



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:47 AM UTC

PDB ID : 1EFK / pdb_00001efk
Title : STRUCTURE OF HUMAN MALIC ENZYME IN COMPLEX WITH KE-
TOMALONATE
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on : 2000-02-09
Resolution : 2.60 Å(reported)

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

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

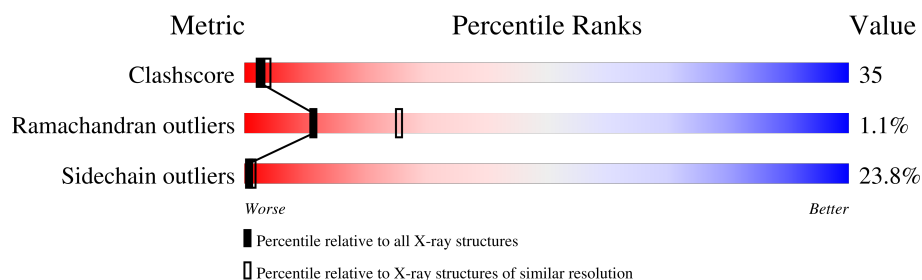
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	
1	C	584	
1	D	584	

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
4	MAK	A	603	-	X	-	-
4	MAK	C	2603	-	X	-	-
4	MAK	D	3603	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17931 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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	modified residue	UNP P23368
A	38	MSE	MET	modified residue	UNP P23368
A	47	MSE	MET	modified residue	UNP P23368
A	75	MSE	MET	modified residue	UNP P23368
A	86	MSE	MET	modified residue	UNP P23368
A	108	MSE	MET	modified residue	UNP P23368
A	177	MSE	MET	modified residue	UNP P23368
A	219	MSE	MET	modified residue	UNP P23368
A	239	MSE	MET	modified residue	UNP P23368
A	325	MSE	MET	modified residue	UNP P23368
A	327	MSE	MET	modified residue	UNP P23368
A	343	MSE	MET	modified residue	UNP P23368
A	407	MSE	MET	modified residue	UNP P23368
A	539	MSE	MET	modified residue	UNP P23368
B	29	MSE	MET	modified residue	UNP P23368
B	38	MSE	MET	modified residue	UNP P23368
B	47	MSE	MET	modified residue	UNP P23368
B	75	MSE	MET	modified residue	UNP P23368
B	86	MSE	MET	modified residue	UNP P23368
B	108	MSE	MET	modified residue	UNP P23368
B	177	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	MSE	MET	modified residue	UNP P23368
B	239	MSE	MET	modified residue	UNP P23368
B	325	MSE	MET	modified residue	UNP P23368
B	327	MSE	MET	modified residue	UNP P23368
B	343	MSE	MET	modified residue	UNP P23368
B	407	MSE	MET	modified residue	UNP P23368
B	539	MSE	MET	modified residue	UNP P23368
C	29	MSE	MET	modified residue	UNP P23368
C	38	MSE	MET	modified residue	UNP P23368
C	47	MSE	MET	modified residue	UNP P23368
C	75	MSE	MET	modified residue	UNP P23368
C	86	MSE	MET	modified residue	UNP P23368
C	108	MSE	MET	modified residue	UNP P23368
C	177	MSE	MET	modified residue	UNP P23368
C	219	MSE	MET	modified residue	UNP P23368
C	239	MSE	MET	modified residue	UNP P23368
C	325	MSE	MET	modified residue	UNP P23368
C	327	MSE	MET	modified residue	UNP P23368
C	343	MSE	MET	modified residue	UNP P23368
C	407	MSE	MET	modified residue	UNP P23368
C	539	MSE	MET	modified residue	UNP P23368
D	29	MSE	MET	modified residue	UNP P23368
D	38	MSE	MET	modified residue	UNP P23368
D	47	MSE	MET	modified residue	UNP P23368
D	75	MSE	MET	modified residue	UNP P23368
D	86	MSE	MET	modified residue	UNP P23368
D	108	MSE	MET	modified residue	UNP P23368
D	177	MSE	MET	modified residue	UNP P23368
D	219	MSE	MET	modified residue	UNP P23368
D	239	MSE	MET	modified residue	UNP P23368
D	325	MSE	MET	modified residue	UNP P23368
D	327	MSE	MET	modified residue	UNP P23368
D	343	MSE	MET	modified residue	UNP P23368
D	407	MSE	MET	modified residue	UNP P23368
D	539	MSE	MET	modified residue	UNP P23368

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

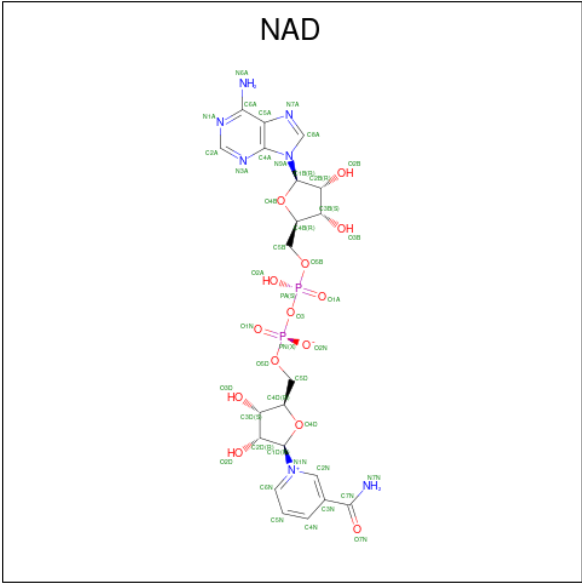
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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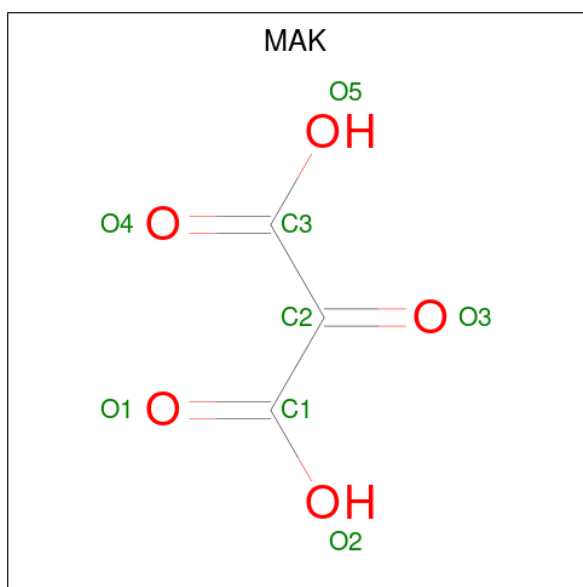
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		

- Molecule 4 is ALPHA-KETOMALONIC ACID (CCD ID: MAK) (formula: C₃H₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	3	5		
4	B	1	Total	C	O	0	0
			8	3	5		
4	C	1	Total	C	O	0	0
			8	3	5		
4	D	1	Total	C	O	0	0
			8	3	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	18	Total	O	0	0
			18	18		
5	C	16	Total	O	0	0
			16	16		
5	D	16	Total	O	0	0
			16	16		

3 Residue-property plots

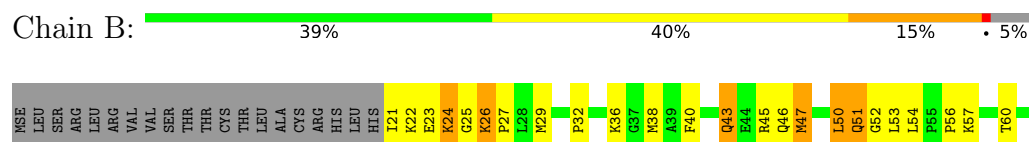
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

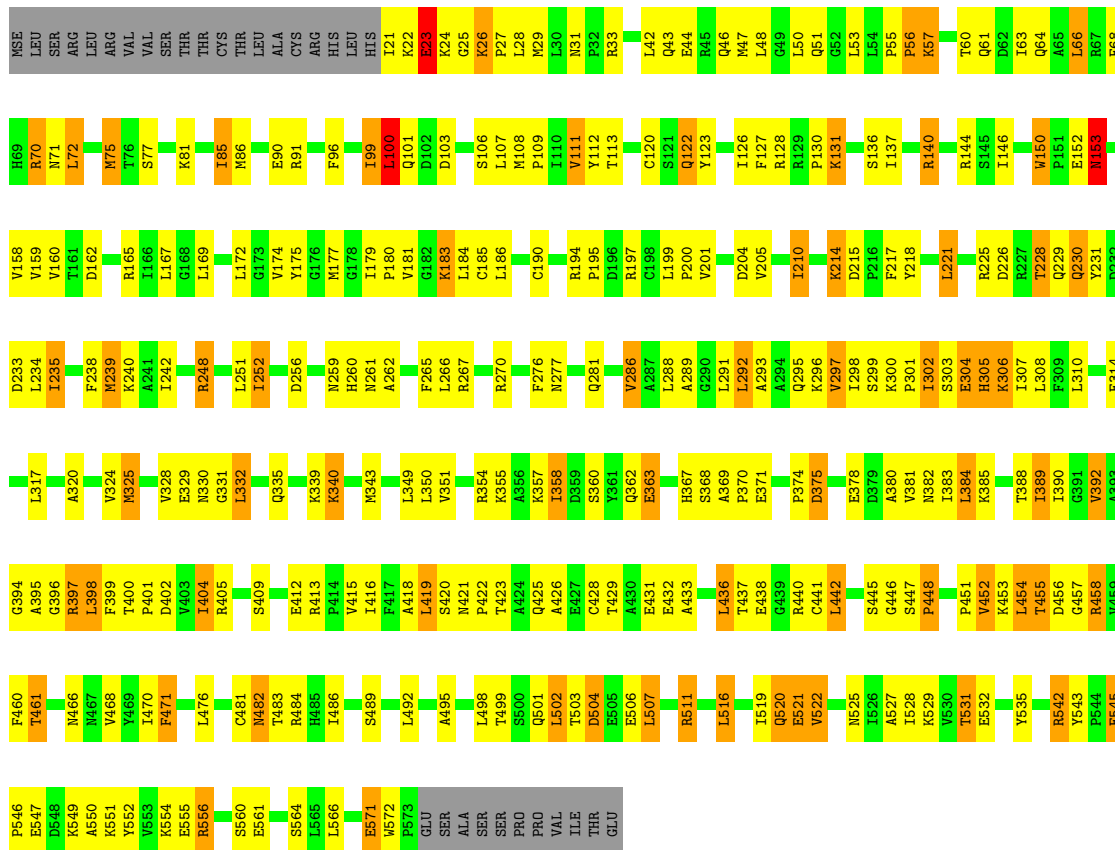
Note EDS was not executed.

