



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:34 PM UTC

PDB ID : 7XHL / pdb_00007xhl
Title : Complex structure of a Glucose 6-Phosphate Dehydrogenase from *Zymomonas mobilis*
Authors : Meng, D.D.; Liu, M.X.; Liu, W.D.; You, C.
Deposited on : 2022-04-08
Resolution : 3.25 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

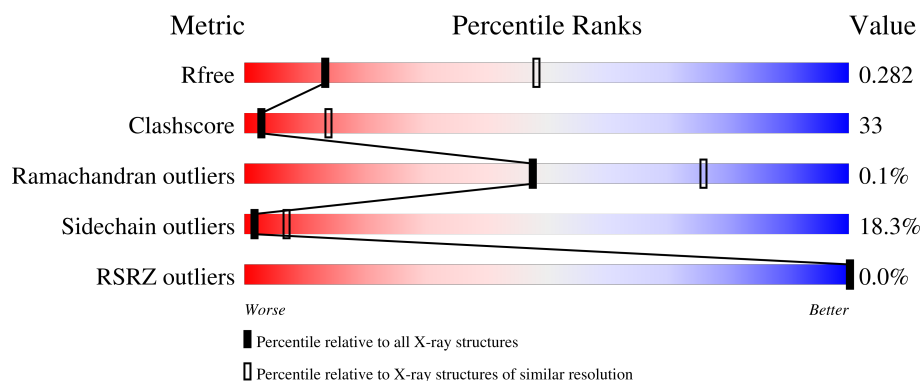
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



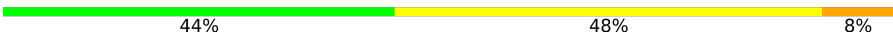
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	487	
1	B	487	
1	C	487	
1	D	487	
1	E	487	

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Mol	Chain	Length	Quality of chain
1	F	487	
1	G	487	
1	H	487	

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
2	NMN	A	501	-	-	X	-

2 Entry composition

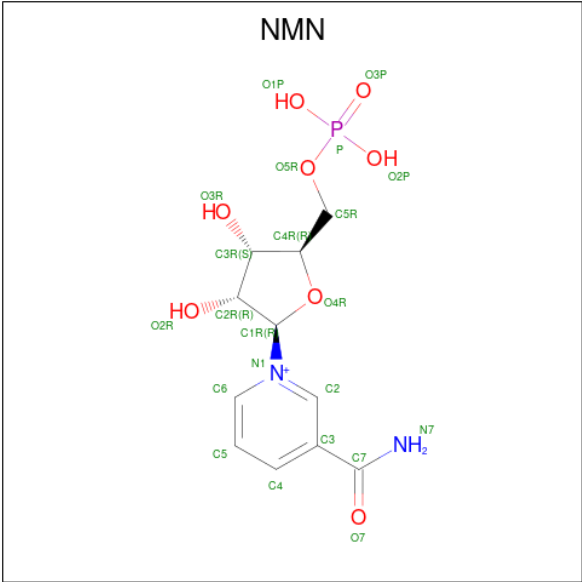
There are 2 unique types of molecules in this entry. The entry contains 28376 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucose 6-Phosphate Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3712	2357	647	698	10			
1	B	479	Total	C	N	O	S	0	0	0
			3625	2294	633	689	9			
1	C	463	Total	C	N	O	S	0	0	0
			3027	1896	552	573	6			
1	D	479	Total	C	N	O	S	0	0	0
			3545	2250	606	679	10			
1	E	476	Total	C	N	O	S	0	0	0
			3587	2276	621	681	9			
1	F	462	Total	C	N	O	S	0	0	0
			3378	2135	600	634	9			
1	G	485	Total	C	N	O	S	0	0	0
			3735	2366	649	710	10			
1	H	481	Total	C	N	O	S	0	0	0
			3679	2336	634	699	10			

- Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (CCD ID: NMN) (formula: C₁₁H₁₆N₂O₈P) (labeled as "Ligand of Interest" by depositor).

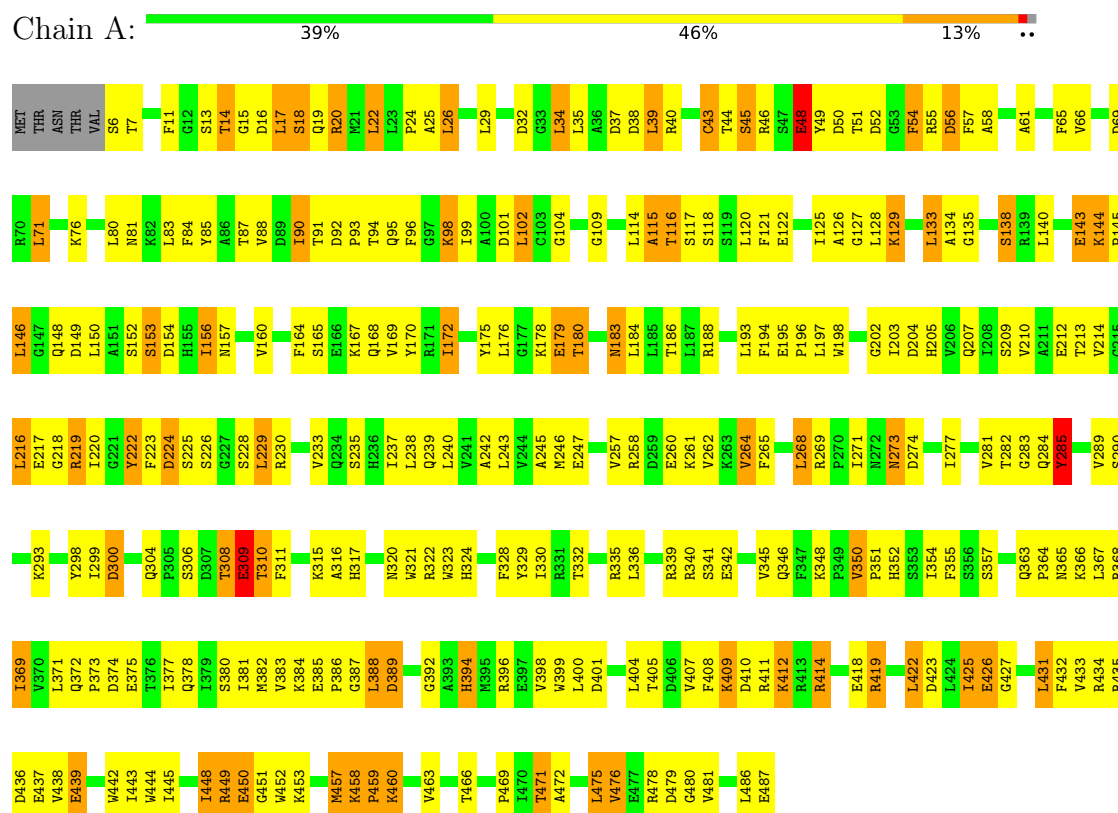


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	G	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

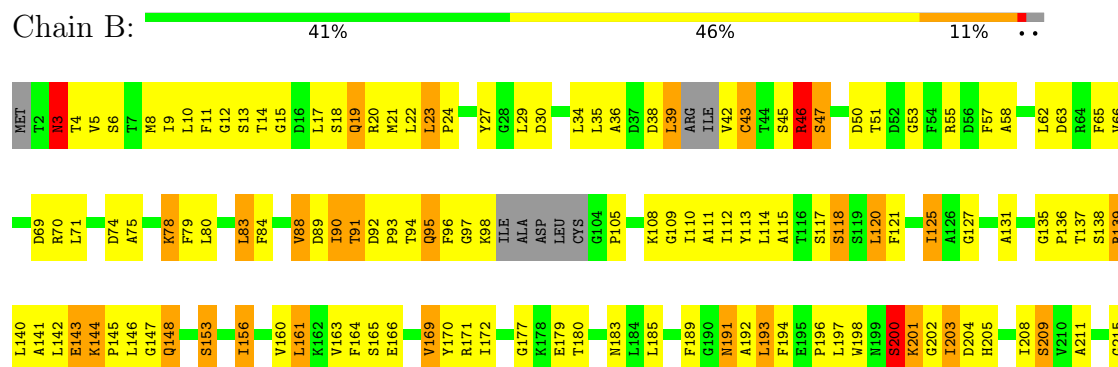
3 Residue-property plots

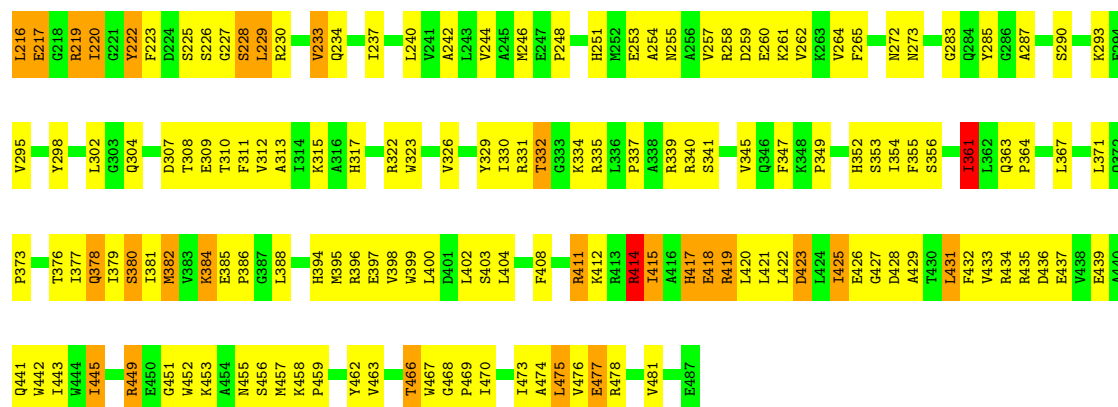
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucose 6-Phosphate Dehydrogenase



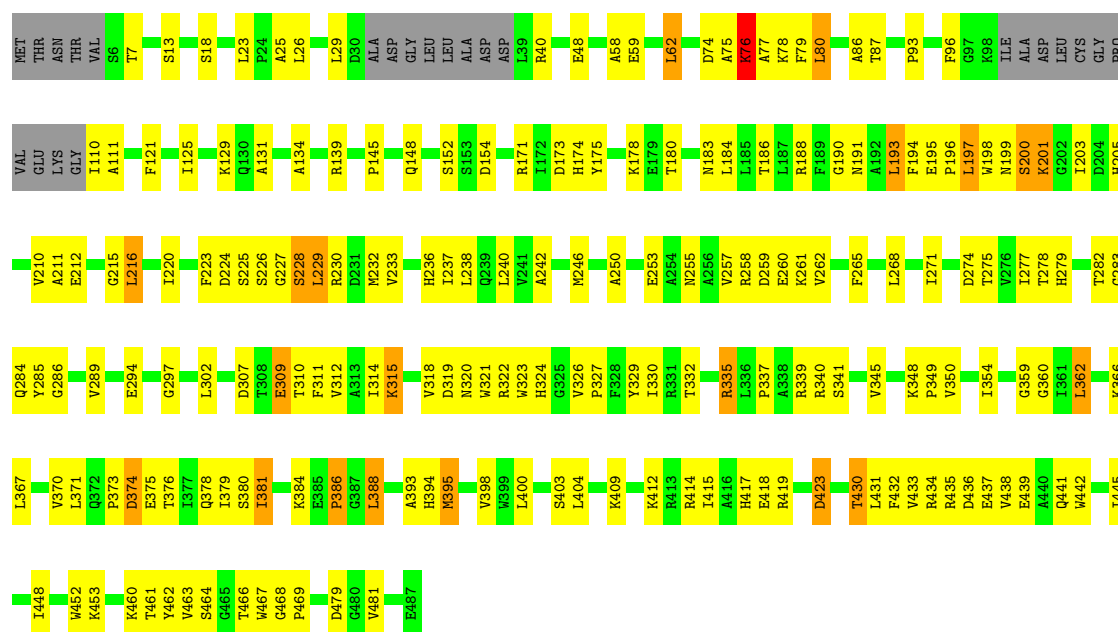
• Molecule 1: Glucose 6-Phosphate Dehydrogenase





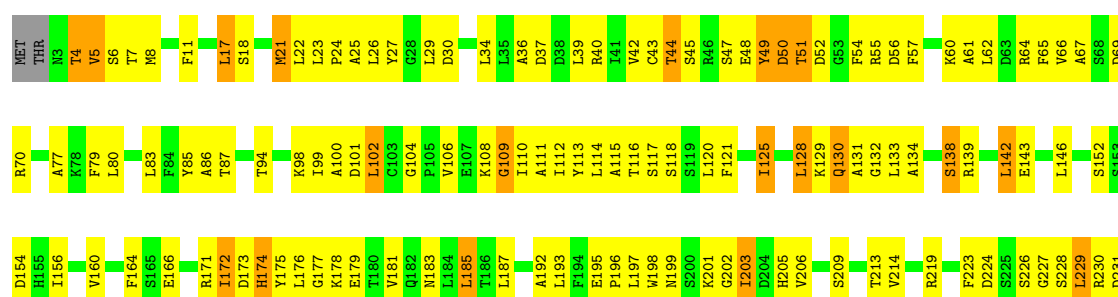
• Molecule 1: Glucose 6-Phosphate Dehydrogenase

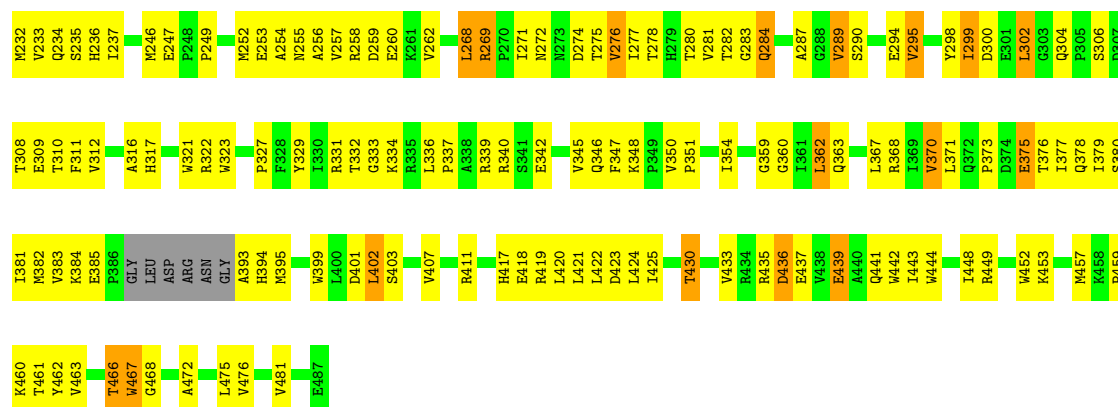
Chain C: 55% 36% 5%



• Molecule 1: Glucose 6-Phosphate Dehydrogenase

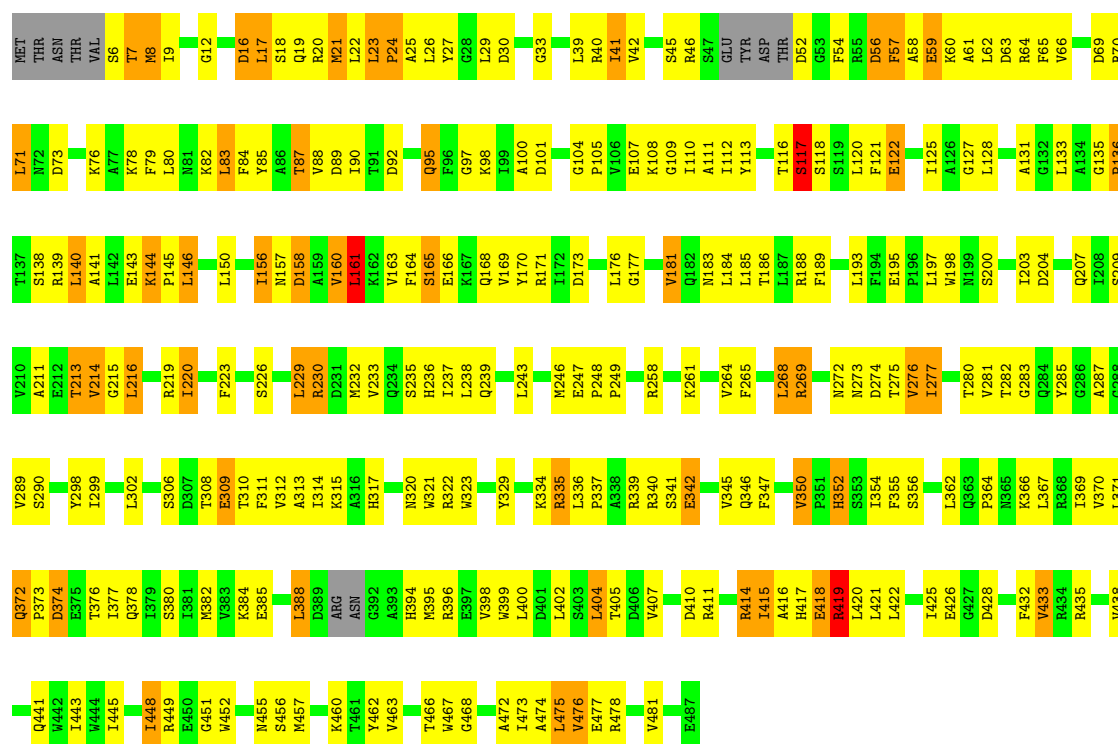
Chain D: 44% 47% 8%





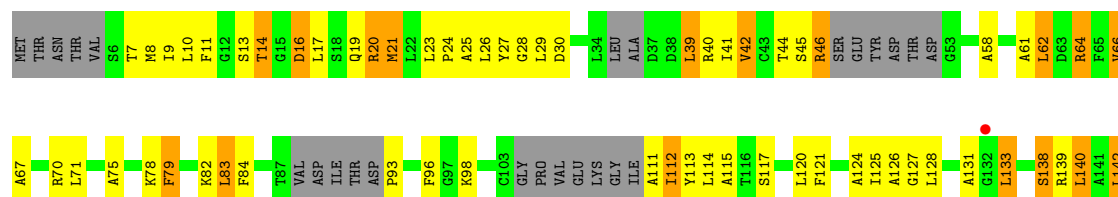
● Molecule 1: Glucose 6-Phosphate Dehydrogenase

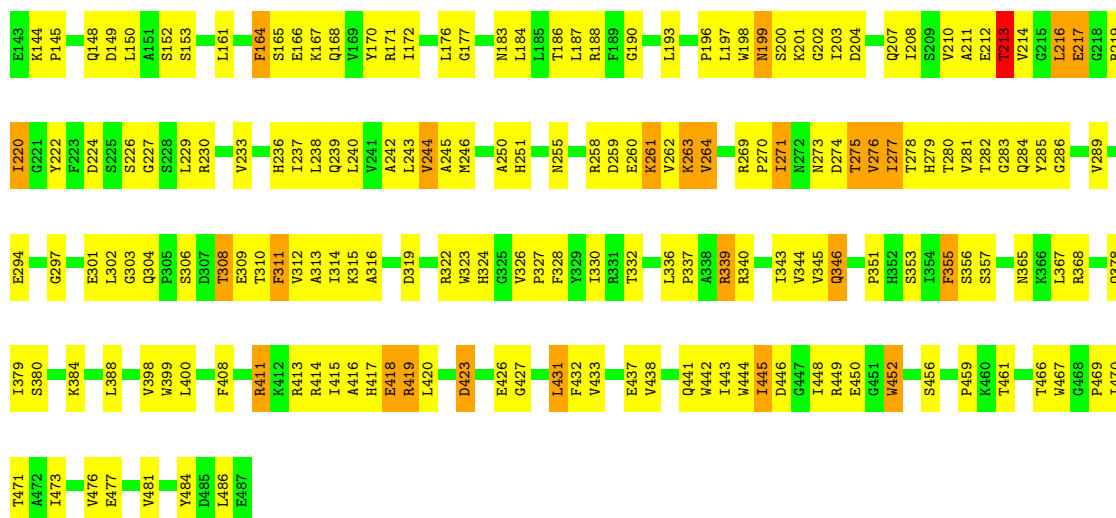
Chain E: 42% 45% 10% ..



● Molecule 1: Glucose 6-Phosphate Dehydrogenase

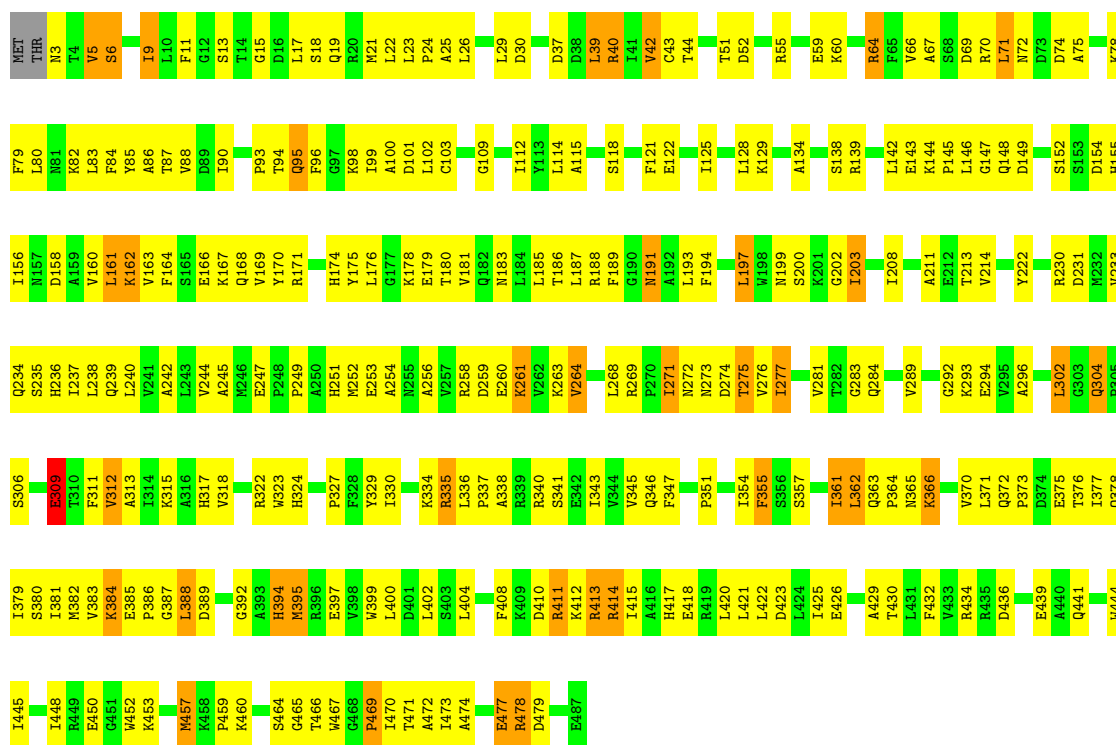
Chain F: 45% 41% 9% 5%





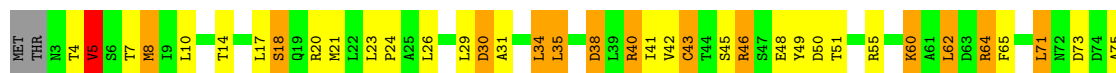
● Molecule 1: Glucose 6-Phosphate Dehydrogenase

Chain G: 44% 48% 8%



● Molecule 1: Glucose 6-Phosphate Dehydrogenase

Chain H: 43% 46% 9%



I443	P373	V295	G227	L156	K76
W444	D374		S228	M157	A77
I445	E375	Y298	L229	A158	K78
D446		I299	R230	A159	F79
	Q378	D300	D231	V160	L80
R449		E301	M232	L161	N81
	M382		V233		K82
W452	V383	T308	G234	F164	L83
K453	K384	E309	S235	S165	F84
	E385	T310	H236	E166	Y85
S456	P386		I237	K167	A86
K457	G387	A313	L238	Q168	T87
K458	L388	I314	G239	V169	
P459	ASP	K315	L240	Y170	F96
K460	ARG		V241	R171	G97
T461	ASN	N320		I172	K98
Y462	GLY	W321	A245		I99
	A393	R322	K246	Y175	A100
T466	H394	W323	E247	L176	D101
W467	K395	H324		G177	L102
G468	R396		M252	K178	C103
P469		P327	E253	E179	G104
I470	W399	F328	A254	T180	
T471	L400	Y329	N255	V181	G109
A472	D401	I330	A256	Q182	I110
I473	L402	R331	V257	N183	A111
A474	S403	T332	R258	L184	I112
L475	L404	G333	D259	L185	Y113
W476	T405	K334	E260	T186	L114
E477	D406	R335	K261	L187	A115
R478	W407	L336	V262		
D479	F408	P337	K263	N191	S118
G480	K409	A338	V264	E195	S119
V481		R339	F265	P196	L120
W482	I415	R340		L197	F121
W483	A416	S341	R269	L198	
	H417	E342	P270	W198	G127
	E418	I343	I271	N199	L128
	R419	V344	N272		K129
	L420	Q346	D274	G202	Q130
	L421	F347	T275	I203	A131
	L422	K348	V276	D204	G132
	D423	P349	I277	Q207	L133
L424	L424	V350	T278	A134	A134
E426	I426	P351	T280	G135	
G427	G427		T281	S209	P136
D428	D428	I354	V281	V210	T137
A429	A429	F355	T282	A211	S138
T430	T430	S356	G283	E212	R139
L431	L431		Q284	T213	L140
F432	F432	G359	Y285	L216	A141
V433	V433	G360	G286		L142
R434	R434	I361	A287	R219	
R435	R435	G288	V289	I220	Q148
D436	D436	P364	N365	G221	D149
E437	E437	L371		Y222	
V438	V438	Q372	K293	F223	S152
E439	E439		E294	D224	S153
					D154
					H155

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.32Å 342.33Å 103.36Å 90.00° 92.66° 90.00°	Depositor
Resolution (Å)	78.11 – 3.25 78.11 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (78.11-3.25) 83.3 (78.11-3.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.237 , 0.297 0.249 , 0.282	Depositor DCC
R_{free} test set	4294 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 111.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
Reported twinning fraction	0.200 for h,-k,-l	Depositor
Outliers	0 of 86165 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28376	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: NMN

