126.83	121.87
1	B	46	TRP	CB-CA-C	5.11	119.36	110.68
1	B	77	GLU	N-CA-CB	5.10	118.20	110.14
1	A	37	ARG	N-CA-C	-5.10	105.63	111.14
1	B	63	GLN	N-CA-CB	5.10	118.78	110.37
1	D	216	TYR	O-C-N	5.09	127.32	122.07
1	A	217	GLN	CA-CB-CG	5.09	124.28	114.10
1	C	30	PHE	CB-CA-C	-5.09	100.92	109.48
1	A	14	ILE	CA-CB-CG1	5.09	119.05	110.40
1	C	27	SER	CA-C-O	5.09	125.64	119.49
1	D	101	ALA	CA-C-O	5.08	125.37	119.32
1	B	242	THR	CA-CB-OG1	5.08	117.22	109.60
1	B	83	ARG	NH1-CZ-NH2	-5.07	112.70	119.30
1	B	56	PRO	N-CA-CB	5.07	108.57	103.25
1	B	271	SER	O-C-N	-5.07	114.30	122.41
1	A	48	ALA	CB-CA-C	-5.07	102.87	110.92
1	D	113	VAL	CA-C-O	5.07	126.08	120.46
1	D	167	GLU	N-CA-C	5.06	116.48	111.07
1	A	31	LYS	CB-CA-C	5.06	118.56	110.16
1	B	94	GLY	N-CA-C	-5.06	104.90	112.89
1	C	193	MET	CB-CG-SD	-5.06	97.53	112.70
1	C	221	LEU	N-CA-C	5.05	116.47	110.97
1	B	214	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	C	195	LYS	O-C-N	-5.04	115.88	122.59
1	C	80	THR	N-CA-CB	5.03	117.61	110.06
1	C	14	ILE	CB-CA-C	-5.03	105.35	112.14
1	D	278	ALA	O-C-N	-5.03	116.11	122.20
1	A	30	PHE	CA-C-O	-5.03	115.53	121.66
1	A	126	LEU	CA-C-N	5.03	126.12	119.84
1	A	126	LEU	C-N-CA	5.03	126.12	119.84
1	B	84	VAL	N-CA-CB	5.03	119.52	111.23
1	A	245	ARG	CB-CG-CD	5.02	122.85	111.30
1	B	66	VAL	CA-C-N	5.02	131.98	121.94
1	B	66	VAL	C-N-CA	5.02	131.98	121.94
1	D	92	GLY	CA-C-N	5.02	130.74	121.85
1	D	92	GLY	C-N-CA	5.02	130.74	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	LEU	CA-C-O	5.02	125.89	120.32
1	A	198	GLY	N-CA-C	-5.01	104.84	112.51
1	D	227	ARG	N-CA-CB	5.01	117.93	110.22
1	B	17	HIS	CA-C-O	-5.01	115.22	120.63
1	C	206	ARG	NE-CZ-NH2	5.01	123.70	119.20
1	C	232	ASN	O-C-N	-5.00	115.25	121.70

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	211	0
1	B	2104	0	2145	170	0
1	C	2179	0	2225	228	0
1	D	2104	0	2145	196	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	9	0
3	C	44	0	24	5	0
3	D	44	0	26	12	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	755	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 44.