• Molecule 1: MALIC ENZYME



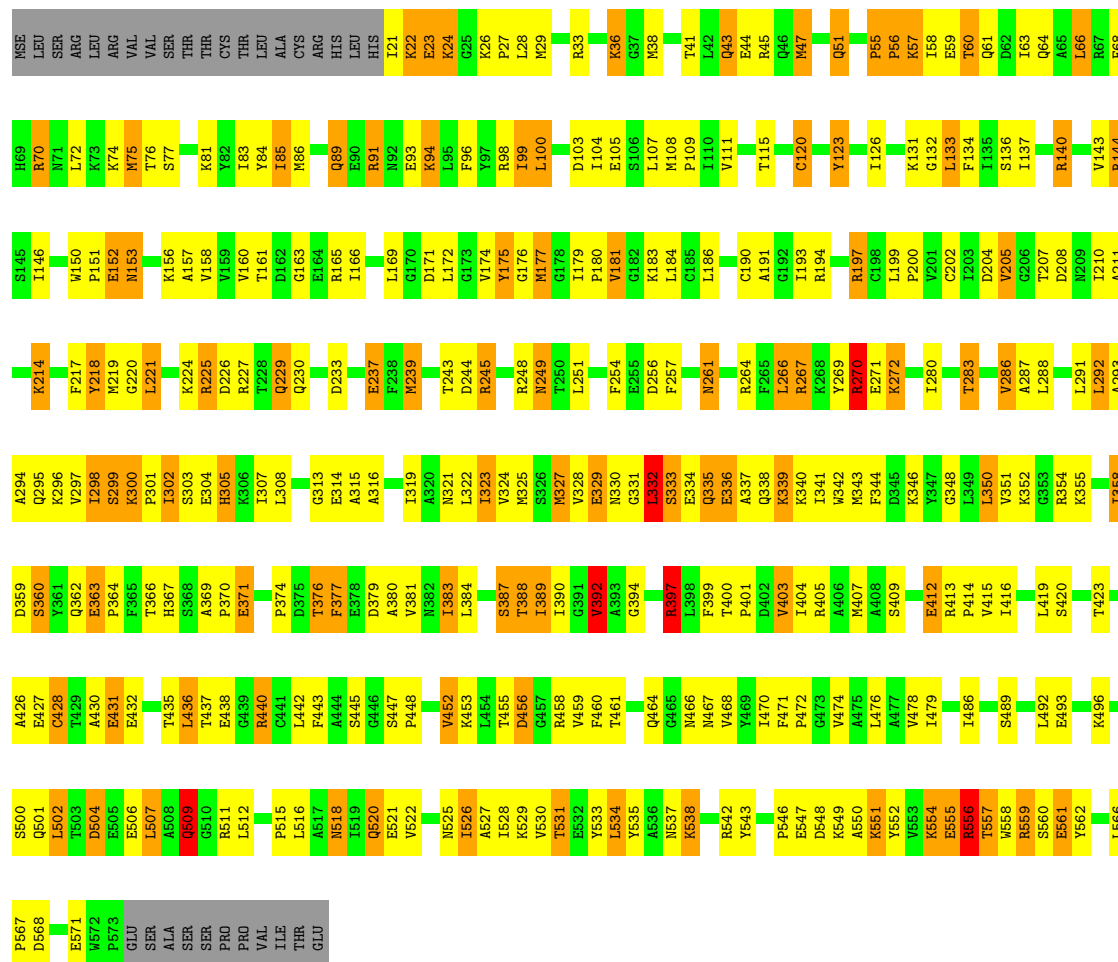
• Molecule 1: MALIC ENZYME





● Molecule 1: MALIC ENZYME

Chain D:  39% 39% 16% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.60Å 118.60Å 113.10Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.0 (20.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17931	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.53	0/4447	1.00	17/5998 (0.3%)
1	B	0.54	0/4447	1.01	20/5998 (0.3%)
1	C	0.55	0/4447	1.01	19/5998 (0.3%)
1	D	0.54	0/4447	0.99	17/5998 (0.3%)
All	All	0.54	0/17788	1.00	73/23992 (0.3%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ILE	N-CA-C	9.26	118.94	111.62
1	D	470	ILE	N-CA-C	9.21	118.90	111.62
1	A	470	ILE	N-CA-C	8.71	118.50	111.62
1	D	556	ARG	N-CA-C	7.66	121.50	112.93
1	C	150	TRP	CA-C-N	7.61	126.88	118.97
1	C	150	TRP	C-N-CA	7.61	126.88	118.97
1	B	185	CYS	N-CA-C	-7.49	103.05	111.07
1	A	556	ARG	N-CA-C	7.43	121.93	113.02
1	D	272	LYS	N-CA-C	-7.09	105.25	114.04
1	D	256	ASP	N-CA-C	6.96	120.99	111.17
1	B	150	TRP	CA-C-N	6.86	128.42	119.84
1	B	150	TRP	C-N-CA	6.86	128.42	119.84
1	B	205	VAL	N-CA-C	-6.38	105.12	111.88
1	C	185	CYS	N-CA-C	-6.38	104.25	111.14
1	B	100	LEU	N-CA-C	-6.38	103.62	111.40
1	D	160	VAL	N-CA-C	6.34	117.61	108.48
1	C	153	ASN	N-CA-C	6.29	120.27	112.59
1	A	256	ASP	N-CA-C	6.22	119.82	111.24
1	B	566	LEU	N-CA-C	6.17	117.42	109.65
1	D	175	TYR	N-CA-C	-6.09	105.94	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	THR	CA-C-N	6.06	125.55	119.24
1	B	400	THR	C-N-CA	6.06	125.55	119.24
1	D	486	ILE	N-CA-C	5.98	116.47	107.80
1	D	509	GLN	N-CA-C	-5.94	106.36	113.97
1	A	310	LEU	N-CA-C	-5.94	98.05	108.20
1	D	55	PRO	CA-C-N	5.90	127.21	119.84
1	D	55	PRO	C-N-CA	5.90	127.21	119.84
1	C	23	GLU	N-CA-C	5.87	118.79	109.81
1	C	215	ASP	CA-C-N	5.86	125.96	119.87
1	C	215	ASP	C-N-CA	5.86	125.96	119.87
1	C	566	LEU	N-CA-C	5.86	117.19	109.93
1	B	358	ILE	N-CA-C	-5.82	99.91	108.99
1	C	522	VAL	N-CA-C	-5.78	104.88	110.42
1	B	506	GLU	N-CA-C	-5.77	105.12	111.82
1	A	457	GLY	N-CA-C	5.63	121.78	115.08
1	A	100	LEU	N-CA-C	-5.62	104.79	111.03
1	A	509	GLN	N-CA-C	-5.59	106.29	114.39
1	C	448	PRO	N-CA-C	5.58	119.84	111.14
1	A	150	TRP	CA-C-N	5.57	126.80	119.84
1	A	150	TRP	C-N-CA	5.57	126.80	119.84
1	C	162	ASP	N-CA-C	-5.57	105.26	113.61
1	B	373	ILE	N-CA-C	5.54	112.60	107.56
1	C	471	PHE	CA-C-N	-5.50	112.95	119.05
1	C	471	PHE	C-N-CA	-5.50	112.95	119.05
1	B	159	VAL	N-CA-C	-5.49	99.60	107.78
1	C	31	ASN	CA-C-N	5.48	125.31	119.28
1	C	31	ASN	C-N-CA	5.48	125.31	119.28
1	C	358	ILE	N-CA-C	-5.46	100.47	108.99
1	D	23	GLU	N-CA-C	5.42	118.54	110.14
1	D	419	LEU	N-CA-C	5.39	119.83	112.88
1	B	175	TYR	N-CA-C	-5.31	106.07	112.54
1	A	512	LEU	N-CA-C	-5.29	106.06	112.88
1	B	167	LEU	CB-CA-C	-5.29	108.94	116.34
1	C	22	LYS	N-CA-C	5.28	119.70	113.16
1	A	175	TYR	N-CA-C	-5.26	106.92	113.19
1	A	31	ASN	CA-C-N	5.26	124.92	119.56
1	A	31	ASN	C-N-CA	5.26	124.92	119.56
1	D	100	LEU	N-CA-C	-5.22	105.24	111.03
1	A	141	GLY	N-CA-C	-5.21	108.14	114.92
1	B	522	VAL	N-CA-C	-5.21	105.42	110.42
1	A	160	VAL	N-CA-C	5.17	116.81	108.85
1	B	419	LEU	N-CA-C	5.16	119.27	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	GLY	CA-C-N	5.16	125.07	119.76
1	B	450	GLY	C-N-CA	5.16	125.07	119.76
1	D	390	ILE	N-CA-C	5.14	114.97	107.37
1	C	100	LEU	N-CA-C	-5.13	105.14	111.40
1	A	357	LYS	N-CA-C	5.12	117.47	110.24
1	D	403	VAL	N-CA-C	-5.08	105.89	110.82
1	B	256	ASP	N-CA-C	5.07	118.38	111.39
1	D	377	PHE	N-CA-C	-5.07	105.94	111.82
1	C	256	ASP	N-CA-C	5.05	118.36	111.39
1	A	448	PRO	N-CA-C	5.03	119.09	111.19
1	D	387	SER	N-CA-C	-5.02	106.33	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4367	0	4407	369	0
1	B	4367	0	4407	324	0
1	C	4367	0	4407	227	0
1	D	4367	0	4407	339	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	88	0	52	4	0
3	B	88	0	52	5	0
3	C	88	0	52	3	0
3	D	88	0	52	3	0
4	A	8	0	0	1	0
4	B	8	0	0	1	0
4	C	8	0	0	1	0
4	D	8	0	0	2	0
5	A	25	0	0	4	0
5	B	18	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	16	0	0	3	0
5	D	16	0	0	1	0
All	All	17931	0	17836	1234	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 35.