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	0.77	1/3790 (0.0%)	1.26	13/5146 (0.3%)
1	B	0.75	1/3696 (0.0%)	1.22	12/5028 (0.2%)
1	C	0.71	0/3079	1.22	10/4224 (0.2%)
1	D	0.71	0/3620	1.18	7/4945 (0.1%)
1	E	0.74	0/3660	1.23	11/4983 (0.2%)
1	F	0.74	0/3444	1.23	8/4692 (0.2%)
1	G	0.69	0/3810	1.13	5/5173 (0.1%)
1	H	0.69	0/3754	1.16	6/5104 (0.1%)
All	All	0.73	2/28853 (0.0%)	1.20	72/39295 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	ILE	CG1-CD1	-6.02	1.28	1.51
1	A	172	ILE	CG1-CD1	-5.72	1.29	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	PRO	N-CA-C	-10.70	99.93	113.84
1	A	309	GLU	N-CA-C	10.10	122.28	111.28
1	C	145	PRO	N-CA-C	-10.03	99.59	113.53
1	C	200	SER	N-CA-C	-9.41	99.92	111.40
1	A	54	PHE	N-CA-C	-9.03	101.20	113.30
1	C	74	ASP	N-CA-C	-8.50	102.62	113.16
1	C	93	PRO	N-CA-C	-8.50	101.72	113.53
1	A	480	GLY	N-CA-C	-7.83	105.17	114.48
1	B	414	ARG	N-CA-C	7.58	119.62	111.36
1	D	177	GLY	N-CA-C	-7.43	103.26	112.77
1	F	310	THR	N-CA-C	-6.98	104.76	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	309	GLU	N-CA-C	6.97	118.52	111.07
1	B	361	ILE	N-CA-C	-6.93	103.45	111.00
1	G	361	ILE	N-CA-C	-6.76	103.72	110.62
1	F	357	SER	N-CA-C	-6.76	104.61	112.92
1	H	430	THR	N-CA-C	-6.73	104.71	113.12
1	B	228	SER	N-CA-C	-6.64	104.05	111.28
1	A	392	GLY	CA-C-O	-6.57	117.70	122.23
1	G	469	PRO	N-CA-C	-6.55	100.80	111.21
1	A	459	PRO	N-CA-C	-6.54	100.95	111.14
1	A	388	LEU	N-CA-C	-6.43	98.76	109.24
1	C	386	PRO	N-CA-C	-6.43	101.11	111.14
1	D	174	HIS	N-CA-C	-6.40	104.30	111.28
1	E	213	THR	N-CA-C	-6.30	105.87	112.93
1	F	227	GLY	CA-C-O	-6.29	117.20	122.29
1	A	115	ALA	N-CA-C	-6.28	105.72	113.19
1	F	213	THR	N-CA-C	-6.18	105.00	112.54
1	H	98	LYS	N-CA-C	-5.96	104.78	111.28
1	E	418	GLU	N-CA-C	-5.90	104.93	111.36
1	E	219	ARG	N-CA-C	-5.87	105.31	112.88
1	A	48	GLU	N-CA-C	5.84	117.13	108.60
1	C	430	THR	N-CA-C	-5.83	105.65	112.89
1	B	3	ASN	CB-CA-C	-5.83	101.11	110.79
1	A	285	TYR	CB-CA-C	5.79	119.34	109.72
1	C	374	ASP	CA-C-N	-5.77	115.33	122.84
1	C	374	ASP	C-N-CA	-5.77	115.33	122.84
1	D	109	GLY	CA-C-O	-5.76	118.25	122.23
1	E	136	PRO	N-CA-C	-5.75	105.53	113.53
1	H	31	ALA	N-CA-C	-5.74	105.03	111.28
1	C	227	GLY	CA-C-O	-5.71	117.27	122.24
1	E	158	ASP	N-CA-C	-5.60	104.39	111.11
1	D	142	LEU	CA-C-N	-5.60	114.44	122.67
1	D	142	LEU	C-N-CA	-5.60	114.44	122.67
1	A	218	GLY	N-CA-C	-5.58	107.94	115.36
1	B	209	SER	N-CA-C	5.57	118.19	107.44
1	D	227	GLY	CA-C-O	-5.56	117.78	122.29
1	H	247	GLU	N-CA-C	-5.55	102.42	110.08
1	E	64	ARG	CA-C-N	-5.54	110.96	121.54
1	E	64	ARG	C-N-CA	-5.54	110.96	121.54
1	C	76	LYS	N-CA-C	-5.51	105.27	111.28
1	G	387	GLY	CA-C-O	-5.47	118.45	122.23
1	E	24	PRO	N-CA-C	-5.46	105.95	113.53
1	B	46	ARG	N-CA-C	-5.45	105.34	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	456	SER	N-CA-C	-5.38	106.01	112.58
1	B	55	ARG	N-CA-C	-5.34	105.46	111.28
1	D	108	LYS	N-CA-C	-5.32	105.48	111.28
1	B	200	SER	N-CA-C	-5.30	105.50	111.28
1	B	4	THR	N-CA-C	-5.30	104.34	111.54
1	G	335	ARG	CB-CG-CD	-5.29	99.12	111.30
1	F	167	LYS	CA-C-N	-5.29	115.39	122.42
1	F	167	LYS	C-N-CA	-5.29	115.39	122.42
1	H	361	ILE	N-CA-C	-5.24	102.83	109.80
1	H	5	VAL	N-CA-C	5.21	115.41	108.11
1	A	101	ASP	N-CA-C	-5.21	106.32	113.56
1	E	419	ARG	N-CA-C	-5.18	106.92	113.18
1	E	161	LEU	N-CA-C	-5.10	107.23	113.50
1	A	264	VAL	N-CA-C	-5.07	105.44	110.62
1	E	60	LYS	N-CA-C	-5.07	105.88	111.71
1	B	466	THR	N-CA-C	5.04	118.51	111.30
1	A	109	GLY	CA-C-O	-5.03	118.22	122.29
1	B	147	GLY	CA-C-O	-5.01	117.88	122.24
1	F	13	SER	N-CA-C	-5.00	105.82	111.28

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	3712	0	3640	259	0
1	B	3625	0	3513	280	0
1	C	3027	0	2453	163	0
1	D	3545	0	3326	214	0
1	E	3587	0	3445	271	0
1	F	3378	0	3145	215	0
1	G	3735	0	3668	232	0
1	H	3679	0	3590	274	0
2	A	22	0	14	16	0
2	B	22	0	14	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	22	0	14	4	0
2	G	22	0	14	5	0
All	All	28376	0	26836	1819	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 33.