All (755) 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
1:D:147:MET:HE1	1:D:262:LEU:HG	1.47	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:D:279:MET:HE2	1:D:283:VAL:HG23	1.50	0.92
1:B:2:ARG:NH1	1:B:83:ARG:HH12	1.68	0.91
1:A:86:VAL:HG21	1:A:244:LEU:HD11	1.51	0.91
1:C:2:ARG:HE	1:C:2:ARG:HA	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:B:147:MET:HE1	1:B:262:LEU:HD23	1.60	0.84
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:HG2	1:C:136:ARG:HH11	1.43	0.82
1:B:174:LEU:HB3	1:B:175:PRO:CD	2.10	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:A:279:MET:HE2	1:A:283:VAL:HG23	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:A:1:ALA:O	1:A:2:ARG:HD2	1.84	0.77
1:B:260:LEU:N	1:B:261:PRO:HD2	2.00	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:16:LEU:HG	1:D:45:LEU:HD23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:D:238:GLU:HA	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:A:279:MET:HE3	1:A:279:MET:HA	1.69	0.74
1:A:185:CYS:HB2	3:A:361:NAD:H5N	1.69	0.74
1:B:76:ARG:HG3	1:B:125:PHE:CZ	2.23	0.73
1:D:136:ARG:NH2	1:D:246:ALA:O	2.16	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
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:C:147:MET:HE1	1:C:262:LEU:HD23	1.70	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:A:122:LEU:HD21	1:A:137:VAL:HG11	1.73	0.71
1:D:9:GLY:HA2	3:D:362:NAD:H1B	1.72	0.71
1:A:157:ALA:HB1	1:B:161:ALA:HB1	1.71	0.70
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: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:B:281:ARG:HG2	1:B:281:ARG:HH11	1.57	0.70
1:C:267:LEU:HD13	1:D:267:LEU:HA	1.72	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:A:107:VAL:HG13	1:A:154:VAL:HG11	1.75	0.69
1:B:92:GLY:CA	3:B:364:NAD:H3D	2.21	0.69
1:A:42:GLN:HE21	1:A:46:TRP:NE1	1.91	0.68
1:A:169:LEU:HD23	1:B:153:ASP:OD2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:LEU:CD2	1:D:245:ARG:HD3	2.23	0.68
1:B:67:ARG:NH1	1:B:109:SER:OG	2.27	0.68
1:B:76:ARG:HG3	1:B:125:PHE:CE2	2.28	0.68
1:C:8:THR:O	1:C:90:ASN:HB3	1.94	0.68
1:C:221:LEU:CD1	1:C:283:VAL:HG22	2.24	0.68
1:C:8:THR:HG23	1:C:121:MET:HE2	1.76	0.68
1:C:86:VAL:HG21	1:C:244:LEU:HD11	1.75	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
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: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:H52N	3:C:363:NAD:H51A	1.77	0.67
1:A:8:THR:HG22	1:A:64:LEU:HD13	1.76	0.67
1:A:234:GLU:O	1:A:237:ALA:HB3	1.95	0.66
1:C:2:ARG:HH22	1:C:81:GLU:HG2	1.60	0.66
1:D:129:MET:HE1	1:D:137:VAL:HG22	1.77	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: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:A:7:ILE:HG12	1:A:88:VAL:HB	1.78	0.66
1:D:35:THR:HG21	1:D:64:LEU:HD13	1.77	0.66
1:C:272:GLY:O	1:C:276:VAL:HG23	1.94	0.65
1:D:130:LYS:HG2	1:D:176:PHE:CD2	2.31	0.65
1:A:210:HIS:O	1:A:213:HIS:HB3	1.96	0.65
1:A:267:LEU:HD23	1:A:267:LEU:N	2.11	0.65
1:B:187:PRO:HG2	1:B:229:ALA:HB3	1.78	0.65
1:C:55:PRO:O	1:C:58:SER:HB2	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:N	1:B:274:ASN:HD22	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:MET:HE3	1:D:282:GLU:HB3	1.77	0.65
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.62	0.64
1:C:139:VAL:HG12	1:C:182:LEU:HD23	1.78	0.64
1:D:266:ARG:HH11	1:D:266:ARG:HG2	1.60	0.64
1:C:261:PRO:HG2	1:C:262:LEU:H	1.62	0.64
1:D:147:MET:CE	1:D:262:LEU:HG	2.25	0.64
1:A:34:ALA:O	1:A:61:THR:HA	1.98	0.64
1:A:267:LEU:O	1:B:267:LEU:HD13	1.98	0.64
1:B:66:VAL:HG22	3:B:364:NAD:H62A	1.62	0.64
1:C:8:THR:CG2	1:C:121:MET:HE2	2.28	0.63
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
1:B:14:ILE:HD12	1:B:236:VAL:HB	1.79	0.63
1:D:279:MET:HE2	1:D:283:VAL:CG2	2.25	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:C:129:MET:O	1:C:130:LYS:C	2.43	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:A:252:ARG:HG3	1:A:252:ARG:HH11	1.65	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: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:D:279:MET:HE3	1:D:279:MET:O	2.01	0.60
1:B:74:ALA:O	1:B:75:ALA:C	2.42	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:HG2	1:A:50:ARG:HH11	1.66	0.60
1:A:68:ASP:HB3	1:A:71:SER:HB3	1.82	0.60
1:B:180:LEU:HD23	1:B:181:SER:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:MET:HE1	1:D:262:LEU:CG	2.25	0.60
1:A:241:LEU:O	1:A:245:ARG:HG3	2.02	0.60
1:A:174:LEU:HB3	1:A:175:PRO:CD	2.32	0.60
1:B:173:LEU:O	1:B:174:LEU:C	2.45	0.60
1:C:87:LEU:HB3	1:C:137:VAL:HG22	1.83	0.60
1:C:150:PRO:HG3	1:D:171:VAL:HG11	1.84	0.60
1:B:39:LEU:O	1:B:42:GLN:HG2	2.02	0.60
1:B:284:PHE:O	1:B:285:GLY:C	2.45	0.60
1:D:99:LEU:HA	1:D:102:LEU:CD1	2.32	0.60
1:B:37:ARG:HH21	3:B:364:NAD:C2B	2.13	0.59
1:B:182:LEU:N	1:B:182:LEU:HD12	2.15	0.59
1:B:2:ARG:CZ	1:B:83:ARG:HH22	2.14	0.59
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.16	0.59
1:B:203:VAL:O	1:B:207:THR:HG22	2.02	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:D:38:ASP:O	1:D:41:THR:HG23	2.02	0.59
1:A:46:TRP:O	1:A:50:ARG:HG3	2.02	0.59
1:D:92:GLY:HA3	3:D:362:NAD:O2D	2.02	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:HG2	1:C:136:ARG:NH1	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:D:105:ASP:O	1:D:106:ALA:C	2.46	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:B:21:ARG:O	1:B:21:ARG:NH1	2.37	0.58
1:C:96:LEU:HD21	1:C:219:LEU:HD21	1.86	0.58
1:C:224:GLN:O	1:C:225:VAL:C	2.46	0.58
1:D:139:VAL:HG11	1:D:162:LEU:HD21	1.86	0.58
1:D:274:ASN:HD22	1:D:274:ASN:N	2.01	0.58
1:C:96:LEU:HD11	1:C:218:TYR:HE2	1.66	0.58
1:A:45:LEU:CD1	1:A:59:LEU:HD21	2.31	0.58
1:A:266:ARG:CB	1:A:267:LEU:HD23	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HH11	1:C:76:ARG:HB3	1.69	0.58
1:D:136:ARG:HH12	1:D:249:PRO:HG3	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:C:74:ALA:O	1:C:75:ALA:C	2.47	0.57
1:B:247:PRO:O	1:B:249:PRO:HD3	2.03	0.57
1:A:190:THR:O	1:A:191:ALA:HB3	2.04	0.57
1:B:260:LEU:CD1	1:B:263:LEU:HD12	2.34	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:C:199:SER:O	1:C:200:PRO:C	2.47	0.57
1:A:274:ASN:N	1:A:274:ASN:HD22	2.02	0.57
1:B:166:CYS:HB3	1:B:180:LEU:HD22	1.87	0.57
1:A:173:LEU:O	1:A:174:LEU:C	2.48	0.57
1:C:263:LEU:HD13	1:C:263:LEU:C	2.29	0.57
1:B:176:PHE:CD1	1:B:176:PHE:N	2.73	0.57
1:C:279:MET:HE3	1:C:282:GLU:HB3	1.86	0.57
1:A:119:VAL:HG22	1:A:165:LEU:HD22	1.87	0.56
1:B:260:LEU:N	1:B:261:PRO:CD	2.67	0.56
1:B:260:LEU:HD11	1:B:263:LEU:HD12	1.87	0.56
1:C:95:LEU:HD12	1:C:197:LEU:HD12	1.86	0.56
1:C:27:SER:O	1:C:28:GLN:C	2.43	0.56
1:C:173:LEU:HD13	1:C:178:VAL:HG12	1.86	0.56
1:A:148:GLY:O	1:A:275:TYR:OH	2.23	0.56
1:A:258:ARG:HH11	1:A:258:ARG:CB	1.99	0.56
1:C:32:VAL:O	1:C:59:LEU:HA	2.06	0.56
1:D:110:VAL:HG13	1:D:114:ASN:HD22	1.70	0.56
1:A:69:SER:HB3	1:B:104:GLU:OE2	2.04	0.56
1:C:150:PRO:HG3	1:D:171:VAL:CG1	2.36	0.56
1:D:89:CYS:SG	1:D:118:THR:HG23	2.46	0.56
1:D:203:VAL:HG13	1:D:207:THR:HG21	1.86	0.56
1:C:232:ASN:HB3	1:C:234:GLU:OE1	2.06	0.56
1:D:20:VAL:CG2	1:D:52:LEU:HD22	2.35	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:D:169:LEU:O	1:D:170:ALA:C	2.48	0.56
1:A:68:ASP:O	1:A:72:VAL:HG23	2.06	0.56
1:A:107:VAL:HG13	1:A:154:VAL:CG1	2.35	0.56
1:D:83:ARG:HG2	1:D:83:ARG:HH11	1.71	0.56
1:B:147:MET:HE3	1:B:275:TYR:OH	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:279:MET:CE	1:D:282:GLU:HB3	2.36	0.55
1:A:136:ARG:HH12	1:A:249:PRO:HG3	1.70	0.55
1:A:260:LEU:N	1:A:261:PRO:HD2	2.21	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:C:68:ASP:CG	1:C:71:SER:H	2.15	0.55
1:A:131:ARG:CZ	1:B:208:ASP:HB3	2.37	0.55
1:C:232:ASN:O	1:C:233:PRO:C	2.50	0.55
1:D:83:ARG:HD2	1:D:85:ASP:OD1	2.06	0.55
1:A:261:PRO:HG2	1:A:262:LEU:H	1.71	0.55
1:C:14:ILE:HD12	1:C:236:VAL:HG11	1.86	0.55
1:C:261:PRO:O	1:C:262:LEU:C	2.49	0.55
1:D:232:ASN:HB2	1:D:235:GLU:HG3	1.89	0.55
1:A:216:TYR:CD2	1:C:200:PRO:HB2	2.42	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:C:252:ARG:HB2	1:D:271:SER:HA	1.88	0.55
1:B:52:LEU:O	1:B:53:ALA:HB3	2.07	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:A:241:LEU:O	1:A:244:LEU:HB3	2.07	0.55
1:B:96:LEU:HD12	1:B:97:GLY:N	2.22	0.55
1:C:252:ARG:HG3	1:C:252:ARG:HH11	1.70	0.55
1:D:66:VAL:HG22	3:D:362:NAD:C6A	2.36	0.55
1:D:67:ARG:HB3	1:D:112:ASP:OD2	2.06	0.55
1:D:266:ARG:HG2	1:D:266:ARG:NH1	2.19	0.55
1:D:103:GLY:O	1:D:106:ALA:N	2.40	0.55
1:B:10:CYS:HA	1:B:15:GLY:HA3	1.90	0.54
1:B:13:GLY:O	1:B:17:HIS:HD2	1.90	0.54
1:B:247:PRO:C	1:B:249:PRO:HD3	2.32	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:B:3:THR:HB	1:B:30:PHE:CD1	2.42	0.54
1:D:24:SER:OG	1:D:52:LEU:HD23	2.06	0.54
1:A:167:GLU:HB2	1:A:251:LEU:HD21	1.90	0.54
1:B:170:ALA:CB	1:B:251:LEU:HD13	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:THR:OG1	1:C:208:ASP:N	2.41	0.54