All (1234) 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:C:210:ILE:H	1:C:210:ILE:HD13	1.00	1.10
1:D:140:ARG:HH22	1:D:233:ASP:HB3	1.15	1.09
1:D:177:MSE:HE1	1:D:181:VAL:HG23	1.34	1.06
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.38	1.06
1:B:354:ARG:HE	1:B:358:ILE:HD11	1.21	1.06
1:D:300:LYS:HE3	1:D:304:GLU:HB2	1.37	1.03
1:D:302:ILE:HG12	1:D:332:LEU:HD11	1.41	1.00
1:C:210:ILE:H	1:C:210:ILE:CD1	1.73	0.96
1:C:378:GLU:O	1:C:381:VAL:HG12	1.65	0.96
1:B:354:ARG:NE	1:B:358:ILE:HD11	1.81	0.96
1:A:86:MSE:HE1	1:A:111:VAL:HG23	1.48	0.95
1:A:492:LEU:HD22	1:A:496:LYS:HE3	1.49	0.94
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.32	0.94
1:B:339:LYS:HA	1:B:367:HIS:CE1	2.03	0.94
1:D:123:TYR:HD2	1:D:219:MSE:HE1	1.32	0.93
1:B:351:VAL:HG11	1:B:369:ALA:HA	1.50	0.93
1:D:371:GLU:CD	1:D:371:GLU:H	1.73	0.93
1:D:374:PRO:HG3	1:D:383:ILE:HG13	1.49	0.92
1:C:454:LEU:HD11	1:C:460:PHE:HE2	1.32	0.91
1:D:137:ILE:HD12	1:D:205:VAL:HG12	1.51	0.91
1:C:210:ILE:HD13	1:C:210:ILE:N	1.86	0.91
1:D:327:MSE:HG2	1:D:332:LEU:HD22	1.49	0.91
1:A:137:ILE:HB	1:A:205:VAL:HG12	1.53	0.90
1:D:261:ASN:HD22	1:D:264:ARG:NH2	1.68	0.90
1:D:527:ALA:O	1:D:531:THR:HG22	1.72	0.90
1:C:61:GLN:HA	1:C:64:GLN:HE21	1.38	0.89
1:B:29:MSE:HE2	1:B:50:LEU:HD22	1.56	0.88
1:B:266:LEU:O	1:B:270:ARG:HG2	1.74	0.87
1:C:527:ALA:O	1:C:531:THR:HG22	1.72	0.87
1:A:389:ILE:HB	1:A:407:MSE:HE2	1.57	0.87
1:C:81:LYS:O	1:C:85:ILE:HG23	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASN:ND2	1:A:264:ARG:HH21	1.72	0.86
1:B:339:LYS:HA	1:B:367:HIS:HE1	1.42	0.85
1:D:379:ASP:O	1:D:383:ILE:HG12	1.75	0.85
1:D:327:MSE:HE3	1:D:337:ALA:HB1	1.56	0.85
1:D:85:ILE:HD11	1:D:111:VAL:HG12	1.58	0.85
1:B:371:GLU:CD	1:B:371:GLU:H	1.84	0.85
1:C:453:LYS:HE3	1:C:457:GLY:HA2	1.58	0.85
1:A:38:MSE:HE3	1:A:59:GLU:CD	2.02	0.85
1:D:332:LEU:HD23	1:D:340:LYS:HE3	1.58	0.85
1:A:220:GLY:HA2	1:B:56:PRO:HG2	1.59	0.84
1:A:211:ALA:O	1:A:214:LYS:HG2	1.76	0.84
1:A:377:PHE:HE2	1:A:389:ILE:HD11	1.42	0.84
1:D:140:ARG:NH2	1:D:233:ASP:HB3	1.92	0.84
1:A:408:ALA:HB2	1:A:437:THR:HG22	1.57	0.84
1:C:520:GLN:H	1:C:520:GLN:HE21	1.24	0.84
1:B:520:GLN:H	1:B:520:GLN:HE21	1.23	0.84
1:D:72:LEU:HD12	1:D:75:MSE:HE2	1.60	0.83
1:B:505:GLU:CD	1:B:505:GLU:H	1.85	0.83
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.61	0.83
1:B:506:GLU:OE2	1:B:515:PRO:HD3	1.78	0.82
1:D:261:ASN:HD22	1:D:264:ARG:HH22	1.25	0.82
1:B:527:ALA:O	1:B:531:THR:HG23	1.80	0.82
1:C:23:GLU:OE1	1:C:23:GLU:HA	1.80	0.82
1:C:239:MSE:HE1	1:C:252:ILE:HD13	1.62	0.82
1:B:478:VAL:HG13	1:B:483:THR:HB	1.61	0.81
1:B:546:PRO:HG2	1:B:549:LYS:HD2	1.60	0.81
1:D:75:MSE:CE	1:D:81:LYS:HA	2.10	0.81
1:D:392:VAL:HG13	1:D:392:VAL:O	1.80	0.81
1:A:177:MSE:HE1	1:A:180:PRO:HB2	1.63	0.81
1:A:163:GLY:HA2	1:A:166:ILE:HD11	1.61	0.81
1:D:468:VAL:HA	1:D:471:PHE:CE2	2.15	0.80
1:C:397:ARG:HH21	1:C:426:ALA:HB3	1.46	0.80
1:A:140:ARG:NH2	1:A:233:ASP:HB3	1.95	0.80
1:B:81:LYS:O	1:B:85:ILE:HG23	1.80	0.80
1:C:349:LEU:HD22	1:C:374:PRO:HG2	1.63	0.80
1:B:466:ASN:HB3	1:B:468:VAL:HG12	1.62	0.80
1:D:123:TYR:CD2	1:D:219:MSE:HE1	2.17	0.80
1:D:437:THR:O	1:D:440:ARG:HG3	1.82	0.79
1:D:324:VAL:O	1:D:328:VAL:HG23	1.83	0.79
1:B:528:ILE:O	1:B:532:GLU:HG3	1.81	0.79
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:GLN:HE21	1:B:51:GLN:HA	1.48	0.79
1:D:556:ARG:CG	1:D:556:ARG:HH11	1.96	0.78
1:D:177:MSE:CE	1:D:181:VAL:HG23	2.13	0.78
1:A:518:ASN:HA	1:A:520:GLN:OE1	1.84	0.78
1:D:91:ARG:HG3	1:D:91:ARG:HH11	1.48	0.78
1:B:208:ASP:O	1:B:210:ILE:HD12	1.83	0.77
1:B:377:PHE:O	1:B:381:VAL:HG23	1.84	0.77
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.46	0.77
1:B:342:TRP:CE3	1:B:349:LEU:HD21	2.19	0.77
1:C:140:ARG:HB2	1:C:140:ARG:NH1	2.00	0.77
1:D:261:ASN:ND2	1:D:264:ARG:NH2	2.33	0.77
1:B:229:GLN:NE2	1:B:232:ASP:HB2	1.99	0.77
1:C:422:PRO:HD2	1:C:425:GLN:NE2	2.00	0.77
1:B:505:GLU:CD	1:B:505:GLU:N	2.40	0.77
1:D:249:ASN:C	1:D:249:ASN:HD22	1.92	0.77
1:B:79:LEU:O	1:B:83:ILE:HG13	1.84	0.77
1:D:377:PHE:HZ	1:D:389:ILE:HD11	1.49	0.77
1:A:43:GLN:HG2	1:A:566:LEU:HD11	1.67	0.76
1:D:548:ASP:OD2	1:D:551:LYS:HB2	1.85	0.76
1:A:260:HIS:O	1:A:264:ARG:HB2	1.85	0.76
1:D:301:PRO:HB2	1:D:304:GLU:HG3	1.65	0.76
1:D:177:MSE:HG2	1:D:202:CYS:HB2	1.67	0.76
1:D:302:ILE:CG1	1:D:332:LEU:HD11	2.14	0.76
1:C:454:LEU:HD11	1:C:460:PHE:CE2	2.18	0.76
1:B:239:MSE:HE1	1:B:252:ILE:HD13	1.68	0.75
1:A:85:ILE:HG12	1:A:86:MSE:HE2	1.68	0.75
1:A:552:TYR:HE1	1:A:556:ARG:NH2	1.85	0.74
1:C:433:ALA:O	1:C:437:THR:HG23	1.87	0.74
1:D:60:THR:O	1:D:63:ILE:HG22	1.87	0.74
1:A:535:TYR:OH	1:A:542:ARG:HB3	1.87	0.74
1:D:43:GLN:OE1	1:D:47:MSE:HE1	1.87	0.74
1:B:422:PRO:HD2	1:B:425:GLN:HE21	1.53	0.74
1:D:175:TYR:CE2	1:D:218:TYR:HA	2.21	0.74
1:D:397:ARG:NH2	1:D:426:ALA:HB3	2.03	0.74
1:D:294:ALA:O	1:D:297:VAL:HG22	1.88	0.74
1:B:229:GLN:HE21	1:B:229:GLN:HA	1.53	0.73
1:C:395:ALA:HB3	1:C:398:LEU:HD21	1.71	0.73
1:D:538:LYS:H	1:D:538:LYS:HZ3	1.34	0.73
1:B:305:HIS:O	1:B:340:LYS:HD3	1.89	0.73
1:D:75:MSE:HE3	1:D:81:LYS:HA	1.70	0.73
1:D:400:THR:OG1	1:D:403:VAL:HG23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:HG2	1:B:220:GLY:HA2	1.69	0.73
1:C:60:THR:OG1	1:C:63:ILE:HG13	1.88	0.73
1:D:377:PHE:CZ	1:D:389:ILE:HD11	2.23	0.73
1:A:392:VAL:O	1:A:392:VAL:HG13	1.88	0.72
1:B:334:GLU:O	1:B:338:GLN:HG3	1.89	0.72
1:A:525:ASN:O	1:A:529:LYS:HG2	1.89	0.72
1:B:177:MSE:O	1:B:180:PRO:HD2	1.89	0.72
1:A:520:GLN:NE2	1:A:521:GLU:N	2.37	0.72
1:B:349:LEU:HD11	1:B:384:LEU:HD11	1.71	0.72
1:B:351:VAL:CG1	1:B:369:ALA:HA	2.19	0.72
1:A:495:ALA:O	1:A:499:THR:HG22	1.89	0.72
1:D:556:ARG:HH11	1:D:556:ARG:HG2	1.52	0.72
1:B:29:MSE:HE2	1:B:50:LEU:CD2	2.19	0.72
1:C:248:ARG:HG3	1:C:248:ARG:HH11	1.54	0.72
1:A:52:GLY:O	1:B:133:LEU:HD23	1.89	0.72
1:B:334:GLU:HG3	1:B:338:GLN:NE2	2.04	0.72
1:B:446:GLY:O	1:B:466:ASN:ND2	2.23	0.72
1:C:378:GLU:OE1	1:C:402:ASP:HB3	1.90	0.72
1:A:225:ARG:HB2	5:A:4041:HOH:O	1.90	0.71
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.03	0.71
1:B:287:ALA:HB3	1:B:319:ILE:HG21	1.72	0.71
1:B:298:ILE:CG2	1:B:300:LYS:HB2	2.21	0.71
1:A:164:GLU:HG3	1:A:225:ARG:CZ	2.20	0.71
1:B:358:ILE:HG12	1:B:366:THR:HG21	1.72	0.71
1:D:94:LYS:HE3	1:D:558:TRP:CZ2	2.25	0.71
1:A:164:GLU:HG3	1:A:225:ARG:NE	2.05	0.71
1:B:184:LEU:HD22	1:B:198:CYS:HB3	1.73	0.71
1:C:382:ASN:O	1:C:385:LYS:HD2	1.91	0.71
1:C:542:ARG:HD2	1:C:552:TYR:OH	1.91	0.71
1:D:153:ASN:H	1:D:153:ASN:ND2	1.87	0.71
1:A:369:ALA:HB1	1:A:373:ILE:HD11	1.72	0.71
1:A:319:ILE:O	1:A:323:ILE:HG13	1.90	0.70
1:A:33:ARG:HD3	1:A:93:GLU:OE2	1.92	0.70
1:A:343:MSE:HB2	1:A:350:LEU:HD12	1.71	0.70
1:B:307:ILE:HD13	1:B:323:ILE:HD13	1.73	0.70
1:B:406:ALA:O	1:B:410:ILE:HD12	1.92	0.70
1:A:177:MSE:CE	1:A:180:PRO:HB2	2.21	0.70
1:A:332:LEU:CD2	1:A:340:LYS:HZ1	2.04	0.70
1:A:431:GLU:O	1:A:435:THR:OG1	2.09	0.70
1:B:137:ILE:O	1:B:140:ARG:HG2	1.91	0.70
1:B:401:PRO:HB2	1:B:405:ARG:HH21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:MSE:O	1:C:48:LEU:HD23	1.91	0.70
1:D:137:ILE:HB	1:D:205:VAL:HG12	1.73	0.70
1:C:451:PRO:HG3	1:C:461:THR:HG23	1.73	0.70
1:A:86:MSE:CE	1:A:111:VAL:HG23	2.21	0.70
1:A:138:SER:OG	1:A:221:LEU:HD21	1.92	0.70
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.38	0.69
1:A:315:ALA:O	1:A:319:ILE:HD12	1.93	0.69
1:D:288:LEU:HG	1:D:292:LEU:HD22	1.73	0.69
1:B:397:ARG:HH21	1:B:426:ALA:HB3	1.58	0.69
1:B:489:SER:HB2	1:B:533:TYR:OH	1.91	0.69
1:A:144:ARG:NH2	1:A:245:ARG:HB2	2.08	0.69
1:A:295:GLN:HE22	1:A:300:LYS:N	1.91	0.69
1:B:315:ALA:O	1:B:319:ILE:HG13	1.91	0.69
1:C:235:ILE:HD13	1:C:265:PHE:CZ	2.28	0.69
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.73	0.69
1:B:267:ARG:HB2	5:B:4022:HOH:O	1.91	0.69
1:B:295:GLN:HA	1:B:295:GLN:OE1	1.93	0.69
1:A:327:MSE:CE	1:A:337:ALA:HB1	2.21	0.68
1:B:518:ASN:O	1:B:522:VAL:HG23	1.93	0.68
1:A:81:LYS:O	1:A:85:ILE:HG23	1.94	0.68
1:B:397:ARG:NH2	1:B:426:ALA:HB3	2.08	0.68
1:D:68:PHE:CD2	1:D:99:ILE:HG13	2.28	0.68
1:D:401:PRO:HB3	1:D:436:LEU:HD21	1.74	0.68
1:A:300:LYS:HZ1	1:A:304:GLU:C	2.02	0.68
1:D:381:VAL:HG21	1:D:403:VAL:HG13	1.75	0.68
1:A:334:GLU:O	1:A:338:GLN:HG3	1.94	0.68
1:C:454:LEU:HD12	1:C:458:ARG:HB2	1.75	0.68
1:B:108:MSE:CE	1:B:516:LEU:HD11	2.24	0.68
1:B:522:VAL:O	1:B:526:ILE:HG13	1.92	0.68
1:C:429:THR:OG1	1:C:432:GLU:HG3	1.93	0.68
1:B:422:PRO:HD2	1:B:425:GLN:NE2	2.09	0.68
1:C:535:TYR:CE2	1:C:545:GLU:HB2	2.29	0.68
1:D:85:ILE:HD11	1:D:111:VAL:CG1	2.24	0.67
1:D:194:ARG:HE	1:D:197:ARG:NH1	1.92	0.67
1:B:96:PHE:O	1:B:100:LEU:HD13	1.94	0.67
1:B:392:VAL:O	1:B:392:VAL:HG22	1.95	0.67
1:B:342:TRP:HE3	1:B:349:LEU:HD21	1.56	0.67
1:D:327:MSE:HE3	1:D:337:ALA:CB	2.24	0.67
1:A:267:ARG:NH1	1:A:361:TYR:OH	2.27	0.67
1:A:300:LYS:HZ3	1:A:304:GLU:HB2	1.59	0.67
1:A:350:LEU:HD22	1:A:358:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ILE:HD13	1:C:550:ALA:HA	1.75	0.67