All (1819) 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:E:54:PHE:CD2	1:E:84:PHE:HA	1.76	1.21
1:E:54:PHE:CE2	1:E:84:PHE:HA	1.84	1.13
1:A:144:LYS:HE3	2:A:501:NMN:C6	1.78	1.12
1:E:54:PHE:HE2	1:E:84:PHE:CB	1.63	1.11
1:E:54:PHE:HE2	1:E:84:PHE:HB3	1.10	1.10
1:E:54:PHE:CE2	1:E:84:PHE:HB3	1.91	1.05
1:E:54:PHE:CE2	1:E:84:PHE:CA	2.40	1.05
1:B:144:LYS:HE2	2:B:501:NMN:HC6	1.38	1.03
1:A:144:LYS:HE3	2:A:501:NMN:C5	1.90	1.00
1:C:211:ALA:HB3	1:C:340:ARG:H	1.28	0.97
1:D:476:VAL:HG22	1:D:481:VAL:HG13	1.47	0.96
1:E:474:ALA:HA	1:E:477:GLU:HB2	1.48	0.95
1:E:40:ARG:HB3	1:E:84:PHE:HE2	1.30	0.94
1:G:400:LEU:HD23	1:H:402:LEU:HB3	1.51	0.92
1:E:54:PHE:CE2	1:E:84:PHE:CB	2.50	0.92
1:E:54:PHE:HE2	1:E:84:PHE:CA	1.77	0.92
1:G:18:SER:HA	1:G:22:LEU:HB2	1.49	0.92
1:C:237:ILE:HA	1:C:240:LEU:HD12	1.52	0.92
1:A:45:SER:HB3	1:A:85:TYR:HE2	1.32	0.91
1:D:229:LEU:HA	1:D:233:VAL:HG12	1.50	0.91
1:A:419:ARG:HG2	1:B:388:LEU:HD22	1.52	0.90
1:D:8:MET:HG3	1:D:111:ALA:HB3	1.50	0.90
1:F:25:ALA:HA	1:F:415:ILE:HD13	1.51	0.90
1:F:144:LYS:HG3	1:F:145:PRO:HD3	1.54	0.88
2:B:501:NMN:H5R1	2:B:501:NMN:HC2	1.55	0.87
1:G:388:LEU:HA	1:H:419:ARG:HE	1.40	0.87
1:E:238:LEU:HD23	1:E:441:GLN:HG2	1.57	0.87
1:G:384:LYS:HB2	1:H:186:THR:HG21	1.56	0.86
1:E:476:VAL:HG22	1:E:481:VAL:HG23	1.56	0.86
1:F:275:THR:HG22	1:F:279:HIS:HD2	1.40	0.86
1:E:20:ARG:HA	1:E:65:PHE:CE2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:VAL:HG22	1:F:437:GLU:HG3	1.58	0.85
1:G:271:ILE:HG13	1:G:448:ILE:HG13	1.58	0.85
1:H:99:ILE:HB	1:H:133:LEU:HD11	1.59	0.84
1:B:198:TRP:HH2	1:B:367:LEU:HD23	1.40	0.84
1:B:452:TRP:HB2	1:B:457:MET:HB2	1.58	0.84
1:A:257:VAL:HG12	1:A:261:LYS:HD2	1.60	0.84
1:G:95:GLN:O	1:G:98:LYS:HG3	1.78	0.84
1:E:233:VAL:O	1:E:238:LEU:HD13	1.78	0.84
1:D:54:PHE:HE2	1:D:83:LEU:HD12	1.40	0.83
1:E:12:GLY:HA2	1:E:46:ARG:HG2	1.59	0.83
1:E:340:ARG:HG2	1:E:372:GLN:HG2	1.60	0.83
1:A:411:ARG:HD3	1:B:386:PRO:HD2	1.61	0.83
1:C:463:VAL:O	1:C:466:THR:HG22	1.77	0.83
1:E:54:PHE:HD2	1:E:84:PHE:HA	1.42	0.82
1:A:479:ASP:HB2	1:A:481:VAL:HG12	1.62	0.82
1:C:154:ASP:HA	1:C:435:ARG:NH2	1.95	0.81
1:E:369:ILE:HG23	1:E:377:ILE:HG12	1.58	0.81
1:E:273:ASN:HA	1:E:451:GLY:CA	2.10	0.81
1:G:281:VAL:HB	1:G:313:ALA:HB3	1.62	0.81
1:G:233:VAL:HG21	1:G:312:VAL:HG11	1.62	0.81
1:H:359:GLY:O	1:H:394:HIS:HD2	1.63	0.81
1:F:114:LEU:HD13	1:F:140:LEU:HD21	1.63	0.80
1:G:17:LEU:HD22	2:G:501:NMN:C2	2.11	0.80
1:B:216:LEU:H	1:B:216:LEU:HD22	1.45	0.80
1:B:229:LEU:HA	1:B:233:VAL:HG13	1.64	0.80
1:B:144:LYS:HG3	1:B:145:PRO:HD3	1.63	0.79
1:A:45:SER:HB3	1:A:85:TYR:CE2	2.16	0.79
1:C:180:THR:HG21	1:C:371:LEU:HA	1.63	0.79
1:E:382:MET:HE2	1:E:395:MET:HE3	1.63	0.79
1:A:125:ILE:HA	1:A:128:LEU:HD12	1.65	0.79
1:C:381:ILE:HD11	1:C:400:LEU:HG	1.64	0.79
1:B:97:GLY:HA2	1:B:131:ALA:HB1	1.64	0.79
1:E:144:LYS:HG3	1:E:145:PRO:HD3	1.61	0.79
1:F:242:ALA:HA	1:F:264:VAL:HG21	1.65	0.78
1:F:306:SER:HB2	1:F:308:THR:HG22	1.66	0.78
1:A:17:LEU:HD22	2:A:501:NMN:H5R2	1.63	0.78
1:A:48:GLU:HB3	1:A:49:TYR:CD1	2.18	0.78
1:B:466:THR:HG23	1:G:289:VAL:HG22	1.66	0.78
1:G:408:PHE:HE1	1:H:385:GLU:HG2	1.47	0.78
1:A:50:ASP:HA	1:A:85:TYR:CE1	2.19	0.78
1:B:429:ALA:HA	1:B:432:PHE:CD1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:476:VAL:HG22	1:H:481:VAL:HG22	1.66	0.77
1:E:370:VAL:HB	1:E:372:GLN:HG3	1.64	0.77
1:D:229:LEU:HA	1:D:233:VAL:CG1	2.14	0.77
1:H:285:TYR:CD1	1:H:335:ARG:HG3	2.20	0.77
1:E:452:TRP:HB2	1:E:457:MET:HB2	1.67	0.77
1:B:88:VAL:HG13	1:B:95:GLN:HB3	1.66	0.77
1:D:312:VAL:HG12	1:D:332:THR:HG22	1.67	0.77
1:G:340:ARG:HA	1:G:373:PRO:HG3	1.67	0.76
1:G:389:ASP:H	1:H:419:ARG:HH21	1.32	0.76
1:H:203:ILE:HD11	1:H:345:VAL:HG13	1.66	0.76
1:A:216:LEU:HD12	1:A:219:ARG:HB2	1.68	0.76
1:D:54:PHE:CE2	1:D:83:LEU:HD12	2.20	0.76
1:B:5:VAL:HG22	1:B:109:GLY:HA3	1.68	0.76
1:B:216:LEU:HB2	1:B:220:ILE:HG23	1.66	0.76
1:G:144:LYS:HB3	1:G:145:PRO:HD3	1.66	0.76
1:A:46:ARG:H	1:A:46:ARG:HD3	1.51	0.76
1:F:10:LEU:HB3	1:F:42:VAL:O	1.85	0.76
1:G:125:ILE:HD12	1:G:160:VAL:HG22	1.66	0.76
1:E:40:ARG:HG3	1:E:105:PRO:HG2	1.66	0.76
1:E:337:PRO:HD2	1:E:467:TRP:CE3	2.21	0.76
1:F:23:LEU:HA	1:F:26:LEU:HD12	1.68	0.76
1:A:377:ILE:HG13	1:A:404:LEU:HD11	1.66	0.75
1:H:30:ASP:HA	1:H:35:LEU:HD11	1.67	0.75
1:A:49:TYR:HB3	1:A:54:PHE:HB2	1.69	0.75
1:E:449:ARG:HA	1:E:452:TRP:CE2	2.21	0.75
1:H:114:LEU:HD13	1:H:140:LEU:HD11	1.68	0.75
1:B:381:ILE:HG13	1:B:398:VAL:HG23	1.67	0.75
1:G:175:TYR:HA	1:G:178:LYS:HD2	1.68	0.75
1:D:23:LEU:HA	1:D:26:LEU:HD12	1.67	0.75
1:E:17:LEU:HB3	2:E:501:NMN:O2P	1.87	0.75
1:C:199:ASN:HB2	1:C:201:LYS:O	1.86	0.75
1:F:112:ILE:HD11	1:F:138:SER:HB2	1.67	0.75
1:E:207:GLN:HG2	1:E:329:TYR:HB2	1.68	0.74
1:G:6:SER:HB2	1:G:109:GLY:C	2.12	0.74
1:B:265:PHE:HE2	1:B:437:GLU:HG2	1.51	0.74
1:H:216:LEU:HD22	1:H:223:PHE:HB2	1.69	0.74
1:B:215:GLY:HA2	1:B:334:LYS:HE3	1.70	0.74
1:D:255:ASN:O	1:D:259:ASP:N	2.20	0.74
1:F:365:ASN:ND2	1:F:380:SER:O	2.20	0.74
1:D:246:MET:HE3	1:D:260:GLU:HB2	1.68	0.73
1:E:273:ASN:HA	1:E:451:GLY:HA3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:HD2	1:B:434:ARG:HB2	1.68	0.73
1:G:222:TYR:OH	2:G:501:NMN:H2RC	1.87	0.73
1:E:9:ILE:HD13	1:E:112:ILE:HG12	1.69	0.73
1:D:152:SER:O	1:D:156:ILE:HG12	1.89	0.73
1:C:381:ILE:HD12	1:C:398:VAL:HG13	1.71	0.73
1:F:8:MET:HE3	1:F:10:LEU:HB2	1.69	0.73
1:C:13:SER:HA	1:C:18:SER:CB	2.20	0.72
1:C:337:PRO:HG2	1:C:467:TRP:CE2	2.25	0.72
1:C:400:LEU:HD23	1:D:402:LEU:HB3	1.71	0.72
1:E:40:ARG:HB3	1:E:84:PHE:CE2	2.20	0.72
1:B:110:ILE:O	1:B:138:SER:HA	1.90	0.72
1:E:135:GLY:CA	1:E:138:SER:HB2	2.19	0.72
1:H:203:ILE:HG21	1:H:323:TRP:HZ3	1.55	0.72
1:E:189:PHE:HE2	1:E:246:MET:HE2	1.55	0.72
1:F:408:PHE:HB3	1:F:411:ARG:HB2	1.72	0.72
1:G:271:ILE:HD11	1:G:444:TRP:O	1.88	0.72
1:B:27:TYR:OH	1:B:71:LEU:HA	1.90	0.71
1:H:233:VAL:O	1:H:238:LEU:HB2	1.90	0.71
1:H:439:GLU:O	1:H:443:ILE:HG13	1.90	0.71
1:G:66:VAL:HG11	1:G:71:LEU:HD13	1.71	0.71
1:A:193:LEU:HA	1:B:197:LEU:HD11	1.71	0.71
1:G:269:ARG:HB3	1:G:317:HIS:HB2	1.73	0.71
1:A:386:PRO:HD2	1:B:408:PHE:CE1	2.26	0.71
1:E:73:ASP:HA	1:E:76:LYS:HD3	1.73	0.71
1:H:265:PHE:HE2	1:H:437:GLU:HB3	1.56	0.71
1:G:118:SER:CB	1:G:146:LEU:HA	2.21	0.71
1:B:312:VAL:HG12	1:B:332:THR:HG22	1.73	0.70
1:C:376:THR:HG22	1:C:403:SER:HA	1.73	0.70
1:A:6:SER:O	1:A:39:LEU:HA	1.91	0.70
1:E:52:ASP:N	1:E:87:THR:HG1	1.89	0.70
1:G:40:ARG:HB3	1:G:84:PHE:CE2	2.26	0.70
1:H:462:TYR:HB2	1:H:466:THR:HG21	1.73	0.70
1:C:18:SER:HA	1:C:23:LEU:H	1.57	0.70
1:C:183:ASN:HB2	1:D:384:LYS:H	1.57	0.70
1:D:77:ALA:HA	1:D:80:LEU:HD12	1.74	0.70
1:F:70:ARG:HH21	1:F:415:ILE:HD12	1.56	0.70
1:H:203:ILE:HA	1:H:347:PHE:HA	1.73	0.70
1:A:165:SER:OG	1:A:167:LYS:NZ	2.24	0.70
1:D:7:THR:O	1:D:110:ILE:HA	1.92	0.70
1:C:210:VAL:HG11	1:C:232:MET:HE2	1.72	0.70
1:E:54:PHE:CD2	1:E:84:PHE:CA	2.61	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:LEU:O	1:F:233:VAL:HG22	1.91	0.70
1:C:190:GLY:HA2	1:D:362:LEU:HD11	1.73	0.69
1:E:166:GLU:HA	1:E:169:VAL:HG22	1.74	0.69
1:B:90:ILE:HA	1:B:96:PHE:CZ	2.27	0.69
1:B:170:TYR:CE2	1:B:429:ALA:HB2	2.27	0.69
1:E:340:ARG:HA	1:E:372:GLN:HB3	1.73	0.69
1:F:114:LEU:HD22	1:F:140:LEU:HD11	1.73	0.69
1:D:302:LEU:HD22	1:D:306:SER:HB2	1.73	0.69
1:A:118:SER:HA	1:A:121:PHE:CD2	2.28	0.69
1:B:97:GLY:HA2	1:B:131:ALA:CB	2.21	0.69
1:E:22:LEU:HD23	1:E:421:LEU:HD11	1.73	0.69
1:A:204:ASP:OD2	1:A:346:GLN:NE2	2.25	0.69
1:H:375:GLU:HB3	1:H:404:LEU:HB2	1.74	0.69
1:B:143:GLU:HB3	1:B:145:PRO:HD2	1.72	0.69
1:D:339:ARG:O	1:D:373:PRO:HD3	1.92	0.69
1:E:165:SER:O	1:E:169:VAL:HG13	1.93	0.69
1:B:422:LEU:O	1:B:426:GLU:HG2	1.93	0.69
1:B:29:LEU:HD22	1:B:422:LEU:HD13	1.75	0.69
1:F:281:VAL:HB	1:F:313:ALA:HB3	1.73	0.68
1:E:63:ASP:HA	1:E:71:LEU:HD21	1.74	0.68
1:F:275:THR:HG22	1:F:279:HIS:CD2	2.25	0.68
1:E:197:LEU:HD11	1:F:193:LEU:HA	1.73	0.68
1:E:213:THR:HG23	1:E:336:LEU:O	1.94	0.68
1:E:283:GLY:HA2	1:E:460:LYS:O	1.93	0.68
1:H:7:THR:OG1	1:H:104:GLY:HA3	1.93	0.68
1:H:169:VAL:C	1:H:170:TYR:HD1	2.01	0.68
1:H:339:ARG:O	1:H:373:PRO:HD3	1.93	0.68
1:B:197:LEU:HB3	1:B:347:PHE:CE1	2.28	0.68
1:A:435:ARG:O	1:A:439:GLU:HG2	1.94	0.68
1:F:9:ILE:HA	1:F:42:VAL:HB	1.76	0.68
1:H:476:VAL:HG13	1:H:481:VAL:O	1.94	0.68
1:G:341:SER:H	1:G:373:PRO:HD3	1.59	0.67
1:B:29:LEU:HB3	1:B:35:LEU:HG	1.75	0.67
1:G:197:LEU:O	1:G:202:GLY:HA3	1.94	0.67
1:B:215:GLY:N	1:B:335:ARG:HD2	2.10	0.67
1:E:166:GLU:O	1:E:169:VAL:HG22	1.94	0.67
1:A:26:LEU:HA	1:A:29:LEU:HD12	1.77	0.67
1:B:170:TYR:HB3	1:B:432:PHE:CD2	2.30	0.67
1:G:203:ILE:HA	1:G:347:PHE:HA	1.77	0.67
1:A:146:LEU:O	1:A:153:SER:HB3	1.95	0.67
1:A:17:LEU:HB2	2:A:501:NMN:O7	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:LEU:HB3	1:H:121:PHE:CE1	2.30	0.66
1:A:143:GLU:HG3	2:A:501:NMN:O4R	1.95	0.66
1:D:18:SER:HA	1:D:22:LEU:HB2	1.75	0.66
1:F:245:ALA:HA	1:F:323:TRP:CZ2	2.30	0.66
1:H:156:ILE:O	1:H:160:VAL:HG23	1.95	0.66
1:G:37:ASP:HA	1:G:82:LYS:HE2	1.77	0.66
1:E:56:ASP:O	1:E:59:GLU:N	2.28	0.66
1:C:183:ASN:OD1	1:D:383:VAL:HG23	1.95	0.66
1:A:224:ASP:O	1:A:308:THR:HG21	1.96	0.66
1:E:265:PHE:HA	1:E:268:LEU:HD12	1.76	0.66
1:A:55:ARG:HB3	1:A:80:LEU:CD2	2.26	0.66
1:E:341:SER:H	1:E:372:GLN:HB3	1.60	0.66
1:G:11:PHE:CZ	1:G:128:LEU:HD21	2.30	0.66
1:B:27:TYR:CD2	1:B:66:VAL:HG21	2.31	0.66
1:F:200:SER:HA	1:F:326:VAL:HG21	1.78	0.65
1:H:169:VAL:HG11	1:H:171:ARG:CZ	2.26	0.65
1:A:140:LEU:HD12	1:A:164:PHE:CD2	2.31	0.65
1:A:207:GLN:HG2	1:A:329:TYR:HB2	1.78	0.65
1:F:112:ILE:HB	1:F:140:LEU:HD23	1.78	0.65
1:G:259:ASP:OD1	1:G:434:ARG:NH1	2.29	0.65
1:A:387:GLY:HA3	1:A:394:HIS:CE1	2.30	0.65
1:B:13:SER:HA	1:B:18:SER:CB	2.27	0.65
1:G:18:SER:HA	1:G:22:LEU:CB	2.24	0.65
1:H:216:LEU:HD22	1:H:223:PHE:CB	2.27	0.65
1:G:25:ALA:HB1	1:G:418:GLU:HG3	1.77	0.65
1:A:411:ARG:CD	1:B:386:PRO:HD2	2.27	0.65
1:E:122:GLU:HA	1:E:125:ILE:HD12	1.77	0.65
1:A:423:ASP:O	1:A:427:GLY:N	2.30	0.65
1:B:265:PHE:CE2	1:B:437:GLU:HG2	2.32	0.65
1:D:117:SER:H	1:D:120:LEU:HD12	1.61	0.65
1:E:110:ILE:O	1:E:138:SER:HA	1.97	0.65
1:A:115:ALA:O	2:A:501:NMN:H4RC	1.97	0.65
1:A:246:MET:HE3	1:A:260:GLU:HB2	1.79	0.65
1:C:25:ALA:HB2	1:C:415:ILE:HD12	1.77	0.65
1:F:9:ILE:HB	1:F:112:ILE:HA	1.79	0.65
1:A:419:ARG:O	1:A:422:LEU:HD23	1.97	0.65
1:A:450:GLU:HA	1:A:453:LYS:HD2	1.76	0.65
1:E:21:MET:O	1:E:22:LEU:HB2	1.97	0.65
1:B:237:ILE:HG21	1:B:330:ILE:HG23	1.80	0.64
1:D:378:GLN:HB2	1:D:399:TRP:CE3	2.32	0.64
1:C:277:ILE:HG23	1:C:278:THR:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASN:HB3	1:B:139:ARG:HH21	1.62	0.64
1:B:337:PRO:HD3	1:B:467:TRP:H	1.62	0.64
1:C:7:THR:O	1:C:110:ILE:HA	1.98	0.64
1:D:233:VAL:HA	1:D:237:ILE:HB	1.80	0.64
1:E:113:TYR:HA	1:E:141:ALA:HB3	1.77	0.64
1:C:282:THR:O	1:C:469:PRO:HG3	1.97	0.64
1:D:40:ARG:NH1	1:D:102:LEU:O	2.30	0.64
1:F:128:LEU:O	1:F:133:LEU:HB3	1.97	0.64
1:H:80:LEU:HA	1:H:83:LEU:HD12	1.78	0.64
1:F:128:LEU:HA	1:F:131:ALA:HB3	1.78	0.64
1:B:5:VAL:HA	1:B:109:GLY:H	1.63	0.64
1:B:229:LEU:HB2	1:B:312:VAL:HG21	1.79	0.64
1:E:281:VAL:HG11	1:E:472:ALA:HB2	1.80	0.64
1:F:58:ALA:O	1:F:62:LEU:HB2	1.97	0.64
1:H:29:LEU:HA	1:H:34:LEU:HD12	1.80	0.64
1:B:161:LEU:HD21	1:B:435:ARG:HE	1.63	0.64
1:E:340:ARG:HG2	1:E:372:GLN:CG	2.28	0.64
1:B:112:ILE:HD11	1:B:138:SER:HB3	1.79	0.63
1:B:449:ARG:HA	1:B:452:TRP:CE2	2.34	0.63
1:C:462:TYR:CD1	1:C:468:GLY:HA2	2.34	0.63
1:D:262:VAL:HG22	1:D:437:GLU:HG3	1.80	0.63
1:F:161:LEU:HG	1:F:166:GLU:HB2	1.79	0.63
1:G:166:GLU:HA	1:G:169:VAL:HG22	1.80	0.63
1:G:389:ASP:H	1:H:419:ARG:NH2	1.95	0.63
1:E:370:VAL:HB	1:E:372:GLN:CG	2.29	0.63
1:H:255:ASN:HA	1:H:434:ARG:NH1	2.13	0.63
1:H:277:ILE:HG23	1:H:278:THR:HG23	1.81	0.63
1:E:372:GLN:HB2	1:E:373:PRO:HD2	1.79	0.63
1:G:112:ILE:HG13	1:G:139:ARG:O	1.98	0.63
1:D:462:TYR:HB2	1:D:466:THR:CG2	2.28	0.63
1:H:254:ALA:HB2	1:H:430:THR:HB	1.80	0.63
1:E:92:ASP:HB2	1:E:95:GLN:CD	2.23	0.63
1:E:372:GLN:NE2	1:E:374:ASP:OD2	2.29	0.63
1:E:462:TYR:HD2	1:E:466:THR:HG22	1.64	0.63
1:G:408:PHE:CE1	1:H:385:GLU:HG2	2.33	0.63
1:B:70:ARG:NH1	1:B:414:ARG:HB2	2.14	0.63
1:F:419:ARG:HE	1:F:431:LEU:HD11	1.62	0.63
1:A:24:PRO:HB3	1:A:66:VAL:HG22	1.80	0.63
1:G:167:LYS:HG3	1:G:168:GLN:HG3	1.81	0.63
1:H:204:ASP:HB3	1:H:346:GLN:HE21	1.64	0.63
1:A:342:GLU:OE2	1:A:368:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ASP:H	1:B:419:ARG:NH1	1.97	0.62
1:G:143:GLU:OE1	2:G:501:NMN:HC6	1.98	0.62
1:G:203:ILE:HG23	1:G:347:PHE:CD1	2.33	0.62
1:A:434:ARG:HB3	1:A:436:ASP:OD1	1.98	0.62
1:B:29:LEU:HD21	1:B:418:GLU:HB2	1.81	0.62
1:B:382:MET:HA	1:B:397:GLU:HA	1.81	0.62
1:C:121:PHE:O	1:C:125:ILE:N	2.28	0.62
1:H:462:TYR:HB2	1:H:466:THR:CG2	2.29	0.62
1:B:118:SER:HA	1:B:121:PHE:CD2	2.35	0.62
1:E:26:LEU:HB3	1:E:79:PHE:CE1	2.34	0.62
1:G:245:ALA:HA	1:G:323:TRP:CZ2	2.34	0.62
1:G:402:LEU:HB3	1:H:400:LEU:HD23	1.81	0.62
1:C:111:ALA:HB1	1:C:139:ARG:CB	2.29	0.62
1:C:438:VAL:HA	1:C:441:GLN:HE21	1.65	0.62
1:F:62:LEU:O	1:F:66:VAL:HB	1.99	0.62
1:F:398:VAL:HG22	1:F:399:TRP:H	1.64	0.62
1:G:139:ARG:HD3	1:G:170:TYR:CZ	2.35	0.62
1:H:75:ALA:HA	1:H:78:LYS:HD2	1.81	0.62
1:H:175:TYR:CD2	1:H:236:HIS:HB3	2.35	0.62
1:A:29:LEU:HA	1:A:34:LEU:HD12	1.82	0.62
1:E:273:ASN:HA	1:E:451:GLY:HA2	1.82	0.62
1:G:118:SER:HB3	1:G:146:LEU:HA	1.80	0.62
1:H:55:ARG:HB3	1:H:80:LEU:HG	1.81	0.62
1:B:202:GLY:O	1:B:347:PHE:HD1	1.83	0.62
1:E:277:ILE:HD11	1:E:455:ASN:CB	2.30	0.62
1:H:170:TYR:HE2	1:H:424:LEU:HA	1.64	0.62
1:A:226:SER:HB2	1:A:230:ARG:HB2	1.81	0.62
1:A:164:PHE:HD1	1:A:168:GLN:OE1	1.82	0.61
1:A:425:ILE:HG12	1:A:426:GLU:N	2.15	0.61
1:B:19:GLN:HE21	1:B:20:ARG:HG3	1.63	0.61
1:B:27:TYR:CE2	1:B:66:VAL:HG21	2.35	0.61
1:D:462:TYR:HB2	1:D:466:THR:HG21	1.82	0.61
1:G:422:LEU:O	1:G:426:GLU:HG3	1.98	0.61
1:B:226:SER:HA	1:B:230:ARG:HE	1.64	0.61
1:C:265:PHE:HE2	1:C:437:GLU:HG2	1.65	0.61
1:G:388:LEU:HD22	1:H:419:ARG:HD3	1.82	0.61
1:A:448:ILE:HD11	1:A:452:TRP:CZ2	2.35	0.61
1:B:209:SER:O	1:B:341:SER:HA	2.01	0.61
1:C:194:PHE:HB3	1:C:198:TRP:CZ3	2.35	0.61
1:E:419:ARG:HD2	1:F:388:LEU:HA	1.82	0.61
1:G:125:ILE:HA	1:G:128:LEU:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:386:PRO:HG3	1:H:408:PHE:HB3	1.81	0.61
1:H:224:ASP:O	1:H:308:THR:HG21	2.00	0.61
1:H:406:ASP:HA	1:H:409:LYS:HD2	1.81	0.61
1:B:180:THR:HG21	1:B:371:LEU:HA	1.82	0.61
1:F:27:TYR:HB2	1:F:79:PHE:CE2	2.36	0.61
1:F:269:ARG:NH2	1:F:319:ASP:OD1	2.33	0.61
1:D:283:GLY:HA2	1:D:460:LYS:O	2.00	0.61
1:E:66:VAL:HG13	1:E:71:LEU:HD22	1.81	0.61
1:D:143:GLU:HG2	1:D:172:ILE:HG23	1.81	0.61
1:H:112:ILE:N	1:H:139:ARG:O	2.23	0.61
1:H:210:VAL:HB	1:H:237:ILE:HD11	1.82	0.61
1:E:415:ILE:O	1:E:418:GLU:HB2	1.99	0.61
1:H:45:SER:O	1:H:46:ARG:HB3	2.00	0.61
1:D:209:SER:HA	1:D:331:ARG:O	2.00	0.61
1:F:282:THR:O	1:F:469:PRO:HG3	2.00	0.61
1:G:370:VAL:CG1	1:G:373:PRO:HG2	2.31	0.61
1:B:198:TRP:CH2	1:B:367:LEU:HD23	2.30	0.61
1:F:229:LEU:HD13	1:F:312:VAL:HG21	1.83	0.61
1:A:175:TYR:HA	1:A:178:LYS:HD2	1.82	0.61
1:C:200:SER:HA	1:C:326:VAL:CG2	2.31	0.61
1:C:284:GLN:HG3	1:C:310:THR:HG23	1.82	0.61
1:E:452:TRP:O	1:E:456:SER:N	2.34	0.61
1:H:170:TYR:HB3	1:H:432:PHE:CD1	2.36	0.61
1:D:213:THR:HG22	1:D:336:LEU:O	2.01	0.60
1:E:12:GLY:HA2	1:E:46:ARG:CG	2.30	0.60
1:E:193:LEU:HD23	1:E:193:LEU:H	1.65	0.60
1:E:246:MET:HE1	1:E:249:PRO:HD3	1.82	0.60
1:G:139:ARG:HA	1:G:168:GLN:O	2.01	0.60
1:B:349:PRO:HG3	1:B:364:PRO:HG3	1.83	0.60
1:H:71:LEU:HD21	1:H:76:LYS:HD3	1.83	0.60
1:H:99:ILE:HB	1:H:133:LEU:CD1	2.31	0.60
1:H:295:VAL:HB	1:H:335:ARG:NH2	2.15	0.60
1:B:246:MET:HA	1:B:264:VAL:HG21	1.83	0.60
1:H:170:TYR:CE2	1:H:424:LEU:HA	2.36	0.60
1:H:460:LYS:HD3	1:H:471:THR:HG23	1.83	0.60
1:A:54:PHE:O	1:A:57:PHE:N	2.34	0.60
1:A:122:GLU:HA	1:A:125:ILE:HD12	1.82	0.60
1:C:479:ASP:HB2	1:C:481:VAL:HG12	1.84	0.60
1:A:90:ILE:HA	1:A:96:PHE:CZ	2.37	0.60
1:C:311:PHE:CD1	1:C:469:PRO:HD2	2.37	0.60
1:H:195:GLU:OE2	1:H:322:ARG:NH1	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PRO:O	1:B:27:TYR:HB3	2.01	0.60
1:F:41:ILE:HB	1:F:83:LEU:HA	1.84	0.60
1:G:11:PHE:HZ	1:G:128:LEU:HD21	1.66	0.60
1:G:26:LEU:HA	1:G:29:LEU:HD12	1.83	0.60
1:G:18:SER:CA	1:G:22:LEU:HB2	2.27	0.60
1:A:40:ARG:CB	1:A:84:PHE:HE2	2.15	0.60
1:A:176:LEU:HD11	1:A:239:GLN:OE1	2.01	0.60
1:D:5:VAL:HG11	1:D:111:ALA:HB2	1.82	0.60
1:E:135:GLY:HA2	1:E:138:SER:HB2	1.83	0.60
1:B:125:ILE:HG23	1:B:163:VAL:HG11	1.82	0.60
1:F:378:GLN:HA	1:F:400:LEU:O	2.02	0.60
1:G:122:GLU:OE1	1:G:155:HIS:NE2	2.35	0.60
1:H:114:LEU:HB3	1:H:121:PHE:HE1	1.66	0.60
1:B:377:ILE:HD12	1:B:404:LEU:HD21	1.82	0.60
1:D:289:VAL:HA	1:D:294:GLU:HA	1.84	0.60
1:B:339:ARG:O	1:B:373:PRO:HD3	2.01	0.59
1:D:172:ILE:HD11	1:D:420:LEU:HD13	1.83	0.59
1:F:216:LEU:HD13	1:F:220:ILE:HG23	1.83	0.59
1:F:67:ALA:HB3	1:F:70:ARG:HG3	1.84	0.59
1:H:272:ASN:HB3	1:H:275:THR:HG23	1.83	0.59
1:A:283:GLY:HA2	1:A:460:LYS:O	2.02	0.59
1:B:451:GLY:O	1:B:455:ASN:HB2	2.02	0.59
1:F:340:ARG:HD2	1:F:368:ARG:NH2	2.16	0.59
1:D:118:SER:HA	1:D:121:PHE:CD2	2.36	0.59
1:E:135:GLY:HA3	1:E:138:SER:HB2	1.83	0.59
1:G:415:ILE:HG22	1:G:417:HIS:H	1.68	0.59
1:A:143:GLU:OE1	2:A:501:NMN:HC6	2.03	0.59
1:C:258:ARG:HD2	1:C:434:ARG:HB2	1.83	0.59
1:E:215:GLY:HA3	1:E:335:ARG:HH11	1.66	0.59
1:G:354:ILE:HG13	1:H:252:MET:HG2	1.84	0.59
1:F:246:MET:HE3	1:F:260:GLU:HB2	1.85	0.59
1:G:40:ARG:HB3	1:G:84:PHE:HE2	1.68	0.59
1:B:216:LEU:HD13	1:B:334:LYS:HE2	1.84	0.59
1:H:203:ILE:HG21	1:H:323:TRP:CZ3	2.38	0.59
1:C:462:TYR:CG	1:C:468:GLY:HA2	2.38	0.58
1:E:29:LEU:HD13	1:E:422:LEU:HG	1.84	0.58
1:A:96:PHE:CG	1:A:127:GLY:HA3	2.39	0.58
1:C:200:SER:N	1:C:322:ARG:O	2.37	0.58
1:H:213:THR:HA	1:H:336:LEU:O	2.03	0.58
1:A:76:LYS:C	1:A:80:LEU:HD12	2.28	0.58
1:A:237:ILE:HG21	1:A:330:ILE:HG23	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:ASP:OD2	1:D:79:PHE:HB2	2.03	0.58
1:E:56:ASP:O	1:E:57:PHE:C	2.46	0.58
1:A:150:LEU:HB2	1:A:442:TRP:HB3	1.86	0.58
1:H:129:LYS:HA	1:H:134:ALA:CB	2.33	0.58
1:H:216:LEU:CD2	1:H:223:PHE:HB2	2.32	0.58
1:A:309:GLU:C	1:A:311:PHE:H	2.11	0.58
1:D:282:THR:OG1	1:D:459:PRO:HA	2.02	0.58
1:E:322:ARG:HD2	1:E:323:TRP:NE1	2.19	0.58
1:F:216:LEU:HD11	1:F:285:TYR:HE2	1.68	0.58
1:H:265:PHE:CE2	1:H:437:GLU:HB3	2.39	0.58
1:D:116:THR:HB	1:D:120:LEU:HD12	1.86	0.58
1:G:191:ASN:HB3	1:H:365:ASN:HD21	1.69	0.58
1:A:156:ILE:O	1:A:160:VAL:HG23	2.03	0.58
1:A:372:GLN:HG2	1:A:373:PRO:HA	1.85	0.58
1:D:44:THR:HB	1:D:99:ILE:HD11	1.85	0.58
1:E:342:GLU:HB3	1:E:370:VAL:HG12	1.86	0.58
1:G:5:VAL:HA	1:G:425:ILE:O	2.04	0.58
1:A:229:LEU:O	1:A:233:VAL:HB	2.04	0.58
1:G:23:LEU:N	1:G:24:PRO:HD2	2.18	0.58
1:H:329:TYR:CE2	1:H:481:VAL:HG11	2.38	0.58
1:A:382:MET:HB2	1:B:191:ASN:OD1	2.03	0.58
1:B:93:PRO:HA	1:B:96:PHE:HD1	1.69	0.58
1:D:43:CYS:O	1:D:85:TYR:HA	2.04	0.58
1:E:18:SER:O	1:E:23:LEU:HB2	2.03	0.58
1:G:178:LYS:HB2	1:G:181:VAL:HG23	1.86	0.58
1:F:29:LEU:HG	1:F:418:GLU:HB3	1.85	0.57
1:A:198:TRP:HH2	1:A:367:LEU:HD23	1.68	0.57
1:A:385:GLU:HB2	1:A:396:ARG:HG3	1.86	0.57
1:D:30:ASP:CG	1:D:79:PHE:HB2	2.29	0.57
1:D:310:THR:O	1:D:333:GLY:HA2	2.04	0.57
1:E:346:GLN:HG2	1:E:364:PRO:HB2	1.86	0.57
1:F:133:LEU:HG	1:F:164:PHE:CZ	2.39	0.57
1:A:235:SER:O	1:A:239:GLN:HG2	2.04	0.57
1:B:171:ARG:NH1	1:B:434:ARG:HA	2.19	0.57
1:C:175:TYR:O	1:C:178:LYS:N	2.32	0.57
1:C:289:VAL:HA	1:C:294:GLU:HA	1.85	0.57
1:D:368:ARG:HB3	1:D:378:GLN:HG3	1.86	0.57
1:E:146:LEU:HD11	1:E:438:VAL:HG11	1.86	0.57
1:F:45:SER:O	1:F:46:ARG:C	2.46	0.57
1:G:44:THR:HB	1:G:86:ALA:O	2.04	0.57
1:C:154:ASP:HA	1:C:435:ARG:HH21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:MET:HA	1:E:111:ALA:O	2.03	0.57
1:E:54:PHE:CD2	1:E:85:TYR:N	2.71	0.57
1:F:96:PHE:CG	1:F:127:GLY:HA3	2.39	0.57
1:B:429:ALA:HA	1:B:432:PHE:HD1	1.70	0.57
1:E:40:ARG:HG3	1:E:105:PRO:CG	2.32	0.57
1:E:281:VAL:HG21	1:E:472:ALA:HA	1.85	0.57
1:C:341:SER:H	1:C:373:PRO:HG2	1.69	0.57
1:E:16:ASP:O	1:E:19:GLN:HG2	2.05	0.57
1:E:345:VAL:O	1:E:366:LYS:HA	2.04	0.57
1:A:383:VAL:HG21	1:B:404:LEU:HD11	1.87	0.57
1:C:188:ARG:HH22	1:C:322:ARG:HH12	1.53	0.57
1:D:37:ASP:N	1:D:37:ASP:OD1	2.35	0.57
1:F:286:GLY:O	1:F:297:GLY:HA2	2.05	0.57
1:H:41:ILE:HD13	1:H:79:PHE:HE1	1.70	0.57
1:H:176:LEU:HD12	1:H:431:LEU:O	2.05	0.57
1:H:271:ILE:HG21	1:H:276:VAL:HG23	1.85	0.57
1:B:215:GLY:CA	1:B:335:ARG:HD2	2.34	0.57
1:C:229:LEU:HD21	1:C:445:ILE:HG23	1.86	0.57
1:E:223:PHE:HZ	1:E:310:THR:HA	1.68	0.57
1:H:209:SER:O	1:H:341:SER:HA	2.04	0.57
1:C:184:LEU:O	1:C:188:ARG:N	2.31	0.57
1:C:200:SER:HA	1:C:326:VAL:HG23	1.87	0.57
1:D:25:ALA:HA	1:D:418:GLU:HG2	1.87	0.57
1:E:156:ILE:HG12	1:E:157:ASN:N	2.19	0.57
1:F:40:ARG:HA	1:F:84:PHE:HD2	1.70	0.57
1:H:230:ARG:HE	1:H:449:ARG:NE	2.02	0.57
1:E:69:ASP:OD1	1:E:70:ARG:HG3	2.04	0.56
1:E:306:SER:OG	1:E:308:THR:HG23	2.04	0.56
1:H:462:TYR:CD1	1:H:469:PRO:HD3	2.40	0.56
1:B:70:ARG:HH11	1:B:414:ARG:HB2	1.67	0.56
1:E:161:LEU:HA	1:E:164:PHE:O	2.04	0.56
1:E:417:HIS:HA	1:E:420:LEU:HB2	1.86	0.56
1:A:400:LEU:HB3	1:B:400:LEU:HB3	1.86	0.56
1:A:463:VAL:O	1:A:466:THR:HG22	2.06	0.56
1:B:20:ARG:HG2	1:B:65:PHE:CZ	2.40	0.56
1:D:247:GLU:HB2	1:D:260:GLU:OE1	2.05	0.56
1:E:334:LYS:O	1:E:462:TYR:OH	2.23	0.56
1:F:258:ARG:O	1:F:262:VAL:HG23	2.04	0.56
1:H:80:LEU:HD12	1:H:83:LEU:HD12	1.86	0.56
1:H:199:ASN:O	1:H:203:ILE:HG22	2.05	0.56
1:H:285:TYR:OH	1:H:301:GLU:OE1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ALA:O	1:E:314:ILE:HG13	2.05	0.56
1:F:70:ARG:HH22	1:F:418:GLU:CD	2.14	0.56
1:H:320:ASN:O	1:H:324:HIS:HB2	2.06	0.56
2:A:501:NMN:C5R	2:A:501:NMN:HC2	2.36	0.56
1:B:423:ASP:OD1	1:B:428:ASP:HB2	2.06	0.56
1:B:452:TRP:O	1:B:456:SER:N	2.39	0.56
1:C:286:GLY:C	1:C:297:GLY:HA2	2.29	0.56
1:C:412:LYS:C	1:C:414:ARG:H	2.13	0.56
1:D:282:THR:HB	1:D:459:PRO:HB3	1.86	0.56
1:G:142:LEU:HD12	1:G:171:ARG:HG2	1.86	0.56
1:H:153:SER:HA	1:H:156:ILE:HD12	1.88	0.56
1:H:475:LEU:HD12	1:H:478:ARG:HH21	1.70	0.56
1:A:188:ARG:NH1	1:A:243:LEU:O	2.38	0.56
1:C:75:ALA:O	1:C:79:PHE:N	2.33	0.56
1:D:129:LYS:HA	1:D:134:ALA:HB3	1.86	0.56
1:G:315:LYS:HE3	1:G:327:PRO:HB3	1.87	0.56
1:H:285:TYR:HD2	1:H:310:THR:HG21	1.71	0.56
1:A:152:SER:O	1:A:156:ILE:HG23	2.05	0.56
1:A:458:LYS:HE3	1:A:459:PRO:HD2	1.86	0.56
1:B:36:ALA:HB3	1:B:39:LEU:HD12	1.88	0.56
1:B:46:ARG:HG3	1:B:120:LEU:HD23	1.87	0.56
1:B:423:ASP:O	1:B:427:GLY:N	2.38	0.56
1:F:144:LYS:HG3	1:F:145:PRO:CD	2.32	0.56
1:F:302:LEU:HG	1:F:303:GLY:H	1.71	0.56
1:H:349:PRO:HG3	1:H:364:PRO:HG3	1.87	0.56
1:A:212:GLU:O	1:A:336:LEU:N	2.35	0.56
1:B:216:LEU:HB3	1:B:219:ARG:HG3	1.86	0.56
1:C:423:ASP:HB3	1:C:430:THR:HG23	1.88	0.56
1:G:272:ASN:HB2	1:G:275:THR:HG23	1.88	0.56
1:G:370:VAL:HG12	1:G:373:PRO:HG2	1.86	0.56
1:E:160:VAL:HG12	1:E:161:LEU:HD12	1.86	0.56
1:A:366:LYS:HB2	1:A:380:SER:OG	2.06	0.56
1:B:9:ILE:HB	1:B:112:ILE:HA	1.88	0.56
1:B:229:LEU:HD23	1:B:230:ARG:HG2	1.87	0.56
1:B:298:TYR:HE2	1:B:308:THR:HB	1.71	0.56
1:D:55:ARG:HD3	1:D:80:LEU:O	2.06	0.56
1:D:202:GLY:O	1:D:347:PHE:HD1	1.89	0.56
1:B:237:ILE:HA	1:B:240:LEU:HD12	1.88	0.55
1:D:197:LEU:O	1:D:203:ILE:HG13	2.06	0.55
1:F:255:ASN:HA	1:F:258:ARG:HB2	1.88	0.55
1:G:378:GLN:HG3	1:G:399:TRP:CE3	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:474:ALA:O	1:G:478:ARG:HG2	2.05	0.55
1:H:175:TYR:CD1	1:H:236:HIS:HD2	2.24	0.55
1:E:8:MET:HG3	1:E:9:ILE:N	2.18	0.55
1:E:90:ILE:HG13	1:E:120:LEU:HD23	1.88	0.55
1:H:216:LEU:HB2	1:H:220:ILE:HG23	1.88	0.55
1:C:148:GLN:H	1:C:152:SER:CB	2.18	0.55
1:F:10:LEU:HD12	1:F:11:PHE:H	1.72	0.55
1:H:5:VAL:HG13	1:H:109:GLY:C	2.31	0.55
1:H:340:ARG:HA	1:H:373:PRO:HD3	1.87	0.55
1:A:183:ASN:O	1:A:184:LEU:C	2.49	0.55
1:B:105:PRO:HG2	1:B:108:LYS:CB	2.36	0.55
1:B:193:LEU:HG	1:B:194:PHE:N	2.20	0.55
1:B:313:ALA:HA	1:B:330:ILE:O	2.06	0.55
1:D:128:LEU:HG	1:D:133:LEU:HD12	1.87	0.55
1:D:463:VAL:O	1:D:466:THR:HB	2.07	0.55
1:E:472:ALA:O	1:E:474:ALA:N	2.39	0.55
1:G:26:LEU:HD21	1:G:421:LEU:HD22	1.88	0.55
1:B:5:VAL:HG22	1:B:109:GLY:CA	2.36	0.55
1:D:7:THR:HB	1:D:109:GLY:O	2.07	0.55
1:E:366:LYS:H	1:E:380:SER:HB2	1.70	0.55
1:A:76:LYS:O	1:A:80:LEU:HD12	2.07	0.55
1:A:262:VAL:HG22	1:A:437:GLU:HG3	1.88	0.55
1:D:309:GLU:HB3	1:D:311:PHE:O	2.06	0.55
1:E:112:ILE:HD11	1:E:138:SER:HB3	1.88	0.55
1:E:125:ILE:HA	1:E:128:LEU:HD12	1.89	0.55
1:F:11:PHE:HA	1:F:44:THR:HB	1.87	0.55
1:G:186:THR:HA	1:H:355:PHE:CZ	2.41	0.55
1:C:381:ILE:CD1	1:C:400:LEU:HG	2.37	0.55
1:D:403:SER:O	1:D:407:VAL:HG23	2.05	0.55
1:F:184:LEU:O	1:F:187:LEU:HB3	2.06	0.55
1:F:353:SER:HB3	1:F:356:SER:HB3	1.89	0.55
1:F:473:ILE:O	1:F:476:VAL:HG12	2.06	0.55
1:G:144:LYS:HD3	1:G:236:HIS:CE1	2.41	0.55
1:H:337:PRO:HG2	1:H:467:TRP:CG	2.41	0.55
1:A:144:LYS:CE	2:A:501:NMN:C5	2.76	0.55
1:B:125:ILE:CG2	1:B:163:VAL:HG21	2.36	0.55
1:E:364:PRO:O	1:E:366:LYS:NZ	2.37	0.55
1:G:355:PHE:CG	1:G:395:MET:HE1	2.42	0.55
1:H:136:PRO:O	1:H:137:THR:HG22	2.07	0.55
1:H:139:ARG:NH2	1:H:427:GLY:HA3	2.22	0.55
1:C:340:ARG:HA	1:C:373:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:GLN:NE2	1:E:441:GLN:HE22	2.05	0.55
1:E:285:TYR:CD1	1:E:335:ARG:HG3	2.42	0.55
1:G:388:LEU:HA	1:H:419:ARG:NE	2.17	0.55
1:A:55:ARG:HB3	1:A:80:LEU:HD22	1.89	0.55
1:A:180:THR:HG21	1:A:371:LEU:HA	1.89	0.55
1:B:117:SER:HB3	1:B:120:LEU:HD22	1.88	0.55
1:B:66:VAL:HG11	1:B:71:LEU:HD13	1.88	0.54
1:B:135:GLY:C	1:B:137:THR:N	2.61	0.54
1:E:135:GLY:N	1:E:136:PRO:HD3	2.22	0.54
1:G:118:SER:HB2	1:G:146:LEU:HA	1.89	0.54
1:G:337:PRO:HD2	1:G:467:TRP:CD2	2.42	0.54
1:H:219:ARG:HB3	1:H:222:TYR:HD1	1.71	0.54
1:B:51:THR:C	1:B:53:GLY:H	2.15	0.54
1:B:135:GLY:H	1:B:138:SER:HB2	1.72	0.54
1:B:148:GLN:HB3	1:B:230:ARG:CZ	2.37	0.54
1:E:419:ARG:HB2	1:F:388:LEU:HD22	1.88	0.54
1:A:345:VAL:O	1:A:366:LYS:HA	2.07	0.54
1:C:265:PHE:CE2	1:C:437:GLU:HG2	2.42	0.54
1:D:156:ILE:O	1:D:160:VAL:HG23	2.07	0.54
1:D:219:ARG:O	1:D:223:PHE:N	2.39	0.54
1:D:232:MET:O	1:D:236:HIS:HB2	2.07	0.54
1:D:435:ARG:O	1:D:439:GLU:HG2	2.07	0.54
1:G:283:GLY:HA2	1:G:460:LYS:O	2.06	0.54
1:A:29:LEU:HG	1:A:418:GLU:HG2	1.90	0.54
1:A:202:GLY:C	1:A:348:LYS:H	2.16	0.54
1:E:209:SER:HB2	1:E:342:GLU:HG3	1.88	0.54
1:F:128:LEU:HB3	1:F:133:LEU:CB	2.38	0.54
1:F:212:GLU:HA	1:F:339:ARG:HA	1.89	0.54
1:A:268:LEU:HD21	1:A:316:ALA:HB1	1.89	0.54
1:E:419:ARG:O	1:E:419:ARG:HG3	2.06	0.54
1:H:46:ARG:O	1:H:46:ARG:HG3	2.06	0.54
1:B:198:TRP:HA	1:B:203:ILE:HD11	1.90	0.54
1:C:278:THR:OG1	1:C:279:HIS:ND1	2.40	0.54
1:D:253:GLU:HB2	1:D:256:ALA:HB3	1.90	0.54
1:E:56:ASP:O	1:E:58:ALA:N	2.41	0.54
1:F:204:ASP:HB3	1:F:346:GLN:HG2	1.89	0.54
1:G:203:ILE:HG22	1:G:346:GLN:O	2.07	0.54
1:A:148:GLN:HG2	1:A:149:ASP:N	2.23	0.54
1:A:352:HIS:HB3	1:D:321:TRP:HA	1.89	0.54
1:E:171:ARG:HD3	1:E:438:VAL:HG21	1.90	0.54
1:F:311:PHE:CZ	1:F:313:ALA:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HB2	2:A:501:NMN:C7	2.38	0.54