1:A:5:VAL:HA	1:A:86:VAL:O	2.08	0.54
1:A:256:THR:HG1	1:A:258:ARG:H	1.55	0.54
1:D:184:GLU:O	1:D:255:THR:HG23	2.06	0.54
1:C:273:SER:O	1:C:274:ASN:C	2.49	0.54
1:C:280:HIS:CG	1:D:174:LEU:HD23	2.43	0.54
1:C:151:PHE:CE2	1:C:215:PHE:HA	2.43	0.53
1:D:2:ARG:HA	1:D:83:ARG:HH21	1.73	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:C:271:SER:HB2	1:D:250:THR:HB	1.89	0.53
1:D:35:THR:HG23	1:D:64:LEU:HB3	1.89	0.53
1:A:76:ARG:HH11	1:A:76:ARG:HB3	1.72	0.53
1:B:119:VAL:O	1:B:123:GLN:HG3	2.09	0.53
1:D:126:LEU:CD2	1:D:178:VAL:HG11	2.38	0.53
1:C:147:MET:HB2	1:C:275:TYR:OH	2.08	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:A:278:ALA:O	1:A:279:MET:C	2.52	0.53
1:C:120:ARG:HA	1:C:123:GLN:HE21	1.72	0.53
1:D:9:GLY:O	1:D:15:GLY:HA3	2.09	0.53
1:D:262:LEU:O	1:D:263:LEU:C	2.50	0.53
1:A:266:ARG:HG2	1:A:267:LEU:CD2	2.39	0.53
1:B:129:MET:O	1:B:130:LYS:C	2.52	0.53
1:D:31:LYS:NZ	1:D:81:GLU:OE2	2.39	0.53
1:A:216:TYR:HA	1:A:219:LEU:HB2	1.91	0.53
1:B:187:PRO:HB3	1:B:226:PHE:CE1	2.42	0.53
1:D:127:PRO:O	1:D:128:ASP:C	2.50	0.53
1:B:93:LEU:HG	1:B:113:VAL:HG11	1.90	0.53
1:C:111:LEU:HD23	1:C:158:SER:HB3	1.90	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:A:78:ARG:HA	1:A:78:ARG:HH11	1.75	0.52
1:A:87:LEU:HD11	1:A:121:MET:HE3	1.91	0.52
1:B:21:ARG:HH12	1:B:25:ASP:HA	1.74	0.52
1:C:105:ASP:O	1:C:108:ALA:HB3	2.09	0.52
1:C:131:ARG:NH1	1:D:208:ASP:HB3	2.23	0.52
1:C:267:LEU:N	1:C:267:LEU:CD2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:GLU:HA	1:C:241:LEU:HD13	1.91	0.52
1:A:141:GLY:HA3	1:A:184:GLU:OE1	2.09	0.52
1:B:68:ASP:O	1:B:69:SER:C	2.52	0.52
1:C:76:ARG:HH11	1:C:76:ARG:CB	2.21	0.52
1:C:221:LEU:O	1:C:222:SER:C	2.53	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: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:A:281:ARG:O	1:A:282:GLU:C	2.52	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:B:274:ASN:N	1:B:274:ASN:ND2	2.57	0.52
1:C:266:ARG:NH2	1:D:167:GLU:OE2	2.41	0.52
1:D:122:LEU:HD21	1:D:137:VAL:HG11	1.92	0.52
1:C:262:LEU:O	1:C:263:LEU:C	2.51	0.51
1:C:120:ARG:NH2	1:D:104:GLU:OE2	2.43	0.51
1:C:174:LEU:HB3	1:C:175:PRO:HD3	1.90	0.51
1:D:203:VAL:HG13	1:D:207:THR:CG2	2.40	0.51
1:C:52:LEU:O	1:C:53:ALA:HB3	2.10	0.51
1:C:237:ALA:O	1:C:241:LEU:HD12	2.11	0.51
1:B:3:THR:HB	1:B:30:PHE:HD1	1.76	0.51
1:C:126:LEU:N	1:C:127:PRO:CD	2.72	0.51
1:C:266:ARG:HH21	1:D:167:GLU:CD	2.18	0.51
1:D:66:VAL:HG22	3:D:362:NAD:H62A	1.73	0.51
1:A:207:THR:OG1	1:A:208:ASP:N	2.44	0.51
1:A:263:LEU:O	1:A:263:LEU:HD22	2.10	0.51
1:A:281:ARG:O	1:A:285:GLY:N	2.43	0.51
1:C:241:LEU:HA	1:C:244:LEU:HB3	1.92	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: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:A:33:TYR:CE2	1:A:79:VAL:HG13	2.45	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:7:ILE:HG23	1:A:88:VAL:HB	1.93	0.51
1:A:96:LEU:HD11	1:A:218:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:O	1:A:237:ALA:C	2.54	0.51
1:C:173:LEU:O	1:C:174:LEU:C	2.54	0.51
1:C:138:LEU:HD13	1:C:240:PHE:HD1	1.76	0.50
1:D:66:VAL:O	1:D:120:ARG:HD2	2.11	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:242:THR:O	1:D:243:ALA:C	2.52	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:C:200:PRO:HA	1:C:203:VAL:HG12	1.92	0.50
1:D:92:GLY:HA2	1:D:114:ASN:OD1	2.11	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: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:OE1	1:C:282:GLU:HA	2.09	0.50
1:D:173:LEU:O	1:D:174:LEU:C	2.54	0.50
1:A:187:PRO:HB3	1:A:226:PHE:CE2	2.47	0.50
1:A:193:MET:HE1	1:A:223:LYS:HE3	1.94	0.50
1:B:38:ASP:HB3	1:B:41:THR:HG23	1.94	0.50
1:D:260:LEU:N	1:D:261:PRO:HD2	2.25	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:A:224:GLN:O	1:A:225:VAL:C	2.52	0.50
1:B:143:VAL:HG13	1:B:144:GLY:N	2.27	0.50
1:A:174:LEU:HB3	1:A:175:PRO:HD2	1.93	0.50
1:B:24:SER:O	1:B:25:ASP:C	2.49	0.50
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:C:182:LEU:HB3	1:C:184:GLU:OE2	2.12	0.50
1:A:264:ARG:O	1:A:265:MET:C	2.54	0.49
1:B:92:GLY:HA3	3:B:364:NAD:C3D	2.37	0.49
1:C:187:PRO:HB3	1:C:226:PHE:CE1	2.47	0.49
1:A:35:THR:HG22	1:A:62:LEU:HD12	1.94	0.49
1:A:183:ILE:HD13	1:A:253:TYR:HB2	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:B:14:ILE:HD12	1:B:236:VAL:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:VAL:HG22	1:B:138:LEU:HB2	1.94	0.49
1:B:277:THR:O	1:B:278:ALA:C	2.53	0.49
1:C:8:THR:HG22	1:C:64:LEU:HD13	1.94	0.49
1:D:17:HIS:CG	1:D:233:PRO:HB2	2.47	0.49
1:D:82:GLY:O	1:D:132:ARG:NH2	2.45	0.49
1:D:147:MET:HG3	1:D:275:TYR:OH	2.13	0.49
1:A:239:VAL:O	1:A:240:PHE:C	2.55	0.49
1:B:184:GLU:OE2	1:B:252:ARG:HG2	2.13	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:A:86:VAL:CG2	1:A:244:LEU:HD11	2.34	0.49
1:A:95:LEU:HG	1:A:102:LEU:HD22	1.93	0.49
1:A:274:ASN:O	1:A:275:TYR:C	2.55	0.49
1:C:281:ARG:HA	1:C:285:GLY:O	2.12	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:C:279:MET:HE3	1:C:279:MET:HA	1.95	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:C:236:VAL:HG22	1:C:255:THR:HG21	1.95	0.48
1:D:261:PRO:O	1:D:265:MET:N	2.35	0.48
1:A:248:LYS:HD2	1:A:249:PRO:HD2	1.95	0.48
1:A:101:ALA:CB	1:A:206:ARG:HB3	2.44	0.48
1:B:59:LEU:HG	1:B:60:GLU:N	2.29	0.48
1:C:16:LEU:O	1:C:19:ALA:HB3	2.14	0.48
1:D:36:LEU:HD22	1:D:42:GLN:HB3	1.95	0.48
1:D:126:LEU:CD2	1:D:173:LEU:HD11	2.43	0.48
1:D:247:PRO:C	1:D:249:PRO:HD3	2.38	0.48
1:C:16:LEU:C	1:C:16:LEU:HD23	2.39	0.48
1:C:202:GLU:OE2	1:C:206:ARG:NH2	2.46	0.48
1:D:155:TYR:O	1:D:158:SER:OG	2.30	0.48
1:A:150:PRO:O	1:A:151:PHE:HB2	2.12	0.48
1:A:187:PRO:O	1:A:230:ALA:HA	2.14	0.48
1:A:236:VAL:HG22	1:A:255:THR:HG21	1.95	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:D:203:VAL:HG12	1:D:212:PHE:CD2	2.49	0.48
1:C:280:HIS:CE1	1:D:175:PRO:HD3	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:MET:O	1:A:280:HIS:C	2.55	0.48
1:C:7:ILE:HG23	1:C:88:VAL:CG1	2.44	0.48
1:C:11:SER:HA	1:C:36:LEU:CD2	2.44	0.48
1:C:67:ARG:CD	4:C:525:HOH:O	2.60	0.48
1:C:260:LEU:N	1:C:261:PRO:HD2	2.29	0.48
1:B:13:GLY:H	1:B:190:THR:HG21	1.79	0.47
1:C:20:VAL:O	1:C:21:ARG:C	2.52	0.47
1:D:98:PRO:HG2	1:D:203:VAL:HG13	1.96	0.47
1:D:143:VAL:HG21	1:D:259:PHE:CB	2.45	0.47
1:A:17:HIS:O	1:A:18:LEU:C	2.57	0.47
1:A:68:ASP:HB3	1:A:71:SER:CB	2.44	0.47
1:A:86:VAL:HA	1:A:136:ARG:O	2.15	0.47
1:B:68:ASP:O	1:B:71:SER:N	2.46	0.47
1:C:42:GLN:HE22	1:C:46:TRP:HE1	1.62	0.47
1:D:190:THR:O	3:D:362:NAD:O2N	2.32	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:B:262:LEU:O	1:B:263:LEU:C	2.56	0.47
1:A:221:LEU:HD13	1:A:221:LEU:C	2.39	0.47
1:A:129:MET:O	1:A:130:LYS:C	2.57	0.47
1:A:165:LEU:O	1:A:169:LEU:HG	2.15	0.47
1:A:274:ASN:N	1:A:274:ASN:ND2	2.62	0.47
1:B:75:ALA:O	1:B:76:ARG:C	2.56	0.47
1:C:42:GLN:NE2	1:C:46:TRP:NE1	2.62	0.47
1:C:89:CYS:N	1:C:138:LEU:O	2.43	0.47
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.58	0.47
1:C:172:LEU:HD21	1:D:211:THR:HG23	1.96	0.47
1:D:275:TYR:O	1:D:276:VAL:C	2.57	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: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:273:SER:HB3	1:B:250:THR:HG22	1.97	0.47
1:B:25:ASP:CG	1:B:26:PRO:HD2	2.40	0.47
1:C:217:GLN:O	1:C:220:ALA:HB3	2.15	0.47
1:D:38:ASP:O	1:D:40:LYS:N	2.47	0.47
1:D:128:ASP:OD2	1:D:132:ARG:NH2	2.47	0.47
1:C:122:LEU:HD21	1:C:137:VAL:HG11	1.97	0.47
1:D:83:ARG:HG2	1:D:83:ARG:NH1	2.29	0.47
1:B:176:PHE:HD1	1:B:176:PHE:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:269:ASP:HA	1:C:270:PRO:HD2	1.64	0.47
1:D:1:ALA:O	1:D:2:ARG:NH2	2.47	0.47
1:B:40:LYS:NZ	4:B:550:HOH:O	2.48	0.46
1:B:48:ALA:O	1:B:52:LEU:N	2.47	0.46
1:C:232:ASN:O	1:C:235:GLU:N	2.48	0.46
1:C:252:ARG:HG3	1:C:252:ARG:NH1	2.30	0.46
1:A:165:LEU:O	1:A:165:LEU:HD12	2.16	0.46
1:A:201:GLU:O	1:A:202:GLU:C	2.58	0.46
1:C:185:CYS:HB2	3:C:363:NAD:C5N	2.46	0.46
1:C:250:THR:HG22	1:D:273:SER:HB3	1.98	0.46
1:D:129:MET:O	1:D:130:LYS:C	2.58	0.46
1:D:143:VAL:HG21	1:D:259:PHE:HB2	1.97	0.46
1:A:95:LEU:HB2	1:A:110:VAL:HG21	1.96	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:A:267:LEU:HD23	1:A:267:LEU:H	1.79	0.46
1:C:25:ASP:OD1	1:C:27:SER:OG	2.34	0.46
1:C:167:GLU:O	1:C:171:VAL:HG23	2.16	0.46
1:C:219:LEU:O	1:C:220:ALA:C	2.55	0.46
1:D:221:LEU:O	1:D:225:VAL:HG23	2.15	0.46
1:A:248:LYS:HD2	1:A:248:LYS:HA	1.33	0.46
1:B:11:SER:O	1:B:16:LEU:HD12	2.15	0.46
1:B:170:ALA:HB2	1:B:251:LEU:HD13	1.98	0.46
1:C:26:PRO:O	1:C:28:GLN:HG3	2.14	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:A:240:PHE:O	1:A:244:LEU:HB2	2.16	0.46
1:B:147:MET:CE	1:B:262:LEU:HD23	2.41	0.46
1:B:166:CYS:HB3	1:B:180:LEU:CD2	2.46	0.46
1:C:65:ASP:OD1	1:C:67:ARG:HB2	2.16	0.46
1:C:179:HIS:HB3	1:C:249:PRO:HG2	1.96	0.46
1:C:208:ASP:CG	1:C:211:THR:HG1	2.21	0.46
1:C:279:MET:CE	1:C:282:GLU:HB3	2.46	0.46