1:A:186:LEU:O	1:A:190:CYS:HB2	1.94	0.67
1:D:397:ARG:NH2	1:D:423:THR:O	2.27	0.67
1:A:492:LEU:O	1:A:496:LYS:HG3	1.95	0.67
1:D:556:ARG:HG2	1:D:556:ARG:NH1	2.09	0.67
1:A:389:ILE:HG22	1:A:416:ILE:HA	1.77	0.67
1:B:492:LEU:O	1:B:496:LYS:HG3	1.94	0.67
1:B:527:ALA:O	1:B:531:THR:CG2	2.43	0.67
1:C:325:MSE:O	1:C:329:GLU:HG3	1.95	0.67
1:A:140:ARG:NH2	1:A:230:GLN:HA	2.10	0.67
1:B:349:LEU:HD23	1:B:350:LEU:N	2.10	0.67
1:B:400:THR:OG1	1:B:403:VAL:HG23	1.95	0.67
1:D:535:TYR:O	1:D:538:LYS:NZ	2.28	0.66
1:A:432:GLU:O	1:A:436:LEU:HB2	1.94	0.66
1:A:64:GLN:NE2	1:A:562:TYR:OH	2.25	0.66
1:A:226:ASP:OD1	1:A:228:THR:HG23	1.95	0.66
1:A:332:LEU:HD23	1:A:340:LYS:HZ1	1.58	0.66
1:B:179:ILE:HB	1:B:180:PRO:HD3	1.77	0.66
1:B:239:MSE:HE1	1:B:252:ILE:CD1	2.25	0.66
1:D:537:ASN:C	1:D:538:LYS:HG2	2.20	0.66
1:A:520:GLN:NE2	1:A:521:GLU:H	1.91	0.66
1:C:546:PRO:HG2	1:C:549:LYS:HD3	1.77	0.66
1:A:288:LEU:HD23	1:A:322:LEU:HD23	1.78	0.66
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.59	0.66
1:D:22:LYS:O	1:D:22:LYS:HD3	1.96	0.66
1:D:75:MSE:HE1	1:D:81:LYS:HA	1.78	0.66
1:A:123:TYR:CD2	1:A:219:MSE:HE1	2.29	0.66
1:B:301:PRO:HG2	1:B:304:GLU:CD	2.21	0.66
1:D:371:GLU:CD	1:D:371:GLU:N	2.51	0.66
1:A:150:TRP:HE1	1:A:152:GLU:CD	2.03	0.66
1:B:297:VAL:HG22	1:B:298:ILE:HD12	1.78	0.66
1:D:298:ILE:CG2	1:D:300:LYS:HB2	2.25	0.66
1:B:414:PRO:O	1:B:442:LEU:HD12	1.96	0.66
1:B:298:ILE:HG22	1:B:300:LYS:N	2.11	0.65
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.31	0.65
1:D:177:MSE:HE3	1:D:177:MSE:O	1.95	0.65
1:D:559:ARG:HG3	1:D:561:GLU:OE1	1.97	0.65
1:A:45:ARG:NH2	1:A:58:ILE:HD13	2.11	0.65
1:A:556:ARG:HH11	1:A:556:ARG:CG	2.09	0.65
1:A:144:ARG:NH2	1:A:245:ARG:HG3	2.11	0.65
1:C:131:LYS:O	1:C:177:MSE:HE3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLY:O	1:B:332:LEU:O	2.15	0.65
1:B:346:LYS:HG2	3:B:1601:NAD:O2B	1.97	0.64
1:B:301:PRO:HG2	1:B:304:GLU:HG3	1.79	0.64
1:D:266:LEU:HD12	1:D:280:ILE:HD12	1.78	0.64
1:A:467:ASN:O	1:A:471:PHE:HD2	1.81	0.64
1:D:363:GLU:HB3	1:D:364:PRO:HD3	1.79	0.64
1:C:317:LEU:HD23	1:C:343:MSE:HE1	1.79	0.64
1:B:261:ASN:ND2	1:B:264:ARG:NH2	2.46	0.64
1:C:331:GLY:O	1:C:332:LEU:O	2.15	0.64
1:A:550:ALA:O	1:A:554:LYS:HG2	1.98	0.64
1:B:29:MSE:HE1	1:B:53:LEU:CD1	2.28	0.64
1:C:546:PRO:O	1:C:549:LYS:NZ	2.31	0.64
1:A:552:TYR:CE1	1:A:556:ARG:NH2	2.65	0.64
1:B:505:GLU:N	1:B:505:GLU:OE2	2.31	0.64
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.81	0.63
1:D:342:TRP:CZ3	1:D:367:HIS:HB2	2.33	0.63
1:A:160:VAL:HG21	1:A:203:ILE:HD11	1.80	0.63
1:C:140:ARG:HH22	1:C:233:ASP:HB2	1.63	0.63
1:D:33:ARG:NH1	1:D:93:GLU:OE2	2.31	0.63
1:B:240:LYS:HE3	1:B:244:ASP:OD2	1.98	0.63
1:B:112:TYR:CD2	1:B:113:THR:HG22	2.34	0.63
1:C:160:VAL:HG12	1:C:201:VAL:HB	1.80	0.63
1:A:21:ILE:HG22	1:A:21:ILE:O	1.98	0.63
1:A:404:ILE:HG22	1:A:437:THR:HG23	1.81	0.63
1:D:316:ALA:HB2	1:D:392:VAL:HG11	1.80	0.63
1:C:56:PRO:HB2	1:D:221:LEU:HD13	1.81	0.62
1:D:298:ILE:HG23	1:D:300:LYS:HB2	1.81	0.62
1:C:85:ILE:HD12	1:C:96:PHE:HE1	1.63	0.62
1:C:297:VAL:HG21	1:C:442:LEU:HD11	1.80	0.62
1:D:343:MSE:O	1:D:350:LEU:HD23	2.00	0.62
1:A:43:GLN:HG3	1:A:566:LEU:HD21	1.82	0.62
1:A:219:MSE:HG2	1:B:38:MSE:HE1	1.81	0.62
1:D:298:ILE:HD12	1:D:442:LEU:HD11	1.81	0.62
1:D:329:GLU:HG2	1:D:330:ASN:ND2	2.14	0.62
1:D:332:LEU:HD12	1:D:332:LEU:N	2.14	0.62
1:D:350:LEU:HD22	1:D:354:ARG:HH12	1.63	0.62
1:D:538:LYS:HZ3	1:D:538:LYS:N	1.97	0.62
1:A:413:ARG:HH21	1:A:440:ARG:C	2.08	0.61
1:A:177:MSE:HE3	1:A:180:PRO:HD2	1.82	0.61
1:B:238:PHE:CE1	1:B:242:ILE:HG13	2.36	0.61
1:B:288:LEU:HG	1:B:292:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ASN:HB3	1:C:468:VAL:HG12	1.82	0.61
1:D:81:LYS:O	1:D:85:ILE:HG23	1.99	0.61
1:D:327:MSE:CE	1:D:337:ALA:HB1	2.28	0.61
1:D:432:GLU:O	1:D:436:LEU:HB2	2.00	0.61
1:D:555:GLU:HB3	1:D:556:ARG:NH1	2.15	0.61
1:A:324:VAL:HA	1:A:327:MSE:HE2	1.81	0.61
1:B:352:LYS:HE3	1:B:366:THR:O	2.00	0.61
1:D:538:LYS:NZ	1:D:538:LYS:N	2.48	0.61
1:B:75:MSE:HG2	1:B:80:GLU:OE1	1.99	0.61
1:B:370:PRO:HD2	1:B:373:ILE:HD12	1.81	0.61
1:B:496:LYS:O	1:B:500:SER:HB3	1.99	0.61
1:C:194:ARG:HB2	1:C:197:ARG:HG3	1.81	0.61
1:D:363:GLU:OE1	1:D:363:GLU:C	2.43	0.61
1:A:108:MSE:N	1:A:109:PRO:HD2	2.16	0.61
1:A:504:ASP:OD2	1:A:504:ASP:N	2.33	0.61
1:B:64:GLN:NE2	1:B:562:TYR:OH	2.34	0.61
1:D:137:ILE:CD1	1:D:205:VAL:HG12	2.29	0.61
1:D:538:LYS:H	1:D:538:LYS:NZ	1.99	0.61
1:B:301:PRO:HG2	1:B:304:GLU:CG	2.31	0.61
1:C:432:GLU:O	1:C:436:LEU:HB2	2.00	0.61
1:C:389:ILE:HG22	1:C:416:ILE:HA	1.82	0.61
1:D:23:GLU:O	1:D:28:LEU:HD21	2.01	0.61
1:A:332:LEU:HD12	1:A:332:LEU:H	1.66	0.60
1:A:548:ASP:OD2	1:A:551:LYS:HB2	2.00	0.60
1:B:239:MSE:HE3	1:B:239:MSE:HA	1.83	0.60
1:D:332:LEU:HD12	1:D:332:LEU:H	1.66	0.60
1:A:324:VAL:HA	1:A:327:MSE:CE	2.30	0.60
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.82	0.60
1:A:570:TYR:HE1	1:A:572:TRP:HE1	1.49	0.60
1:C:140:ARG:NH2	1:C:233:ASP:HB2	2.16	0.60
1:A:525:ASN:HA	1:A:528:ILE:HD12	1.82	0.60
1:B:229:GLN:NE2	1:B:229:GLN:HA	2.15	0.60
1:D:137:ILE:HD12	1:D:205:VAL:CG1	2.29	0.60
1:D:33:ARG:HD3	1:D:93:GLU:OE2	2.02	0.60
1:D:174:VAL:HG12	1:D:219:MSE:HE2	1.83	0.60
1:B:36:LYS:NZ	1:B:562:TYR:HB3	2.17	0.60
1:D:506:GLU:HG2	1:D:511:ARG:HD2	1.83	0.60
1:D:297:VAL:HG21	1:D:442:LEU:HD21	1.82	0.60
1:D:506:GLU:CB	1:D:511:ARG:HD2	2.32	0.60
1:B:108:MSE:HE2	1:B:516:LEU:HD11	1.84	0.59
1:C:551:LYS:O	1:C:555:GLU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LYS:HE3	1:D:562:TYR:HB3	1.84	0.59
1:D:153:ASN:H	1:D:153:ASN:HD22	1.48	0.59
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.37	0.59
1:B:480:LEU:HD22	1:B:556:ARG:HD3	1.85	0.59
1:D:59:GLU:HB3	1:D:63:ILE:HG21	1.83	0.59
1:A:332:LEU:HG	1:A:336:GLU:CD	2.28	0.59
1:B:75:MSE:HG2	1:B:80:GLU:CD	2.26	0.59
1:B:315:ALA:HB3	1:B:392:VAL:HG21	1.82	0.59
1:C:306:LYS:HZ3	1:C:306:LYS:HB2	1.66	0.59
1:A:472:PRO:HG2	5:A:4021:HOH:O	2.03	0.59
1:A:401:PRO:HA	1:A:404:ILE:HD12	1.83	0.59
1:B:29:MSE:HE1	1:B:53:LEU:HD12	1.85	0.59
1:B:310:LEU:HD21	1:B:398:LEU:HD23	1.84	0.59
1:D:261:ASN:ND2	1:D:264:ARG:HH21	2.01	0.59
1:A:79:LEU:O	1:A:83:ILE:HG13	2.02	0.59
1:A:144:ARG:NH2	1:A:245:ARG:CB	2.65	0.59
1:C:546:PRO:HG2	1:C:549:LYS:CD	2.32	0.59
1:A:47:MSE:SE	1:C:47:MSE:HE2	2.53	0.59
1:B:400:THR:HB	1:B:401:PRO:HD2	1.83	0.59
1:C:140:ARG:NH2	1:C:230:GLN:O	2.34	0.59
1:C:286:VAL:HG11	1:C:466:ASN:O	2.03	0.59
1:A:466:ASN:HB3	1:A:468:VAL:HG12	1.84	0.59
1:B:60:THR:OG1	1:B:63:ILE:HG13	2.03	0.59
1:B:287:ALA:HB3	1:B:319:ILE:CG2	2.31	0.59
1:B:503:THR:HA	5:B:4040:HOH:O	2.01	0.59
1:C:289:ALA:CB	1:C:498:LEU:HD23	2.33	0.59
1:D:186:LEU:HD13	1:D:468:VAL:HG23	1.85	0.59
1:C:43:GLN:O	1:C:47:MSE:HB2	2.02	0.58
1:D:286:VAL:HG11	1:D:466:ASN:O	2.03	0.58
1:D:412:GLU:HG3	1:D:413:ARG:HG2	1.85	0.58
1:A:316:ALA:HB2	1:A:392:VAL:HG11	1.85	0.58
1:B:307:ILE:HG23	1:B:388:THR:HB	1.85	0.58
1:C:305:HIS:O	1:C:340:LYS:HB3	2.03	0.58
1:D:374:PRO:HB3	1:D:379:ASP:HB2	1.84	0.58
1:D:389:ILE:HG22	1:D:416:ILE:HA	1.84	0.58
1:B:136:SER:HA	1:B:204:ASP:O	2.04	0.58
1:C:179:ILE:HB	1:C:180:PRO:HD3	1.85	0.58
1:D:331:GLY:O	1:D:332:LEU:O	2.21	0.58
1:C:42:LEU:O	1:C:46:GLN:HG3	2.03	0.58
1:C:153:ASN:C	1:C:153:ASN:HD22	2.11	0.58
1:D:175:TYR:HE2	1:D:218:TYR:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:MSE:HE3	1:A:59:GLU:OE1	2.03	0.58
1:A:456:ASP:CG	1:A:458:ARG:HH11	2.10	0.58
1:C:66:LEU:HD22	1:C:70:ARG:NH1	2.18	0.58
1:D:506:GLU:HB3	1:D:511:ARG:HD2	1.85	0.58
1:B:131:LYS:O	1:B:177:MSE:HE3	2.03	0.58
1:B:323:ILE:HG22	1:B:324:VAL:N	2.18	0.58
1:B:351:VAL:HG11	1:B:370:PRO:HD3	1.85	0.58
1:C:85:ILE:HG13	1:C:86:MSE:N	2.17	0.58
1:C:301:PRO:O	1:C:304:GLU:HG2	2.04	0.58
1:C:481:CYS:O	1:C:482:ASN:HB2	2.02	0.58
1:D:324:VAL:HA	1:D:327:MSE:HE2	1.86	0.58
1:D:392:VAL:O	1:D:392:VAL:CG1	2.52	0.58
1:A:154:HIS:O	1:A:197:ARG:HG3	2.04	0.58
1:A:239:MSE:HE1	1:A:254:PHE:HE1	1.68	0.58
1:C:33:ARG:HH21	1:C:152:GLU:HG3	1.69	0.58
1:D:502:LEU:CD1	1:D:507:LEU:HG	2.34	0.58
1:A:85:ILE:HA	1:A:88:ILE:HD12	1.86	0.58
1:B:363:GLU:HG2	1:B:364:PRO:N	2.19	0.58
1:B:418:ALA:HB1	1:B:427:GLU:HB2	1.85	0.58
1:D:551:LYS:O	1:D:555:GLU:HB2	2.04	0.58
1:A:332:LEU:HD23	1:A:340:LYS:NZ	2.19	0.58
1:D:41:THR:O	1:D:45:ARG:HG3	2.04	0.58
1:A:295:GLN:HE22	1:A:299:SER:CA	2.17	0.58
1:A:300:LYS:HB3	1:A:300:LYS:HZ2	1.68	0.58
1:B:260:HIS:CE1	1:B:264:ARG:NE	2.72	0.58
1:C:392:VAL:HG13	1:C:392:VAL:O	2.03	0.58
1:D:329:GLU:HG2	1:D:330:ASN:HD22	1.69	0.58
1:D:456:ASP:OD1	1:D:458:ARG:HG3	2.04	0.58
1:D:38:MSE:HE3	1:D:59:GLU:CD	2.28	0.57
1:D:550:ALA:O	1:D:554:LYS:HG2	2.04	0.57
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.84	0.57
1:B:152:GLU:HG2	1:B:196:ASP:HB2	1.85	0.57
1:B:210:ILE:O	1:B:214:LYS:HG2	2.04	0.57
1:B:504:ASP:HB2	1:B:505:GLU:OE2	2.03	0.57
1:C:401:PRO:HB2	1:C:405:ARG:NH2	2.20	0.57
1:D:269:TYR:O	1:D:271:GLU:N	2.37	0.57