1:A:140:LEU:HD12	1:A:164:PHE:HD2	1.72	0.54
1:C:7:THR:HA	1:C:40:ARG:O	2.08	0.54
1:C:246:MET:HE3	1:C:260:GLU:HB2	1.89	0.54
1:C:319:ASP:HB3	1:C:324:HIS:ND1	2.22	0.54
1:D:112:ILE:HD13	1:D:128:LEU:CD2	2.37	0.54
1:E:183:ASN:O	1:E:184:LEU:C	2.51	0.54
1:F:337:PRO:HG2	1:F:467:TRP:CD1	2.42	0.54
1:G:236:HIS:O	1:G:240:LEU:HD13	2.07	0.54
1:H:207:GLN:HG2	1:H:329:TYR:HB2	1.90	0.54
1:B:3:ASN:HB2	1:B:5:VAL:HG23	1.89	0.54
1:B:5:VAL:HA	1:B:109:GLY:N	2.22	0.54
1:D:61:ALA:HA	1:D:64:ARG:HG2	1.89	0.54
1:E:161:LEU:HG	1:E:164:PHE:O	2.08	0.54
1:E:164:PHE:HD2	1:E:168:GLN:HB2	1.72	0.54
1:F:8:MET:HG2	1:F:41:ILE:HG23	1.90	0.54
1:F:240:LEU:O	1:F:244:VAL:HG23	2.08	0.54
1:F:415:ILE:HG22	1:F:417:HIS:H	1.73	0.54
1:A:195:GLU:HA	1:A:198:TRP:HB2	1.90	0.54
1:B:161:LEU:CD2	1:B:435:ARG:HE	2.21	0.54
1:B:228:SER:H	1:B:309:GLU:HG2	1.72	0.54
1:A:143:GLU:HG3	2:A:501:NMN:C1R	2.38	0.53
1:A:386:PRO:HD2	1:B:408:PHE:CD1	2.43	0.53
1:D:224:ASP:O	1:D:308:THR:HG21	2.08	0.53
1:E:54:PHE:CE2	1:E:85:TYR:N	2.76	0.53
1:F:210:VAL:O	1:F:332:THR:HA	2.07	0.53
1:G:93:PRO:O	1:G:96:PHE:HB2	2.08	0.53
1:H:203:ILE:HD13	1:H:323:TRP:CZ3	2.43	0.53
1:A:17:LEU:CD2	2:A:501:NMN:H5R2	2.35	0.53
1:A:90:ILE:H	1:A:90:ILE:HD13	1.72	0.53
1:A:351:PRO:HD2	1:D:321:TRP:CZ2	2.43	0.53
1:E:189:PHE:CE2	1:E:246:MET:HE2	2.41	0.53
1:E:475:LEU:HG	1:E:478:ARG:HH21	1.73	0.53
1:F:112:ILE:HD12	1:F:139:ARG:C	2.34	0.53
1:G:9:ILE:HG23	1:G:42:VAL:HB	1.90	0.53
1:H:42:VAL:HA	1:H:84:PHE:O	2.07	0.53
1:A:143:GLU:OE1	2:A:501:NMN:C6	2.55	0.53
1:B:58:ALA:O	1:B:62:LEU:N	2.34	0.53
1:C:354:ILE:O	1:D:252:MET:HG2	2.08	0.53
1:D:226:SER:O	1:D:230:ARG:HB2	2.08	0.53
1:E:377:ILE:C	1:E:378:GLN:HG3	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:TYR:HD1	1:F:79:PHE:CD2	2.26	0.53
1:F:142:LEU:N	1:F:170:TYR:O	2.42	0.53
1:G:146:LEU:HD23	1:G:146:LEU:H	1.73	0.53
1:H:336:LEU:HD22	1:H:467:TRP:CE3	2.43	0.53
1:A:475:LEU:HD12	1:A:478:ARG:HH21	1.71	0.53
1:C:58:ALA:O	1:C:62:LEU:N	2.36	0.53
1:C:86:ALA:O	1:C:87:THR:C	2.50	0.53
1:C:378:GLN:HA	1:C:400:LEU:O	2.09	0.53
1:D:336:LEU:HD13	1:D:467:TRP:CZ3	2.44	0.53
1:E:30:ASP:O	1:E:33:GLY:N	2.35	0.53
1:G:208:ILE:HG23	1:G:343:ILE:HG12	1.89	0.53
1:G:434:ARG:HH21	1:G:436:ASP:CG	2.15	0.53
1:H:479:ASP:HB2	1:H:481:VAL:HG12	1.91	0.53
1:C:259:ASP:OD1	1:C:434:ARG:NH2	2.34	0.53
1:E:370:VAL:HG22	1:E:376:THR:O	2.09	0.53
1:G:284:GLN:HA	1:G:309:GLU:O	2.09	0.53
1:D:49:TYR:CD2	1:D:54:PHE:HA	2.43	0.53
1:D:175:TYR:O	1:D:176:LEU:HB2	2.09	0.53
1:D:254:ALA:O	1:D:258:ARG:HG3	2.09	0.53
1:B:283:GLY:O	1:B:309:GLU:HA	2.09	0.53
1:B:287:ALA:O	1:B:463:VAL:HG23	2.09	0.53
1:E:6:SER:HA	1:E:109:GLY:O	2.08	0.53
1:F:128:LEU:HB3	1:F:133:LEU:HD13	1.90	0.53
1:F:289:VAL:HA	1:F:294:GLU:HA	1.90	0.53
2:A:501:NMN:HC2	2:A:501:NMN:H5R1	1.90	0.53
1:C:197:LEU:HD21	1:D:193:LEU:HA	1.91	0.53
1:F:27:TYR:HB2	1:F:62:LEU:HD21	1.91	0.53
1:F:27:TYR:CE2	1:F:71:LEU:HA	2.43	0.53
1:G:118:SER:CB	1:G:147:GLY:H	2.22	0.53
1:C:436:ASP:HA	1:C:439:GLU:OE2	2.08	0.53
1:E:161:LEU:HD21	1:E:166:GLU:HB2	1.90	0.53
1:F:188:ARG:NH2	1:F:322:ARG:HH12	2.07	0.53
1:A:401:ASP:O	1:B:400:LEU:HA	2.09	0.53
1:D:205:HIS:CD2	1:D:481:VAL:HG21	2.44	0.53
1:G:434:ARG:NH2	1:G:436:ASP:OD2	2.35	0.53
1:H:203:ILE:HD13	1:H:323:TRP:HZ3	1.74	0.53
1:A:128:LEU:HB3	1:A:133:LEU:HB2	1.91	0.52
1:A:242:ALA:O	1:A:246:MET:HB3	2.09	0.52
1:B:222:TYR:OH	2:B:501:NMN:H2RC	2.09	0.52
1:C:129:LYS:CB	1:C:134:ALA:HB2	2.39	0.52
1:E:40:ARG:HG3	1:E:105:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:LEU:HD23	1:F:304:GLN:O	2.09	0.52
1:A:205:HIS:NE2	1:A:481:VAL:HG23	2.24	0.52
1:B:462:TYR:CD2	1:B:469:PRO:HD3	2.44	0.52
1:C:466:THR:OG1	1:C:467:TRP:N	2.40	0.52
1:F:415:ILE:N	1:F:418:GLU:OE1	2.43	0.52
1:H:167:LYS:O	1:H:170:TYR:HE1	1.91	0.52
1:A:93:PRO:HA	1:A:96:PHE:CD1	2.44	0.52
1:A:134:ALA:HA	1:A:164:PHE:CZ	2.43	0.52
1:B:70:ARG:HD2	1:B:414:ARG:HE	1.75	0.52
1:B:144:LYS:CE	2:B:501:NMN:HC6	2.27	0.52
1:H:175:TYR:CE1	1:H:236:HIS:HD2	2.27	0.52
1:A:242:ALA:HA	1:A:264:VAL:HG11	1.91	0.52
1:B:166:GLU:CD	1:B:171:ARG:HH22	2.17	0.52
1:B:307:ASP:OD2	1:B:458:LYS:HD2	2.10	0.52
1:D:67:ALA:HB3	1:D:70:ARG:HG2	1.91	0.52
1:A:386:PRO:HG2	1:B:411:ARG:HG3	1.90	0.52
1:G:100:ALA:O	1:G:103:CYS:HB2	2.10	0.52
1:G:233:VAL:HG22	1:G:237:ILE:HD12	1.91	0.52
1:A:55:ARG:HB3	1:A:80:LEU:HD23	1.91	0.52
1:B:378:GLN:HB2	1:B:399:TRP:CE3	2.45	0.52
1:D:113:TYR:OH	1:D:143:GLU:HB2	2.10	0.52
1:E:313:ALA:C	1:E:314:ILE:HG13	2.33	0.52
1:F:150:LEU:HD22	1:F:443:ILE:HD13	1.91	0.52
1:F:245:ALA:HA	1:F:323:TRP:HZ2	1.72	0.52
1:G:79:PHE:O	1:G:83:LEU:HD13	2.09	0.52
1:H:7:THR:O	1:H:110:ILE:HA	2.09	0.52
1:H:172:ILE:HG23	1:H:420:LEU:HD13	1.91	0.52
1:H:202:GLY:O	1:H:347:PHE:HD1	1.93	0.52
1:A:48:GLU:HB3	1:A:49:TYR:CE1	2.44	0.52
1:E:177:GLY:HA3	1:E:420:LEU:HD21	1.92	0.52
1:F:322:ARG:HD2	1:F:323:TRP:NE1	2.24	0.52
1:A:183:ASN:O	1:A:186:THR:N	2.42	0.52
1:A:320:ASN:HD21	1:A:323:TRP:HD1	1.55	0.52
1:G:327:PRO:HB2	1:G:329:TYR:CE2	2.45	0.52
1:D:142:LEU:O	1:D:172:ILE:HG22	2.10	0.52
1:F:484:TYR:OH	1:F:486:LEU:HD23	2.10	0.52
1:A:242:ALA:HB2	1:A:265:PHE:CE1	2.45	0.52
1:D:287:ALA:O	1:D:463:VAL:HG13	2.10	0.52
1:F:476:VAL:HG13	1:F:477:GLU:N	2.24	0.52
1:G:5:VAL:O	1:G:425:ILE:HG23	2.09	0.52
1:C:409:LYS:HE2	1:C:409:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:LEU:HD21	1:F:239:GLN:HB3	1.93	0.51
1:G:185:LEU:HD22	1:G:189:PHE:CE2	2.45	0.51
1:G:271:ILE:HG13	1:G:448:ILE:CG1	2.37	0.51
1:A:96:PHE:CD2	1:A:127:GLY:HA3	2.44	0.51
1:B:153:SER:O	1:B:156:ILE:HG12	2.11	0.51
1:D:281:VAL:HG11	1:D:472:ALA:HB2	1.91	0.51
1:D:462:TYR:CD1	1:D:468:GLY:HA2	2.46	0.51
1:E:160:VAL:O	1:E:164:PHE:HB2	2.10	0.51
1:F:177:GLY:HA3	1:F:420:LEU:HD11	1.90	0.51
1:H:232:MET:HB2	1:H:332:THR:HG21	1.91	0.51
1:H:329:TYR:HB3	1:H:483:TRP:CH2	2.45	0.51
1:D:23:LEU:HD23	1:D:26:LEU:HD12	1.91	0.51
1:F:196:PRO:C	1:F:199:ASN:HD21	2.18	0.51
1:G:156:ILE:O	1:G:160:VAL:HG23	2.11	0.51
1:G:166:GLU:O	1:G:169:VAL:HG22	2.09	0.51
1:B:307:ASP:O	1:B:459:PRO:HG3	2.11	0.51
1:E:29:LEU:HD21	1:E:418:GLU:O	2.11	0.51
1:E:376:THR:HG23	1:E:402:LEU:O	2.10	0.51
1:F:284:GLN:HB2	1:F:459:PRO:HB2	1.91	0.51
1:A:486:LEU:O	1:A:487:GLU:HB2	2.09	0.51
1:B:353:SER:C	1:B:355:PHE:H	2.16	0.51
1:D:337:PRO:HG2	1:D:467:TRP:CD1	2.46	0.51
1:G:75:ALA:HA	1:G:78:LYS:HD2	1.92	0.51
1:A:369:ILE:HG23	1:A:377:ILE:HG12	1.92	0.51
1:B:96:PHE:CD1	1:B:127:GLY:HA3	2.45	0.51
1:B:257:VAL:O	1:B:261:LYS:HG3	2.11	0.51
1:D:449:ARG:HA	1:D:452:TRP:CD1	2.45	0.51
1:E:276:VAL:HG11	1:E:452:TRP:CA	2.41	0.51
1:F:276:VAL:HA	1:F:280:THR:HG23	1.92	0.51
1:G:166:GLU:CD	1:G:171:ARG:HH22	2.19	0.51
1:A:371:LEU:H	1:A:371:LEU:HD12	1.76	0.51
1:A:386:PRO:HA	1:B:179:GLU:OE2	2.11	0.51
1:C:314:ILE:HB	1:C:330:ILE:HD12	1.91	0.51
1:F:7:THR:O	1:F:111:ALA:N	2.43	0.51
1:H:35:LEU:HD13	1:H:82:LYS:HE2	1.91	0.51
1:H:237:ILE:HG21	1:H:330:ILE:HG23	1.92	0.51
1:A:268:LEU:HD23	1:A:317:HIS:O	2.11	0.51
1:A:431:LEU:C	1:A:432:PHE:CD2	2.88	0.51
1:D:154:ASP:HA	1:D:435:ARG:HH12	1.76	0.51
1:D:193:LEU:O	1:D:196:PRO:HG2	2.11	0.51
1:F:226:SER:O	1:F:230:ARG:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:ALA:N	1:F:328:PHE:O	2.40	0.51
1:G:271:ILE:HD13	1:G:271:ILE:H	1.76	0.51
1:G:385:GLU:CG	1:G:386:PRO:HD2	2.40	0.51
1:A:138:SER:HB2	1:A:164:PHE:CE1	2.46	0.51
1:A:188:ARG:NH1	1:A:246:MET:HG2	2.25	0.51
1:B:62:LEU:O	1:B:66:VAL:HG12	2.10	0.51
1:C:59:GLU:HA	1:C:62:LEU:HB2	1.91	0.51
1:C:452:TRP:HD1	1:C:453:LYS:N	2.09	0.51
1:D:118:SER:HA	1:D:121:PHE:CG	2.45	0.51
1:D:393:ALA:C	1:D:394:HIS:HD1	2.18	0.51
1:E:216:LEU:HD23	1:E:334:LYS:HD2	1.92	0.51
1:E:466:THR:O	1:E:468:GLY:N	2.38	0.51
1:G:197:LEU:C	1:G:199:ASN:H	2.19	0.51
1:G:452:TRP:HA	1:G:457:MET:HG3	1.92	0.51
1:H:359:GLY:HA3	1:H:393:ALA:O	2.11	0.51
1:B:262:VAL:HG21	1:B:436:ASP:OD2	2.10	0.51
1:D:85:TYR:CG	1:D:86:ALA:N	2.79	0.51
1:F:213:THR:HA	1:F:336:LEU:O	2.11	0.51
1:G:234:GLN:HG2	1:G:445:ILE:HG13	1.92	0.51
1:G:379:ILE:O	1:G:399:TRP:HA	2.11	0.51
1:G:381:ILE:HB	1:H:191:ASN:ND2	2.26	0.51
1:A:223:PHE:CE2	1:A:310:THR:HG22	2.46	0.50
1:E:166:GLU:CA	1:E:169:VAL:HG22	2.40	0.50
1:F:302:LEU:HG	1:F:303:GLY:N	2.25	0.50
1:G:43:CYS:O	1:G:85:TYR:HA	2.11	0.50
1:H:24:PRO:HA	1:H:62:LEU:HD23	1.93	0.50
1:A:144:LYS:HB3	2:A:501:NMN:HC6	1.94	0.50
1:C:205:HIS:HB3	1:C:327:PRO:HG2	1.93	0.50
1:D:327:PRO:HB2	1:D:329:TYR:CZ	2.46	0.50
1:F:470:ILE:O	1:F:473:ILE:N	2.44	0.50
1:A:154:ASP:HA	1:A:157:ASN:HB2	1.93	0.50
1:B:11:PHE:O	1:B:115:ALA:HB3	2.11	0.50
1:B:23:LEU:N	1:B:24:PRO:HD2	2.25	0.50
1:E:52:ASP:N	1:E:87:THR:OG1	2.44	0.50
1:E:135:GLY:HA2	1:E:138:SER:CB	2.42	0.50
1:F:16:ASP:O	1:F:17:LEU:C	2.54	0.50
1:G:17:LEU:HD22	2:G:501:NMN:N1	2.25	0.50
1:G:281:VAL:HG11	1:G:472:ALA:HB2	1.92	0.50
1:H:21:MET:C	1:H:24:PRO:HD2	2.37	0.50
1:B:198:TRP:CH2	1:B:345:VAL:HG21	2.46	0.50
1:E:419:ARG:HA	1:F:388:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:PRO:HD3	1:G:467:TRP:HA	1.94	0.50
1:B:79:PHE:O	1:B:83:LEU:HD22	2.11	0.50
1:B:337:PRO:HD2	1:B:467:TRP:CE3	2.47	0.50
1:C:171:ARG:O	1:C:432:PHE:HD1	1.93	0.50
1:C:195:GLU:N	1:C:196:PRO:HD2	2.26	0.50
1:D:17:LEU:HD12	1:D:21:MET:HB2	1.93	0.50
1:D:262:VAL:CG2	1:D:437:GLU:HG3	2.41	0.50
1:E:25:ALA:HA	1:E:418:GLU:HG3	1.93	0.50
1:G:322:ARG:HD2	1:G:323:TRP:NE1	2.26	0.50
1:H:170:TYR:OH	1:H:427:GLY:HA2	2.12	0.50
1:A:52:ASP:OD1	1:A:84:PHE:HA	2.12	0.50
1:E:176:LEU:HA	1:E:181:VAL:HG11	1.94	0.50
1:E:186:THR:HA	1:F:355:PHE:CZ	2.47	0.50
1:G:337:PRO:HG3	1:G:465:GLY:O	2.12	0.50
1:A:213:THR:O	1:A:290:SER:OG	2.27	0.50
1:D:199:ASN:O	1:D:203:ILE:HB	2.12	0.50
1:E:276:VAL:HG22	1:E:280:THR:HG21	1.92	0.50
1:F:343:ILE:O	1:F:368:ARG:HA	2.11	0.50
1:G:183:ASN:OD1	1:H:383:VAL:HG23	2.12	0.50
1:H:449:ARG:O	1:H:453:LYS:HG2	2.11	0.50
1:B:3:ASN:HB2	1:B:5:VAL:CG2	2.41	0.50
1:B:197:LEU:O	1:B:203:ILE:HG13	2.11	0.50
1:B:198:TRP:CZ2	1:B:345:VAL:HG21	2.47	0.50
1:B:273:ASN:O	1:B:455:ASN:ND2	2.45	0.50
1:F:27:TYR:HE2	1:F:71:LEU:HA	1.77	0.50
1:D:254:ALA:HA	1:D:430:THR:HG22	1.93	0.50
1:D:276:VAL:HG22	1:D:280:THR:HG21	1.94	0.50
1:E:112:ILE:HB	1:E:140:LEU:HD23	1.93	0.50
1:E:203:ILE:HA	1:E:347:PHE:HA	1.93	0.50
1:E:238:LEU:HD23	1:E:441:GLN:CG	2.35	0.50
1:F:351:PRO:O	1:G:324:HIS:HB3	2.12	0.50
1:G:355:PHE:CD2	1:G:395:MET:HE1	2.47	0.50
1:H:127:GLY:O	1:H:131:ALA:N	2.44	0.50
1:A:383:VAL:HG23	1:B:183:ASN:OD1	2.11	0.49
1:C:191:ASN:HD21	1:D:382:MET:H	1.59	0.49
1:D:462:TYR:CE1	1:D:468:GLY:HA2	2.46	0.49
1:E:101:ASP:HA	1:E:104:GLY:O	2.12	0.49
1:F:271:ILE:HG13	1:F:448:ILE:HG12	1.93	0.49
1:H:99:ILE:O	1:H:100:ALA:HB3	2.11	0.49
1:H:148:GLN:O	1:H:230:ARG:HD3	2.12	0.49
1:H:276:VAL:HG22	1:H:280:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:TYR:N	1:H:310:THR:OG1	2.44	0.49
1:E:27:TYR:HB2	1:E:62:LEU:HD11	1.94	0.49
1:F:172:ILE:HG12	1:F:432:PHE:CE2	2.47	0.49
1:G:365:ASN:ND2	1:H:191:ASN:OD1	2.44	0.49
1:H:258:ARG:HA	1:H:261:LYS:HD2	1.94	0.49
1:H:423:ASP:HB3	1:H:428:ASP:OD2	2.13	0.49
1:H:460:LYS:HD3	1:H:471:THR:CG2	2.43	0.49
1:A:118:SER:O	1:A:121:PHE:HB2	2.11	0.49
1:A:445:ILE:O	1:A:448:ILE:HG23	2.12	0.49
1:B:415:ILE:HG22	1:B:418:GLU:HG2	1.93	0.49
1:B:417:HIS:O	1:B:421:LEU:HG	2.13	0.49
1:E:45:SER:HB3	1:E:85:TYR:OH	2.12	0.49
1:E:183:ASN:O	1:E:186:THR:N	2.46	0.49
1:E:370:VAL:CG2	1:E:376:THR:H	2.25	0.49
1:F:112:ILE:HG21	1:F:128:LEU:HD13	1.93	0.49
1:H:99:ILE:HD12	1:H:133:LEU:HG	1.94	0.49
1:A:237:ILE:HG21	1:A:330:ILE:CG2	2.42	0.49
1:A:442:TRP:HA	1:A:442:TRP:CE3	2.47	0.49
1:C:337:PRO:HD3	1:C:466:THR:O	2.13	0.49
1:H:18:SER:O	1:H:23:LEU:HG	2.13	0.49
1:H:288:GLY:O	1:H:295:VAL:N	2.26	0.49
1:C:433:VAL:HG12	1:C:438:VAL:HG23	1.94	0.49
1:E:203:ILE:HG12	1:E:347:PHE:CD1	2.48	0.49
1:F:121:PHE:O	1:F:125:ILE:HG13	2.11	0.49
1:F:283:GLY:O	1:F:309:GLU:HA	2.13	0.49
1:B:3:ASN:HB3	1:B:139:ARG:NH2	2.26	0.49
1:B:53:GLY:O	1:B:57:PHE:N	2.43	0.49
1:C:203:ILE:O	1:C:348:LYS:NZ	2.44	0.49
1:D:290:SER:H	1:D:295:VAL:HG13	1.78	0.49
1:D:385:GLU:HB3	1:D:394:HIS:O	2.13	0.49
1:E:276:VAL:HG11	1:E:452:TRP:N	2.28	0.49
1:E:277:ILE:HD11	1:E:455:ASN:HB3	1.93	0.49
1:F:21:MET:C	1:F:24:PRO:HD2	2.37	0.49
1:H:96:PHE:C	1:H:98:LYS:H	2.21	0.49
1:H:334:LYS:O	1:H:335:ARG:HB2	2.13	0.49
1:H:378:GLN:HG3	1:H:399:TRP:CZ3	2.48	0.49
1:A:273:ASN:HA	1:A:451:GLY:HA2	1.95	0.49
1:B:139:ARG:NH1	1:B:427:GLY:HA2	2.28	0.49
1:B:476:VAL:HB	1:B:481:VAL:O	2.12	0.49
1:D:27:TYR:CE2	1:D:66:VAL:HG11	2.48	0.49
1:D:272:ASN:H	1:D:275:THR:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:LEU:HD23	1:D:422:LEU:O	2.12	0.49
1:F:261:LYS:HB3	1:F:261:LYS:HE3	1.57	0.49
1:G:179:GLU:OE1	1:H:386:PRO:HA	2.12	0.49
1:H:359:GLY:O	1:H:394:HIS:CD2	2.54	0.49
1:B:216:LEU:HD13	1:B:334:LYS:CE	2.43	0.49
1:B:229:LEU:HG	1:B:445:ILE:HD11	1.93	0.49
1:B:415:ILE:HG22	1:B:418:GLU:CD	2.37	0.49
1:B:470:ILE:O	1:B:473:ILE:HG12	2.12	0.49
1:C:367:LEU:HD13	1:C:379:ILE:HG12	1.95	0.49
1:D:444:TRP:O	1:D:448:ILE:HG13	2.13	0.49
1:E:226:SER:HA	1:E:230:ARG:NH1	2.27	0.49
1:F:197:LEU:O	1:F:202:GLY:HA3	2.13	0.49
1:F:408:PHE:CD1	1:F:411:ARG:HD3	2.48	0.49
1:C:285:TYR:CD1	1:C:335:ARG:HG3	2.48	0.49
1:D:114:LEU:HD21	1:D:121:PHE:CG	2.47	0.49
1:E:7:THR:O	1:E:8:MET:HB3	2.11	0.49
1:F:144:LYS:HD3	1:F:236:HIS:CE1	2.47	0.49
1:F:423:ASP:O	1:F:427:GLY:N	2.45	0.49
1:H:258:ARG:NH1	1:H:429:ALA:O	2.46	0.49
1:B:29:LEU:CD2	1:B:418:GLU:HB2	2.43	0.49
1:D:195:GLU:OE2	1:D:322:ARG:NH1	2.27	0.49
1:E:29:LEU:HG	1:E:418:GLU:HG2	1.95	0.49
1:G:64:ARG:HB2	1:G:64:ARG:HH11	1.78	0.49
1:G:149:ASP:OD1	1:G:149:ASP:N	2.43	0.49
1:H:429:ALA:HA	1:H:432:PHE:HD2	1.77	0.49
1:B:211:ALA:HB3	1:B:340:ARG:H	1.76	0.48
1:B:315:LYS:HE2	1:B:317:HIS:NE2	2.28	0.48
1:C:268:LEU:HD23	1:C:318:VAL:HG22	1.94	0.48
1:C:415:ILE:HB	1:C:418:GLU:HG3	1.95	0.48
1:D:114:LEU:HD23	1:D:142:LEU:HD23	1.95	0.48
1:D:199:ASN:OD1	1:D:201:LYS:O	2.31	0.48
1:H:227:GLY:O	1:H:231:ASP:HB2	2.13	0.48
1:H:460:LYS:HZ3	1:H:470:ILE:HG13	1.78	0.48
1:C:362:LEU:HD23	1:C:362:LEU:HA	1.70	0.48
1:D:45:SER:HB3	1:D:85:TYR:HE2	1.77	0.48
1:D:336:LEU:HD13	1:D:467:TRP:HZ3	1.77	0.48
1:E:315:LYS:HG3	1:E:329:TYR:CE1	2.48	0.48
1:F:262:VAL:HG22	1:F:437:GLU:CG	2.39	0.48
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.67	0.48
1:E:69:ASP:OD1	1:E:70:ARG:N	2.45	0.48
1:E:157:ASN:O	1:E:158:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:GLU:HG2	1:E:248:PRO:HD2	1.95	0.48
1:E:273:ASN:CB	1:E:451:GLY:HA2	2.43	0.48
1:F:14:THR:HG21	1:F:46:ARG:C	2.37	0.48
1:F:150:LEU:HD22	1:F:443:ILE:CD1	2.44	0.48
1:G:185:LEU:HD22	1:G:189:PHE:HE2	1.79	0.48
1:H:158:ASP:C	1:H:160:VAL:H	2.21	0.48
1:H:282:THR:HG23	1:H:309:GLU:HB3	1.95	0.48
1:A:164:PHE:CD1	1:A:168:GLN:OE1	2.65	0.48
1:A:168:GLN:HA	1:A:170:TYR:HE1	1.78	0.48
1:D:342:GLU:HA	1:D:370:VAL:HA	1.95	0.48
1:D:472:ALA:O	1:D:475:LEU:N	2.44	0.48
1:E:188:ARG:HD3	1:E:243:LEU:O	2.14	0.48
1:E:384:LYS:HG2	1:E:385:GLU:O	2.13	0.48
1:H:286:GLY:N	1:H:462:TYR:O	2.42	0.48
1:A:321:TRP:CH2	1:D:350:VAL:HB	2.48	0.48
1:A:365:ASN:C	1:A:366:LYS:HG3	2.39	0.48
1:A:409:LYS:HG2	1:A:410:ASP:N	2.28	0.48
1:F:128:LEU:C	1:F:133:LEU:HB3	2.38	0.48
1:F:200:SER:HA	1:F:326:VAL:CG2	2.43	0.48
1:G:178:LYS:HB2	1:G:181:VAL:CG2	2.44	0.48
1:H:80:LEU:O	1:H:83:LEU:HB2	2.14	0.48
1:B:436:ASP:HA	1:B:439:GLU:OE2	2.13	0.48
1:C:435:ARG:HH11	1:C:439:GLU:CD	2.20	0.48
1:E:65:PHE:O	1:E:66:VAL:C	2.57	0.48
1:E:107:GLU:O	1:E:108:LYS:C	2.56	0.48
1:E:309:GLU:O	1:E:311:PHE:N	2.41	0.48
1:E:337:PRO:HD2	1:E:467:TRP:CZ3	2.48	0.48
1:F:198:TRP:HH2	1:F:367:LEU:CD2	2.26	0.48
1:G:40:ARG:HD3	1:G:84:PHE:CE2	2.49	0.48
1:G:296:ALA:O	1:G:335:ARG:NH1	2.33	0.48
1:A:203:ILE:O	1:A:348:LYS:HE3	2.14	0.48
1:A:316:ALA:HB3	1:A:328:PHE:HB2	1.96	0.48
1:C:340:ARG:HA	1:C:373:PRO:CG	2.44	0.48
1:D:67:ALA:HB3	1:D:70:ARG:CG	2.44	0.48
1:E:16:ASP:HA	1:E:19:GLN:CD	2.39	0.48
1:E:189:PHE:CE1	1:E:248:PRO:HD3	2.49	0.48
1:E:352:HIS:CE1	1:F:250:ALA:O	2.67	0.48
1:F:188:ARG:HH22	1:F:322:ARG:HH12	1.61	0.48
1:H:99:ILE:HG21	1:H:131:ALA:O	2.13	0.48
1:B:12:GLY:HA3	1:B:115:ALA:O	2.14	0.48
1:B:233:VAL:HG22	1:B:445:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:LEU:H	1:E:193:LEU:CD2	2.27	0.48
1:E:415:ILE:HG23	1:E:418:GLU:OE2	2.13	0.48
1:F:207:GLN:O	1:F:343:ILE:HA	2.13	0.48
1:H:50:ASP:O	1:H:51:THR:C	2.57	0.48
1:H:167:LYS:HE3	1:H:168:GLN:HG2	1.95	0.48
1:A:20:ARG:O	1:A:24:PRO:HG2	2.14	0.48
1:A:210:VAL:O	1:A:332:THR:HA	2.14	0.48
1:A:412:LYS:HG2	1:A:414:ARG:HG3	1.96	0.48
1:B:197:LEU:HD13	1:B:347:PHE:CD1	2.49	0.48
1:B:309:GLU:HB2	1:B:311:PHE:O	2.14	0.48
1:D:249:PRO:HG3	1:D:257:VAL:HG22	1.96	0.48
1:D:271:ILE:HG22	1:D:276:VAL:HG23	1.95	0.48
1:E:261:LYS:O	1:E:264:VAL:HB	2.14	0.48
1:G:211:ALA:HB3	1:G:340:ARG:N	2.29	0.48
1:H:8:MET:O	1:H:41:ILE:HA	2.14	0.48
1:A:114:LEU:HB3	1:A:121:PHE:CE1	2.48	0.48
1:B:412:LYS:C	1:B:414:ARG:HH22	2.21	0.48
1:D:106:VAL:O	1:D:109:GLY:N	2.47	0.48
1:F:204:ASP:CB	1:F:346:GLN:HG2	2.44	0.48
1:F:379:ILE:O	1:F:399:TRP:HA	2.14	0.48
1:H:433:VAL:HG12	1:H:434:ARG:H	1.78	0.48
1:A:54:PHE:CE1	1:A:85:TYR:HB2	2.48	0.47
1:B:193:LEU:O	1:B:196:PRO:HD2	2.12	0.47
1:B:378:GLN:HB2	1:B:399:TRP:HE3	1.78	0.47
1:E:52:ASP:HB3	1:E:85:TYR:HE2	1.78	0.47
1:E:320:ASN:HD21	1:E:322:ARG:HB3	1.79	0.47
1:F:148:GLN:HG3	1:F:149:ASP:OD1	2.13	0.47
1:F:281:VAL:HG12	1:F:311:PHE:HE1	1.79	0.47
1:H:10:LEU:O	1:H:43:CYS:HA	2.14	0.47
1:B:93:PRO:HA	1:B:96:PHE:CD1	2.49	0.47
1:B:200:SER:N	1:B:322:ARG:O	2.47	0.47
1:E:215:GLY:HA3	1:E:335:ARG:NH1	2.29	0.47
1:E:476:VAL:HG13	1:E:481:VAL:O	2.14	0.47
1:F:11:PHE:CE2	1:F:44:THR:HG21	2.49	0.47
1:G:335:ARG:HD2	1:G:464:SER:OG	2.14	0.47
1:H:211:ALA:O	1:H:339:ARG:HA	2.14	0.47
1:A:90:ILE:HA	1:A:96:PHE:HZ	1.79	0.47
1:B:144:LYS:HE2	2:B:501:NMN:C6	2.27	0.47
1:C:255:ASN:OD1	1:C:434:ARG:NH1	2.47	0.47
1:F:117:SER:H	1:F:120:LEU:HB2	1.79	0.47
1:F:172:ILE:HG12	1:F:432:PHE:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:ASN:CG	1:H:383:VAL:HG23	2.39	0.47
1:G:337:PRO:CD	1:G:467:TRP:HA	2.44	0.47
1:H:178:LYS:O	1:H:182:GLN:HG3	2.15	0.47
1:B:43:CYS:HB2	1:B:84:PHE:O	2.15	0.47
1:B:217:GLU:O	1:B:220:ILE:HG12	2.15	0.47
1:C:417:HIS:O	1:C:418:GLU:C	2.54	0.47
1:G:213:THR:HG22	1:G:336:LEU:O	2.14	0.47
1:G:230:ARG:HA	1:G:234:GLN:HB2	1.96	0.47
1:G:289:VAL:HG13	1:G:292:GLY:O	2.15	0.47
1:H:237:ILE:HD12	1:H:332:THR:HB	1.96	0.47
1:H:285:TYR:CD2	1:H:310:THR:HG21	2.48	0.47
1:A:88:VAL:HG22	1:A:98:LYS:HD2	1.96	0.47
1:A:419:ARG:O	1:A:419:ARG:HD2	2.15	0.47
1:A:469:PRO:HB2	1:A:471:THR:OG1	2.14	0.47
1:B:121:PHE:HZ	1:B:143:GLU:HB2	1.80	0.47
1:B:142:LEU:O	1:B:172:ILE:HB	2.14	0.47
1:C:210:VAL:O	1:C:332:THR:HA	2.14	0.47
1:C:285:TYR:H	1:C:310:THR:HG21	1.79	0.47
1:D:284:GLN:CB	1:D:461:THR:HG22	2.45	0.47
1:E:143:GLU:HB3	2:E:501:NMN:H1RC	1.95	0.47
1:G:214:VAL:O	1:G:334:LYS:HB3	2.13	0.47
1:G:337:PRO:HG2	1:G:467:TRP:CD1	2.50	0.47
1:G:365:ASN:ND2	1:G:380:SER:O	2.48	0.47
1:A:126:ALA:O	1:A:129:LYS:HG3	2.14	0.47
1:A:339:ARG:O	1:A:373:PRO:HD3	2.15	0.47
1:B:30:ASP:HA	1:B:35:LEU:HB2	1.96	0.47
1:C:229:LEU:O	1:C:233:VAL:HG12	2.14	0.47
1:C:345:VAL:O	1:C:366:LYS:HA	2.14	0.47
1:D:195:GLU:HA	1:D:198:TRP:HB2	1.96	0.47
1:E:456:SER:O	1:E:457:MET:C	2.56	0.47
1:H:14:THR:HB	1:H:45:SER:OG	2.14	0.47
1:A:214:VAL:O	1:A:335:ARG:N	2.46	0.47
1:B:3:ASN:HB3	1:B:425:ILE:O	2.15	0.47
1:B:201:LYS:HB3	1:C:201:LYS:HE3	1.96	0.47
1:B:329:TYR:CZ	1:B:481:VAL:HG11	2.49	0.47
1:B:421:LEU:O	1:B:422:LEU:C	2.58	0.47
1:B:428:ASP:O	1:B:429:ALA:HB3	2.15	0.47
1:C:212:GLU:HA	1:C:339:ARG:CB	2.45	0.47
1:C:226:SER:O	1:C:230:ARG:HB2	2.14	0.47
1:C:261:LYS:HE2	1:C:437:GLU:OE2	2.15	0.47
1:C:360:GLY:HA3	1:C:395:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:PRO:HD2	1:D:411:ARG:NH1	2.29	0.47
1:D:50:ASP:OD1	1:D:52:ASP:HB2	2.15	0.47
1:E:161:LEU:C	1:E:163:VAL:N	2.72	0.47
1:E:287:ALA:O	1:E:463:VAL:HG13	2.14	0.47
1:E:472:ALA:O	1:E:475:LEU:N	2.43	0.47
1:H:20:ARG:HH11	1:H:65:PHE:HE1	1.62	0.47
1:H:337:PRO:HG2	1:H:467:TRP:CD1	2.50	0.47
1:H:378:GLN:HA	1:H:400:LEU:O	2.14	0.47
1:H:415:ILE:HB	1:H:418:GLU:HG3	1.95	0.47
1:A:54:PHE:C	1:A:56:ASP:N	2.72	0.47
1:C:154:ASP:HA	1:C:435:ARG:HH22	1.76	0.47
1:C:285:TYR:CG	1:C:335:ARG:HG3	2.50	0.47
1:E:354:ILE:O	1:F:251:HIS:CD2	2.67	0.47
1:F:19:GLN:HA	1:F:23:LEU:HD12	1.96	0.47
1:B:3:ASN:CB	1:B:139:ARG:HH21	2.26	0.47
1:B:78:LYS:HB2	1:B:78:LYS:HE2	1.71	0.47
1:C:242:ALA:HB2	1:C:265:PHE:CE1	2.50	0.47
1:E:213:THR:HA	1:E:336:LEU:H	1.79	0.47
1:E:341:SER:N	1:E:372:GLN:HB3	2.28	0.47
1:G:138:SER:O	1:G:168:GLN:HB3	2.14	0.47
1:H:78:LYS:HA	1:H:81:ASN:ND2	2.30	0.47
1:H:120:LEU:HD23	1:H:120:LEU:HA	1.77	0.47
1:H:198:TRP:CH2	1:H:345:VAL:HG21	2.50	0.47
1:H:284:GLN:HB2	1:H:459:PRO:HB2	1.97	0.47
1:A:15:GLY:N	1:A:46:ARG:HH12	2.13	0.47
1:A:135:GLY:N	1:A:164:PHE:CE1	2.82	0.47
1:B:143:GLU:O	1:B:146:LEU:HD23	2.15	0.47
1:B:402:LEU:HD12	1:B:403:SER:H	1.80	0.47
1:H:272:ASN:N	1:H:275:THR:OG1	2.48	0.47
1:A:7:THR:HG21	1:A:104:GLY:N	2.30	0.46
1:A:13:SER:HB2	1:A:43:CYS:HB3	1.96	0.46
1:C:262:VAL:HG22	1:C:437:GLU:HA	1.97	0.46
1:D:130:GLN:H	1:D:130:GLN:HG2	1.35	0.46
1:F:260:GLU:HA	1:F:263:LYS:HD3	1.97	0.46
1:F:322:ARG:HD2	1:F:323:TRP:CE2	2.49	0.46
1:G:191:ASN:HB3	1:H:365:ASN:ND2	2.29	0.46
1:G:377:ILE:HG22	1:H:400:LEU:HD21	1.97	0.46
1:H:26:LEU:HD21	1:H:421:LEU:HD22	1.97	0.46
1:H:272:ASN:CB	1:H:275:THR:HG23	2.44	0.46
1:A:114:LEU:C	1:A:116:THR:H	2.21	0.46
1:A:258:ARG:O	1:A:261:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ALA:HA	1:B:477:GLU:HB2	1.97	0.46
1:D:417:HIS:O	1:D:421:LEU:HD23	2.16	0.46
1:D:437:GLU:O	1:D:441:GLN:HG3	2.16	0.46
1:E:185:LEU:O	1:F:355:PHE:HZ	1.97	0.46
1:E:203:ILE:HG12	1:E:347:PHE:CE1	2.50	0.46
1:F:140:LEU:HB2	1:F:164:PHE:CE1	2.51	0.46
1:G:44:THR:HB	1:G:99:ILE:HD11	1.96	0.46
1:G:235:SER:O	1:G:239:GLN:N	2.40	0.46
1:G:245:ALA:O	1:G:323:TRP:NE1	2.43	0.46
1:G:417:HIS:HA	1:G:420:LEU:HD12	1.97	0.46
1:H:329:TYR:CZ	1:H:481:VAL:HG11	2.49	0.46
1:A:320:ASN:O	1:A:324:HIS:HB2	2.15	0.46
1:B:5:VAL:HG13	1:B:109:GLY:O	2.14	0.46
1:B:457:MET:HE2	1:B:457:MET:HB3	1.70	0.46
1:B:463:VAL:HG11	1:G:294:GLU:HG3	1.97	0.46
1:E:236:HIS:O	1:E:239:GLN:N	2.45	0.46
1:E:388:LEU:HD21	1:F:414:ARG:NE	2.31	0.46
1:F:216:LEU:H	1:F:216:LEU:HG	1.49	0.46
1:F:438:VAL:CG1	1:F:442:TRP:HD1	2.29	0.46
1:G:6:SER:HB2	1:G:109:GLY:CA	2.45	0.46
1:H:4:THR:HA	1:H:425:ILE:O	2.16	0.46
1:H:30:ASP:HA	1:H:35:LEU:CD1	2.41	0.46
1:H:60:LYS:HD3	1:H:60:LYS:HA	1.60	0.46
1:H:385:GLU:OE1	1:H:396:ARG:HD3	2.15	0.46
1:H:419:ARG:O	1:H:422:LEU:N	2.47	0.46
1:A:7:THR:HG21	1:A:104:GLY:H	1.81	0.46
1:D:5:VAL:HG23	1:D:109:GLY:C	2.40	0.46
1:D:214:VAL:O	1:D:334:LYS:HB3	2.15	0.46
1:G:249:PRO:HB2	1:G:251:HIS:O	2.16	0.46
1:H:293:LYS:HD3	1:H:293:LYS:HA	1.45	0.46
1:A:85:TYR:CD1	1:A:85:TYR:C	2.94	0.46
1:B:15:GLY:C	1:B:17:LEU:H	2.23	0.46
1:B:216:LEU:HD13	1:B:334:LYS:NZ	2.30	0.46
1:B:227:GLY:H	1:B:230:ARG:HG3	1.81	0.46
1:C:25:ALA:HB1	1:C:418:GLU:CG	2.46	0.46
1:C:250:ALA:O	1:D:354:ILE:HG22	2.16	0.46
1:C:431:LEU:HD12	1:C:431:LEU:O	2.14	0.46
1:D:7:THR:CG2	1:D:104:GLY:H	2.29	0.46
1:E:20:ARG:HA	1:E:65:PHE:CD2	2.48	0.46
1:E:52:ASP:HB3	1:E:85:TYR:CE2	2.50	0.46
1:E:299:ILE:O	1:E:302:LEU:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:VAL:HG13	1:F:437:GLU:HA	1.98	0.46
1:G:309:GLU:HB2	1:G:311:PHE:H	1.80	0.46
1:H:466:THR:O	1:H:467:TRP:HB2	2.15	0.46
1:B:113:TYR:HE2	1:B:172:ILE:HG13	1.81	0.46
1:B:148:GLN:HB3	1:B:230:ARG:NH2	2.30	0.46
1:C:48:GLU:CB	1:C:87:THR:HA	2.46	0.46
1:C:242:ALA:HB1	1:C:261:LYS:HG2	1.98	0.46
1:D:152:SER:O	1:D:156:ILE:N	2.34	0.46
1:E:355:PHE:CZ	1:F:186:THR:HA	2.50	0.46
1:F:28:GLY:HA3	1:F:70:ARG:NH2	2.30	0.46
1:F:208:ILE:HG23	1:F:343:ILE:HG12	1.96	0.46
1:F:415:ILE:O	1:F:418:GLU:HG3	2.16	0.46
1:G:187:LEU:HG	1:G:194:PHE:CE2	2.51	0.46
1:A:11:PHE:CE1	1:A:128:LEU:HD21	2.50	0.46
1:A:285:TYR:CD2	1:A:298:TYR:HB2	2.50	0.46
1:A:340:ARG:NH1	1:A:342:GLU:OE1	2.49	0.46
1:A:389:ASP:H	1:B:419:ARG:HH12	1.64	0.46
1:B:63:ASP:HA	1:B:71:LEU:HD21	1.98	0.46
1:C:183:ASN:HB2	1:D:384:LYS:N	2.27	0.46
1:C:386:PRO:HA	1:D:179:GLU:HG3	1.98	0.46
1:D:98:LYS:HA	1:D:101:ASP:OD2	2.15	0.46
1:G:70:ARG:NH1	1:G:413:ARG:O	2.49	0.46
1:G:86:ALA:O	1:G:99:ILE:HD11	2.16	0.46
1:H:197:LEU:O	1:H:199:ASN:N	2.47	0.46
1:H:210:VAL:O	1:H:332:THR:HA	2.16	0.46
1:A:157:ASN:HB3	1:A:435:ARG:HE	1.80	0.46
1:B:172:ILE:HD11	1:B:432:PHE:CE2	2.51	0.46
1:E:276:VAL:HG13	1:E:457:MET:SD	2.56	0.46
1:F:297:GLY:O	1:F:301:GLU:N	2.48	0.46
1:G:15:GLY:O	1:G:19:GLN:HG3	2.16	0.46
1:G:412:LYS:HG2	1:G:414:ARG:HG2	1.98	0.46
1:H:176:LEU:CD1	1:H:431:LEU:O	2.63	0.46
1:A:7:THR:HG21	1:A:104:GLY:CA	2.46	0.46
1:A:20:ARG:HB3	1:A:65:PHE:CE1	2.50	0.46
1:A:146:LEU:HD22	1:A:438:VAL:HG11	1.98	0.46
1:A:247:GLU:HB2	1:A:260:GLU:OE1	2.16	0.46
1:A:378:GLN:HA	1:A:400:LEU:O	2.15	0.46
1:B:215:GLY:H	1:B:335:ARG:HD2	1.81	0.46
1:C:230:ARG:HD3	1:C:442:TRP:HH2	1.81	0.46
1:E:23:LEU:H	1:E:24:PRO:CD	2.29	0.46
1:E:355:PHE:HE2	1:F:190:GLY:HA2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ASP:HA	1:F:19:GLN:CG	2.45	0.46
1:G:6:SER:HB2	1:G:109:GLY:HA3	1.97	0.46
1:G:55:ARG:HD3	1:G:80:LEU:HB3	1.98	0.46
1:G:366:LYS:HE2	1:G:366:LYS:HB2	1.38	0.46
1:H:263:LYS:HB3	1:H:263:LYS:HE2	1.63	0.46
1:H:415:ILE:HD12	1:H:415:ILE:N	2.31	0.46
1:A:17:LEU:HD13	2:A:501:NMN:C3	2.46	0.46
1:B:62:LEU:O	1:B:63:ASP:C	2.60	0.46
1:C:360:GLY:N	1:C:394:HIS:HA	2.31	0.46
1:E:246:MET:CE	1:E:249:PRO:HD3	2.44	0.46
1:E:367:LEU:HG	1:E:369:ILE:HD11	1.97	0.46
1:E:370:VAL:HG23	1:E:376:THR:H	1.81	0.46
1:G:37:ASP:HA	1:G:82:LYS:CE	2.43	0.46
1:G:148:GLN:N	1:G:152:SER:OG	2.42	0.46
1:H:161:LEU:HA	1:H:164:PHE:O	2.15	0.46
1:A:315:LYS:HD2	1:A:478:ARG:NH2	2.31	0.45
1:E:414:ARG:HG3	1:E:418:GLU:CD	2.41	0.45
1:F:198:TRP:HH2	1:F:367:LEU:HD23	1.80	0.45
1:F:211:ALA:O	1:F:339:ARG:HA	2.16	0.45
1:G:340:ARG:HA	1:G:373:PRO:CG	2.41	0.45
1:H:172:ILE:HG12	1:H:432:PHE:HE1	1.81	0.45
1:B:14:THR:HG23	1:B:45:SER:HB2	1.97	0.45
1:B:380:SER:HB2	1:B:399:TRP:CE2	2.51	0.45
1:C:283:GLY:HA2	1:C:460:LYS:O	2.16	0.45
1:C:341:SER:H	1:C:373:PRO:CG	2.29	0.45
1:D:322:ARG:HD2	1:D:323:TRP:NE1	2.31	0.45
1:E:143:GLU:OE1	2:E:501:NMN:HC6	2.14	0.45
1:E:269:ARG:HB3	1:E:317:HIS:HB2	1.98	0.45
1:E:455:ASN:O	1:E:456:SER:HB2	2.16	0.45
1:F:470:ILE:O	1:F:471:THR:C	2.59	0.45
1:G:11:PHE:HB2	1:G:114:LEU:HA	1.97	0.45
1:A:444:TRP:O	1:A:448:ILE:HG22	2.16	0.45
1:B:90:ILE:HD13	1:B:90:ILE:H	1.80	0.45
1:D:11:PHE:HB2	1:D:113:TYR:O	2.15	0.45
1:E:97:GLY:HA2	1:E:131:ALA:HB1	1.98	0.45
1:E:473:ILE:O	1:E:477:GLU:HG3	2.17	0.45
1:F:188:ARG:HH22	1:F:322:ARG:NH1	2.14	0.45
1:F:398:VAL:HG22	1:F:399:TRP:N	2.31	0.45
1:G:80:LEU:O	1:G:83:LEU:HB2	2.17	0.45
1:G:240:LEU:O	1:G:244:VAL:HG23	2.16	0.45