1:A:203:VAL:HG21	1:A:215:PHE:CE2	2.51	0.46
1:A:242:THR:O	1:A:243:ALA:C	2.59	0.46
1:C:166:CYS:SG	1:C:180:LEU:HD21	2.56	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:264:ARG:O	1:C:265:MET:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LYS:O	1:D:131:ARG:C	2.59	0.46
1:B:226:PHE:O	1:B:230:ALA:N	2.42	0.46
1:C:2:ARG:NE	1:C:83:ARG:HH22	2.14	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:187:PRO:HG2	1:D:229:ALA:CB	2.47	0.45
1:D:279:MET:O	1:D:279:MET:HG3	2.16	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:159:LYS:HD2	1:A:159:LYS:HA	1.43	0.45
1:C:163:GLU:CD	1:C:182:LEU:HD13	2.41	0.45
1:A:7:ILE:HD13	1:A:18:LEU:HG	1.98	0.45
1:A:265:MET:SD	1:A:275:TYR:HA	2.56	0.45
1:D:89:CYS:CB	1:D:139:VAL:HG22	2.42	0.45
1:A:50:ARG:O	1:A:51:ALA:C	2.58	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:C:202:GLU:O	1:C:203:VAL:C	2.60	0.45
1:A:44:ARG:NH2	2:A:401:SO4:S	2.89	0.45
1:A:262:LEU:O	1:A:263:LEU:C	2.56	0.45
1:B:207:THR:OG1	1:B:208:ASP:N	2.49	0.45
1:D:245:ARG:HE	1:D:245:ARG:HB2	1.51	0.45
1:A:96:LEU:HB3	1:A:196:VAL:HG12	1.97	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:D:86:VAL:HG12	1:D:88:VAL:HG23	1.99	0.45
1:D:236:VAL:O	1:D:239:VAL:N	2.47	0.45
1:B:17:HIS:CG	1:B:233:PRO:HB2	2.52	0.45
1:D:281:ARG:NH1	1:D:281:ARG:HG2	2.32	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:280:HIS:CB	1:D:174:LEU:HD23	2.47	0.45
1:D:110:VAL:O	1:D:114:ASN:HB2	2.17	0.45
1:A:271:SER:OG	1:A:273:SER:OG	2.31	0.44
1:C:100:GLU:OE2	1:D:130:LYS:NZ	2.48	0.44
1:C:190:THR:O	1:C:191:ALA:HB3	2.16	0.44
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:C:17:HIS:O	1:C:18:LEU:C	2.58	0.44
1:C:68:ASP:HB3	1:C:71:SER:CB	2.44	0.44
1:D:185:CYS:HB2	3:D:362:NAD:H5N	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:GLN:NE2	1:D:255:THR:O	2.41	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:HD12	1:B:262:LEU:HA	1.81	0.44
1:C:73:ALA:O	1:C:74:ALA:C	2.59	0.44
1:C:95:LEU:HG	1:C:102:LEU:HD22	2.00	0.44
1:A:210:HIS:O	1:A:214:ARG:HG2	2.17	0.44
1:C:193:MET:O	1:C:194:GLU:C	2.61	0.44
1:D:95:LEU:HD12	1:D:95:LEU:HA	1.74	0.44
1:D:139:VAL:CG1	1:D:162:LEU:HD21	2.47	0.44
1:A:8:THR:HG23	1:A:121:MET:HE2	1.98	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:A:183:ILE:O	1:A:183:ILE:HG22	2.18	0.44
1:B:107:VAL:HG13	1:B:154:VAL:HG11	2.00	0.44
1:B:143:VAL:CG1	1:B:144:GLY:N	2.81	0.44
1:C:126:LEU:N	1:C:127:PRO:HD2	2.33	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:A:24:SER:O	1:A:25:ASP:C	2.59	0.44
1:A:226:PHE:CD1	1:A:230:ALA:HB2	2.53	0.44
1:B:87:LEU:HD11	1:B:121:MET:HE3	1.99	0.44
1:B:229:ALA:O	1:B:230:ALA:C	2.61	0.44
1:C:11:SER:HA	1:C:36:LEU:HD21	2.00	0.44
1:C:172:LEU:HD12	1:C:172:LEU:O	2.18	0.44
1:D:260:LEU:HD12	1:D:260:LEU:HA	1.85	0.44
1:B:38:ASP:OD2	1:B:40:LYS:HG3	2.18	0.43
1:C:42:GLN:HE21	1:C:42:GLN:HB2	1.53	0.43
1:B:133:GLY:HA2	1:B:176:PHE:O	2.19	0.43
1:D:33:TYR:HE1	1:D:81:GLU:OE1	2.01	0.43
1:D:129:MET:HE1	1:D:137:VAL:CG2	2.46	0.43
1:A:22:LEU:O	1:A:23:ALA:C	2.58	0.43
1:A:189:HIS:NE2	1:A:226:PHE:HD1	2.17	0.43
1:A:213:HIS:NE2	1:C:209:ILE:HD12	2.33	0.43
1:A:279:MET:HA	1:A:279:MET:CE	2.45	0.43
1:C:185:CYS:HB2	3:C:363:NAD:H5N	1.99	0.43
1:A:166:CYS:HB2	1:A:182:LEU:HD11	1.99	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: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:D:74:ALA:O	1:D:75:ALA:C	2.62	0.43
1:A:174:LEU:CB	1:A:175:PRO:CD	2.93	0.43
1:A:149:LEU:O	1:A:150:PRO:C	2.59	0.43
1:B:67:ARG:HG2	1:B:112:ASP:OD2	2.19	0.43
1:C:99:LEU:HD11	1:D:119:VAL:HG13	2.01	0.43
1:A:126:LEU:N	1:A:127:PRO:CD	2.82	0.43
1:A:275:TYR:O	1:A:276:VAL:C	2.59	0.43
1:C:10:CYS:O	1:C:16:LEU:HB2	2.19	0.43
1:C:25:ASP:HA	1:C:26:PRO:HD2	1.73	0.43
1:C:107:VAL:HG13	1:C:154:VAL:HG11	2.01	0.43
1:D:75:ALA:O	1:D:76:ARG:C	2.61	0.43
1:A:76:ARG:HG3	1:A:125:PHE:CE1	2.54	0.43
1:A:109:SER:O	1:A:110:VAL:C	2.61	0.43
1:B:33:TYR:CE1	1:B:79:VAL:HG13	2.54	0.43
1:C:266:ARG:O	1:C:267:LEU:C	2.61	0.43
1:D:146:LEU:HD23	1:D:146:LEU:HA	1.83	0.43
1:D:152:ASN:O	1:D:156:CYS:HB2	2.19	0.43
1:D:2:ARG:HA	1:D:83:ARG:NH2	2.34	0.42
1:D:138:LEU:CD2	1:D:181:SER:HB2	2.48	0.42
1:D:281:ARG:HG2	1:D:281:ARG:HH11	1.83	0.42
1:A:149:LEU:HA	1:A:150:PRO:HD2	1.85	0.42
1:B:278:ALA:HA	1:B:281:ARG:CZ	2.48	0.42
1:C:41:THR:HG22	1:C:41:THR:O	2.19	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:265:MET:HE2	1:B:265:MET:HB2	1.88	0.42
1:D:9:GLY:CA	3:D:362:NAD:H1B	2.46	0.42
1:C:223:LYS:O	1:C:224:GLN:C	2.62	0.42
1:D:202:GLU:O	1:D:206:ARG:N	2.32	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:92:GLY:HA3	3:C:363:NAD:H3D	2.01	0.42
1:A:271:SER:HG	1:A:273:SER:HG	1.64	0.42
1:C:265:MET:O	1:C:266:ARG:C	2.62	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:96:LEU:HD21	1:B:219:LEU:HD21	2.02	0.42
1:C:2:ARG:O	1:C:83:ARG:NH2	2.52	0.42
1:C:18:LEU:HD23	1:C:88:VAL:HG11	2.01	0.42
1:C:21:ARG:HG2	1:C:241:LEU:HD11	2.01	0.42
1:D:252:ARG:HH11	1:D:252:ARG:HD2	1.66	0.42
1:B:81:GLU:H	1:B:81:GLU:CD	2.25	0.42
1:C:99:LEU:HD12	1:C:102:LEU:CD1	2.46	0.42
1:A:161:ALA:HB2	1:B:161:ALA:HB2	2.01	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:B:244:LEU:O	1:B:244:LEU:HD12	2.20	0.42
1:C:25:ASP:OD1	1:C:25:ASP:C	2.62	0.42
1:C:50:ARG:O	1:C:51:ALA:C	2.60	0.42
1:C:70:LYS:O	1:C:71:SER:C	2.62	0.42
1:D:7:ILE:O	1:D:35:THR:HB	2.20	0.42
1:C:199:SER:O	1:C:202:GLU:N	2.53	0.42
1:C:200:PRO:O	1:C:201:GLU:C	2.63	0.42
1:D:83:ARG:HA	1:D:132:ARG:HH21	1.85	0.42
1:B:65:ASP:O	1:B:67:ARG:N	2.53	0.41
1:C:136:ARG:NH2	1:C:246:ALA:O	2.48	0.41
1:A:257:GLU:O	1:A:260:LEU:HB2	2.19	0.41
1:B:210:HIS:O	1:B:211:THR:C	2.63	0.41
1:C:50:ARG:HG3	1:C:50:ARG:NH1	2.35	0.41
1:C:120:ARG:HH21	1:D:104:GLU:CD	2.28	0.41
1:C:160:PHE:HB3	1:D:160:PHE:O	2.21	0.41
1:D:90:ASN:HB2	1:D:140:THR:OG1	2.19	0.41
1:D:132:ARG:HG2	1:D:132:ARG:NH1	2.34	0.41
1:B:110:VAL:HG13	1:B:114:ASN:ND2	2.35	0.41
1:B:240:PHE:O	1:B:243:ALA:HB3	2.20	0.41
1:C:37:ARG:HA	1:C:64:LEU:O	2.21	0.41
1:C:121:MET:O	1:C:124:ALA:N	2.52	0.41
1:D:52:LEU:HD12	1:D:52:LEU:HA	1.92	0.41
1:A:37:ARG:O	1:A:63:GLN:HG3	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:C:54:CYS:O	1:C:55:PRO:C	2.63	0.41
1:C:208:ASP:OD2	1:C:210:HIS:HB2	2.19	0.41
1:D:66:VAL:HG22	3:D:362:NAD:N1A	2.35	0.41
1:D:263:LEU:O	1:D:264:ARG:C	2.63	0.41
1:B:27:SER:O	1:B:28:GLN:C	2.62	0.41
1:B:122:LEU:HD13	1:B:169:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASP:O	1:C:69:SER:C	2.60	0.41
1:A:18:LEU:O	1:A:18:LEU:HD12	2.21	0.41
1:C:76:ARG:HD2	1:C:125:PHE:CD2	2.55	0.41
1:C:261:PRO:HG2	1:C:262:LEU:N	2.32	0.41
1:C:262:LEU:HA	1:C:262:LEU:HD12	1.70	0.41
1:D:155:TYR:CE1	1:D:159:LYS:HD2	2.56	0.41
1:D:218:TYR:CD2	1:D:218:TYR:C	2.97	0.41
1:A:172:LEU:HD13	1:B:151:PHE:CZ	2.55	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:245:ARG:O	1:C:246:ALA:C	2.63	0.41
1:A:14:ILE:HD12	1:A:236:VAL:CG1	2.50	0.41
1:C:2:ARG:NH2	1:C:81:GLU:HG2	2.33	0.41
1:A:15:GLY:O	1:A:16:LEU:C	2.64	0.41
1:A:32:VAL:O	1:A:59:LEU:HA	2.20	0.41
1:A:81:GLU:H	1:A:81:GLU:CD	2.28	0.41
1:A:252:ARG:NH1	1:A:252:ARG:CG	2.81	0.41
1:A:261:PRO:O	1:A:264:ARG:N	2.54	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:C:173:LEU:HD22	1:C:178:VAL:HG11	2.01	0.41
1:A:219:LEU:O	1:A:223:LYS:HD3	2.21	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: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:D:38:ASP:OD1	1:D:40:LYS:HE3	2.20	0.41
1:D:73:ALA:O	1:D:74:ALA:C	2.63	0.41
1:D:187:PRO:HG2	1:D:229:ALA:HB3	2.03	0.41
1:D:213:HIS:O	1:D:214:ARG:C	2.62	0.41
1:B:16:LEU:HD23	1:B:16:LEU:C	2.45	0.40
1:B:67:ARG:NH1	4:B:514:HOH:O	2.53	0.40
1:B:135:GLY:O	1:B:178:VAL:HG13	2.21	0.40
1:B:143:VAL:O	1:B:146:LEU:HB2	2.20	0.40
1:B:260:LEU:HD12	1:B:263:LEU:HB2	2.03	0.40
1:C:169:LEU:O	1:C:170:ALA:C	2.65	0.40
1:C:221:LEU:HD22	1:C:221:LEU:C	2.46	0.40
1:D:281:ARG:O	1:D:282:GLU:C	2.63	0.40
1:C:35:THR:CG2	1:C:62:LEU:HD12	2.51	0.40
1:C:39:LEU:HG	1:C:63:GLN:HB2	2.02	0.40
1:D:49:ALA:O	1:D:50:ARG:C	2.64	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:B:11:SER:HB3	1:B:36:LEU:HD23	2.03	0.40
1:B:20:VAL:O	1:B:21:ARG:C	2.63	0.40
1:B:182:LEU:HD12	1:B:182:LEU:H	1.85	0.40
1:B:269:ASP:HA	1:B:270:PRO:HD2	1.72	0.40
1:C:11:SER:CA	1:C:36:LEU:HD23	2.50	0.40
1:C:33:TYR:CE2	1:C:79:VAL:HG22	2.56	0.40
1:C:119:VAL:HG12	1:C:123:GLN:NE2	2.37	0.40
1:C:211:THR:OG1	1:D:130:LYS:HE2	2.21	0.40
1:C:260:LEU:HA	1:C:263:LEU:HB3	2.03	0.40
1:D:239:VAL:HG21	1:D:255:THR:HA	2.04	0.40
1:A:257:GLU:CG	1:A:260:LEU:HD22	2.47	0.40
1:B:242:THR:O	1:B:243:ALA:C	2.64	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%)	11	39
1	B	271/327 (83%)	244 (90%)	24 (9%)	3 (1%)	11	39
1	C	283/327 (86%)	235 (83%)	40 (14%)	8 (3%)	4	20
1	D	271/327 (83%)	239 (88%)	26 (10%)	6 (2%)	5	24
All	All	1108/1308 (85%)	964 (87%)	124 (11%)	20 (2%)	6	28