1:A:343:MSE:HE3	1:A:350:LEU:CD1	2.34	0.57
1:A:343:MSE:HE3	1:A:350:LEU:HD11	1.86	0.57
1:B:322:LEU:HG	1:B:492:LEU:HD23	1.86	0.57
1:D:89:GLN:HG2	1:D:131:LYS:HZ3	1.69	0.57
1:D:300:LYS:HE3	1:D:304:GLU:CB	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MSE:HE1	1:A:488:ASP:HB2	1.85	0.57
1:D:316:ALA:HB2	1:D:392:VAL:CG1	2.35	0.57
1:A:166:ILE:HG13	1:A:172:LEU:HB2	1.86	0.57
1:A:503:THR:OG1	1:A:506:GLU:HG2	2.03	0.57
1:B:229:GLN:HE21	1:B:229:GLN:CA	2.18	0.57
1:D:191:ALA:HB3	1:D:193:ILE:HD12	1.87	0.57
1:A:295:GLN:NE2	1:A:299:SER:HA	2.19	0.57
1:B:358:ILE:HG23	1:B:362:GLN:HB2	1.86	0.57
1:C:504:ASP:HA	1:C:507:LEU:HB2	1.85	0.57
1:D:388:THR:HG23	1:D:415:VAL:HB	1.86	0.57
1:A:293:ALA:O	1:A:296:LYS:HB2	2.05	0.56
1:B:431:GLU:O	1:B:435:THR:HG23	2.04	0.56
1:D:165:ARG:NH2	4:D:3603:MAK:O1	2.38	0.56
1:A:157:ALA:HB1	1:A:187:TYR:HE2	1.71	0.56
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.87	0.56
1:A:392:VAL:O	1:A:392:VAL:CG1	2.52	0.56
1:B:456:ASP:OD2	1:B:458:ARG:NH1	2.38	0.56
1:D:431:GLU:HA	1:D:452:VAL:HG11	1.86	0.56
1:A:140:ARG:O	1:A:140:ARG:HG3	2.05	0.56
1:B:229:GLN:HE21	1:B:232:ASP:HB2	1.69	0.56
1:D:153:ASN:ND2	1:D:153:ASN:N	2.50	0.56
1:D:352:LYS:HG3	1:D:366:THR:HG22	1.86	0.56
1:D:471:PHE:CG	1:D:472:PRO:HD3	2.40	0.56
1:B:177:MSE:C	1:B:180:PRO:HD2	2.28	0.56
1:C:277:ASN:N	1:C:281:GLN:OE1	2.25	0.56
1:D:229:GLN:O	1:D:229:GLN:HG2	2.05	0.56
1:D:333:SER:HB3	1:D:336:GLU:HG3	1.87	0.56
1:B:430:ALA:HB3	5:B:4069:HOH:O	2.04	0.56
1:A:26:LYS:HG3	1:B:151:PRO:HG2	1.87	0.56
1:A:160:VAL:CG2	1:A:203:ILE:HD11	2.35	0.56
1:C:422:PRO:HD2	1:C:425:GLN:HE21	1.69	0.56
1:A:468:VAL:HA	1:A:471:PHE:HE2	1.71	0.56
1:B:86:MSE:CE	1:B:111:VAL:HG23	2.36	0.56
1:B:306:LYS:NZ	1:B:384:LEU:O	2.38	0.56
1:C:167:LEU:HD22	1:C:421:ASN:HB2	1.86	0.56
1:D:150:TRP:NE1	1:D:152:GLU:HG2	2.21	0.56
1:D:293:ALA:HA	1:D:296:LYS:HE2	1.86	0.56
1:A:219:MSE:HG2	1:B:38:MSE:CE	2.35	0.56
1:A:344:PHE:CE2	1:A:348:GLY:HA2	2.40	0.56
1:B:293:ALA:O	1:B:296:LYS:HB2	2.05	0.56
1:B:298:ILE:HG21	1:B:300:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:LEU:HD12	1:D:200:PRO:HG3	1.88	0.56
1:C:295:GLN:OE1	1:C:295:GLN:HA	2.06	0.56
1:D:186:LEU:HD12	1:D:471:PHE:HZ	1.71	0.56
1:A:183:LYS:HA	1:A:186:LEU:HD12	1.89	0.56
1:A:552:TYR:CE1	1:A:556:ARG:CZ	2.89	0.56
1:B:332:LEU:HD12	1:B:332:LEU:H	1.70	0.56
1:D:334:GLU:O	1:D:338:GLN:HG3	2.06	0.56
1:A:527:ALA:O	1:A:531:THR:HG23	2.05	0.55
1:B:24:LYS:O	1:D:22:LYS:NZ	2.36	0.55
1:A:106:SER:OG	1:A:107:LEU:HD12	2.06	0.55
1:A:528:ILE:O	1:A:532:GLU:HG3	2.05	0.55
1:D:298:ILE:HD11	1:D:413:ARG:HB2	1.88	0.55
1:B:284:ALA:HA	1:B:319:ILE:HG23	1.87	0.55
1:C:455:THR:HG22	5:C:4002:HOH:O	2.06	0.55
1:A:22:LYS:HD2	1:A:22:LYS:O	2.06	0.55
1:A:227:ARG:HH11	1:A:227:ARG:CG	2.11	0.55
1:D:143:VAL:HG21	1:D:237:GLU:HG2	1.88	0.55
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.89	0.55
1:A:120:CYS:O	1:A:175:TYR:HB3	2.06	0.55
1:A:300:LYS:NZ	1:A:305:HIS:HD2	2.04	0.55
1:A:542:ARG:HD2	1:A:552:TYR:OH	2.06	0.55
1:B:551:LYS:O	1:B:555:GLU:HB2	2.06	0.55
1:D:530:VAL:O	1:D:534:LEU:HG	2.07	0.55
1:A:140:ARG:HH22	1:A:230:GLN:HA	1.70	0.55
1:C:140:ARG:HB2	1:C:140:ARG:HH11	1.72	0.55
1:B:36:LYS:HZ2	1:B:562:TYR:HB3	1.72	0.55
1:B:335:GLN:O	1:B:339:LYS:HD2	2.07	0.55
1:D:332:LEU:HA	1:D:336:GLU:OE2	2.06	0.55
1:C:358:ILE:HG23	1:C:362:GLN:HB2	1.89	0.55
1:D:528:ILE:O	1:D:531:THR:HG23	2.07	0.55
1:A:104:ILE:HD13	1:A:519:ILE:HG21	1.89	0.55
1:A:215:ASP:OD1	1:A:216:PRO:HD2	2.06	0.55
1:A:261:ASN:ND2	1:A:264:ARG:NH2	2.50	0.55
1:A:401:PRO:CB	1:A:436:LEU:HD21	2.37	0.55
1:D:370:PRO:HB2	1:D:371:GLU:OE1	2.07	0.55
1:D:530:VAL:HG12	1:D:534:LEU:HD21	1.90	0.55
1:A:343:MSE:HB2	1:A:350:LEU:CD1	2.35	0.54
1:B:45:ARG:HA	1:B:50:LEU:HD12	1.89	0.54
1:B:69:HIS:HE1	1:B:102:ASP:OD2	1.90	0.54
1:C:535:TYR:HE2	1:C:545:GLU:HB2	1.70	0.54
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LYS:O	1:A:500:SER:HB3	2.07	0.54
1:D:207:THR:O	1:D:224:LYS:HA	2.07	0.54
1:D:401:PRO:HA	1:D:436:LEU:HD23	1.89	0.54
1:A:350:LEU:HD23	1:A:354:ARG:NH1	2.23	0.54
1:C:456:ASP:OD1	1:C:456:ASP:C	2.50	0.54
1:D:166:ILE:HG13	1:D:172:LEU:HB2	1.89	0.54
1:A:226:ASP:OD1	1:A:226:ASP:C	2.48	0.54
1:B:518:ASN:HB3	1:B:521:GLU:OE2	2.07	0.54
1:A:419:LEU:O	3:A:601:NAD:H2N	2.08	0.54
1:B:21:ILE:HG13	1:B:23:GLU:H	1.73	0.54
1:B:130:PRO:O	1:B:131:LYS:HG3	2.07	0.54
1:A:358:ILE:HD12	1:A:366:THR:OG1	2.08	0.54
1:B:467:ASN:ND2	4:B:1603:MAK:O5	2.41	0.54
1:C:33:ARG:HH21	1:C:152:GLU:CG	2.21	0.54
1:C:91:ARG:NE	5:C:4011:HOH:O	2.39	0.54
1:C:276:PHE:HB3	1:C:486:ILE:HD12	1.90	0.54
1:C:388:THR:HG22	1:C:389:ILE:N	2.23	0.54
1:C:571:GLU:OE2	1:C:572:TRP:O	2.26	0.54
1:D:461:THR:HB	1:D:509:GLN:HB3	1.90	0.54
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.90	0.54
1:A:187:TYR:HE1	1:A:471:PHE:HD1	1.54	0.54
1:D:64:GLN:NE2	1:D:562:TYR:OH	2.24	0.54
1:A:534:LEU:CD2	1:A:539:MSE:HE2	2.38	0.54
1:A:546:PRO:HG3	1:A:552:TYR:CD2	2.43	0.54
1:B:296:LYS:HZ2	1:B:507:LEU:HD11	1.73	0.54
1:C:127:PHE:CD2	1:D:38:MSE:HE2	2.43	0.54
1:D:329:GLU:C	1:D:330:ASN:HD22	2.16	0.54
1:B:516:LEU:HD12	1:B:516:LEU:O	2.08	0.54
1:D:51:GLN:HE21	1:D:51:GLN:HA	1.72	0.54
1:D:59:GLU:HB3	1:D:63:ILE:CG2	2.37	0.54
1:C:47:MSE:C	1:C:48:LEU:HD23	2.33	0.53
1:A:175:TYR:CE2	1:A:218:TYR:HA	2.42	0.53
1:A:177:MSE:O	1:A:177:MSE:HG3	2.08	0.53
1:C:61:GLN:HA	1:C:64:GLN:NE2	2.15	0.53
1:C:140:ARG:HE	1:C:230:GLN:HG2	1.73	0.53
1:D:453:LYS:HG3	1:D:459:VAL:HG22	1.89	0.53
1:A:183:LYS:HG3	1:A:471:PHE:CZ	2.43	0.53
1:A:387:SER:HA	1:A:411:ASN:OD1	2.08	0.53
1:C:248:ARG:HH11	1:C:248:ARG:CG	2.20	0.53
1:C:546:PRO:HG2	1:C:549:LYS:HE3	1.91	0.53
1:D:75:MSE:HE3	1:D:81:LYS:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ILE:O	1:B:373:ILE:HG22	2.08	0.53
1:D:248:ARG:NH1	1:D:272:LYS:O	2.41	0.53
1:A:302:ILE:HG21	1:A:332:LEU:HD13	1.91	0.53
1:C:140:ARG:HB2	1:C:140:ARG:CZ	2.36	0.53
1:C:350:LEU:HD23	1:C:354:ARG:NH1	2.23	0.53
1:C:441:CYS:C	1:C:442:LEU:HD23	2.34	0.53
1:D:226:ASP:C	1:D:226:ASP:OD1	2.49	0.53
1:A:174:VAL:C	1:A:176:GLY:H	2.16	0.53
1:A:297:VAL:CG2	1:A:442:LEU:HD11	2.39	0.53
1:A:300:LYS:HZ2	1:A:305:HIS:HD2	1.57	0.53
1:B:324:VAL:HG13	1:B:337:ALA:HB3	1.91	0.53
1:B:354:ARG:HE	1:B:358:ILE:CD1	2.09	0.53
1:C:56:PRO:HG2	1:D:220:GLY:HA2	1.89	0.53
1:C:174:VAL:HG12	1:C:174:VAL:O	2.09	0.53
1:D:177:MSE:SE	5:D:4017:HOH:O	2.76	0.53
1:D:531:THR:HA	1:D:534:LEU:HG	1.90	0.53
1:A:153:ASN:HB3	1:A:245:ARG:HH21	1.74	0.53
1:A:518:ASN:OD1	1:A:518:ASN:N	2.42	0.53
1:B:276:PHE:CD1	1:B:276:PHE:C	2.87	0.53
1:C:503:THR:OG1	1:C:506:GLU:HG3	2.09	0.53
1:D:399:PHE:HB2	1:D:428:CYS:HB3	1.90	0.53
1:D:466:ASN:HB3	1:D:468:VAL:HG12	1.91	0.53
1:B:86:MSE:HE2	1:B:111:VAL:HG23	1.90	0.53
1:B:525:ASN:HA	1:B:528:ILE:HG13	1.91	0.53
1:D:120:CYS:O	1:D:175:TYR:HB3	2.09	0.53
1:D:295:GLN:HE21	1:D:305:HIS:HE1	1.57	0.53
1:A:153:ASN:H	1:A:153:ASN:ND2	2.07	0.53
1:D:83:ILE:HD11	1:D:126:ILE:CG2	2.38	0.53
1:B:43:GLN:HG2	1:B:47:MSE:HE1	1.89	0.52
1:B:324:VAL:HG13	1:B:337:ALA:CB	2.39	0.52
1:C:351:VAL:CG1	1:C:369:ALA:HA	2.39	0.52
1:A:97:TYR:HA	1:A:100:LEU:HD22	1.91	0.52
1:A:295:GLN:HE22	1:A:299:SER:C	2.17	0.52
1:B:112:TYR:CE2	1:B:113:THR:HG22	2.43	0.52
1:B:389:ILE:HG23	1:B:399:PHE:CE1	2.45	0.52
1:D:26:LYS:HB3	1:D:27:PRO:HD3	1.91	0.52
1:A:177:MSE:CE	1:A:200:PRO:HB2	2.39	0.52
1:B:415:VAL:C	1:B:416:ILE:HD12	2.34	0.52
1:C:418:ALA:O	1:C:445:SER:HA	2.10	0.52
1:A:288:LEU:CD2	1:A:322:LEU:HD23	2.40	0.52
1:B:75:MSE:HG2	1:B:80:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD12	1:B:377:PHE:CD1	2.44	0.52
1:B:349:LEU:CD1	1:B:384:LEU:HD11	2.38	0.52
1:B:166:ILE:HA	1:B:256:ASP:OD2	2.09	0.52
1:C:288:LEU:O	1:C:292:LEU:HD22	2.09	0.52
1:D:61:GLN:OE1	1:D:98:ARG:NH1	2.42	0.52
1:D:150:TRP:O	1:D:245:ARG:NH2	2.41	0.52
1:D:374:PRO:HB3	1:D:380:ALA:N	2.24	0.52
1:A:456:ASP:OD2	1:A:458:ARG:NH1	2.41	0.52
1:B:26:LYS:HA	1:B:29:MSE:HE3	1.91	0.52
1:B:194:ARG:HB2	1:B:197:ARG:HG3	1.92	0.52
1:D:363:GLU:OE1	1:D:363:GLU:O	2.28	0.52
1:C:90:GLU:OE1	1:C:131:LYS:HD2	2.09	0.52
1:D:94:LYS:HG3	1:D:560:SER:O	2.09	0.52
1:D:161:THR:HA	1:D:257:PHE:CE1	2.45	0.52
1:D:327:MSE:HE3	1:D:337:ALA:CA	2.40	0.52
1:B:298:ILE:HG22	1:B:300:LYS:H	1.73	0.52
1:C:137:ILE:O	1:C:140:ARG:HG2	2.10	0.52
1:C:504:ASP:OD2	1:C:504:ASP:N	2.42	0.52
1:A:46:GLN:HG3	1:A:51:GLN:HG3	1.92	0.52
1:A:377:PHE:CE2	1:A:389:ILE:HD11	2.33	0.52
1:A:552:TYR:HE1	1:A:556:ARG:CZ	2.23	0.52
1:D:307:ILE:HD13	1:D:388:THR:OG1	2.10	0.52
1:D:518:ASN:ND2	1:D:518:ASN:N	2.57	0.52
1:C:144:ARG:HD2	1:C:144:ARG:O	2.10	0.52
1:A:374:PRO:HB3	1:A:380:ALA:N	2.25	0.51
1:A:518:ASN:O	1:A:522:VAL:HG23	2.10	0.51
1:C:297:VAL:CG2	1:C:442:LEU:HD11	2.39	0.51
1:D:140:ARG:NH2	1:D:230:GLN:O	2.43	0.51
1:D:174:VAL:C	1:D:176:GLY:H	2.17	0.51
1:A:183:LYS:HG3	1:A:471:PHE:CE1	2.45	0.51
1:A:251:LEU:HD22	1:A:252:ILE:N	2.25	0.51
1:C:218:TYR:O	1:D:57:LYS:HE2	2.11	0.51