1:H:175:TYR:CD1	1:H:236:HIS:CD2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:378:GLN:HB2	1:H:399:TRP:HE3	1.81	0.45
1:A:188:ARG:HH12	1:A:246:MET:HG2	1.81	0.45
1:A:258:ARG:HA	1:A:261:LYS:HD3	1.99	0.45
1:C:320:ASN:OD1	1:C:323:TRP:N	2.47	0.45
1:D:173:ASP:OD1	1:D:235:SER:HB2	2.16	0.45
1:D:302:LEU:CD2	1:D:306:SER:HB2	2.43	0.45
1:E:166:GLU:HA	1:E:169:VAL:CG2	2.44	0.45
1:E:350:VAL:HG13	1:E:362:LEU:CD2	2.47	0.45
1:F:261:LYS:O	1:F:264:VAL:HG13	2.16	0.45
1:H:76:LYS:HB3	1:H:76:LYS:HE3	1.80	0.45
1:A:32:ASP:HB2	1:A:34:LEU:HG	1.99	0.45
1:A:195:GLU:N	1:A:196:PRO:HD2	2.32	0.45
1:B:229:LEU:O	1:B:233:VAL:HG22	2.16	0.45
1:C:220:ILE:O	1:C:224:ASP:N	2.46	0.45
1:C:452:TRP:CD1	1:C:452:TRP:C	2.95	0.45
1:D:393:ALA:C	1:D:394:HIS:ND1	2.74	0.45
1:D:462:TYR:HB2	1:D:466:THR:HG22	1.98	0.45
1:E:377:ILE:HG13	1:E:404:LEU:HD21	1.99	0.45
1:F:449:ARG:HA	1:F:452:TRP:CE2	2.51	0.45
1:H:309:GLU:CD	1:H:309:GLU:H	2.24	0.45
1:A:118:SER:HA	1:A:121:PHE:CG	2.51	0.45
1:B:74:ASP:O	1:B:75:ALA:C	2.60	0.45
1:B:166:GLU:O	1:B:169:VAL:HG22	2.17	0.45
1:B:198:TRP:HA	1:B:203:ILE:CD1	2.46	0.45
1:B:309:GLU:HG2	1:B:309:GLU:O	2.16	0.45
1:C:96:PHE:CB	1:C:131:ALA:HB3	2.47	0.45
1:D:114:LEU:HD21	1:D:121:PHE:CD1	2.52	0.45
1:E:229:LEU:HA	1:E:233:VAL:HG23	1.97	0.45
1:E:416:ALA:O	1:E:417:HIS:HB2	2.17	0.45
1:F:233:VAL:HG23	1:F:445:ILE:HD11	1.97	0.45
1:F:324:HIS:HB3	1:G:351:PRO:O	2.17	0.45
1:C:194:PHE:HB3	1:C:198:TRP:CE3	2.52	0.45
1:C:285:TYR:CB	1:C:335:ARG:HB2	2.47	0.45
1:C:412:LYS:C	1:C:414:ARG:N	2.75	0.45
1:C:435:ARG:NH1	1:C:439:GLU:CD	2.75	0.45
1:D:27:TYR:CD2	1:D:66:VAL:HG11	2.52	0.45
1:E:23:LEU:N	1:E:24:PRO:CD	2.80	0.45
1:F:279:HIS:CE1	1:F:315:LYS:HD3	2.52	0.45
1:F:344:VAL:HG22	1:F:368:ARG:HG3	1.99	0.45
1:G:88:VAL:CB	1:G:95:GLN:HB2	2.46	0.45
1:G:271:ILE:CG1	1:G:448:ILE:HG13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:ASP:HB2	1:H:35:LEU:HD11	1.98	0.45
1:H:198:TRP:O	1:H:322:ARG:HD3	2.16	0.45
1:A:99:ILE:O	1:A:102:LEU:HB2	2.17	0.45
1:A:144:LYS:N	1:A:145:PRO:HD2	2.32	0.45
1:A:273:ASN:HA	1:A:451:GLY:CA	2.47	0.45
1:B:382:MET:HE3	1:B:382:MET:HB3	1.56	0.45
1:B:466:THR:C	1:B:468:GLY:H	2.25	0.45
1:D:29:LEU:HD23	1:D:34:LEU:HD12	1.97	0.45
1:D:205:HIS:NE2	1:D:481:VAL:HG21	2.32	0.45
1:F:62:LEU:O	1:F:66:VAL:N	2.49	0.45
1:F:242:ALA:CA	1:F:264:VAL:HG21	2.43	0.45
1:F:246:MET:HE3	1:F:260:GLU:CB	2.47	0.45
1:H:84:PHE:HB3	1:H:102:LEU:CB	2.47	0.45
1:H:211:ALA:HA	1:H:336:LEU:CD1	2.47	0.45
1:H:271:ILE:CG2	1:H:276:VAL:HG23	2.46	0.45
1:A:198:TRP:O	1:A:322:ARG:HD3	2.16	0.45
1:A:219:ARG:HB3	1:A:222:TYR:CZ	2.52	0.45
1:B:34:LEU:HB3	1:B:422:LEU:HD21	1.98	0.45
1:B:139:ARG:HH12	1:B:427:GLY:HA2	1.82	0.45
1:B:293:LYS:HE2	1:B:293:LYS:HB2	1.61	0.45
1:C:337:PRO:HG2	1:C:467:TRP:NE1	2.32	0.45
1:D:359:GLY:O	1:D:360:GLY:C	2.60	0.45
1:E:171:ARG:O	1:E:433:VAL:N	2.47	0.45
1:F:416:ALA:O	1:F:420:LEU:HD12	2.16	0.45
1:G:474:ALA:HA	1:G:477:GLU:HB2	1.98	0.45
1:H:269:ARG:O	1:H:444:TRP:NE1	2.43	0.45
1:H:435:ARG:C	1:H:435:ARG:HD3	2.42	0.45
1:A:283:GLY:O	1:A:309:GLU:O	2.35	0.45
1:A:381:ILE:HD13	1:A:400:LEU:HD11	1.98	0.45
1:C:271:ILE:HA	1:C:275:THR:HB	1.99	0.45
1:F:8:MET:HB3	1:F:40:ARG:O	2.17	0.45
1:F:26:LEU:HB2	1:F:79:PHE:HZ	1.82	0.45
1:F:219:ARG:HB3	1:F:222:TYR:CZ	2.52	0.45
1:F:233:VAL:O	1:F:238:LEU:HD13	2.17	0.45
1:G:284:GLN:HB2	1:G:459:PRO:HB2	1.97	0.45
1:A:354:ILE:O	1:B:251:HIS:HA	2.16	0.44
1:D:449:ARG:HA	1:D:452:TRP:NE1	2.33	0.44
1:F:96:PHE:CZ	1:F:124:ALA:HA	2.52	0.44
1:F:183:ASN:O	1:F:187:LEU:N	2.45	0.44
1:G:242:ALA:HA	1:G:264:VAL:HG11	2.00	0.44
1:G:382:MET:N	1:H:191:ASN:HD21	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:372:GLN:HG2	1:H:373:PRO:HA	1.99	0.44
1:A:51:THR:O	1:A:54:PHE:HB3	2.16	0.44
1:A:233:VAL:O	1:A:238:LEU:HG	2.16	0.44
1:A:285:TYR:CD1	1:A:335:ARG:HG3	2.52	0.44
1:B:38:ASP:O	1:B:39:LEU:C	2.60	0.44
1:B:255:ASN:O	1:B:259:ASP:N	2.43	0.44
1:C:286:GLY:O	1:C:464:SER:OG	2.31	0.44
1:D:299:ILE:HD12	1:D:304:GLN:O	2.18	0.44
1:E:204:ASP:HB2	1:E:347:PHE:O	2.17	0.44
1:E:298:TYR:HE2	1:E:308:THR:HG1	1.63	0.44
1:E:415:ILE:HG12	1:E:418:GLU:HG3	2.00	0.44
1:G:382:MET:H	1:H:191:ASN:HD21	1.65	0.44
1:A:363:GLN:HA	1:A:364:PRO:HD3	1.86	0.44
1:B:165:SER:O	1:B:169:VAL:HG13	2.17	0.44
1:D:51:THR:O	1:D:55:ARG:HG3	2.16	0.44
1:D:205:HIS:CD2	1:D:346:GLN:CD	2.95	0.44
1:D:298:TYR:CZ	1:D:302:LEU:HD13	2.52	0.44
1:D:467:TRP:HA	1:D:467:TRP:CE3	2.53	0.44
1:E:157:ASN:HA	1:E:160:VAL:HB	1.99	0.44
1:F:445:ILE:HA	1:F:448:ILE:HD12	1.99	0.44
1:G:247:GLU:HB2	1:G:260:GLU:OE1	2.17	0.44
1:G:381:ILE:HB	1:H:191:ASN:HD21	1.80	0.44
1:G:429:ALA:HA	1:G:432:PHE:CD1	2.52	0.44
1:H:422:LEU:O	1:H:426:GLU:HG2	2.17	0.44
1:H:475:LEU:HA	1:H:478:ARG:HE	1.81	0.44
1:B:75:ALA:O	1:B:78:LYS:HG3	2.17	0.44
1:C:359:GLY:HA3	1:C:393:ALA:O	2.17	0.44
1:D:64:ARG:HG3	1:D:65:PHE:CD2	2.52	0.44
1:D:378:GLN:HB2	1:D:399:TRP:HE3	1.82	0.44
1:E:26:LEU:HD13	1:E:41:ILE:HD12	2.00	0.44
1:E:156:ILE:O	1:E:160:VAL:N	2.49	0.44
1:E:340:ARG:CA	1:E:372:GLN:HB3	2.44	0.44
1:F:23:LEU:HB2	1:F:24:PRO:HD3	2.00	0.44
1:F:61:ALA:HA	1:F:64:ARG:HE	1.83	0.44
1:F:233:VAL:HA	1:F:237:ILE:HB	1.99	0.44
1:G:154:ASP:O	1:G:158:ASP:N	2.37	0.44
1:G:203:ILE:HG21	1:G:345:VAL:CG1	2.48	0.44
1:G:234:GLN:HA	1:G:445:ILE:HD11	2.00	0.44
1:H:237:ILE:O	1:H:241:VAL:HG23	2.17	0.44
1:H:460:LYS:NZ	1:H:470:ILE:HG13	2.33	0.44
1:A:7:THR:HG21	1:A:104:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ILE:HG12	1:A:432:PHE:CE1	2.52	0.44
1:A:423:ASP:HA	1:A:426:GLU:HB2	1.99	0.44
1:A:433:VAL:CG1	1:A:437:GLU:HB3	2.47	0.44
1:B:189:PHE:CE1	1:B:248:PRO:HG3	2.53	0.44
1:D:21:MET:HE3	1:D:21:MET:HB3	1.71	0.44
1:F:217:GLU:H	1:F:217:GLU:HG2	1.60	0.44
1:G:121:PHE:O	1:G:125:ILE:HG13	2.16	0.44
1:G:385:GLU:HG2	1:G:386:PRO:HD2	1.99	0.44
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.58	0.44
1:A:449:ARG:HH11	1:A:453:LYS:HZ1	1.66	0.44
1:B:51:THR:C	1:B:53:GLY:N	2.76	0.44
1:B:203:ILE:HD13	1:B:345:VAL:CG1	2.48	0.44
1:B:352:HIS:HB3	1:C:321:TRP:HA	1.99	0.44
1:B:361:ILE:HB	1:B:363:GLN:HG2	1.99	0.44
1:B:411:ARG:HA	1:B:411:ARG:HD2	1.76	0.44
1:D:100:ALA:HB2	1:D:131:ALA:HB1	1.99	0.44
1:E:127:GLY:O	1:E:131:ALA:N	2.50	0.44
1:E:410:ASP:O	1:E:411:ARG:C	2.61	0.44
1:F:229:LEU:HG	1:F:445:ILE:HD11	1.99	0.44
1:G:420:LEU:O	1:G:423:ASP:HB2	2.17	0.44
1:H:170:TYR:HB3	1:H:432:PHE:CG	2.52	0.44
1:H:245:ALA:HA	1:H:323:TRP:HE1	1.83	0.44
1:H:254:ALA:HB2	1:H:430:THR:CB	2.47	0.44
1:A:14:THR:HG23	1:A:45:SER:OG	2.18	0.44
1:B:246:MET:HA	1:B:264:VAL:CG2	2.48	0.44
1:E:220:ILE:H	1:E:220:ILE:HG12	1.38	0.44
1:E:398:VAL:HG22	1:E:399:TRP:H	1.82	0.44
1:F:171:ARG:HB2	1:F:433:VAL:HB	1.99	0.44
1:F:220:ILE:H	1:F:220:ILE:HG12	1.51	0.44
1:G:302:LEU:HG	1:G:304:GLN:HG2	2.00	0.44
1:H:142:LEU:HB2	1:H:171:ARG:HA	2.00	0.44
1:H:148:GLN:NE2	1:H:149:ASP:OD1	2.51	0.44
1:A:202:GLY:O	1:A:348:LYS:N	2.47	0.44
1:A:298:TYR:HE2	1:A:306:SER:OG	2.01	0.44
1:A:394:HIS:H	1:A:394:HIS:CD2	2.35	0.44
1:B:20:ARG:HG2	1:B:65:PHE:CE1	2.52	0.44
1:B:222:TYR:C	1:B:222:TYR:CD1	2.95	0.44
1:B:290:SER:HB3	1:B:295:VAL:HG11	2.00	0.44
1:B:352:HIS:HD2	1:B:354:ILE:CG2	2.30	0.44
1:B:376:THR:HG23	1:B:402:LEU:O	2.17	0.44
1:C:395:MET:HE2	1:C:395:MET:HB2	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:GLN:HG3	1:D:442:TRP:CZ3	2.53	0.44
1:E:116:THR:H	1:E:121:PHE:HE1	1.64	0.44
1:F:282:THR:OG1	1:F:459:PRO:HA	2.18	0.44
1:F:337:PRO:HG2	1:F:467:TRP:NE1	2.33	0.44
1:G:11:PHE:O	1:G:115:ALA:HB3	2.18	0.44
1:G:386:PRO:HD3	1:H:408:PHE:CD2	2.53	0.44
1:G:388:LEU:CD2	1:H:419:ARG:HD3	2.48	0.44
1:H:180:THR:CG2	1:H:371:LEU:HA	2.48	0.44
1:A:293:LYS:HA	1:A:293:LYS:HD3	1.85	0.44
1:B:14:THR:HG21	1:B:47:SER:O	2.18	0.44
1:B:114:LEU:HD21	1:B:140:LEU:HD11	1.99	0.44
1:B:285:TYR:N	1:B:310:THR:OG1	2.51	0.44
1:D:11:PHE:CD1	1:D:113:TYR:O	2.71	0.44
1:E:214:VAL:O	1:E:334:LYS:HD3	2.18	0.44
1:E:448:ILE:H	1:E:448:ILE:HG13	1.57	0.44
1:G:93:PRO:O	1:G:94:THR:C	2.61	0.44
1:H:212:GLU:O	1:H:336:LEU:N	2.49	0.44
1:A:281:VAL:HG11	1:A:472:ALA:HB2	1.99	0.43
1:C:253:GLU:O	1:C:257:VAL:HG23	2.18	0.43
1:D:268:LEU:HD21	1:D:316:ALA:HB1	1.99	0.43
1:E:350:VAL:HG13	1:E:362:LEU:HD21	1.98	0.43
1:G:144:LYS:HD2	1:G:231:ASP:O	2.18	0.43
1:G:179:GLU:OE1	1:H:384:LYS:NZ	2.51	0.43
1:H:170:TYR:HA	1:H:432:PHE:HB3	2.00	0.43
1:H:219:ARG:HB3	1:H:222:TYR:CD1	2.51	0.43
1:H:382:MET:HE3	1:H:382:MET:HB3	1.83	0.43
1:A:80:LEU:HA	1:A:83:LEU:HD12	2.00	0.43
1:A:289:VAL:HA	1:A:293:LYS:O	2.18	0.43
1:A:439:GLU:O	1:A:443:ILE:HG22	2.18	0.43
1:B:246:MET:HE3	1:B:260:GLU:HB2	1.99	0.43
1:C:315:LYS:HE2	1:C:327:PRO:HB3	2.01	0.43
1:C:438:VAL:HA	1:C:441:GLN:NE2	2.31	0.43
1:D:202:GLY:CA	1:D:348:LYS:HB2	2.49	0.43
1:G:39:LEU:O	1:G:82:LYS:HD3	2.18	0.43
1:G:167:LYS:HG3	1:G:168:GLN:N	2.33	0.43
1:G:364:PRO:O	1:G:366:LYS:NZ	2.51	0.43
1:H:165:SER:H	1:H:168:GLN:HG3	1.83	0.43
1:H:449:ARG:HA	1:H:452:TRP:HB2	2.00	0.43
1:B:89:ASP:OD2	1:B:91:THR:HB	2.18	0.43
1:B:215:GLY:H	1:B:335:ARG:NE	2.16	0.43
1:C:193:LEU:H	1:C:193:LEU:HG	1.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:THR:HA	1:D:425:ILE:O	2.19	0.43
1:D:377:ILE:HB	1:D:402:LEU:HD23	1.99	0.43
1:E:211:ALA:HB3	1:E:340:ARG:H	1.83	0.43
1:G:147:GLY:HA3	1:G:152:SER:OG	2.18	0.43
1:H:235:SER:HG	1:H:236:HIS:H	1.66	0.43
1:A:114:LEU:C	1:A:116:THR:N	2.76	0.43
1:B:13:SER:HA	1:B:18:SER:HB2	1.98	0.43
1:B:415:ILE:HG22	1:B:418:GLU:CG	2.48	0.43
1:B:475:LEU:HD12	1:B:478:ARG:HE	1.83	0.43
1:C:62:LEU:HD12	1:C:76:LYS:HA	1.99	0.43
1:C:258:ARG:HE	1:C:434:ARG:HD3	1.83	0.43
1:C:388:LEU:HA	1:D:419:ARG:HD2	2.00	0.43
1:D:36:ALA:O	1:D:39:LEU:HB2	2.18	0.43
1:D:128:LEU:HD23	1:D:133:LEU:HB2	1.99	0.43
1:F:277:ILE:H	1:F:277:ILE:HG13	1.61	0.43
1:G:211:ALA:HB1	1:G:338:ALA:O	2.18	0.43
1:G:361:ILE:O	1:G:362:LEU:C	2.60	0.43
1:H:149:ASP:HB2	1:H:446:ASP:OD2	2.18	0.43
1:A:34:LEU:HD11	1:A:414:ARG:HH22	1.83	0.43
1:A:92:ASP:HB3	1:A:95:GLN:NE2	2.34	0.43
1:A:321:TRP:CZ2	1:D:351:PRO:HD2	2.53	0.43
1:B:10:LEU:HB3	1:B:42:VAL:O	2.19	0.43
1:B:216:LEU:HB2	1:B:220:ILE:CG2	2.43	0.43
1:B:420:LEU:HD23	1:B:431:LEU:HD13	1.99	0.43
1:C:223:PHE:HE2	1:C:228:SER:HA	1.83	0.43
1:D:146:LEU:HD12	1:D:146:LEU:O	2.18	0.43
1:D:340:ARG:HH11	1:D:368:ARG:HH22	1.66	0.43
1:D:370:VAL:O	1:D:375:GLU:HA	2.18	0.43
1:E:173:ASP:OD2	1:E:235:SER:C	2.61	0.43
1:F:40:ARG:HA	1:F:84:PHE:CD2	2.51	0.43
1:G:254:ALA:HB2	1:G:430:THR:HG22	1.99	0.43
1:G:404:LEU:HD21	1:H:383:VAL:HG21	2.00	0.43
1:H:5:VAL:HA	1:H:109:GLY:HA3	2.01	0.43
1:H:460:LYS:NZ	1:H:471:THR:HG23	2.33	0.43
1:H:476:VAL:HG22	1:H:481:VAL:CG2	2.42	0.43
1:A:194:PHE:C	1:A:196:PRO:HD2	2.43	0.43
1:A:309:GLU:C	1:A:311:PHE:N	2.74	0.43
1:B:215:GLY:HA3	1:B:335:ARG:HD2	2.00	0.43
1:B:311:PHE:HB2	1:B:462:TYR:OH	2.19	0.43
1:G:450:GLU:O	1:G:453:LYS:N	2.50	0.43
1:H:118:SER:HA	1:H:121:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:LYS:HA	1:H:134:ALA:HB3	1.99	0.43
1:H:313:ALA:HA	1:H:330:ILE:O	2.18	0.43
1:A:29:LEU:HD23	1:A:34:LEU:HD12	2.01	0.43
1:B:70:ARG:HH11	1:B:414:ARG:CB	2.30	0.43
1:B:177:GLY:HA3	1:B:420:LEU:HD11	2.00	0.43
1:B:240:LEU:O	1:B:244:VAL:HG23	2.18	0.43
1:C:237:ILE:O	1:C:238:LEU:C	2.62	0.43
1:D:185:LEU:HD22	1:D:185:LEU:HA	1.76	0.43
1:E:41:ILE:HB	1:E:83:LEU:HD12	2.00	0.43
1:E:89:ASP:H	1:E:95:GLN:HG3	1.83	0.43
1:E:166:GLU:C	1:E:169:VAL:HG22	2.44	0.43
1:E:229:LEU:HB2	1:E:312:VAL:HG11	2.01	0.43
1:E:299:ILE:HD13	1:E:299:ILE:HA	1.82	0.43
1:G:17:LEU:HG	1:G:22:LEU:CD2	2.48	0.43
1:G:67:ALA:O	1:G:71:LEU:HB2	2.18	0.43
1:G:118:SER:HB3	1:G:145:PRO:O	2.18	0.43
1:G:197:LEU:C	1:G:199:ASN:N	2.75	0.43
1:H:24:PRO:HA	1:H:62:LEU:CD2	2.49	0.43
1:H:64:ARG:H	1:H:64:ARG:HG3	1.56	0.43
1:H:384:LYS:HE2	1:H:384:LYS:HB3	1.71	0.43
1:A:114:LEU:HD23	1:A:121:PHE:CD1	2.53	0.43
1:B:3:ASN:H	1:B:3:ASN:HD22	1.66	0.43
1:B:259:ASP:HA	1:B:434:ARG:HH22	1.84	0.43
1:D:24:PRO:HA	1:D:66:VAL:HG22	2.00	0.43
1:D:203:ILE:HG12	1:D:347:PHE:CD1	2.54	0.43
1:E:161:LEU:C	1:E:163:VAL:H	2.26	0.43
1:E:342:GLU:HA	1:E:370:VAL:HA	2.00	0.43
1:F:8:MET:N	1:F:40:ARG:O	2.43	0.43
1:F:27:TYR:OH	1:F:75:ALA:HB3	2.18	0.43
1:F:149:ASP:HA	1:F:446:ASP:OD1	2.18	0.43
1:G:161:LEU:HA	1:G:164:PHE:O	2.18	0.43
1:H:139:ARG:NH1	1:H:425:ILE:O	2.47	0.43
1:H:415:ILE:HG22	1:H:417:HIS:H	1.84	0.43
1:A:25:ALA:HB1	1:A:418:GLU:HG3	2.00	0.43
1:A:216:LEU:HD13	1:A:216:LEU:HA	1.87	0.43
1:A:265:PHE:HE2	1:A:437:GLU:HG2	1.83	0.43
1:A:350:VAL:HA	1:B:192:ALA:HB2	2.01	0.43
1:B:385:GLU:HG2	1:B:396:ARG:HB2	2.01	0.43
1:C:25:ALA:HB1	1:C:418:GLU:HG2	2.01	0.43
1:H:285:TYR:CE1	1:H:335:ARG:HG3	2.53	0.43
1:B:272:ASN:HB3	1:B:273:ASN:H	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:H	1:B:361:ILE:HG12	1.50	0.43
1:C:315:LYS:HG2	1:C:329:TYR:CE1	2.54	0.43
1:D:110:ILE:O	1:D:138:SER:HA	2.19	0.43
1:D:176:LEU:HA	1:D:181:VAL:HG11	2.00	0.43
1:D:466:THR:O	1:D:467:TRP:HB2	2.18	0.43
1:E:40:ARG:HG3	1:E:105:PRO:HD2	2.01	0.43
1:G:392:GLY:HA3	1:G:394:HIS:NE2	2.33	0.43
1:H:172:ILE:HG12	1:H:432:PHE:CE1	2.54	0.43
1:A:66:VAL:HB	1:A:71:LEU:HD22	1.99	0.42
1:A:169:VAL:C	1:A:170:TYR:HD1	2.27	0.42
1:A:389:ASP:N	1:A:389:ASP:OD1	2.52	0.42
1:D:79:PHE:O	1:D:83:LEU:HD23	2.19	0.42
1:D:299:ILE:O	1:D:300:ASP:C	2.61	0.42
1:E:100:ALA:O	1:E:104:GLY:N	2.44	0.42
1:E:139:ARG:HD3	1:E:170:TYR:CZ	2.54	0.42
1:E:282:THR:HG22	1:E:283:GLY:H	1.83	0.42
1:F:219:ARG:HD2	1:F:222:TYR:CE2	2.54	0.42
1:G:273:ASN:O	1:G:276:VAL:HG12	2.19	0.42
1:A:54:PHE:O	1:A:57:PHE:HB3	2.19	0.42
1:A:176:LEU:HD21	1:A:239:GLN:HB3	2.00	0.42
1:C:77:ALA:HA	1:C:80:LEU:HD12	2.00	0.42
1:D:45:SER:HB3	1:D:85:TYR:CE2	2.55	0.42
1:D:269:ARG:N	1:D:317:HIS:O	2.44	0.42
1:E:54:PHE:CE2	1:E:84:PHE:C	2.95	0.42
1:E:277:ILE:HD11	1:E:455:ASN:CG	2.44	0.42
1:F:39:LEU:HD23	1:F:40:ARG:H	1.83	0.42
1:G:237:ILE:HG21	1:G:330:ILE:HG23	2.00	0.42
1:H:152:SER:O	1:H:156:ILE:HG13	2.19	0.42
1:A:186:THR:HG21	1:B:384:LYS:N	2.35	0.42
1:B:9:ILE:HG12	1:B:111:ALA:O	2.18	0.42
1:D:121:PHE:O	1:D:125:ILE:HG13	2.18	0.42
1:E:272:ASN:H	1:E:275:THR:HB	1.84	0.42
1:F:9:ILE:O	1:F:113:TYR:N	2.48	0.42
1:F:113:TYR:CE1	1:F:115:ALA:HB2	2.54	0.42
1:F:148:GLN:HA	1:F:230:ARG:HD3	2.01	0.42
1:G:176:LEU:HD23	1:G:176:LEU:HA	1.80	0.42
1:G:252:MET:HG2	1:H:354:ILE:HD12	2.02	0.42
1:H:235:SER:HG	1:H:236:HIS:CE1	2.29	0.42
1:A:229:LEU:HG	1:A:230:ARG:N	2.34	0.42
1:A:385:GLU:CD	1:B:411:ARG:HE	2.26	0.42
1:B:215:GLY:CA	1:B:334:LYS:HE3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:O	1:B:246:MET:N	2.49	0.42
1:C:215:GLY:HA2	1:C:335:ARG:HG2	2.01	0.42
1:C:285:TYR:HB2	1:C:335:ARG:HB2	2.01	0.42
1:E:273:ASN:CA	1:E:451:GLY:HA2	2.48	0.42
1:E:422:LEU:HA	1:E:425:ILE:HD12	2.02	0.42
1:F:315:LYS:HE2	1:F:327:PRO:HB3	2.00	0.42
1:B:216:LEU:H	1:B:216:LEU:CD2	2.23	0.42
1:B:451:GLY:O	1:B:455:ASN:N	2.50	0.42
1:C:75:ALA:HA	1:C:78:LYS:CB	2.49	0.42
1:C:350:VAL:HG12	1:D:192:ALA:HB2	2.01	0.42
1:D:5:VAL:HG21	1:D:111:ALA:N	2.35	0.42
1:D:62:LEU:HA	1:D:66:VAL:HG23	2.02	0.42
1:D:85:TYR:CD1	1:D:86:ALA:N	2.87	0.42
1:E:385:GLU:HB2	1:E:394:HIS:O	2.18	0.42
1:E:438:VAL:O	1:E:441:GLN:HB2	2.18	0.42
1:G:234:GLN:OE1	1:G:441:GLN:HB3	2.19	0.42
1:G:283:GLY:O	1:G:309:GLU:O	2.37	0.42
1:H:183:ASN:OD1	1:H:183:ASN:C	2.63	0.42
1:H:314:ILE:O	1:H:329:TYR:HA	2.19	0.42
1:H:449:ARG:NH1	1:H:453:LYS:NZ	2.68	0.42
1:B:23:LEU:HD22	1:B:23:LEU:HA	1.82	0.42
1:C:348:LYS:HA	1:C:349:PRO:HD3	1.86	0.42
1:C:375:GLU:HB3	1:C:404:LEU:CB	2.48	0.42
1:D:269:ARG:HB2	1:D:317:HIS:HB2	2.02	0.42
1:E:346:GLN:CD	1:E:364:PRO:HG2	2.45	0.42
1:F:152:SER:OG	1:F:153:SER:N	2.53	0.42
1:G:187:LEU:HG	1:G:194:PHE:HE2	1.85	0.42
1:A:153:SER:O	1:A:156:ILE:HG12	2.19	0.42
1:A:169:VAL:C	1:A:170:TYR:CD1	2.98	0.42
1:A:388:LEU:HD22	1:B:419:ARG:CG	2.49	0.42
1:A:476:VAL:HG22	1:A:481:VAL:HG22	2.02	0.42
1:B:255:ASN:O	1:B:434:ARG:NH1	2.51	0.42
1:C:76:LYS:HE3	1:C:76:LYS:HB2	1.66	0.42
1:D:56:ASP:O	1:D:60:LYS:HG3	2.19	0.42
1:E:258:ARG:NH1	1:E:432:PHE:O	2.53	0.42
1:F:70:ARG:NH2	1:F:415:ILE:HD12	2.30	0.42
1:F:188:ARG:NH2	1:F:322:ARG:NH1	2.68	0.42
1:F:238:LEU:HD23	1:F:441:GLN:HG2	2.01	0.42
1:G:277:ILE:H	1:G:277:ILE:HD13	1.84	0.42
1:A:129:LYS:HB2	1:A:129:LYS:HE2	1.42	0.42
1:A:202:GLY:C	1:A:348:LYS:HB2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ARG:NH2	1:C:322:ARG:HH12	2.16	0.42
1:C:197:LEU:O	1:C:199:ASN:N	2.53	0.42
1:C:230:ARG:HD3	1:C:442:TRP:CH2	2.54	0.42
1:D:25:ALA:CB	1:D:418:GLU:HG2	2.49	0.42
1:D:138:SER:O	1:D:164:PHE:HE2	2.03	0.42
1:D:452:TRP:HB2	1:D:457:MET:SD	2.60	0.42
1:E:372:GLN:HG3	1:E:372:GLN:H	1.45	0.42
1:E:419:ARG:CB	1:F:388:LEU:HD22	2.50	0.42
1:F:142:LEU:HB2	1:F:171:ARG:HA	2.02	0.42
1:F:226:SER:HA	1:F:230:ARG:HH11	1.85	0.42
1:G:162:LYS:HE3	1:G:162:LYS:HB3	1.51	0.42
1:H:284:GLN:NE2	1:H:298:TYR:HD2	2.17	0.42
1:B:3:ASN:H	1:B:3:ASN:ND2	2.18	0.42
1:B:197:LEU:HB3	1:B:347:PHE:HE1	1.80	0.42
1:C:186:THR:HG21	1:D:395:MET:HG2	2.02	0.42
1:C:236:HIS:O	1:C:240:LEU:HG	2.20	0.42
1:D:246:MET:CE	1:D:249:PRO:HD3	2.50	0.42
1:D:247:GLU:OE2	1:D:322:ARG:NE	2.53	0.42
1:D:436:ASP:HA	1:D:439:GLU:OE2	2.19	0.42
1:F:476:VAL:CG1	1:F:477:GLU:N	2.83	0.42
1:G:5:VAL:O	1:G:425:ILE:CG2	2.67	0.42
1:H:113:TYR:CE1	1:H:115:ALA:HB2	2.55	0.42
1:H:420:LEU:O	1:H:432:PHE:HZ	2.03	0.42
1:A:18:SER:HA	1:A:22:LEU:HB2	2.02	0.42
1:A:55:ARG:NH1	1:A:81:ASN:HA	2.35	0.42
1:A:309:GLU:CD	1:A:309:GLU:H	2.23	0.42
1:B:92:ASP:HB3	1:B:95:GLN:NE2	2.34	0.42
1:B:197:LEU:HB3	1:B:347:PHE:CD1	2.54	0.42
1:B:204:ASP:O	1:B:205:HIS:HB3	2.20	0.42
1:B:223:PHE:O	1:B:225:SER:N	2.53	0.42
1:B:432:PHE:CD1	1:B:432:PHE:N	2.87	0.42
1:C:183:ASN:CG	1:D:383:VAL:HG23	2.44	0.42
1:D:5:VAL:HG12	1:D:425:ILE:HA	2.02	0.42
1:D:48:GLU:HA	1:D:87:THR:OG1	2.20	0.42
1:D:449:ARG:O	1:D:453:LYS:N	2.44	0.42
1:E:385:GLU:OE2	1:E:396:ARG:HG3	2.20	0.42
1:E:422:LEU:HA	1:E:422:LEU:HD23	1.78	0.42
1:G:144:LYS:HD3	1:G:236:HIS:NE2	2.35	0.42
1:G:411:ARG:NH1	1:G:411:ARG:H	2.17	0.42
1:H:38:ASP:HA	1:H:40:ARG:HH21	1.85	0.42
1:H:99:ILE:CB	1:H:133:LEU:HD11	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:THR:HG23	1:B:395:MET:HE3	2.02	0.41
1:B:90:ILE:HG13	1:B:120:LEU:HG	2.02	0.41
1:B:222:TYR:CE2	2:B:501:NMN:O3P	2.73	0.41
1:B:418:GLU:HG2	1:B:418:GLU:H	1.65	0.41
1:D:439:GLU:HG2	1:D:439:GLU:H	1.69	0.41
1:F:29:LEU:CG	1:F:418:GLU:HB3	2.50	0.41
1:A:29:LEU:HB3	1:A:35:LEU:HG	2.02	0.41
1:A:179:GLU:HG3	1:B:386:PRO:HB3	2.02	0.41
1:B:160:VAL:O	1:B:164:PHE:N	2.42	0.41
1:B:234:GLN:O	1:B:441:GLN:NE2	2.53	0.41
1:B:415:ILE:HG23	1:B:417:HIS:H	1.85	0.41
1:C:274:ASP:O	1:C:277:ILE:HG22	2.20	0.41
1:C:435:ARG:NH1	1:C:439:GLU:OE1	2.53	0.41
1:D:11:PHE:CE1	1:D:112:ILE:HG23	2.55	0.41
1:D:128:LEU:O	1:D:132:GLY:N	2.51	0.41
1:D:422:LEU:O	1:D:423:ASP:C	2.63	0.41
1:E:19:GLN:HB2	1:E:61:ALA:HB1	2.02	0.41
1:E:107:GLU:C	1:E:109:GLY:N	2.77	0.41
1:F:125:ILE:O	1:F:126:ALA:C	2.62	0.41
1:F:237:ILE:HG21	1:F:330:ILE:HG23	2.01	0.41
1:G:174:HIS:CD2	1:G:236:HIS:NE2	2.88	0.41
1:G:258:ARG:HD2	1:G:434:ARG:HB2	2.01	0.41
1:G:311:PHE:CZ	1:G:469:PRO:HD2	2.55	0.41
1:G:436:ASP:HA	1:G:439:GLU:HG2	2.03	0.41
1:H:48:GLU:HA	1:H:87:THR:OG1	2.20	0.41
1:H:183:ASN:HA	1:H:186:THR:HG23	2.01	0.41
1:H:315:LYS:HE3	1:H:327:PRO:HB3	2.01	0.41
1:H:354:ILE:HG13	1:H:355:PHE:N	2.35	0.41
1:A:90:ILE:HG13	1:A:120:LEU:HG	2.02	0.41
1:A:439:GLU:HG2	1:A:439:GLU:H	1.60	0.41
1:B:322:ARG:HD2	1:B:323:TRP:NE1	2.36	0.41
1:G:318:VAL:HB	1:G:323:TRP:CB	2.49	0.41
1:H:236:HIS:ND1	1:H:236:HIS:N	2.67	0.41
1:H:282:THR:CG2	1:H:309:GLU:HB3	2.51	0.41
1:H:425:ILE:H	1:H:425:ILE:HG12	1.61	0.41
1:A:149:ASP:OD1	1:A:152:SER:HB3	2.20	0.41
1:C:173:ASP:O	1:C:174:HIS:C	2.63	0.41
1:C:205:HIS:CB	1:C:327:PRO:HG2	2.50	0.41
1:C:216:LEU:N	1:C:285:TYR:OH	2.43	0.41
1:C:258:ARG:O	1:C:262:VAL:HG23	2.20	0.41
1:D:70:ARG:HG2	1:D:70:ARG:H	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:HIS:HB3	1:D:421:LEU:HD23	2.03	0.41
1:E:116:THR:O	1:E:117:SER:HB3	2.19	0.41
1:F:127:GLY:O	1:F:131:ALA:N	2.53	0.41
1:G:258:ARG:HA	1:G:261:LYS:HG3	2.01	0.41
1:H:204:ASP:CB	1:H:346:GLN:HE21	2.32	0.41
1:A:281:VAL:HG11	1:A:472:ALA:N	2.35	0.41
1:A:300:ASP:OD1	1:A:300:ASP:N	2.52	0.41
1:A:398:VAL:HG22	1:A:399:TRP:H	1.86	0.41
1:B:113:TYR:CD2	1:B:141:ALA:HB3	2.55	0.41
1:C:360:GLY:HA2	1:C:395:MET:H	1.86	0.41
1:C:370:VAL:HG11	1:C:374:ASP:OD1	2.20	0.41
1:D:25:ALA:CA	1:D:418:GLU:HG2	2.50	0.41
1:D:246:MET:HE3	1:D:260:GLU:CB	2.44	0.41
1:E:116:THR:HB	1:E:120:LEU:HD22	2.03	0.41
1:E:400:LEU:HB3	1:F:400:LEU:HB3	2.03	0.41
1:F:39:LEU:HD23	1:F:40:ARG:N	2.36	0.41
1:F:270:PRO:HA	1:F:444:TRP:CD1	2.56	0.41
1:G:44:THR:CB	1:G:86:ALA:O	2.67	0.41
1:H:51:THR:HA	1:H:85:TYR:CB	2.50	0.41
1:H:254:ALA:O	1:H:255:ASN:HB2	2.20	0.41
1:H:256:ALA:HA	1:H:259:ASP:HB2	2.03	0.41
1:H:289:VAL:HG23	1:H:293:LYS:N	2.35	0.41
1:H:343:ILE:HD11	1:H:371:LEU:HD11	2.02	0.41
1:A:245:ALA:HA	1:A:323:TRP:CZ2	2.55	0.41
1:C:186:THR:O	1:C:190:GLY:N	2.39	0.41
1:C:237:ILE:O	1:C:240:LEU:N	2.53	0.41
1:D:57:PHE:HA	1:D:60:LYS:HD2	2.03	0.41
1:D:246:MET:HE2	1:D:249:PRO:HD3	2.02	0.41
1:F:233:VAL:O	1:F:238:LEU:HB2	2.20	0.41
1:F:259:ASP:O	1:F:263:LYS:HG3	2.20	0.41
1:F:476:VAL:CG2	1:F:481:VAL:HG13	2.50	0.41
1:G:271:ILE:HD13	1:G:271:ILE:N	2.36	0.41
1:G:340:ARG:NH2	1:G:467:TRP:HZ2	2.18	0.41
1:H:220:ILE:HG22	1:H:298:TYR:HE1	1.85	0.41
1:H:476:VAL:O	1:H:481:VAL:HG13	2.21	0.41
1:A:149:ASP:CG	1:A:152:SER:HB3	2.45	0.41
1:A:281:VAL:HG22	1:A:471:THR:HB	2.03	0.41
1:B:144:LYS:N	1:B:145:PRO:CD	2.84	0.41
1:C:228:SER:HB2	1:C:309:GLU:O	2.20	0.41
1:C:320:ASN:O	1:C:321:TRP:C	2.63	0.41
1:D:102:LEU:HD12	1:D:102:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:SER:HB2	1:E:342:GLU:CG	2.50	0.41
1:E:321:TRP:CE2	1:H:351:PRO:HD2	2.55	0.41
1:F:314:ILE:HB	1:F:330:ILE:HD12	2.03	0.41
1:B:34:LEU:O	1:B:422:LEU:HD11	2.21	0.41
1:D:42:VAL:HG13	1:D:102:LEU:HD23	2.01	0.41
1:D:47:SER:O	1:D:85:TYR:OH	2.38	0.41
1:D:466:THR:O	1:D:466:THR:HG23	2.20	0.41
1:E:26:LEU:HA	1:E:26:LEU:HD23	1.79	0.41
1:E:195:GLU:HA	1:E:198:TRP:HB2	2.02	0.41
1:G:302:LEU:HD23	1:G:306:SER:CB	2.51	0.41
1:H:154:ASP:OD1	1:H:435:ARG:NH2	2.53	0.41
1:A:20:ARG:HB3	1:A:65:PHE:CZ	2.56	0.41
1:A:58:ALA:O	1:A:61:ALA:HB3	2.21	0.41
1:A:309:GLU:HB3	1:A:311:PHE:O	2.21	0.41
1:A:408:PHE:O	1:A:409:LYS:C	2.64	0.41
1:B:262:VAL:HG22	1:B:437:GLU:HA	2.02	0.41
1:B:323:TRP:HZ3	1:B:326:VAL:HG11	1.86	0.41
1:B:361:ILE:HG12	1:B:382:MET:HE1	2.01	0.41
1:B:415:ILE:HG23	1:B:417:HIS:N	2.36	0.41
1:C:13:SER:O	1:C:18:SER:O	2.39	0.41
1:D:336:LEU:HD23	1:D:336:LEU:HA	1.73	0.41
1:E:26:LEU:HB3	1:E:79:PHE:HE1	1.82	0.41
1:E:112:ILE:CD1	1:E:138:SER:HB3	2.51	0.41
1:E:226:SER:O	1:E:230:ARG:HB2	2.21	0.41
1:E:233:VAL:HG22	1:E:237:ILE:HD12	2.01	0.41
1:E:238:LEU:HB3	1:E:441:GLN:HE21	1.85	0.41
1:E:382:MET:HE3	1:E:382:MET:HB3	1.78	0.41
1:F:78:LYS:O	1:F:82:LYS:N	2.45	0.41
1:F:112:ILE:HD12	1:F:139:ARG:O	2.20	0.41
1:F:279:HIS:ND1	1:F:315:LYS:HB3	2.36	0.41
1:F:365:ASN:HA	1:F:380:SER:HB2	2.03	0.41
1:G:180:THR:HG23	1:G:375:GLU:HG2	2.02	0.41
1:G:271:ILE:HG12	1:G:271:ILE:O	2.21	0.41
1:G:415:ILE:C	1:G:417:HIS:N	2.77	0.41
1:H:101:ASP:O	1:H:102:LEU:C	2.64	0.41
1:H:185:LEU:HD22	1:H:185:LEU:HA	1.78	0.41
1:H:228:SER:O	1:H:229:LEU:C	2.63	0.41
1:H:240:LEU:HD21	1:H:371:LEU:HD12	2.03	0.41
1:H:456:SER:HB3	1:H:458:LYS:HE2	2.02	0.41
1:A:92:ASP:HB3	1:A:95:GLN:HE21	1.86	0.41
1:A:458:LYS:O	1:A:459:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ASN:HB3	1:B:193:LEU:HD23	2.03	0.41
1:B:219:ARG:HB3	1:B:222:TYR:CE2	2.55	0.41
1:C:216:LEU:HD13	1:C:216:LEU:HA	1.76	0.41
1:D:121:PHE:CD1	1:D:121:PHE:N	2.89	0.41
1:D:206:VAL:HG22	1:D:345:VAL:HG13	2.03	0.41
1:F:16:ASP:O	1:F:20:ARG:N	2.47	0.41
1:F:476:VAL:HG22	1:F:481:VAL:C	2.46	0.41
1:G:129:LYS:HA	1:G:134:ALA:HB2	2.03	0.41
1:H:41:ILE:HD13	1:H:79:PHE:CE1	2.53	0.41
1:H:435:ARG:HD3	1:H:435:ARG:O	2.21	0.41
1:A:128:LEU:CD2	1:A:133:LEU:HD12	2.51	0.40
1:A:180:THR:HG23	1:A:375:GLU:HB3	2.01	0.40
1:B:304:GLN:H	1:B:304:GLN:CD	2.26	0.40
1:B:353:SER:C	1:B:355:PHE:N	2.79	0.40
1:E:29:LEU:HD11	1:E:418:GLU:O	2.21	0.40
1:E:89:ASP:HB3	1:E:95:GLN:HE21	1.86	0.40
1:E:117:SER:HA	2:E:501:NMN:O3R	2.21	0.40
1:E:475:LEU:O	1:E:478:ARG:HG2	2.19	0.40
1:F:203:ILE:HG23	1:F:346:GLN:O	2.21	0.40
1:G:253:GLU:HB3	1:G:256:ALA:HB3	2.02	0.40
1:G:376:THR:HG22	1:G:377:ILE:N	2.36	0.40
1:A:197:LEU:HA	1:A:197:LEU:HD23	1.70	0.40
1:C:26:LEU:O	1:C:29:LEU:N	2.50	0.40
1:D:11:PHE:O	1:D:115:ALA:HB3	2.21	0.40
1:D:226:SER:C	1:D:230:ARG:HB2	2.46	0.40
1:E:200:SER:N	1:E:322:ARG:O	2.54	0.40
1:E:472:ALA:O	1:E:473:ILE:C	2.65	0.40
1:G:37:ASP:O	1:G:40:ARG:NH2	2.54	0.40
1:G:146:LEU:HD23	1:G:146:LEU:N	2.35	0.40
1:G:238:LEU:HA	1:G:238:LEU:HD12	1.68	0.40
1:G:470:ILE:H	1:G:470:ILE:HG12	1.69	0.40
1:A:197:LEU:HD22	1:A:202:GLY:HA3	2.03	0.40
1:A:387:GLY:HA3	1:A:394:HIS:HE1	1.83	0.40
1:A:457:MET:HE3	1:A:457:MET:HB3	1.61	0.40
1:B:10:LEU:HD12	1:B:11:PHE:H	1.87	0.40
1:B:192:ALA:O	1:B:196:PRO:HD3	2.21	0.40
1:B:311:PHE:CE1	1:B:469:PRO:HD2	2.56	0.40
1:B:352:HIS:CD2	1:B:354:ILE:HG22	2.56	0.40
1:D:269:ARG:CB	1:D:317:HIS:HB2	2.51	0.40
1:E:472:ALA:C	1:E:474:ALA:N	2.78	0.40
1:G:144:LYS:HE2	2:G:501:NMN:C5	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:LEU:HD23	1:G:268:LEU:HA	1.83	0.40
1:G:382:MET:H	1:H:191:ASN:ND2	2.19	0.40
1:G:457:MET:HE3	1:G:457:MET:HB3	1.78	0.40
1:H:5:VAL:HG22	1:H:109:GLY:CA	2.51	0.40
1:H:30:ASP:CA	1:H:35:LEU:HD11	2.43	0.40
1:H:112:ILE:O	1:H:140:LEU:HA	2.21	0.40
1:H:299:ILE:H	1:H:299:ILE:HG12	1.60	0.40
1:H:323:TRP:O	1:H:324:HIS:C	2.64	0.40
1:A:209:SER:O	1:A:341:SER:HA	2.20	0.40
1:A:260:GLU:O	1:A:264:VAL:HG23	2.22	0.40
1:C:448:ILE:HG22	1:C:452:TRP:CE3	2.56	0.40
1:F:16:ASP:HA	1:F:19:GLN:HE21	1.86	0.40
1:F:419:ARG:CZ	1:F:431:LEU:HD21	2.51	0.40
1:G:5:VAL:O	1:G:6:SER:CB	2.69	0.40
1:G:21:MET:HB3	1:G:417:HIS:ND1	2.37	0.40
1:G:388:LEU:CD1	1:H:34:LEU:HD13	2.52	0.40
1:H:158:ASP:C	1:H:160:VAL:N	2.78	0.40
1:H:419:ARG:HG3	1:H:431:LEU:CD1	2.52	0.40
1:A:329:TYR:CE2	1:A:481:VAL:HG11	2.57	0.40
1:B:253:GLU:O	1:B:254:ALA:C	2.64	0.40
1:B:442:TRP:O	1:B:443:ILE:C	2.64	0.40
1:D:5:VAL:HG23	1:D:109:GLY:O	2.21	0.40
1:D:378:GLN:HB3	1:D:401:ASP:OD1	2.22	0.40
1:E:25:ALA:HA	1:E:418:GLU:CG	2.51	0.40
1:H:180:THR:HG21	1:H:371:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/487 (99%)	446 (93%)	34 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	473/487 (97%)	438 (93%)	35 (7%)	0	100	100
1	C	457/487 (94%)	408 (89%)	49 (11%)	0	100	100
1	D	475/487 (98%)	430 (90%)	45 (10%)	0	100	100
1	E	470/487 (96%)	423 (90%)	45 (10%)	2 (0%)	30	59
1	F	452/487 (93%)	413 (91%)	39 (9%)	0	100	100
1	G	483/487 (99%)	453 (94%)	30 (6%)	0	100	100
1	H	477/487 (98%)	431 (90%)	46 (10%)	0	100	100
All	All	3767/3896 (97%)	3442 (91%)	323 (9%)	2 (0%)	48	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	57	PHE
1	E	117	SER