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
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%)	182 (77%)	53 (23%)	1	4
1	B	227/258 (88%)	191 (84%)	36 (16%)	2	12
1	C	235/258 (91%)	192 (82%)	43 (18%)	2	8
1	D	227/258 (88%)	179 (79%)	48 (21%)	1	5
All	All	924/1032 (90%)	744 (80%)	180 (20%)	1	6

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	5	VAL

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Mol	Chain	Res	Type
1	A	7	ILE
1	A	11	SER
1	A	30	PHE
1	A	31	LYS
1	A	35	THR
1	A	70	LYS
1	A	72	VAL
1	A	76	ARG
1	A	78	ARG
1	A	80	THR
1	A	87	LEU
1	A	105	ASP
1	A	109	SER
1	A	114	ASN
1	A	115	VAL
1	A	121	MET
1	A	127	PRO
1	A	128	ASP
1	A	129	MET
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	210	HIS
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

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Mol	Chain	Res	Type
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	B	20	VAL
1	B	28	GLN
1	B	40	LYS
1	B	41	THR
1	B	45	LEU
1	B	64	LEU
1	B	69	SER
1	B	80	THR
1	B	109	SER
1	B	116	VAL
1	B	123	GLN
1	B	132	ARG
1	B	147	MET
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	209	ILE
1	B	221	LEU
1	B	239	VAL
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	260	LEU
1	B	262	LEU
1	B	263	LEU
1	B	265	MET
1	B	271	SER

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Mol	Chain	Res	Type
1	B	273	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
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	178	VAL
1	C	180	LEU
1	C	193	MET
1	C	195	LYS
1	C	196	VAL
1	C	203	VAL
1	C	204	LEU
1	C	206	ARG
1	C	209	ILE
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	256	THR
1	C	257	GLU
1	C	260	LEU
1	C	267	LEU
1	C	268	ASP

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Mol	Chain	Res	Type
1	C	273	SER
1	C	281	ARG
1	C	282	GLU
1	C	283	VAL
1	D	14	ILE
1	D	20	VAL
1	D	35	THR
1	D	37	ARG
1	D	41	THR
1	D	45	LEU
1	D	47	GLU
1	D	50	ARG
1	D	64	LEU
1	D	67	ARG
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	121	MET
1	D	123	GLN
1	D	142	SER
1	D	143	VAL
1	D	147	MET
1	D	149	LEU
1	D	153	ASP
1	D	159	LYS
1	D	162	LEU
1	D	178	VAL
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

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Mol	Chain	Res	Type
1	D	239	VAL
1	D	241	LEU
1	D	244	LEU
1	D	245	ARG
1	D	260	LEU
1	D	262	LEU
1	D	265	MET
1	D	266	ARG
1	D	277	THR
1	D	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	42	GLN
1	A	123	GLN
1	A	152	ASN
1	A	217	GLN
1	A	231	GLN
1	A	274	ASN
1	A	280	HIS
1	B	17	HIS
1	B	42	GLN
1	B	123	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 oligosaccharides 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$
2	SO4	B	400	-	4,4,4	0.66	0	6,6,6	0.26	0
2	SO4	D	402	-	4,4,4	0.68	0	6,6,6	0.35	0
2	SO4	A	401	-	4,4,4	0.64	0	6,6,6	0.37	0
3	NAD	B	364	-	46,48,48	1.58	6 (13%)	64,73,73	1.99	18 (28%)
3	NAD	D	362	-	46,48,48	1.60	6 (13%)	64,73,73	1.90	17 (26%)
2	SO4	C	403	-	4,4,4	0.70	0	6,6,6	0.25	0
3	NAD	C	363	-	46,48,48	1.69	7 (15%)	64,73,73	2.26	22 (34%)
3	NAD	A	361	-	46,48,48	1.86	8 (17%)	64,73,73	2.16	21 (32%)

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	D	362	-	-	11/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	363	-	-	8/30/62/62	0/5/5/5
3	NAD	B	364	-	1/1/11/11	7/30/62/62	0/5/5/5
3	NAD	A	361	-	1/1/11/11	10/30/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361	NAD	C2N-N1N	7.26	1.43	1.35
3	C	363	NAD	C2N-N1N	6.67	1.42	1.35
3	D	362	NAD	C2N-N1N	5.97	1.41	1.35
3	B	364	NAD	C2N-N1N	5.86	1.41	1.35
3	D	362	NAD	O4D-C1D	5.19	1.47	1.40
3	B	364	NAD	O4D-C1D	4.52	1.46	1.40
3	A	361	NAD	O4D-C1D	4.29	1.46	1.40
3	A	361	NAD	PN-O3	3.91	1.63	1.59
3	C	363	NAD	O4D-C1D	3.90	1.46	1.40
3	A	361	NAD	PA-O3	3.82	1.63	1.59
3	A	361	NAD	C5A-N7A	-3.57	1.32	1.39
3	B	364	NAD	C5A-N7A	-3.49	1.32	1.39
3	D	362	NAD	C5A-N7A	-3.43	1.32	1.39
3	C	363	NAD	C5A-N7A	-3.28	1.33	1.39
3	A	361	NAD	C6N-N1N	3.24	1.42	1.35
3	C	363	NAD	C6N-N1N	3.11	1.42	1.35
3	D	362	NAD	C6N-N1N	2.88	1.41	1.35
3	B	364	NAD	PN-O3	2.63	1.62	1.59
3	D	362	NAD	C3N-C7N	2.39	1.54	1.50
3	A	361	NAD	PN-O2N	-2.36	1.44	1.55
3	B	364	NAD	C7N-N7N	2.35	1.37	1.33
3	D	362	NAD	C8A-N9A	-2.35	1.33	1.37
3	A	361	NAD	C4A-N9A	-2.35	1.32	1.37
3	C	363	NAD	C8A-N9A	-2.25	1.33	1.37
3	C	363	NAD	C3N-C7N	2.14	1.53	1.50
3	B	364	NAD	C6N-N1N	2.13	1.40	1.35
3	C	363	NAD	PA-O2A	-2.10	1.45	1.55