1:B:196:ASP:OD1	1:B:197:ARG:HG2	2.11	0.51
1:B:533:TYR:CZ	1:B:537:ASN:ND2	2.78	0.51
1:C:374:PRO:HG3	1:C:383:ILE:HD12	1.92	0.51
1:D:551:LYS:HD2	1:D:555:GLU:OE1	2.11	0.51
1:A:389:ILE:O	1:A:390:ILE:HD13	2.10	0.51
1:A:533:TYR:O	1:A:537:ASN:ND2	2.43	0.51
1:B:493:GLU:HG3	1:B:533:TYR:CD1	2.45	0.51
1:A:297:VAL:HG21	1:A:442:LEU:HD11	1.93	0.51
1:C:528:ILE:HA	1:C:531:THR:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:501:GLN:HE22	1:D:525:ASN:HB2	1.74	0.51
1:B:228:THR:OG1	1:B:230:GLN:HG3	2.10	0.51
1:A:453:LYS:NZ	1:A:457:GLY:HA2	2.24	0.51
1:B:43:GLN:O	1:B:47:MSE:HE3	2.11	0.51
1:B:354:ARG:CD	1:B:358:ILE:HD11	2.40	0.51
1:D:163:GLY:HA2	1:D:166:ILE:HD11	1.93	0.51
1:A:144:ARG:HH21	1:A:245:ARG:HG3	1.75	0.51
1:A:328:VAL:C	1:A:330:ASN:H	2.19	0.51
1:A:453:LYS:HZ3	1:A:457:GLY:HA2	1.76	0.51
1:B:137:ILE:HA	1:B:234:LEU:HD22	1.93	0.51
1:B:401:PRO:HB3	1:B:436:LEU:HD21	1.92	0.51
1:C:167:LEU:HD23	4:C:2603:MAK:C1	2.41	0.51
1:C:288:LEU:HG	1:C:292:LEU:HD22	1.93	0.51
1:A:263:PHE:CZ	1:A:314:GLU:HA	2.46	0.51
1:B:296:LYS:NZ	1:B:507:LEU:HD11	2.25	0.51
1:B:505:GLU:O	1:B:509:GLN:HG2	2.11	0.51
1:D:283:THR:HA	1:D:286:VAL:HG23	1.92	0.51
1:A:61:GLN:HG3	1:A:562:TYR:CE1	2.46	0.50
1:A:239:MSE:O	1:A:243:THR:HG23	2.12	0.50
1:B:182:GLY:O	1:B:185:CYS:HB2	2.11	0.50
1:B:431:GLU:N	5:B:4069:HOH:O	2.44	0.50
1:A:350:LEU:HD22	1:A:358:ILE:CD1	2.40	0.50
1:C:441:CYS:O	1:C:442:LEU:HD23	2.11	0.50
1:D:108:MSE:HA	1:D:111:VAL:HG22	1.93	0.50
1:D:140:ARG:HG3	1:D:140:ARG:O	2.11	0.50
1:A:68:PHE:CD2	1:A:99:ILE:HD11	2.47	0.50
1:A:305:HIS:O	1:A:340:LYS:HD2	2.12	0.50
1:A:412:GLU:O	1:A:440:ARG:NH1	2.44	0.50
1:A:418:ALA:O	1:A:445:SER:HA	2.11	0.50
1:B:447:SER:HB3	1:B:448:PRO:HD2	1.93	0.50
1:C:160:VAL:HG11	1:C:238:PHE:CZ	2.46	0.50
1:D:191:ALA:O	1:D:476:LEU:HD22	2.10	0.50
1:B:251:LEU:HD23	1:B:252:ILE:N	2.27	0.50
1:B:418:ALA:CB	1:B:427:GLU:HB2	2.41	0.50
1:C:446:GLY:O	1:C:466:ASN:ND2	2.42	0.50
1:A:319:ILE:HG22	1:A:323:ILE:HD11	1.93	0.50
1:C:127:PHE:CE2	1:D:38:MSE:HE2	2.47	0.50
1:C:286:VAL:HG13	1:C:470:ILE:HG12	1.93	0.50
1:A:354:ARG:NE	1:A:356:ALA:O	2.44	0.50
1:A:413:ARG:HA	1:A:440:ARG:O	2.12	0.50
1:B:144:ARG:HH12	1:B:244:ASP:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LYS:HE2	1:D:301:PRO:N	2.26	0.50
1:D:351:VAL:HB	1:D:369:ALA:HB2	1.94	0.50
1:A:26:LYS:HG3	1:B:151:PRO:CG	2.41	0.50
1:B:165:ARG:HH21	1:B:167:LEU:CA	2.24	0.50
1:C:358:ILE:HG23	1:C:362:GLN:HE21	1.76	0.50
1:C:396:GLY:HA2	1:C:425:GLN:HA	1.93	0.50
1:D:314:GLU:HB2	3:D:3601:NAD:O1N	2.12	0.50
1:B:94:LYS:HE2	1:B:558:TRP:CZ2	2.46	0.50
1:B:287:ALA:CB	1:B:319:ILE:HG21	2.39	0.50
1:A:404:ILE:HD13	1:A:436:LEU:HD23	1.94	0.49
1:B:359:ASP:O	1:B:360:SER:C	2.54	0.49
1:D:194:ARG:HE	1:D:197:ARG:HH11	1.59	0.49
1:D:404:ILE:CG2	1:D:436:LEU:HB3	2.42	0.49
1:A:295:GLN:HE22	1:A:299:SER:HA	1.77	0.49
1:C:210:ILE:O	1:C:214:LYS:HG2	2.12	0.49
1:D:394:GLY:HA2	1:D:420:SER:HB3	1.94	0.49
1:D:557:THR:O	1:D:559:ARG:NH2	2.45	0.49
1:A:243:THR:HG21	1:A:273:TYR:CE2	2.46	0.49
1:D:186:LEU:HD13	1:D:468:VAL:CG2	2.42	0.49
1:D:437:THR:O	1:D:438:GLU:HB2	2.12	0.49
1:A:294:ALA:O	1:A:297:VAL:HG13	2.12	0.49
1:B:174:VAL:HG12	1:B:174:VAL:O	2.10	0.49
1:B:370:PRO:HD2	1:B:373:ILE:CD1	2.42	0.49
1:D:177:MSE:HE1	1:D:181:VAL:CG2	2.24	0.49
1:A:61:GLN:HA	1:A:64:GLN:NE2	2.26	0.49
1:A:529:LYS:NZ	1:A:532:GLU:OE1	2.46	0.49
1:D:321:ASN:O	1:D:325:MSE:HG3	2.13	0.49
1:D:447:SER:HB3	1:D:448:PRO:HD2	1.95	0.49
1:A:482:ASN:HD21	3:A:602:NAD:H4B	1.78	0.49
1:C:85:ILE:HD12	1:C:85:ILE:C	2.38	0.49
1:D:91:ARG:HH11	1:D:91:ARG:CG	2.23	0.49
1:A:174:VAL:HG12	1:A:219:MSE:HE2	1.95	0.49
1:A:461:THR:O	1:A:511:ARG:HG2	2.12	0.49
1:B:334:GLU:HG3	1:B:338:GLN:HE21	1.74	0.49
1:B:370:PRO:HG2	1:B:372:SER:O	2.12	0.49
1:D:132:GLY:HA2	1:D:200:PRO:HD2	1.93	0.49
1:C:130:PRO:C	1:C:131:LYS:HG2	2.38	0.49
1:A:478:VAL:HG13	1:A:483:THR:HB	1.95	0.49
1:B:75:MSE:HG2	1:B:80:GLU:CG	2.43	0.49
1:B:320:ALA:O	1:B:324:VAL:HG23	2.13	0.49
1:C:128:ARG:HG2	1:D:91:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:PHE:CE1	1:C:242:ILE:HG13	2.47	0.49
1:C:476:LEU:HD23	1:C:527:ALA:CB	2.43	0.49
1:C:495:ALA:O	1:C:499:THR:HG22	2.13	0.49
1:C:552:TYR:CD1	1:C:556:ARG:NH1	2.81	0.49
1:D:287:ALA:HB3	1:D:319:ILE:HG23	1.95	0.48
1:D:506:GLU:O	1:D:511:ARG:HG2	2.13	0.48
1:C:529:LYS:O	1:C:532:GLU:HB2	2.14	0.48
1:D:239:MSE:O	1:D:243:THR:HG23	2.12	0.48
1:A:64:GLN:HB3	1:A:95:LEU:HD22	1.94	0.48
1:A:227:ARG:NH1	1:A:227:ARG:CG	2.71	0.48
1:B:144:ARG:HH12	1:B:244:ASP:CB	2.26	0.48
1:B:481:CYS:SG	1:B:531:THR:HB	2.53	0.48
1:C:351:VAL:HG11	1:C:369:ALA:HA	1.96	0.48
1:D:104:ILE:O	1:D:108:MSE:HB2	2.13	0.48
1:D:115:THR:HG22	1:D:115:THR:O	2.13	0.48
1:A:261:ASN:HD22	1:A:264:ARG:NE	2.09	0.48
1:A:261:ASN:HD21	1:A:264:ARG:HH21	1.59	0.48
1:A:300:LYS:NZ	1:A:304:GLU:HB2	2.28	0.48
1:A:300:LYS:NZ	1:A:304:GLU:O	2.44	0.48
1:A:551:LYS:HB3	1:A:551:LYS:HZ2	1.77	0.48
1:B:323:ILE:HG21	1:B:341:ILE:HD11	1.95	0.48
1:C:33:ARG:NH2	1:C:152:GLU:HG3	2.27	0.48
1:C:184:LEU:HD12	1:C:200:PRO:HG3	1.95	0.48
1:D:208:ASP:OD1	1:D:225:ARG:HG3	2.14	0.48
1:D:287:ALA:CB	1:D:319:ILE:HD13	2.43	0.48
1:D:397:ARG:HA	1:D:427:GLU:O	2.12	0.48
1:A:166:ILE:HG23	1:A:179:ILE:HG13	1.96	0.48
1:A:369:ALA:HB1	1:A:373:ILE:CD1	2.41	0.48
1:C:46:GLN:HG2	1:C:51:GLN:HG3	1.95	0.48
1:C:286:VAL:HG11	1:C:466:ASN:C	2.38	0.48
1:C:351:VAL:HA	1:C:367:HIS:O	2.14	0.48
1:C:400:THR:O	1:C:404:ILE:HG12	2.13	0.48
1:D:502:LEU:HD11	1:D:507:LEU:HG	1.95	0.48
1:A:285:ALA:HB1	1:A:470:ILE:HD12	1.94	0.48
1:D:197:ARG:HH11	1:D:197:ARG:HG2	1.78	0.48
1:D:211:ALA:HA	1:D:214:LYS:HE3	1.95	0.48
1:D:359:ASP:O	1:D:360:SER:C	2.56	0.48
1:D:404:ILE:HG21	1:D:436:LEU:HB3	1.95	0.48
1:D:474:VAL:O	1:D:478:VAL:HG23	2.14	0.48
1:D:506:GLU:CG	1:D:511:ARG:HD2	2.43	0.48
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:CD2	1:A:340:LYS:NZ	2.75	0.48
1:B:297:VAL:HG21	1:B:442:LEU:HD21	1.95	0.48
1:D:91:ARG:HG3	1:D:91:ARG:NH1	2.23	0.48
1:A:144:ARG:NH2	1:A:245:ARG:CG	2.77	0.48
1:A:331:GLY:O	1:A:332:LEU:O	2.31	0.48
1:D:157:ALA:HB2	1:D:479:ILE:HD11	1.96	0.48
1:D:506:GLU:O	1:D:511:ARG:CG	2.62	0.48
1:A:174:VAL:C	1:A:176:GLY:N	2.71	0.48
1:B:533:TYR:CE1	1:B:537:ASN:ND2	2.80	0.48
1:C:260:HIS:C	1:C:260:HIS:CD2	2.92	0.48
1:C:447:SER:HB3	1:C:448:PRO:HD2	1.96	0.48
1:D:298:ILE:O	1:D:299:SER:C	2.57	0.48
1:A:204:ASP:OD2	1:A:221:LEU:HB2	2.14	0.48
1:B:389:ILE:HG22	1:B:416:ILE:HA	1.96	0.48
1:D:555:GLU:HB3	1:D:556:ARG:HH11	1.79	0.48
1:A:253:GLN:HB2	1:A:276:PHE:CE2	2.49	0.47
1:A:396:GLY:O	1:A:398:LEU:HD23	2.14	0.47
1:B:69:HIS:CE1	1:B:102:ASP:OD2	2.67	0.47
1:B:401:PRO:HA	1:B:436:LEU:CD2	2.44	0.47
1:D:344:PHE:CZ	1:D:348:GLY:HA2	2.49	0.47
1:A:503:THR:HG23	1:A:506:GLU:CD	2.39	0.47
1:B:410:ILE:HG22	1:B:411:ASN:CG	2.39	0.47
1:B:549:LYS:HD3	1:B:549:LYS:N	2.28	0.47
1:C:177:MSE:O	1:C:181:VAL:HG23	2.14	0.47
1:D:144:ARG:HH12	1:D:244:ASP:HB2	1.79	0.47
1:D:329:GLU:CG	1:D:330:ASN:ND2	2.78	0.47
1:B:51:GLN:HA	1:B:51:GLN:NE2	2.24	0.47
1:B:416:ILE:HD12	1:B:416:ILE:N	2.29	0.47
1:C:23:GLU:CD	1:C:24:LYS:H	2.22	0.47
1:C:521:GLU:HG3	1:C:522:VAL:N	2.28	0.47
1:D:204:ASP:OD2	1:D:221:LEU:HD22	2.13	0.47
1:D:301:PRO:O	1:D:302:ILE:C	2.57	0.47
1:D:557:THR:OG1	1:D:559:ARG:NH1	2.47	0.47
1:A:108:MSE:HG3	1:A:112:TYR:HB3	1.96	0.47
1:A:549:LYS:H	1:A:549:LYS:HD3	1.79	0.47
1:B:497:ALA:O	1:B:501:GLN:HG3	2.14	0.47
1:D:174:VAL:C	1:D:176:GLY:N	2.71	0.47
1:C:228:THR:OG1	1:C:230:GLN:HB2	2.14	0.47
1:C:546:PRO:O	1:C:549:LYS:CE	2.63	0.47
1:D:438:GLU:O	1:D:458:ARG:NH2	2.47	0.47
1:D:530:VAL:CG1	1:D:534:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:PRO:HB2	1:B:304:GLU:HG3	1.97	0.47
1:D:104:ILE:HG13	1:D:108:MSE:HE2	1.96	0.47
1:D:186:LEU:O	1:D:190:CYS:HB2	2.13	0.47
1:A:404:ILE:HG23	1:A:416:ILE:HD13	1.97	0.47
1:B:163:GLY:HA2	1:B:166:ILE:HD11	1.96	0.47
1:B:231:TYR:HE2	1:B:265:PHE:CZ	2.33	0.47
1:B:504:ASP:O	1:B:508:ALA:N	2.47	0.47
1:B:506:GLU:HA	1:B:509:GLN:HG3	1.97	0.47
1:C:400:THR:HB	1:C:401:PRO:HD2	1.96	0.47
1:C:525:ASN:O	1:C:529:LYS:HG2	2.15	0.47
1:D:43:GLN:O	1:D:47:MSE:HE3	2.14	0.47
1:D:136:SER:HB2	1:D:221:LEU:HD22	1.96	0.47
1:A:57:LYS:HD3	1:B:218:TYR:O	2.15	0.47
1:A:209:ASN:OD1	1:A:211:ALA:HB3	2.15	0.47
1:D:288:LEU:HG	1:D:292:LEU:CD2	2.42	0.47
1:D:344:PHE:C	1:D:344:PHE:CD2	2.92	0.47
1:A:93:GLU:O	1:A:96:PHE:HB3	2.15	0.47
1:A:392:VAL:CG1	5:A:4006:HOH:O	2.63	0.47
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.71	0.47
1:C:165:ARG:NH1	3:C:2601:NAD:O1N	2.45	0.47
1:D:68:PHE:CG	1:D:99:ILE:HG13	2.49	0.47
1:D:107:LEU:O	1:D:111:VAL:HG13	2.15	0.47
1:B:550:ALA:O	1:B:554:LYS:HG3	2.14	0.47
1:C:394:GLY:HA2	1:C:420:SER:HB3	1.97	0.47
1:B:302:ILE:HG13	1:B:332:LEU:HD11	1.97	0.46
1:B:419:LEU:O	3:B:1601:NAD:H2N	2.15	0.46
1:B:559:ARG:HB3	1:B:561:GLU:OE1	2.15	0.46
1:C:150:TRP:CE2	1:C:199:LEU:HD13	2.50	0.46
1:C:259:ASN:O	1:C:262:ALA:HB3	2.15	0.46