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	386/409 (94%)	295 (76%)	91 (24%)	1	3
1	B	372/409 (91%)	301 (81%)	71 (19%)	1	6
1	C	214/409 (52%)	189 (88%)	25 (12%)	5	21
1	D	352/409 (86%)	293 (83%)	59 (17%)	2	10
1	E	364/409 (89%)	292 (80%)	72 (20%)	1	5
1	F	321/409 (78%)	259 (81%)	62 (19%)	1	6
1	G	392/409 (96%)	324 (83%)	68 (17%)	2	9
1	H	383/409 (94%)	322 (84%)	61 (16%)	2	11
All	All	2784/3272 (85%)	2275 (82%)	509 (18%)	2	7

All (509) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	16	ASP
1	A	17	LEU
1	A	18	SER
1	A	19	GLN
1	A	20	ARG
1	A	22	LEU
1	A	26	LEU
1	A	34	LEU
1	A	37	ASP
1	A	38	ASP
1	A	39	LEU
1	A	43	CYS
1	A	44	THR
1	A	45	SER
1	A	48	GLU
1	A	56	ASP
1	A	69	ASP
1	A	71	LEU
1	A	87	THR
1	A	90	ILE
1	A	91	THR
1	A	94	THR
1	A	98	LYS
1	A	102	LEU
1	A	116	THR
1	A	117	SER
1	A	129	LYS
1	A	133	LEU
1	A	138	SER
1	A	143	GLU
1	A	144	LYS
1	A	146	LEU
1	A	153	SER
1	A	156	ILE
1	A	179	GLU
1	A	180	THR
1	A	183	ASN
1	A	216	LEU
1	A	217	GLU
1	A	219	ARG
1	A	220	ILE
1	A	222	TYR