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361	NAD	O4B-C1B-N9A	10.24	127.76	108.09
3	B	364	NAD	O7N-C7N-C3N	6.01	126.95	119.60
3	C	363	NAD	C5A-C4A-N3A	-5.57	119.05	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	361	NAD	C5A-C4A-N3A	-5.24	119.51	126.72
3	B	364	NAD	O4B-C1B-N9A	5.21	118.09	108.09
3	C	363	NAD	O7N-C7N-C3N	5.14	125.88	119.60
3	C	363	NAD	O5D-C5D-C4D	5.06	126.22	108.99
3	C	363	NAD	C6N-N1N-C2N	-4.84	117.76	121.88
3	B	364	NAD	N3A-C2A-N1A	-4.68	121.49	128.58
3	D	362	NAD	O7N-C7N-C3N	4.63	125.26	119.60
3	B	364	NAD	C5A-C4A-N3A	-4.62	120.35	126.72
3	C	363	NAD	N3A-C4A-N9A	4.58	134.95	127.17
3	C	363	NAD	O4B-C1B-C2B	-4.53	96.92	106.62
3	D	362	NAD	C5A-C4A-N3A	-4.43	120.61	126.72
3	C	363	NAD	O4B-C1B-N9A	4.15	116.06	108.09
3	D	362	NAD	C3N-C7N-N7N	-4.15	112.63	117.74
3	C	363	NAD	C2A-N3A-C4A	3.99	121.59	111.83
3	C	363	NAD	N3A-C2A-N1A	-3.98	122.56	128.58
3	B	364	NAD	C4D-O4D-C1D	-3.90	106.35	109.92
3	D	362	NAD	O2B-C2B-C3B	-3.74	99.83	111.82
3	D	362	NAD	N3A-C2A-N1A	-3.68	123.02	128.58
3	B	364	NAD	O2B-C2B-C3B	-3.54	100.47	111.82
3	B	364	NAD	C2A-N3A-C4A	3.49	120.35	111.83
3	D	362	NAD	N3A-C4A-N9A	3.46	133.05	127.17
3	C	363	NAD	C3N-C7N-N7N	-3.45	113.48	117.74
3	A	361	NAD	N3A-C2A-N1A	-3.45	123.36	128.58
3	B	364	NAD	N3A-C4A-N9A	3.30	132.79	127.17
3	A	361	NAD	C2A-N3A-C4A	3.27	119.81	111.83
3	D	362	NAD	C4D-O4D-C1D	-3.15	107.04	109.92
3	A	361	NAD	N3A-C4A-N9A	3.13	132.48	127.17
3	A	361	NAD	O2N-PN-O1N	3.10	126.89	112.44
3	D	362	NAD	O3B-C3B-C2B	-3.06	102.02	111.82
3	B	364	NAD	C2B-C1B-N9A	3.04	120.86	113.30
3	D	362	NAD	C2A-N3A-C4A	2.99	119.14	111.83
3	D	362	NAD	O2D-C2D-C3D	-2.94	102.38	111.82
3	D	362	NAD	O4B-C1B-N9A	2.89	113.64	108.09
3	A	361	NAD	C5A-N7A-C8A	2.85	107.93	103.45
3	C	363	NAD	C5B-C4B-C3B	2.84	125.42	115.21
3	C	363	NAD	N9A-C8A-N7A	-2.83	109.92	113.94
3	D	362	NAD	O2N-PN-O3	2.83	114.92	107.27
3	A	361	NAD	C4A-C5A-N7A	-2.79	107.40	110.58
3	A	361	NAD	O7N-C7N-C3N	2.79	123.00	119.60
3	A	361	NAD	N9A-C8A-N7A	-2.76	110.02	113.94
3	C	363	NAD	C4B-O4B-C1B	-2.75	103.39	109.47
3	B	364	NAD	C3N-C7N-N7N	-2.74	114.37	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	364	NAD	O7N-C7N-N7N	-2.74	118.66	122.62
3	D	362	NAD	N9A-C8A-N7A	-2.71	110.09	113.94
3	C	363	NAD	O4D-C4D-C5D	2.68	117.92	109.33
3	C	363	NAD	C5D-C4D-C3D	2.65	124.77	115.21
3	C	363	NAD	O2N-PN-O1N	2.61	124.57	112.44
3	C	363	NAD	O3-PA-O1A	-2.60	102.89	110.70
3	B	364	NAD	O3B-C3B-C2B	-2.57	103.59	111.82
3	C	363	NAD	O2A-PA-O1A	2.52	124.17	112.44
3	D	362	NAD	C5A-N7A-C8A	2.48	107.35	103.45
3	C	363	NAD	C5A-N7A-C8A	2.48	107.34	103.45
3	C	363	NAD	C4A-N9A-C8A	2.43	108.28	105.74
3	A	361	NAD	O2A-PA-O1A	2.42	123.70	112.44
3	B	364	NAD	O5B-C5B-C4B	2.39	117.14	108.99
3	C	363	NAD	C2D-C3D-C4D	-2.34	98.08	102.61
3	B	364	NAD	C5N-C4N-C3N	2.33	122.66	120.36
3	D	362	NAD	C2D-C3D-C4D	-2.28	98.20	102.61
3	A	361	NAD	C2B-C1B-N9A	2.26	118.92	113.30
3	A	361	NAD	C3N-C7N-N7N	-2.26	114.95	117.74
3	A	361	NAD	O2B-C2B-C3B	-2.25	104.59	111.82
3	A	361	NAD	C6N-N1N-C2N	-2.25	119.96	121.88
3	A	361	NAD	C5N-C4N-C3N	2.24	122.57	120.36
3	C	363	NAD	O5B-C5B-C4B	2.23	116.59	108.99
3	B	364	NAD	C5N-C6N-N1N	-2.15	117.45	120.38
3	D	362	NAD	C4A-N9A-C8A	2.15	107.99	105.74
3	A	361	NAD	C3B-C2B-C1B	2.14	105.52	101.46
3	A	361	NAD	C2N-N1N-C1D	2.12	123.80	119.13
3	B	364	NAD	C5A-N7A-C8A	2.06	106.69	103.45
3	D	362	NAD	C4A-C5A-N7A	-2.05	108.24	110.58
3	A	361	NAD	C6N-N1N-C1D	-2.03	115.74	119.73
3	B	364	NAD	O2N-PN-O1N	2.02	121.82	112.44
3	A	361	NAD	C5A-C4A-N9A	2.01	108.01	105.81
3	A	361	NAD	O3-PA-O1A	-2.01	104.65	110.70
3	B	364	NAD	N9A-C8A-N7A	-2.00	111.09	113.94

All (2) chirality outliers are listed below:

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

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	361	NAD	PN-O3-PA-O5B
3	A	361	NAD	C5D-O5D-PN-O3
3	A	361	NAD	C5D-O5D-PN-O1N
3	A	361	NAD	O4D-C1D-N1N-C2N
3	A	361	NAD	O4D-C1D-N1N-C6N
3	A	361	NAD	C2D-C1D-N1N-C6N
3	B	364	NAD	C5B-O5B-PA-O2A
3	B	364	NAD	C5B-O5B-PA-O3
3	C	363	NAD	C5B-O5B-PA-O2A
3	C	363	NAD	PN-O3-PA-O5B
3	C	363	NAD	C5D-O5D-PN-O3
3	C	363	NAD	C5D-O5D-PN-O2N
3	C	363	NAD	O4D-C1D-N1N-C2N
3	C	363	NAD	O4D-C1D-N1N-C6N
3	D	362	NAD	C5B-O5B-PA-O3
3	D	362	NAD	C5D-O5D-PN-O1N
3	D	362	NAD	O4D-C4D-C5D-O5D
3	D	362	NAD	O4D-C1D-N1N-C2N
3	D	362	NAD	O4D-C1D-N1N-C6N
3	B	364	NAD	O4D-C4D-C5D-O5D
3	D	362	NAD	C3D-C4D-C5D-O5D
3	B	364	NAD	C3D-C4D-C5D-O5D
3	A	361	NAD	PA-O3-PN-O1N
3	A	361	NAD	C5D-O5D-PN-O2N
3	C	363	NAD	C5B-O5B-PA-O3
3	D	362	NAD	C5B-O5B-PA-O2A
3	D	362	NAD	C5D-O5D-PN-O3
3	B	364	NAD	PN-O3-PA-O1A
3	A	361	NAD	O4B-C1B-N9A-C8A
3	C	363	NAD	C4B-C5B-O5B-PA
3	D	362	NAD	PN-O3-PA-O1A
3	B	364	NAD	C4D-C5D-O5D-PN
3	B	364	NAD	PN-O3-PA-O2A
3	D	362	NAD	PN-O3-PA-O2A
3	A	361	NAD	PA-O3-PN-O2N
3	D	362	NAD	PA-O3-PN-O2N

There are no ring outliers.

5 monomers are involved in 33 short contacts:

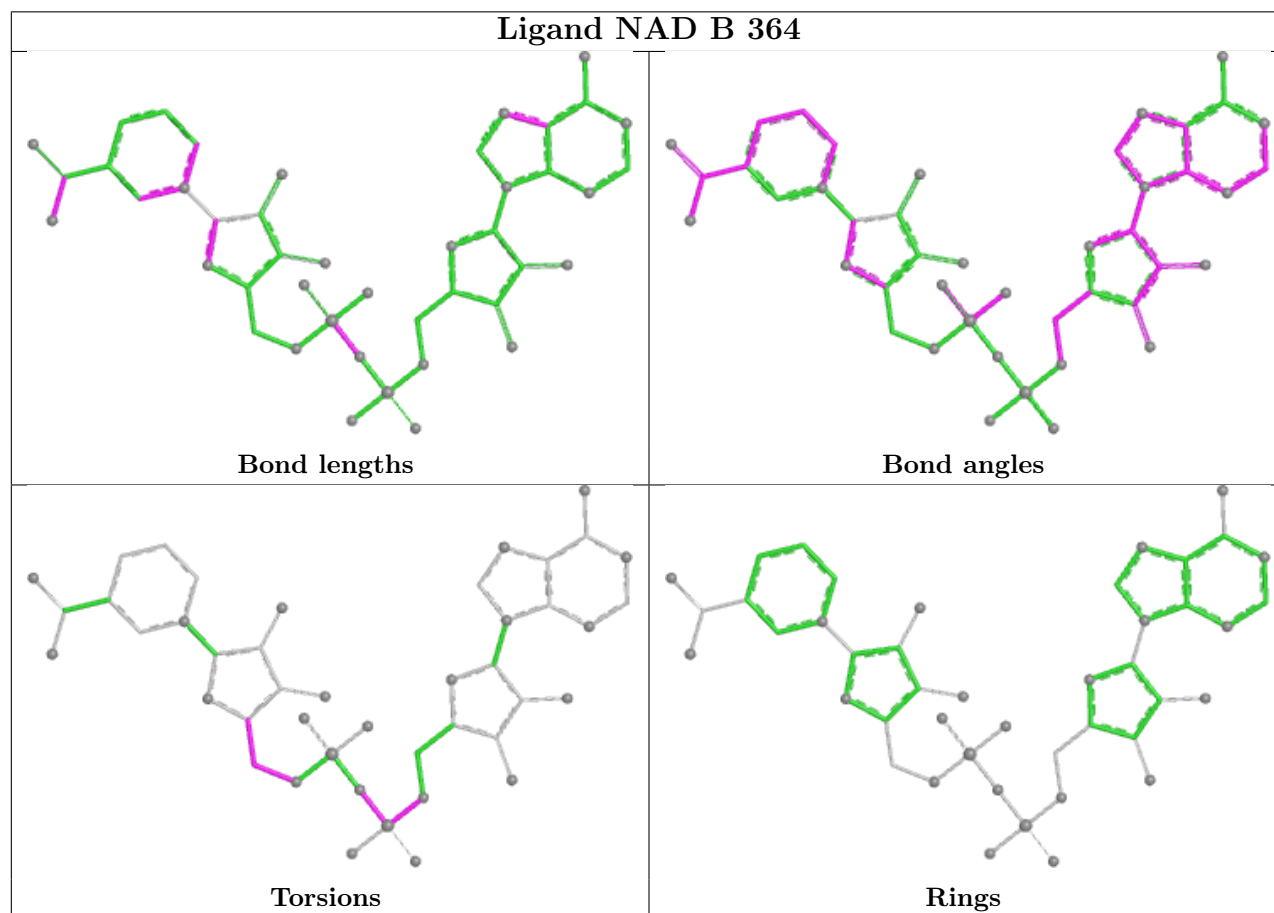
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0
3	B	364	NAD	9	0