1:D:339:LYS:HA	1:D:367:HIS:NE2	2.31	0.46
1:A:96:PHE:O	1:A:100:LEU:HD22	2.15	0.46
1:B:23:GLU:HG3	1:B:24:LYS:N	2.30	0.46
1:B:165:ARG:HH21	1:B:167:LEU:HA	1.80	0.46
1:D:184:LEU:HD12	1:D:200:PRO:CG	2.44	0.46
1:A:175:TYR:CZ	1:A:218:TYR:HA	2.50	0.46
1:A:255:GLU:OE2	1:A:278:ASP:HB3	2.15	0.46
1:A:349:LEU:HD23	1:A:351:VAL:CG1	2.45	0.46
1:C:396:GLY:O	1:C:398:LEU:HD22	2.14	0.46
1:D:22:LYS:HD3	1:D:22:LYS:C	2.40	0.46
1:D:217:PHE:O	1:D:218:TYR:C	2.59	0.46
1:D:267:ARG:CZ	1:D:267:ARG:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASN:HD22	1:D:330:ASN:N	2.13	0.46
1:A:209:ASN:OD1	1:A:209:ASN:C	2.58	0.46
1:B:211:ALA:O	1:B:214:LYS:HG3	2.16	0.46
1:C:25:GLY:C	1:C:27:PRO:HD2	2.40	0.46
1:C:68:PHE:CD2	1:C:99:ILE:CG1	2.99	0.46
1:C:302:ILE:HG23	1:C:303:SER:N	2.31	0.46
1:C:516:LEU:HD12	1:C:516:LEU:O	2.16	0.46
1:A:142:HIS:HB3	1:D:568:ASP:OD1	2.16	0.46
1:A:372:SER:O	1:A:374:PRO:HD3	2.16	0.46
1:B:43:GLN:O	1:B:47:MSE:HB2	2.16	0.46
1:A:42:LEU:HD11	1:A:46:GLN:NE2	2.30	0.46
1:A:108:MSE:N	1:A:109:PRO:CD	2.78	0.46
1:B:333:SER:H	1:B:336:GLU:CG	2.28	0.46
1:C:293:ALA:O	1:C:296:LYS:HB2	2.16	0.46
1:A:183:LYS:HE2	1:A:255:GLU:OE1	2.15	0.46
1:A:301:PRO:O	1:A:302:ILE:C	2.56	0.46
1:B:401:PRO:HA	1:B:436:LEU:HD23	1.97	0.46
1:B:456:ASP:OD1	1:B:456:ASP:C	2.59	0.46
1:C:298:ILE:HD11	1:C:413:ARG:O	2.16	0.46
1:D:535:TYR:OH	1:D:542:ARG:HB3	2.15	0.46
1:A:207:THR:O	1:A:224:LYS:HA	2.16	0.46
1:A:251:LEU:HD22	1:A:252:ILE:H	1.81	0.46
1:C:72:LEU:HA	1:C:75:MSE:HG3	1.97	0.46
1:C:106:SER:O	1:C:109:PRO:HD2	2.16	0.46
1:C:308:LEU:HD13	1:C:384:LEU:HD23	1.97	0.46
1:D:55:PRO:HA	1:D:56:PRO:HD3	1.86	0.46
1:D:520:GLN:H	1:D:520:GLN:HE21	1.64	0.46
1:A:150:TRP:NE1	1:A:152:GLU:CD	2.74	0.46
1:A:171:ASP:OD1	1:A:207:THR:OG1	2.30	0.46
1:A:177:MSE:HE3	1:A:177:MSE:O	2.15	0.46
1:A:177:MSE:HE3	1:A:180:PRO:CG	2.45	0.46
1:B:32:PRO:HG3	1:B:90:GLU:O	2.15	0.46
1:B:404:ILE:HD12	1:B:436:LEU:HD22	1.98	0.46
1:A:72:LEU:HA	1:A:75:MSE:HG3	1.97	0.46
1:A:420:SER:HA	3:A:601:NAD:H1D	1.98	0.46
1:C:158:VAL:HG12	1:C:160:VAL:HG13	1.98	0.46
1:C:320:ALA:O	1:C:324:VAL:HG23	2.15	0.45
1:C:431:GLU:HA	1:C:452:VAL:HG11	1.98	0.45
1:D:502:LEU:HD13	1:D:507:LEU:HG	1.99	0.45
1:A:161:THR:HA	1:A:257:PHE:CE1	2.52	0.45
1:A:188:THR:HG21	1:A:195:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLN:NE2	1:A:299:SER:CA	2.79	0.45
1:B:36:LYS:HB2	1:B:40:PHE:CE1	2.51	0.45
1:B:156:LYS:HG3	1:B:197:ARG:CD	2.46	0.45
1:B:504:ASP:HA	1:B:507:LEU:HB2	1.98	0.45
1:D:338:GLN:HB2	1:D:339:LYS:NZ	2.31	0.45
1:D:397:ARG:H	1:D:397:ARG:HG2	1.63	0.45
1:A:295:GLN:HE22	1:A:300:LYS:H	1.63	0.45
1:A:332:LEU:H	1:A:332:LEU:CD1	2.28	0.45
1:D:249:ASN:C	1:D:249:ASN:ND2	2.65	0.45
1:A:522:VAL:O	1:A:526:ILE:HG12	2.17	0.45
1:B:323:ILE:HG23	1:B:327:MSE:HE3	1.99	0.45
1:D:358:ILE:HG12	1:D:366:THR:OG1	2.16	0.45
1:D:552:TYR:CE1	1:D:556:ARG:CZ	2.99	0.45
1:A:167:LEU:HD23	4:A:603:MAK:O1	2.17	0.45
1:A:382:ASN:O	1:A:385:LYS:NZ	2.42	0.45
1:A:404:ILE:CD1	1:A:436:LEU:HD23	2.46	0.45
1:B:194:ARG:HG3	3:B:1602:NAD:C6A	2.45	0.45
1:D:77:SER:O	1:D:81:LYS:HG3	2.16	0.45
1:A:43:GLN:OE1	1:A:43:GLN:HA	2.17	0.45
1:A:95:LEU:O	1:A:95:LEU:HD12	2.17	0.45
1:A:140:ARG:HB3	1:A:234:LEU:HD13	1.98	0.45
1:C:310:LEU:HD21	1:C:398:LEU:HD23	1.99	0.45
1:D:191:ALA:HB1	1:D:476:LEU:HD22	1.97	0.45
1:D:533:TYR:C	1:D:533:TYR:CD2	2.95	0.45
1:D:534:LEU:N	1:D:534:LEU:HD23	2.31	0.45
1:A:392:VAL:O	3:A:601:NAD:H51N	2.17	0.45
1:A:467:ASN:O	1:A:471:PHE:CD2	2.67	0.45
1:B:229:GLN:NE2	1:B:232:ASP:CB	2.74	0.45
1:B:387:SER:HA	1:B:411:ASN:OD1	2.16	0.45
1:B:397:ARG:HA	1:B:427:GLU:O	2.15	0.45
1:B:210:ILE:HD12	1:B:210:ILE:H	1.81	0.45
1:B:346:LYS:NZ	1:B:346:LYS:HB2	2.32	0.45
1:B:524:ILE:O	1:B:528:ILE:CG1	2.64	0.45
1:C:217:PHE:O	1:C:218:TYR:C	2.59	0.45
1:A:438:GLU:O	1:A:458:ARG:NH2	2.50	0.45
1:C:375:ASP:N	1:C:375:ASP:OD1	2.49	0.45
1:D:89:GLN:HG2	1:D:131:LYS:NZ	2.31	0.45
1:D:171:ASP:OD2	1:D:225:ARG:NE	2.43	0.45
1:D:471:PHE:N	1:D:472:PRO:CD	2.80	0.45
1:A:551:LYS:O	1:A:555:GLU:HG3	2.16	0.45
1:B:130:PRO:C	1:B:131:LYS:HG3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ILE:HG22	1:B:300:LYS:HB2	1.97	0.45
1:B:302:ILE:HD12	1:B:305:HIS:ND1	2.32	0.45
1:B:456:ASP:OD1	1:B:458:ARG:HD3	2.17	0.45
1:B:524:ILE:O	1:B:528:ILE:HG12	2.17	0.45
1:C:325:MSE:HE1	1:C:489:SER:HA	1.99	0.45
1:D:22:LYS:O	1:D:22:LYS:CD	2.65	0.45
1:D:108:MSE:N	1:D:109:PRO:CD	2.80	0.45
1:A:26:LYS:O	1:A:27:PRO:C	2.58	0.44
1:A:160:VAL:CG2	1:A:203:ILE:CD1	2.95	0.44
1:A:400:THR:O	1:A:403:VAL:HB	2.17	0.44
1:B:373:ILE:O	1:B:373:ILE:CG2	2.65	0.44
1:D:313:GLY:HA3	3:D:3601:NAD:O5B	2.17	0.44
1:D:374:PRO:HB3	1:D:379:ASP:CB	2.47	0.44
1:A:177:MSE:HE3	1:A:180:PRO:CD	2.45	0.44
1:A:305:HIS:O	1:A:340:LYS:CD	2.65	0.44
1:B:65:ALA:HA	1:B:99:ILE:HD11	1.98	0.44
1:B:259:ASN:OD1	1:B:263:PHE:HE1	2.00	0.44
1:B:298:ILE:HD11	1:B:442:LEU:CD1	2.47	0.44
1:B:342:TRP:CZ3	1:B:349:LEU:HD21	2.50	0.44
1:B:349:LEU:HD22	1:B:351:VAL:HG13	2.00	0.44
1:C:120:CYS:C	1:C:122:GLN:H	2.25	0.44
1:C:546:PRO:O	1:C:549:LYS:HE3	2.18	0.44
1:D:554:LYS:HG2	1:D:554:LYS:H	1.59	0.44
1:D:561:GLU:H	1:D:561:GLU:CD	2.25	0.44
1:A:97:TYR:HA	1:A:100:LEU:CD2	2.47	0.44
1:A:177:MSE:CE	1:A:177:MSE:O	2.66	0.44
1:A:261:ASN:ND2	1:A:264:ARG:HE	2.10	0.44
1:A:554:LYS:HB3	1:A:554:LYS:HE2	1.61	0.44
1:B:36:LYS:HB2	1:B:40:PHE:CD1	2.53	0.44
1:C:107:LEU:C	1:C:109:PRO:HD2	2.42	0.44
1:C:388:THR:CG2	1:C:389:ILE:N	2.80	0.44
1:D:266:LEU:O	1:D:270:ARG:HG2	2.18	0.44
1:A:96:PHE:O	1:A:99:ILE:HG22	2.17	0.44
1:B:321:ASN:O	1:B:325:MSE:HG3	2.17	0.44
1:B:358:ILE:HA	1:B:362:GLN:HE21	1.81	0.44
1:C:295:GLN:O	1:C:299:SER:N	2.45	0.44
1:C:412:GLU:O	1:C:440:ARG:HD2	2.17	0.44
1:D:83:ILE:HD11	1:D:126:ILE:HG21	1.99	0.44
1:D:346:LYS:HG2	3:D:3601:NAD:O2B	2.16	0.44
1:A:29:MSE:HE2	1:A:29:MSE:HB3	1.83	0.44
1:A:108:MSE:HE2	1:A:108:MSE:HB2	1.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:CD2	1:A:151:PRO:HD2	2.53	0.44
1:A:398:LEU:N	1:A:398:LEU:CD2	2.80	0.44
1:B:29:MSE:HE1	1:B:53:LEU:HD13	2.00	0.44
1:B:132:GLY:HA3	1:B:200:PRO:HG2	2.00	0.44
1:C:186:LEU:HD13	1:C:468:VAL:CG2	2.48	0.44
1:D:23:GLU:OE1	1:D:24:LYS:N	2.44	0.44
1:D:150:TRP:CE2	1:D:199:LEU:HD13	2.53	0.44
1:A:174:VAL:HG23	1:A:204:ASP:OD1	2.18	0.44
1:B:108:MSE:N	1:B:109:PRO:HD2	2.33	0.44
1:B:447:SER:HB3	1:B:448:PRO:CD	2.48	0.44
1:C:502:LEU:HD13	1:C:507:LEU:HG	2.00	0.44
1:D:293:ALA:O	1:D:296:LYS:HB2	2.18	0.44
1:D:559:ARG:HA	1:D:559:ARG:HD3	1.82	0.44
1:A:219:MSE:HE2	1:A:219:MSE:HB2	1.84	0.44
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.82	0.44
1:C:248:ARG:CG	1:C:248:ARG:NH1	2.80	0.44
1:A:46:GLN:HG3	1:A:51:GLN:CG	2.47	0.44
1:A:239:MSE:HE1	1:A:254:PHE:CE1	2.52	0.44
1:B:349:LEU:HD23	1:B:349:LEU:C	2.43	0.44
1:C:172:LEU:O	1:C:175:TYR:HB2	2.17	0.44
1:C:186:LEU:O	1:C:190:CYS:HB2	2.18	0.44
1:C:455:THR:CG2	5:C:4002:HOH:O	2.66	0.44
1:D:75:MSE:HE1	1:D:84:TYR:CB	2.48	0.44
1:D:359:ASP:OD2	1:D:359:ASP:C	2.61	0.44
1:B:25:GLY:C	1:B:27:PRO:HD2	2.43	0.44
1:B:229:GLN:NE2	1:B:229:GLN:CA	2.79	0.44
1:B:401:PRO:O	1:B:405:ARG:HB2	2.18	0.44
1:B:477:ALA:CB	1:B:531:THR:HG22	2.47	0.44
1:C:136:SER:HB2	1:C:221:LEU:HD22	2.00	0.44
1:A:470:ILE:C	1:A:472:PRO:HD2	2.43	0.43
1:A:498:LEU:HB2	1:A:526:ILE:HD11	2.00	0.43
1:B:288:LEU:O	1:B:292:LEU:HD22	2.17	0.43
1:B:319:ILE:HG13	1:B:319:ILE:H	1.55	0.43
1:D:467:ASN:OD1	4:D:3603:MAK:O5	2.36	0.43
1:A:85:ILE:HG12	1:A:86:MSE:N	2.33	0.43
1:A:188:THR:HG23	1:A:193:ILE:O	2.18	0.43
1:C:261:ASN:HB3	1:C:265:PHE:CE1	2.54	0.43
1:D:197:ARG:NH1	1:D:197:ARG:HG2	2.33	0.43
1:A:341:ILE:O	1:A:367:HIS:NE2	2.50	0.43
1:A:549:LYS:O	1:A:552:TYR:HB3	2.18	0.43
1:B:350:LEU:N	1:B:350:LEU:HD23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LYS:H	1:B:357:LYS:HG2	1.36	0.43
1:D:300:LYS:HE2	1:D:300:LYS:C	2.43	0.43
1:D:328:VAL:HA	1:D:332:LEU:O	2.18	0.43
1:A:388:THR:CG2	1:A:390:ILE:HD11	2.48	0.43
1:C:68:PHE:CG	1:C:99:ILE:HG12	2.53	0.43
1:C:103:ASP:C	1:C:103:ASP:OD1	2.61	0.43
1:D:413:ARG:HA	1:D:440:ARG:O	2.18	0.43
1:A:46:GLN:CG	1:A:51:GLN:HG3	2.49	0.43
1:A:453:LYS:HE2	1:A:459:VAL:HG22	2.01	0.43
1:B:350:LEU:HD22	1:B:354:ARG:NH2	2.33	0.43
1:C:266:LEU:O	1:C:270:ARG:HG2	2.19	0.43
1:D:177:MSE:O	1:D:180:PRO:HD2	2.19	0.43
1:D:350:LEU:HD22	1:D:354:ARG:NH1	2.29	0.43
1:A:103:ASP:O	1:A:107:LEU:HD13	2.18	0.43
1:C:229:GLN:O	1:C:229:GLN:HG3	2.18	0.43
1:C:288:LEU:HG	1:C:292:LEU:CD2	2.48	0.43
1:C:381:VAL:CG1	1:C:382:ASN:N	2.81	0.43
1:C:453:LYS:HE3	1:C:457:GLY:CA	2.38	0.43
1:C:506:GLU:HB3	1:C:511:ARG:CD	2.49	0.43
1:D:286:VAL:HG21	1:D:467:ASN:HA	1.99	0.43
1:D:323:ILE:HG22	1:D:324:VAL:N	2.33	0.43
1:A:343:MSE:HE1	1:A:362:GLN:HG2	2.01	0.43
1:B:466:ASN:C	1:B:468:VAL:H	2.27	0.43
1:B:482:ASN:HD22	1:B:482:ASN:HA	1.61	0.43
1:B:524:ILE:N	1:B:524:ILE:CD1	2.80	0.43
1:C:26:LYS:HD3	1:D:151:PRO:CG	2.49	0.43
1:D:137:ILE:HB	1:D:205:VAL:CG1	2.46	0.43