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Mol	Chain	Res	Type
1	A	224	ASP
1	A	225	SER
1	A	228	SER
1	A	229	LEU
1	A	240	LEU
1	A	268	LEU
1	A	269	ARG
1	A	271	ILE
1	A	273	ASN
1	A	274	ASP
1	A	277	ILE
1	A	282	THR
1	A	284	GLN
1	A	285	TYR
1	A	299	ILE
1	A	300	ASP
1	A	304	GLN
1	A	308	THR
1	A	309	GLU
1	A	310	THR
1	A	350	VAL
1	A	355	PHE
1	A	357	SER
1	A	369	ILE
1	A	374	ASP
1	A	384	LYS
1	A	389	ASP
1	A	394	HIS
1	A	405	THR
1	A	407	VAL
1	A	409	LYS
1	A	412	LYS
1	A	414	ARG
1	A	419	ARG
1	A	422	LEU
1	A	425	ILE
1	A	426	GLU
1	A	431	LEU
1	A	439	GLU
1	A	448	ILE
1	A	449	ARG
1	A	450	GLU

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Mol	Chain	Res	Type
1	A	457	MET
1	A	458	LYS
1	A	460	LYS
1	A	471	THR
1	A	475	LEU
1	A	476	VAL
1	B	3	ASN
1	B	6	SER
1	B	8	MET
1	B	19	GLN
1	B	21	MET
1	B	22	LEU
1	B	23	LEU
1	B	39	LEU
1	B	43	CYS
1	B	46	ARG
1	B	47	SER
1	B	50	ASP
1	B	69	ASP
1	B	78	LYS
1	B	80	LEU
1	B	83	LEU
1	B	88	VAL
1	B	90	ILE
1	B	91	THR
1	B	94	THR
1	B	95	GLN
1	B	98	LYS
1	B	118	SER
1	B	120	LEU
1	B	125	ILE
1	B	139	ARG
1	B	143	GLU
1	B	144	LYS
1	B	148	GLN
1	B	153	SER
1	B	156	ILE
1	B	161	LEU
1	B	169	VAL
1	B	191	ASN
1	B	193	LEU
1	B	200	SER

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Mol	Chain	Res	Type
1	B	201	LYS
1	B	203	ILE
1	B	216	LEU
1	B	217	GLU
1	B	219	ARG
1	B	220	ILE
1	B	222	TYR
1	B	229	LEU
1	B	233	VAL
1	B	302	LEU
1	B	331	ARG
1	B	332	THR
1	B	356	SER
1	B	361	ILE
1	B	378	GLN
1	B	379	ILE
1	B	380	SER
1	B	382	MET
1	B	384	LYS
1	B	394	HIS
1	B	411	ARG
1	B	414	ARG
1	B	415	ILE
1	B	417	HIS
1	B	418	GLU
1	B	419	ARG
1	B	423	ASP
1	B	425	ILE
1	B	431	LEU
1	B	433	VAL
1	B	445	ILE
1	B	449	ARG
1	B	453	LYS
1	B	475	LEU
1	B	477	GLU
1	C	62	LEU
1	C	76	LYS
1	C	80	LEU
1	C	193	LEU
1	C	197	LEU
1	C	201	LYS
1	C	216	LEU

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Mol	Chain	Res	Type
1	C	225	SER
1	C	228	SER
1	C	229	LEU
1	C	302	LEU
1	C	307	ASP
1	C	309	GLU
1	C	312	VAL
1	C	315	LYS
1	C	335	ARG
1	C	362	LEU
1	C	380	SER
1	C	381	ILE
1	C	384	LYS
1	C	388	LEU
1	C	395	MET
1	C	419	ARG
1	C	423	ASP
1	C	461	THR
1	D	4	THR
1	D	5	VAL
1	D	6	SER
1	D	17	LEU
1	D	21	MET
1	D	44	THR
1	D	49	TYR
1	D	50	ASP
1	D	51	THR
1	D	69	ASP
1	D	94	THR
1	D	102	LEU
1	D	125	ILE
1	D	128	LEU
1	D	130	GLN
1	D	138	SER
1	D	139	ARG
1	D	166	GLU
1	D	171	ARG
1	D	172	ILE
1	D	174	HIS
1	D	178	LYS
1	D	183	ASN
1	D	185	LEU

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Mol	Chain	Res	Type
1	D	187	LEU
1	D	203	ILE
1	D	228	SER
1	D	229	LEU
1	D	231	ASP
1	D	268	LEU
1	D	269	ARG
1	D	274	ASP
1	D	276	VAL
1	D	277	ILE
1	D	278	THR
1	D	284	GLN
1	D	289	VAL
1	D	295	VAL
1	D	299	ILE
1	D	302	LEU
1	D	362	LEU
1	D	363	GLN
1	D	367	LEU
1	D	370	VAL
1	D	371	LEU
1	D	375	GLU
1	D	376	THR
1	D	379	ILE
1	D	380	SER
1	D	381	ILE
1	D	402	LEU
1	D	424	LEU
1	D	430	THR
1	D	433	VAL
1	D	436	ASP
1	D	439	GLU
1	D	443	ILE
1	D	466	THR
1	D	467	TRP
1	E	7	THR
1	E	8	MET
1	E	16	ASP
1	E	17	LEU
1	E	21	MET
1	E	23	LEU
1	E	39	LEU

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Mol	Chain	Res	Type
1	E	41	ILE
1	E	42	VAL
1	E	56	ASP
1	E	59	GLU
1	E	71	LEU
1	E	78	LYS
1	E	80	LEU
1	E	82	LYS
1	E	83	LEU
1	E	87	THR
1	E	88	VAL
1	E	95	GLN
1	E	98	LYS
1	E	117	SER
1	E	118	SER
1	E	122	GLU
1	E	133	LEU
1	E	140	LEU
1	E	144	LYS
1	E	146	LEU
1	E	150	LEU
1	E	156	ILE
1	E	160	VAL
1	E	161	LEU
1	E	165	SER
1	E	181	VAL
1	E	214	VAL
1	E	216	LEU
1	E	220	ILE
1	E	229	LEU
1	E	230	ARG
1	E	232	MET
1	E	268	LEU
1	E	269	ARG
1	E	274	ASP
1	E	276	VAL
1	E	277	ILE
1	E	289	VAL
1	E	290	SER
1	E	309	GLU
1	E	335	ARG
1	E	339	ARG

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Mol	Chain	Res	Type
1	E	342	GLU
1	E	350	VAL
1	E	352	HIS
1	E	356	SER
1	E	371	LEU
1	E	372	GLN
1	E	374	ASP
1	E	388	LEU
1	E	404	LEU
1	E	405	THR
1	E	407	VAL
1	E	414	ARG
1	E	415	ILE
1	E	419	ARG
1	E	426	GLU
1	E	428	ASP
1	E	433	VAL
1	E	435	ARG
1	E	443	ILE
1	E	445	ILE
1	E	448	ILE
1	E	475	LEU
1	E	476	VAL
1	F	14	THR
1	F	16	ASP
1	F	20	ARG
1	F	21	MET
1	F	30	ASP
1	F	39	LEU
1	F	42	VAL
1	F	46	ARG
1	F	62	LEU
1	F	64	ARG
1	F	66	VAL
1	F	79	PHE
1	F	83	LEU
1	F	93	PRO
1	F	98	LYS
1	F	112	ILE
1	F	133	LEU
1	F	138	SER
1	F	140	LEU

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Mol	Chain	Res	Type
1	F	142	LEU
1	F	164	PHE
1	F	165	SER
1	F	168	GLN
1	F	199	ASN
1	F	201	LYS
1	F	213	THR
1	F	214	VAL
1	F	216	LEU
1	F	217	GLU
1	F	220	ILE
1	F	224	ASP
1	F	243	LEU
1	F	244	VAL
1	F	261	LYS
1	F	263	LYS
1	F	264	VAL
1	F	271	ILE
1	F	273	ASN
1	F	274	ASP
1	F	275	THR
1	F	276	VAL
1	F	277	ILE
1	F	278	THR
1	F	308	THR
1	F	311	PHE
1	F	339	ARG
1	F	345	VAL
1	F	346	GLN
1	F	355	PHE
1	F	384	LYS
1	F	411	ARG
1	F	413	ARG
1	F	418	GLU
1	F	419	ARG
1	F	423	ASP
1	F	426	GLU
1	F	431	LEU
1	F	445	ILE
1	F	450	GLU
1	F	452	TRP
1	F	461	THR

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Mol	Chain	Res	Type
1	F	466	THR
1	G	3	ASN
1	G	5	VAL
1	G	6	SER
1	G	9	ILE
1	G	13	SER
1	G	30	ASP
1	G	39	LEU
1	G	40	ARG
1	G	42	VAL
1	G	51	THR
1	G	52	ASP
1	G	59	GLU
1	G	60	LYS
1	G	64	ARG
1	G	69	ASP
1	G	71	LEU
1	G	72	ASN
1	G	74	ASP
1	G	87	THR
1	G	90	ILE
1	G	95	GLN
1	G	101	ASP
1	G	102	LEU
1	G	161	LEU
1	G	162	LYS
1	G	163	VAL
1	G	188	ARG
1	G	191	ASN
1	G	193	LEU
1	G	197	LEU
1	G	200	SER
1	G	203	ILE
1	G	261	LYS
1	G	263	LYS
1	G	264	VAL
1	G	271	ILE
1	G	274	ASP
1	G	275	THR
1	G	277	ILE
1	G	293	LYS
1	G	302	LEU

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Mol	Chain	Res	Type
1	G	304	GLN
1	G	309	GLU
1	G	312	VAL
1	G	355	PHE
1	G	357	SER
1	G	362	LEU
1	G	363	GLN
1	G	366	LYS
1	G	371	LEU
1	G	372	GLN
1	G	383	VAL
1	G	384	LYS
1	G	388	LEU
1	G	394	HIS
1	G	395	MET
1	G	397	GLU
1	G	410	ASP
1	G	411	ARG
1	G	413	ARG
1	G	414	ARG
1	G	457	MET
1	G	466	THR
1	G	471	THR
1	G	473	ILE
1	G	477	GLU
1	G	478	ARG
1	G	479	ASP
1	H	5	VAL
1	H	8	MET
1	H	17	LEU
1	H	18	SER
1	H	30	ASP
1	H	34	LEU
1	H	35	LEU
1	H	38	ASP
1	H	40	ARG
1	H	43	CYS
1	H	46	ARG
1	H	49	TYR
1	H	60	LYS
1	H	62	LEU
1	H	64	ARG

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Mol	Chain	Res	Type
1	H	71	LEU
1	H	73	ASP
1	H	76	LYS
1	H	80	LEU
1	H	82	LYS
1	H	99	ILE
1	H	133	LEU
1	H	155	HIS
1	H	156	ILE
1	H	165	SER
1	H	168	GLN
1	H	185	LEU
1	H	186	THR
1	H	187	LEU
1	H	220	ILE
1	H	222	TYR
1	H	271	ILE
1	H	274	ASP
1	H	276	VAL
1	H	289	VAL
1	H	290	SER
1	H	293	LYS
1	H	334	LYS
1	H	340	ARG
1	H	356	SER
1	H	374	ASP
1	H	375	GLU
1	H	385	GLU
1	H	388	LEU
1	H	402	LEU
1	H	403	SER
1	H	405	THR
1	H	409	LYS
1	H	422	LEU
1	H	424	LEU
1	H	425	ILE
1	H	426	GLU
1	H	430	THR
1	H	466	THR
1	H	473	ILE
1	H	475	LEU
1	H	476	VAL

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Mol	Chain	Res	Type
1	H	477	GLU
1	H	481	VAL
1	H	486	LEU
1	H	487	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	174	HIS
1	A	365	ASN
1	A	394	HIS
1	A	441	GLN
1	A	455	ASN
1	B	19	GLN
1	B	81	ASN
1	B	155	HIS
1	B	199	ASN
1	B	205	HIS
1	B	352	HIS
1	C	207	GLN
1	C	365	ASN
1	D	157	ASN
1	D	174	HIS
1	D	199	ASN
1	D	205	HIS
1	D	251	HIS
1	D	324	HIS
1	D	346	GLN
1	D	378	GLN
1	D	455	ASN
1	E	19	GLN
1	E	72	ASN
1	E	155	HIS
1	E	324	HIS
1	E	346	GLN
1	E	365	ASN
1	E	441	GLN
1	F	19	GLN
1	F	183	ASN
1	F	234	GLN
1	F	236	HIS