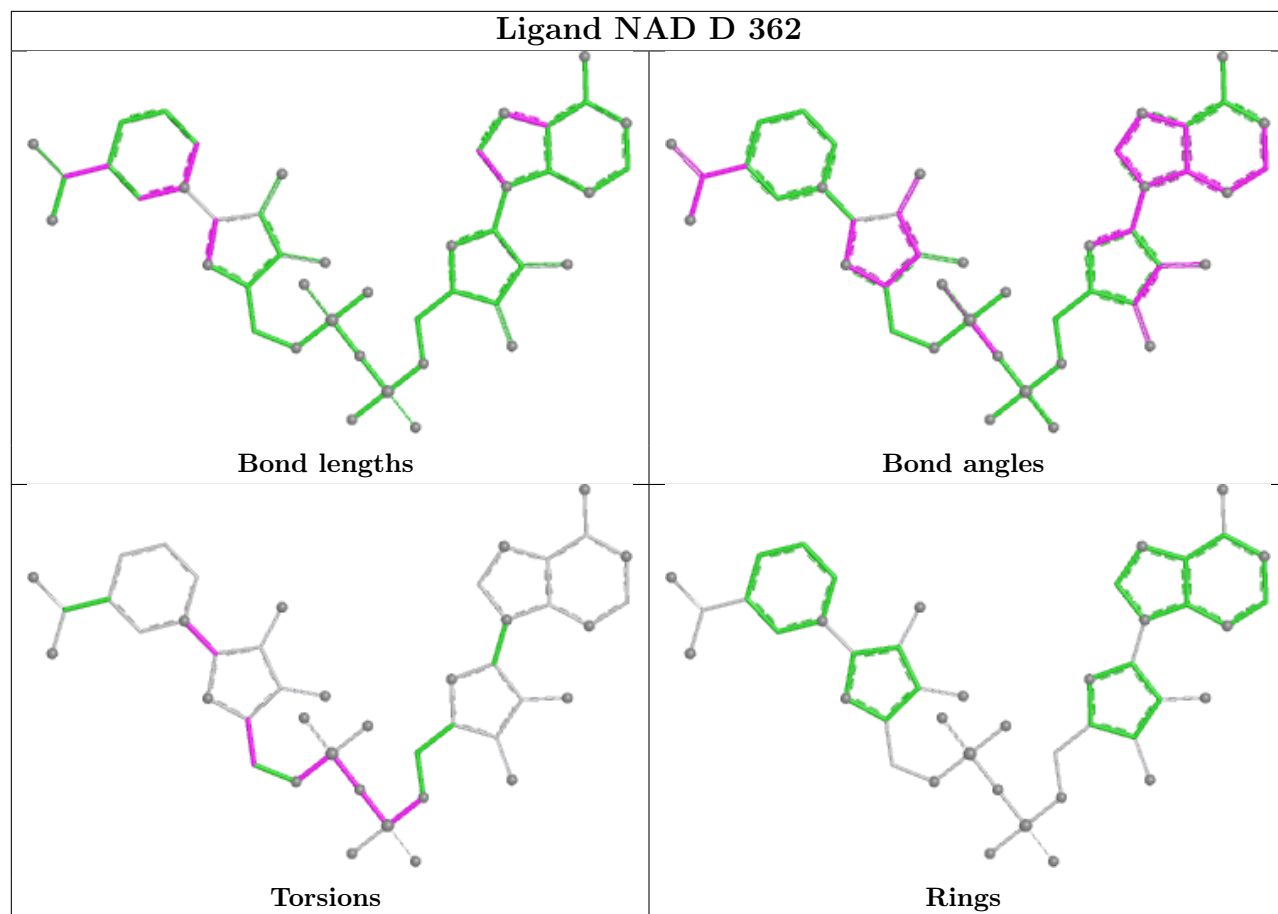
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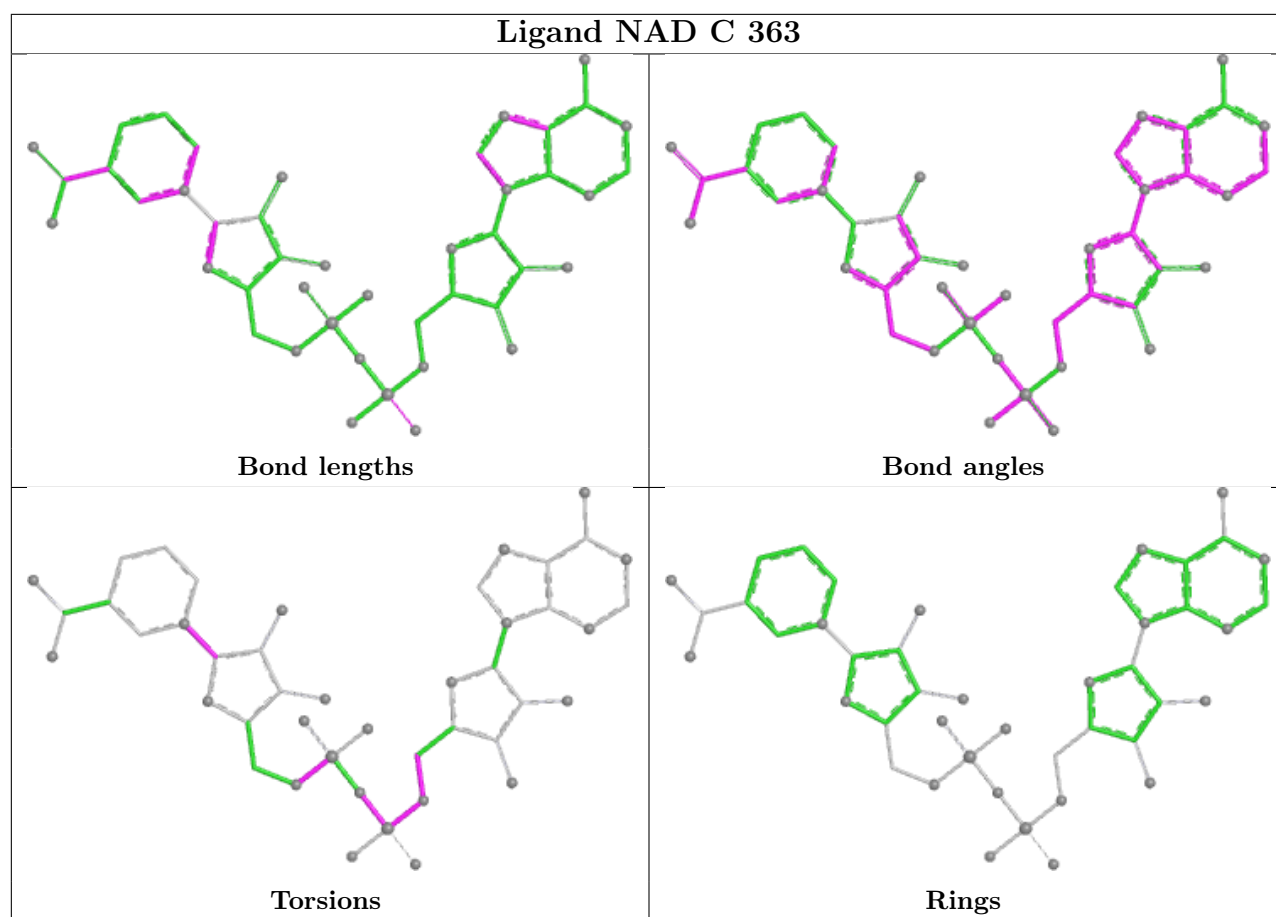
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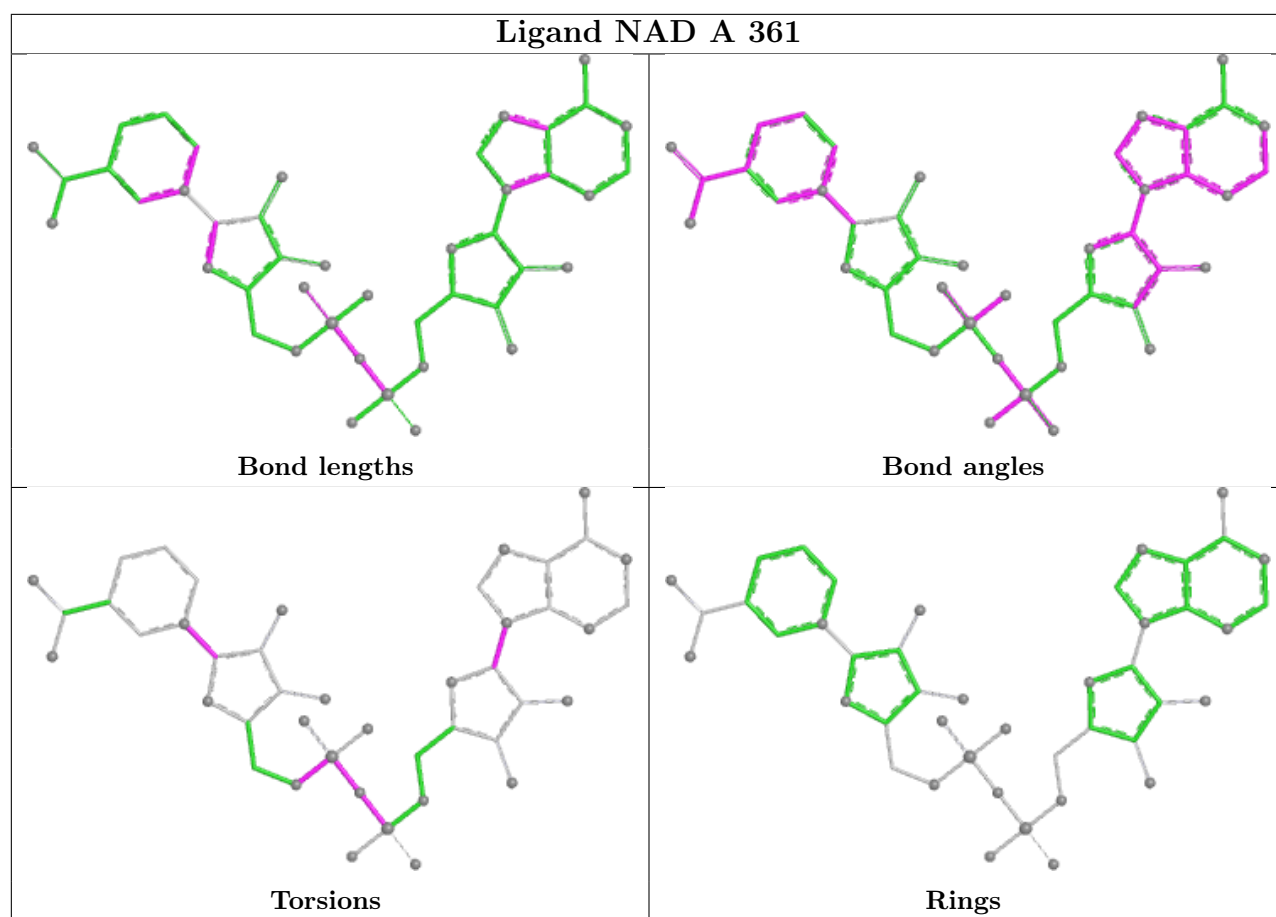
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	362	NAD	12	0
3	C	363	NAD	5	0
3	A	361	NAD	6	0

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	285/327 (87%)	-0.15	8 (2%) 55 34	8, 22, 22, 22	16 (5%)
1	B	275/327 (84%)	-0.23	2 (0%) 84 68	11, 22, 22, 22	8 (2%)
1	C	285/327 (87%)	-0.02	14 (4%) 35 18	7, 22, 22, 22	16 (5%)
1	D	275/327 (84%)	-0.16	7 (2%) 58 37	8, 22, 22, 22	10 (3%)
All	All	1120/1308 (85%)	-0.14	31 (2%) 55 34	7, 22, 22, 22	50 (4%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	LYS	5.6
1	C	264	ARG	5.5
1	A	264	ARG	5.4
1	C	259	PHE	5.3
1	C	196	VAL	5.1
1	D	206	ARG	5.0
1	C	199	SER	4.7
1	B	269	ASP	4.6
1	C	77	GLU	4.5
1	A	199	SER	4.3
1	C	260	LEU	3.8
1	A	195	LYS	3.8
1	D	131	ARG	3.5
1	D	269	ASP	3.4
1	A	227	ARG	3.1
1	A	201	GLU	3.1
1	C	227	ARG	3.0
1	D	286	ASP	2.8
1	A	196	VAL	2.8
1	D	190	THR	2.7
1	B	264	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	2.6
1	C	228	GLU	2.4
1	D	267	LEU	2.4
1	A	285	GLY	2.3
1	C	195	LYS	2.3
1	C	205	ASP	2.3
1	D	264	ARG	2.2
1	C	269	ASP	2.2
1	C	104	GLU	2.1
1	A	47	GLU	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

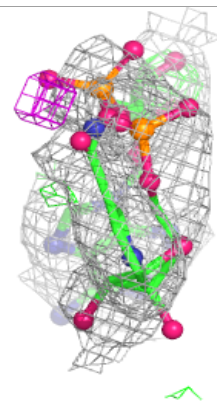
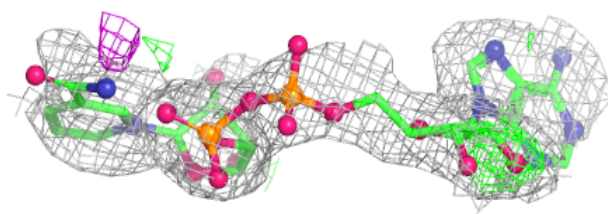
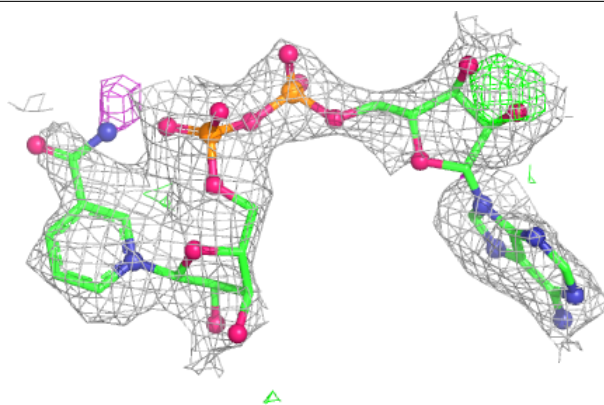
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	D	362	44/44	0.83	0.15	22,22,22,22	44
3	NAD	B	364	44/44	0.87	0.17	22,22,22,22	44
2	SO4	D	402	5/5	0.94	0.10	22,22,22,22	5
2	SO4	B	400	5/5	0.95	0.22	22,22,22,22	5
3	NAD	A	361	44/44	0.95	0.08	22,22,22,22	0
2	SO4	A	401	5/5	0.96	0.13	22,22,22,22	5
3	NAD	C	363	44/44	0.96	0.08	22,22,22,22	0
2	SO4	C	403	5/5	0.96	0.10	22,22,22,22	5

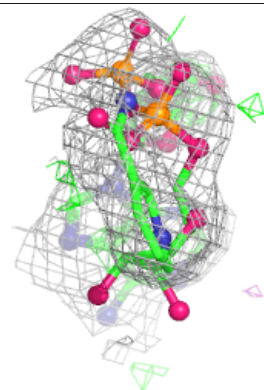
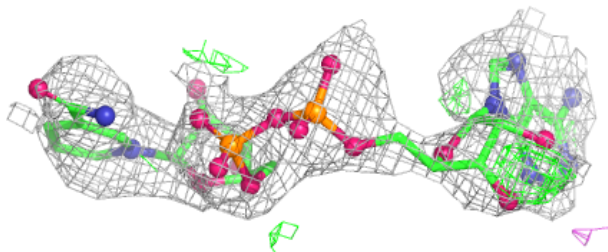
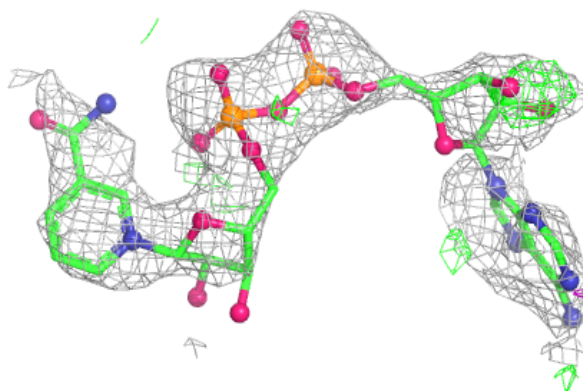
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 362:

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

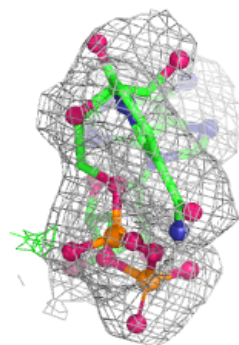
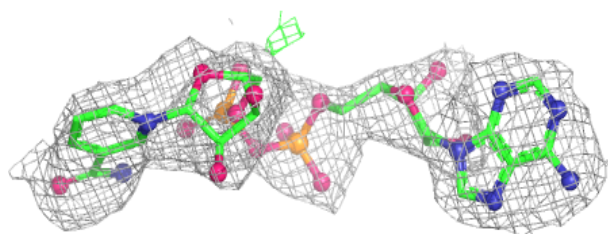
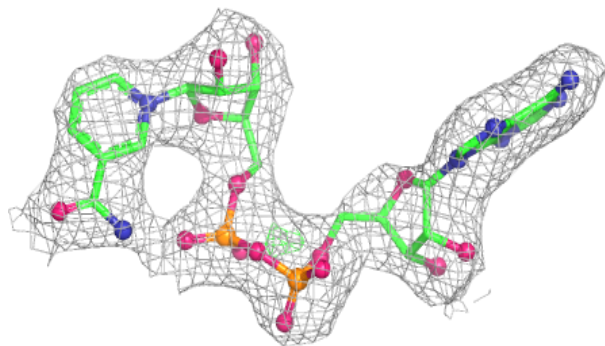
**Electron density around NAD B 364:**

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

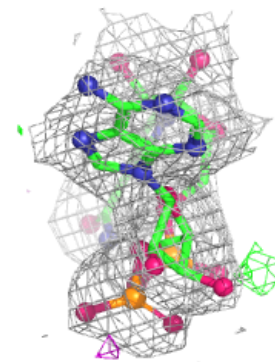
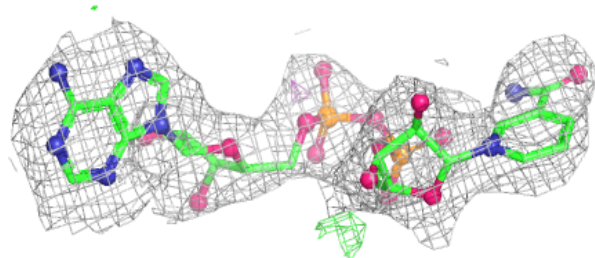
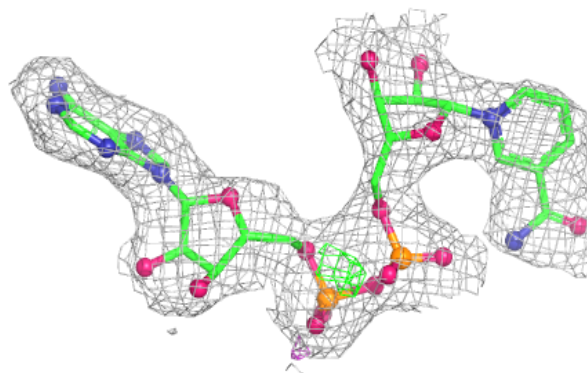


Electron density around NAD A 361:

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

**Electron density around NAD C 363:**

$2mF_o-DF_c$ (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.