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Mol	Chain	Res	Type
1	F	279	HIS
1	F	346	GLN
1	G	3	ASN
1	G	19	GLN
1	G	81	ASN
1	G	168	GLN
1	G	174	HIS
1	G	284	GLN
1	H	19	GLN
1	H	81	ASN
1	H	130	GLN
1	H	284	GLN
1	H	346	GLN
1	H	394	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	NMN	G	501	-	21,23,23	0.96	2 (9%)	27,34,34	1.09	2 (7%)
2	NMN	E	501	-	21,23,23	0.91	2 (9%)	27,34,34	0.97	2 (7%)
2	NMN	B	501	-	21,23,23	1.02	2 (9%)	27,34,34	1.12	3 (11%)
2	NMN	A	501	-	21,23,23	0.96	2 (9%)	27,34,34	1.23	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMN	G	501	-	-	1/14/30/30	0/2/2/2
2	NMN	E	501	-	-	6/14/30/30	0/2/2/2
2	NMN	B	501	-	-	2/14/30/30	0/2/2/2
2	NMN	A	501	-	-	3/14/30/30	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NMN	O4R-C1R	3.20	1.45	1.40
2	B	501	NMN	C2-N1	2.75	1.38	1.35
2	A	501	NMN	O4R-C1R	2.65	1.44	1.40
2	G	501	NMN	C2-N1	2.64	1.37	1.35
2	E	501	NMN	C2-N1	2.59	1.37	1.35
2	E	501	NMN	O4R-C1R	2.41	1.44	1.40
2	A	501	NMN	C2-N1	2.17	1.37	1.35
2	G	501	NMN	P-O5R	2.00	1.66	1.60

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	NMN	O3R-C3R-C2R	-3.85	99.49	111.82
2	B	501	NMN	C6-N1-C2	-3.12	119.22	121.88
2	E	501	NMN	C2-C3-C4	2.53	121.21	118.26
2	A	501	NMN	C6-N1-C2	-2.49	119.76	121.88
2	A	501	NMN	C2-C3-C7	-2.30	112.83	119.46
2	E	501	NMN	C4R-O4R-C1R	-2.18	107.93	109.92
2	B	501	NMN	O4R-C4R-C3R	-2.15	100.89	105.15
2	A	501	NMN	C2-C3-C4	2.13	120.73	118.26
2	G	501	NMN	C6-N1-C2	-2.09	120.10	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NMN	C2R-C3R-C4R	-2.06	98.63	102.61

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NMN	O4R-C1R-N1-C2
2	E	501	NMN	O4R-C1R-N1-C2
2	E	501	NMN	O4R-C1R-N1-C6
2	E	501	NMN	C2R-C1R-N1-C2
2	E	501	NMN	C2R-C1R-N1-C6
2	A	501	NMN	C3R-C4R-C5R-O5R
2	G	501	NMN	C4R-C5R-O5R-P
2	A	501	NMN	O4R-C4R-C5R-O5R
2	A	501	NMN	O4R-C1R-N1-C6
2	B	501	NMN	O4R-C1R-N1-C6
2	E	501	NMN	O4R-C4R-C5R-O5R
2	E	501	NMN	C3R-C4R-C5R-O5R

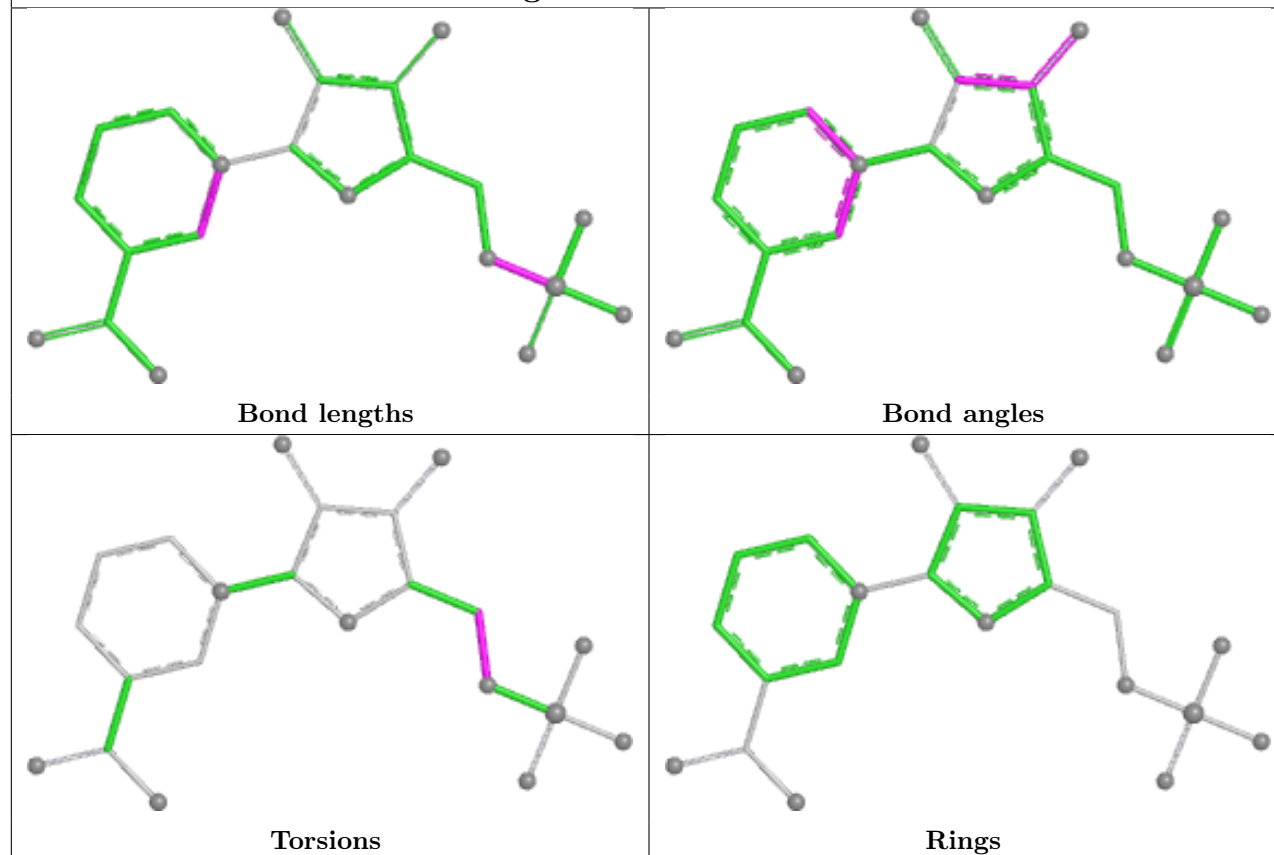
There are no ring outliers.

4 monomers are involved in 31 short contacts:

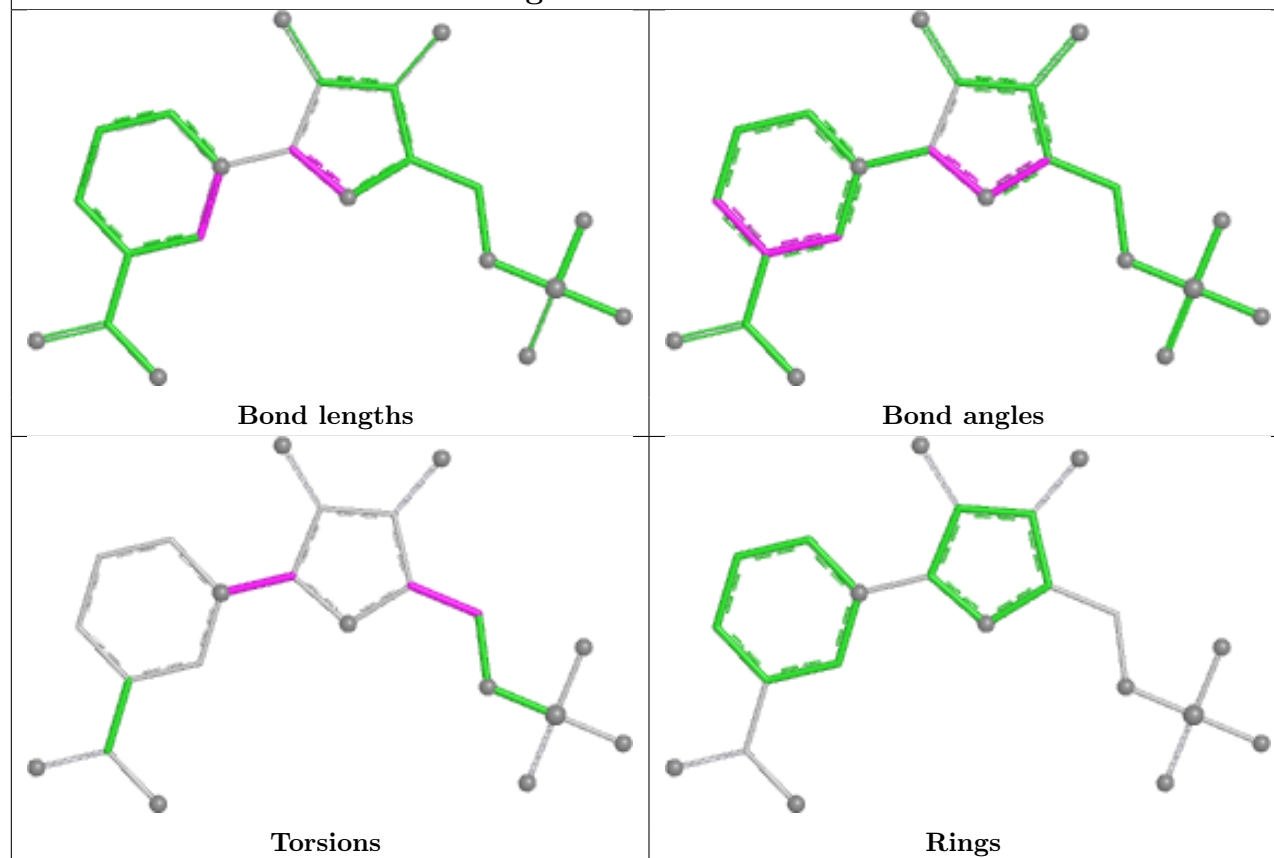
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	NMN	5	0
2	E	501	NMN	4	0
2	B	501	NMN	6	0
2	A	501	NMN	16	0

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.

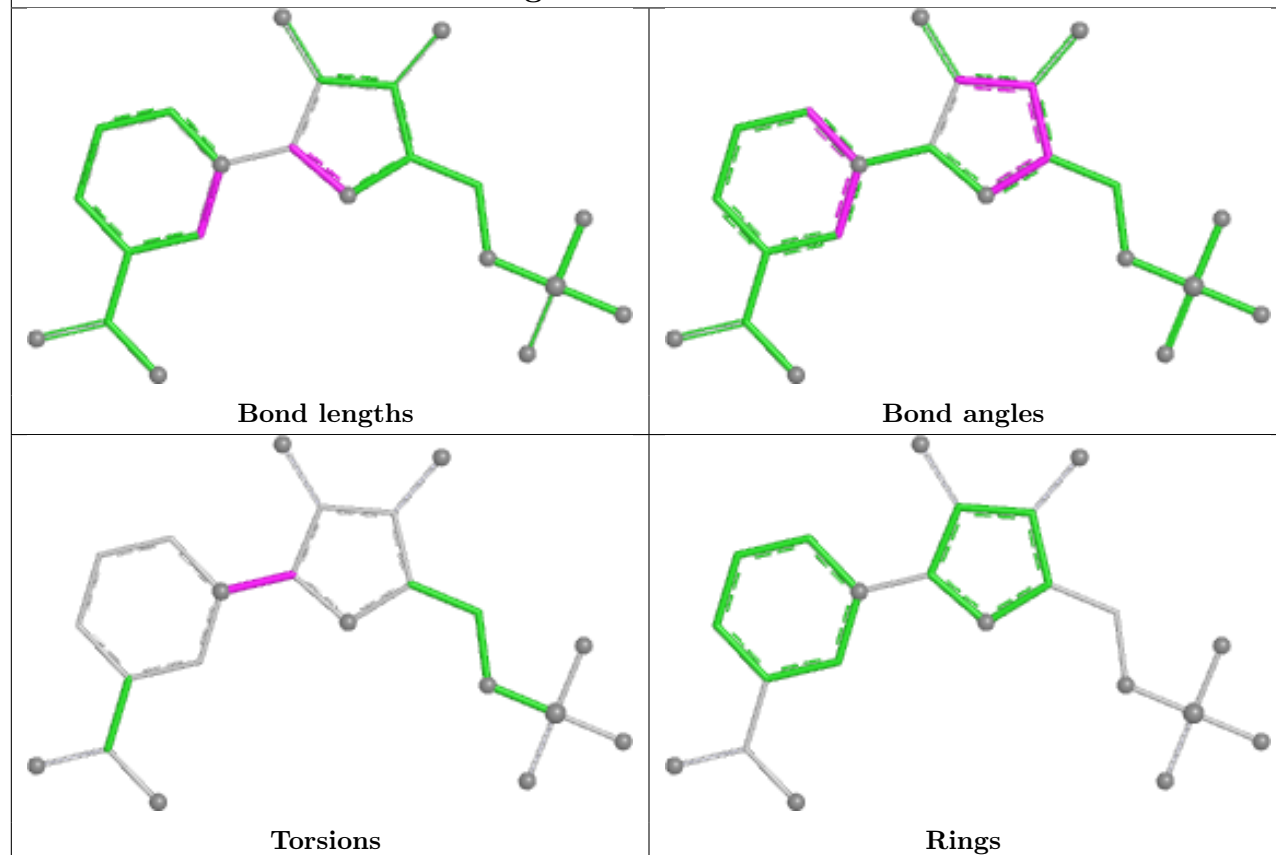
Ligand NMN G 501



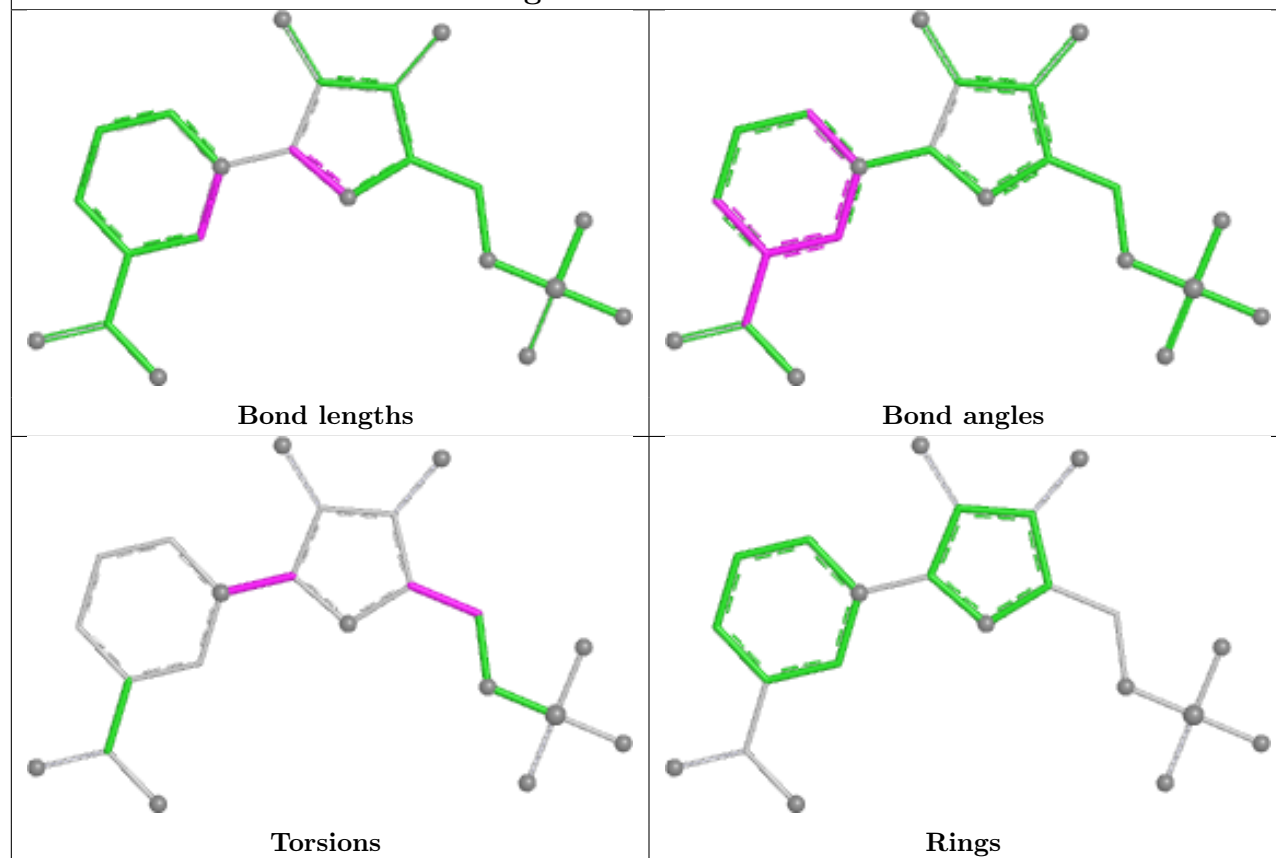
Ligand NMN E 501



Ligand NMN B 501



Ligand NMN A 501



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	482/487 (98%)	-1.33	0 100 100	31, 65, 96, 135	0
1	B	479/487 (98%)	-1.25	0 100 100	26, 63, 129, 151	0
1	C	463/487 (95%)	-1.12	0 100 100	49, 95, 152, 209	0
1	D	479/487 (98%)	-1.31	0 100 100	48, 83, 113, 166	0
1	E	476/487 (97%)	-1.28	0 100 100	40, 81, 116, 139	0
1	F	462/487 (94%)	-1.22	1 (0%) 91 85	42, 82, 173, 204	0
1	G	485/487 (99%)	-1.35	0 100 100	27, 64, 103, 142	0
1	H	481/487 (98%)	-1.34	0 100 100	33, 68, 106, 137	0
All	All	3807/3896 (97%)	-1.28	1 (0%) 100 100	26, 76, 130, 209	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	132	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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,

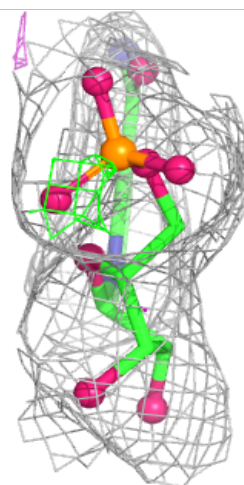
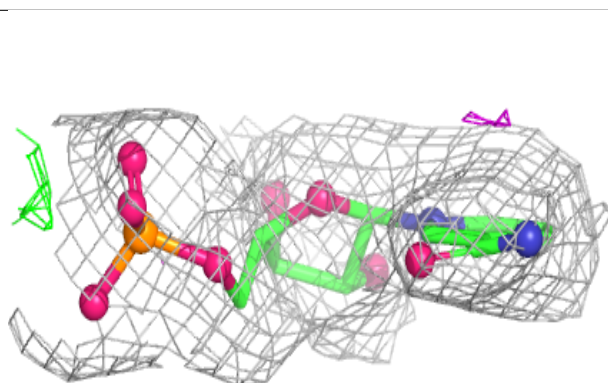
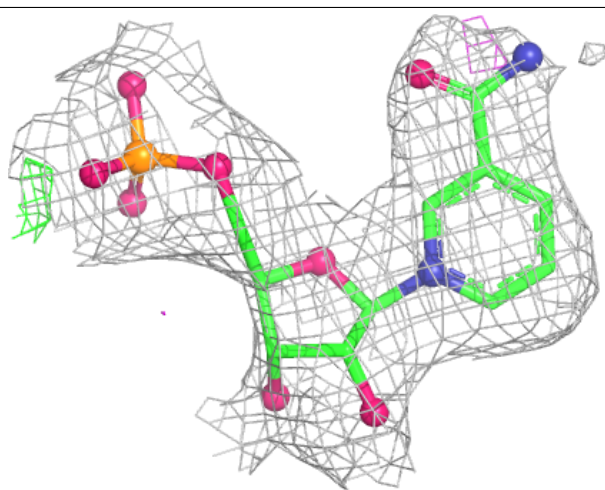
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NMN	G	501	22/22	0.98	0.05	59,71,81,92	0
2	NMN	B	501	22/22	0.99	0.06	87,100,104,172	0
2	NMN	E	501	22/22	0.99	0.03	76,88,102,162	0
2	NMN	A	501	22/22	0.99	0.04	66,73,78,87	0

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

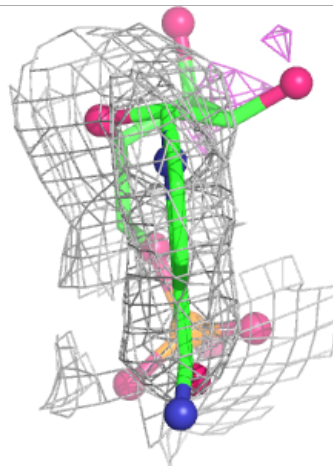
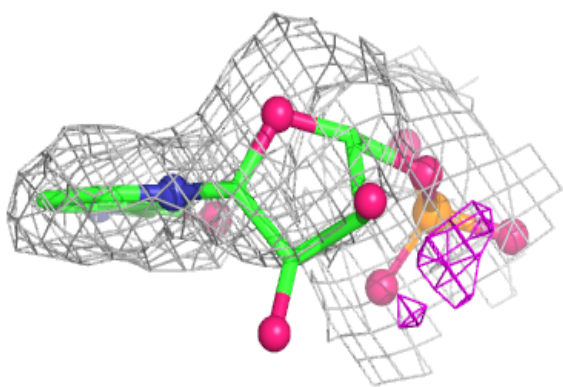
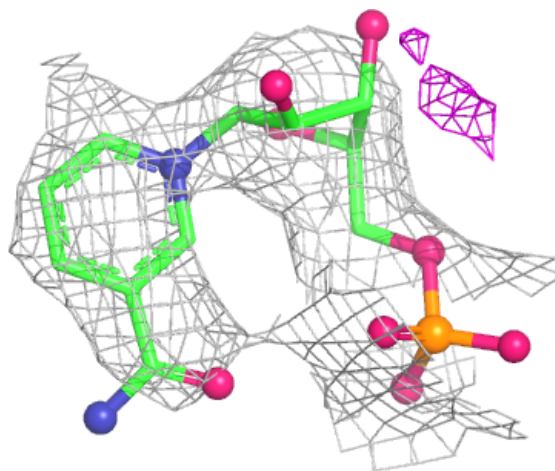
Electron density around NMN G 501:

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



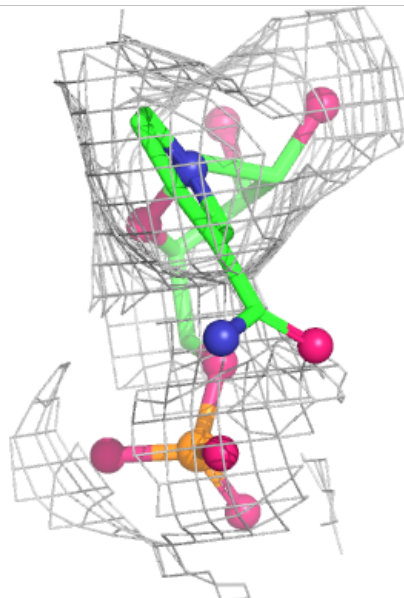
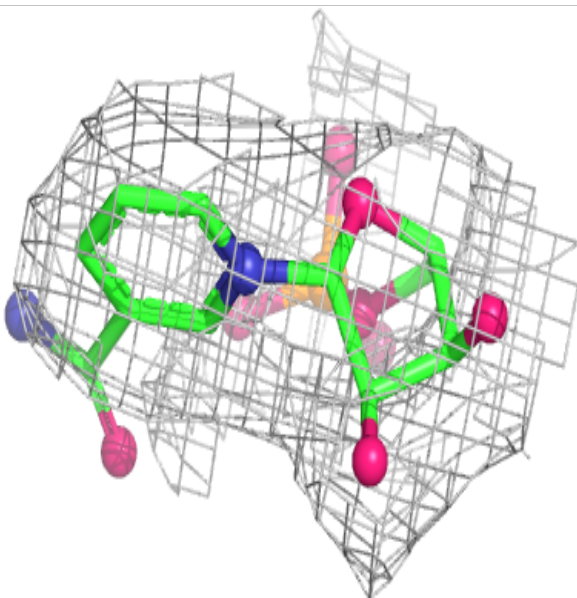
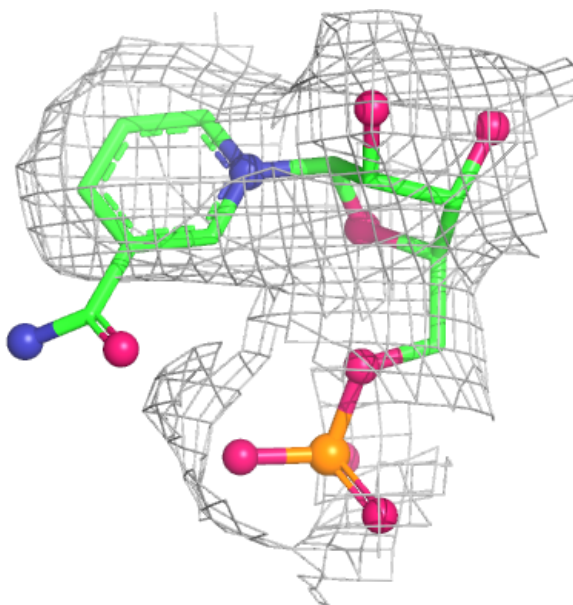
Electron density around NMN B 501:

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



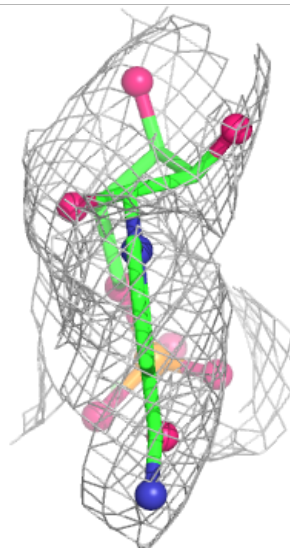
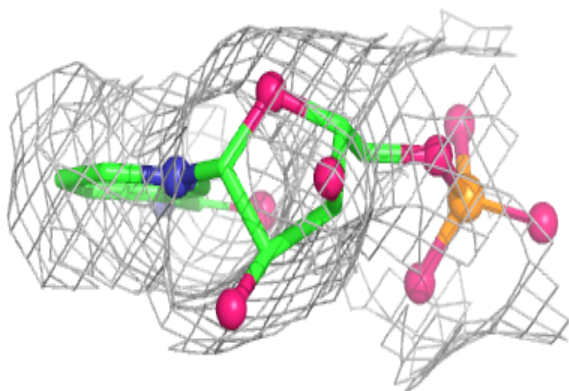
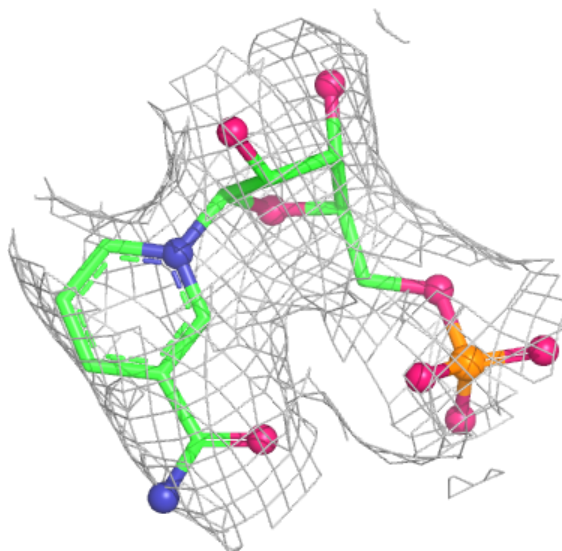
Electron density around NMN E 501:

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



Electron density around NMN A 501:

$2mF_o-DF_c$ (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.