1:D:551:LYS:HE2	1:D:551:LYS:HB3	1.79	0.43
1:A:316:ALA:HB2	1:A:392:VAL:CG1	2.48	0.43
1:A:328:VAL:C	1:A:330:ASN:N	2.77	0.43
1:B:250:THR:O	1:B:252:ILE:HD12	2.19	0.43
1:B:288:LEU:HG	1:B:292:LEU:CD2	2.46	0.43
1:B:345:ASP:HB2	3:B:1601:NAD:O2B	2.19	0.43
1:C:304:GLU:HG2	1:C:304:GLU:H	1.55	0.43
1:D:75:MSE:HE3	1:D:81:LYS:CA	2.45	0.43
1:A:352:LYS:N	1:A:367:HIS:O	2.42	0.43
1:B:343:MSE:HB2	1:B:350:LEU:HG	2.01	0.43
1:C:159:VAL:HG23	1:C:184:LEU:HD21	2.00	0.43
1:C:401:PRO:HA	1:C:404:ILE:HG13	2.01	0.43
1:D:308:LEU:O	1:D:389:ILE:HD13	2.18	0.43
1:D:389:ILE:HD13	1:D:389:ILE:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASN:ND2	1:A:74:LYS:NZ	2.66	0.43
1:A:412:GLU:HG3	1:A:413:ARG:HG2	2.00	0.43
1:B:43:GLN:HG2	1:B:47:MSE:CE	2.49	0.43
1:B:184:LEU:HD12	1:B:200:PRO:HB3	2.01	0.43
1:B:186:LEU:O	1:B:187:TYR:C	2.62	0.43
1:D:546:PRO:HG2	1:D:552:TYR:CD2	2.54	0.43
1:A:29:MSE:O	1:A:35:ASN:ND2	2.51	0.42
1:A:177:MSE:O	1:A:180:PRO:HD2	2.19	0.42
1:A:389:ILE:CG2	1:A:416:ILE:HA	2.48	0.42
1:B:91:ARG:HH11	1:B:91:ARG:CG	2.32	0.42
1:B:161:THR:HA	1:B:257:PHE:CE1	2.54	0.42
1:B:286:VAL:HG11	1:B:466:ASN:O	2.19	0.42
1:B:513:TYR:O	1:B:514:PRO:C	2.61	0.42
1:C:68:PHE:CD2	1:C:99:ILE:HG13	2.54	0.42
1:C:136:SER:HA	1:C:204:ASP:O	2.19	0.42
1:D:315:ALA:O	1:D:319:ILE:HG13	2.19	0.42
1:D:552:TYR:O	1:D:556:ARG:NH1	2.52	0.42
1:A:73:LYS:HD2	1:A:73:LYS:HA	1.79	0.42
1:A:77:SER:OG	1:A:80:GLU:HB3	2.19	0.42
1:A:310:LEU:HD21	1:A:398:LEU:CB	2.49	0.42
1:A:503:THR:HG23	1:A:506:GLU:CG	2.49	0.42
1:B:46:GLN:HG2	1:B:51:GLN:HG3	2.01	0.42
1:B:301:PRO:CG	1:B:304:GLU:HG3	2.47	0.42
1:B:535:TYR:HE2	1:B:545:GLU:HB2	1.84	0.42
1:C:29:MSE:SE	1:C:50:LEU:HD22	2.70	0.42
1:C:546:PRO:HG2	1:C:549:LYS:CE	2.49	0.42
1:D:85:ILE:HG13	1:D:86:MSE:N	2.31	0.42
1:A:295:GLN:OE1	1:A:295:GLN:HA	2.20	0.42
1:A:559:ARG:HA	1:A:559:ARG:HD3	1.84	0.42
1:B:260:HIS:CE1	1:B:264:ARG:HE	2.37	0.42
1:B:483:THR:CG2	1:B:484:ARG:N	2.82	0.42
1:B:524:ILE:HG22	1:B:528:ILE:HD11	2.01	0.42
1:C:194:ARG:HA	1:C:195:PRO:HD3	1.91	0.42
1:D:430:ALA:HA	1:D:443:PHE:CE2	2.55	0.42
1:D:456:ASP:OD1	1:D:458:ARG:NH1	2.53	0.42
1:B:143:VAL:HG11	1:B:238:PHE:HA	2.02	0.42
1:B:243:THR:HG21	1:B:273:TYR:CE2	2.55	0.42
1:B:300:LYS:HA	1:B:301:PRO:HD2	1.91	0.42
1:B:325:MSE:HE2	1:B:325:MSE:HB3	1.91	0.42
1:B:346:LYS:HB2	1:B:346:LYS:HZ3	1.84	0.42
1:B:528:ILE:HG23	1:B:550:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:GLU:O	1:D:435:THR:HB	2.20	0.42
1:D:566:LEU:HA	1:D:567:PRO:HD3	1.86	0.42
1:A:22:LYS:HE3	1:C:24:LYS:O	2.19	0.42
1:A:43:GLN:HG3	1:A:47:MSE:CE	2.50	0.42
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.89	0.42
1:A:390:ILE:CD1	1:A:417:PHE:HB2	2.50	0.42
1:A:484:ARG:CZ	1:D:543:TYR:CD2	3.02	0.42
1:B:166:ILE:O	1:B:167:LEU:HB2	2.20	0.42
1:B:260:HIS:ND1	1:B:264:ARG:NE	2.67	0.42
1:C:128:ARG:HE	1:C:128:ARG:HB2	1.64	0.42
1:C:499:THR:C	1:C:501:GLN:H	2.27	0.42
1:D:66:LEU:HD22	1:D:70:ARG:CD	2.50	0.42
1:D:412:GLU:HG3	1:D:413:ARG:CG	2.48	0.42
1:A:137:ILE:O	1:A:137:ILE:HG13	2.18	0.42
1:A:253:GLN:NE2	1:A:278:ASP:OD2	2.52	0.42
1:A:561:GLU:N	1:A:561:GLU:CD	2.78	0.42
1:B:94:LYS:HE2	1:B:558:TRP:HZ2	1.84	0.42
1:B:150:TRP:HA	1:B:151:PRO:HD3	1.82	0.42
1:B:400:THR:O	1:B:403:VAL:HB	2.19	0.42
1:B:520:GLN:O	1:B:524:ILE:HD13	2.18	0.42
1:D:104:ILE:O	1:D:104:ILE:HG13	2.19	0.42
1:D:136:SER:HB2	1:D:221:LEU:CD2	2.49	0.42
1:A:53:LEU:N	1:A:53:LEU:HD23	2.34	0.42
1:A:55:PRO:C	1:A:57:LYS:H	2.27	0.42
1:A:201:VAL:HG12	1:A:202:CYS:N	2.35	0.42
1:B:345:ASP:OD2	1:B:347:TYR:N	2.49	0.42
1:B:397:ARG:H	1:B:397:ARG:HG2	1.40	0.42
1:C:55:PRO:C	1:C:57:LYS:H	2.28	0.42
1:C:128:ARG:CG	1:D:91:ARG:NE	2.81	0.42
1:D:63:ILE:CG2	1:D:64:GLN:N	2.83	0.42
1:A:24:LYS:HA	1:A:28:LEU:CD1	2.50	0.42
1:A:434:TYR:CZ	1:A:443:PHE:HB3	2.55	0.42
1:A:507:LEU:C	1:A:509:GLN:H	2.28	0.42
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.91	0.42
1:B:313:GLY:O	1:B:317:LEU:HD12	2.20	0.42
1:B:314:GLU:HB2	3:B:1601:NAD:O1N	2.19	0.42
1:B:518:ASN:N	1:B:518:ASN:ND2	2.67	0.42
1:B:520:GLN:H	1:B:520:GLN:NE2	2.04	0.42
1:C:362:GLN:O	1:C:363:GLU:C	2.62	0.42
1:C:420:SER:HA	3:C:2601:NAD:H1D	2.02	0.42
1:D:407:MSE:HG3	1:D:414:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLU:C	1:A:330:ASN:HD22	2.27	0.42
1:B:252:ILE:O	1:B:252:ILE:HG22	2.20	0.42
1:B:288:LEU:HD23	1:B:495:ALA:CB	2.49	0.42
1:B:358:ILE:CG2	1:B:359:ASP:N	2.82	0.42
1:C:60:THR:O	1:C:64:GLN:HG3	2.20	0.42
1:D:239:MSE:HE1	1:D:254:PHE:HE1	1.85	0.42
1:C:226:ASP:OD1	1:C:226:ASP:C	2.62	0.42
1:C:307:ILE:HG22	1:C:308:LEU:N	2.34	0.42
1:C:419:LEU:O	3:C:2601:NAD:H2N	2.19	0.42
1:C:422:PRO:O	1:C:423:THR:C	2.63	0.42
1:D:68:PHE:CZ	1:D:72:LEU:HD13	2.55	0.42
1:D:72:LEU:HD12	1:D:75:MSE:CE	2.42	0.42
1:D:75:MSE:HE1	1:D:84:TYR:HB3	2.02	0.42
1:D:239:MSE:HE1	1:D:254:PHE:CE1	2.55	0.42
1:D:530:VAL:O	1:D:533:TYR:HB3	2.20	0.42
1:C:44:GLU:O	1:C:48:LEU:HG	2.20	0.41
1:C:165:ARG:O	1:C:165:ARG:NE	2.53	0.41
1:D:115:THR:O	1:D:115:THR:CG2	2.68	0.41
1:A:43:GLN:HG3	1:A:47:MSE:HE3	2.02	0.41
1:A:47:MSE:HE3	1:A:47:MSE:HB2	1.82	0.41
1:A:300:LYS:HB3	1:A:300:LYS:NZ	2.28	0.41
1:A:505:GLU:N	1:A:505:GLU:CD	2.78	0.41
1:A:518:ASN:HB3	1:A:521:GLU:OE2	2.20	0.41
1:B:162:ASP:OD2	1:B:257:PHE:CD2	2.73	0.41
1:A:57:LYS:HE3	1:B:222:TYR:OH	2.20	0.41
1:A:394:GLY:HA2	1:A:420:SER:CB	2.50	0.41
1:A:398:LEU:N	1:A:398:LEU:HD22	2.34	0.41
1:B:368:SER:O	1:B:369:ALA:C	2.62	0.41
1:C:108:MSE:N	1:C:109:PRO:HD2	2.35	0.41
1:C:549:LYS:HD3	1:C:549:LYS:HA	1.76	0.41
1:D:36:LYS:NZ	1:D:44:GLU:OE2	2.53	0.41
1:D:506:GLU:CD	1:D:515:PRO:HD3	2.46	0.41
1:A:135:ILE:O	1:A:203:ILE:HA	2.20	0.41
1:A:136:SER:HA	1:A:204:ASP:O	2.19	0.41
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.93	0.41
1:A:454:LEU:HD22	1:A:454:LEU:HA	1.72	0.41
1:B:345:ASP:OD1	1:B:350:LEU:HD21	2.20	0.41
1:B:365:PHE:O	1:B:367:HIS:CD2	2.73	0.41
1:C:85:ILE:HD11	1:C:111:VAL:CG1	2.50	0.41
1:C:369:ALA:HA	1:C:370:PRO:HD3	1.82	0.41
1:D:133:LEU:HD23	1:D:133:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:O	1:A:268:LYS:HG2	2.20	0.41
1:A:331:GLY:O	1:A:332:LEU:C	2.64	0.41
1:B:501:GLN:NE2	1:B:522:VAL:HG12	2.36	0.41
1:C:109:PRO:HA	1:C:113:THR:O	2.20	0.41
1:C:205:VAL:HG11	1:C:231:TYR:HD1	1.86	0.41
1:C:328:VAL:C	1:C:330:ASN:N	2.78	0.41
1:D:85:ILE:HG13	1:D:86:MSE:HE2	2.01	0.41
1:A:45:ARG:CZ	1:A:58:ILE:HD13	2.50	0.41
1:A:122:GLN:O	1:A:125:HIS:HB2	2.21	0.41
1:A:130:PRO:HG3	1:B:54:LEU:HD23	2.02	0.41
1:A:492:LEU:CD2	1:A:496:LYS:HE3	2.35	0.41
1:B:144:ARG:NH1	1:B:244:ASP:HB2	2.36	0.41
1:B:315:ALA:HB3	1:B:392:VAL:CG2	2.49	0.41
1:D:43:GLN:O	1:D:47:MSE:HB2	2.21	0.41
1:D:105:GLU:HG3	1:D:516:LEU:HD23	2.02	0.41
1:D:177:MSE:HG2	1:D:202:CYS:CB	2.43	0.41
1:A:29:MSE:HE1	1:A:54:LEU:CD2	2.51	0.41
1:A:191:ALA:O	1:A:476:LEU:HD22	2.21	0.41
1:A:392:VAL:HG13	5:A:4006:HOH:O	2.20	0.41
1:B:152:GLU:CG	1:B:196:ASP:HB2	2.50	0.41
1:B:358:ILE:HA	1:B:362:GLN:NE2	2.36	0.41
1:D:504:ASP:OD1	1:D:504:ASP:N	2.51	0.41
1:A:26:LYS:HA	1:A:29:MSE:HG3	2.02	0.41
1:A:300:LYS:HZ2	1:A:305:HIS:CD2	2.36	0.41
1:A:371:GLU:OE2	1:A:371:GLU:N	2.36	0.41
1:B:164:GLU:OE1	1:B:225:ARG:HD3	2.21	0.41
1:B:394:GLY:HA2	1:B:420:SER:HB3	2.02	0.41
1:C:50:LEU:HA	1:C:53:LEU:HD12	2.02	0.41
1:C:90:GLU:OE1	1:C:131:LYS:CD	2.68	0.41
1:C:99:ILE:HG22	1:C:100:LEU:HD13	2.03	0.41
1:C:112:TYR:CG	1:C:113:THR:N	2.89	0.41
1:C:374:PRO:HB3	1:C:380:ALA:N	2.35	0.41
1:C:397:ARG:NH2	1:C:423:THR:O	2.54	0.41
1:D:407:MSE:HE2	1:D:407:MSE:HB2	1.92	0.41
1:D:493:GLU:HG2	1:D:533:TYR:CD1	2.55	0.41
1:A:79:LEU:O	1:A:79:LEU:HG	2.19	0.41
1:A:221:LEU:HD12	1:A:221:LEU:HA	1.92	0.41
1:A:401:PRO:O	1:A:405:ARG:HG3	2.21	0.41
1:A:446:GLY:O	1:A:466:ASN:ND2	2.46	0.41
1:A:466:ASN:C	1:A:468:VAL:H	2.29	0.41
1:A:502:LEU:HD21	1:A:506:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:VAL:CG1	1:B:483:THR:HB	2.40	0.41
1:B:528:ILE:CG2	1:B:550:ALA:HA	2.51	0.41
1:C:177:MSE:C	1:C:180:PRO:HD2	2.45	0.41
1:C:358:ILE:CG2	1:C:362:GLN:HB2	2.51	0.41
1:D:93:GLU:O	1:D:96:PHE:HB3	2.20	0.41
1:D:302:ILE:HD11	1:D:332:LEU:CD2	2.50	0.41
1:D:518:ASN:O	1:D:522:VAL:HG23	2.21	0.41
1:A:317:LEU:HD13	1:A:361:TYR:HB2	2.03	0.41
1:A:343:MSE:CE	1:A:362:GLN:HG2	2.51	0.41
1:B:379:ASP:O	1:B:380:ALA:C	2.61	0.41
1:B:535:TYR:CE2	1:B:545:GLU:HB2	2.56	0.41
1:C:183:LYS:HG3	1:C:471:PHE:CZ	2.55	0.41
1:D:376:THR:HG23	1:D:379:ASP:OD2	2.21	0.41
1:D:458:ARG:HB2	1:D:460:PHE:HE2	1.86	0.41
1:A:29:MSE:HE1	1:A:54:LEU:HD21	2.03	0.40
1:A:85:ILE:HG12	1:A:86:MSE:CE	2.45	0.40
1:B:333:SER:H	1:B:336:GLU:CD	2.29	0.40
1:C:55:PRO:HG3	1:D:134:PHE:CZ	2.56	0.40
1:C:546:PRO:CD	1:C:549:LYS:HE3	2.51	0.40
1:D:522:VAL:HG12	1:D:526:ILE:HD12	2.03	0.40
1:A:112:TYR:O	1:A:116:VAL:HG12	2.21	0.40
1:A:303:SER:OG	1:A:304:GLU:HG3	2.22	0.40
1:A:503:THR:HG23	1:A:506:GLU:OE1	2.21	0.40
1:B:85:ILE:HA	1:B:88:ILE:HG13	2.03	0.40
1:B:270:ARG:HE	1:B:270:ARG:HB2	1.65	0.40
1:B:454:LEU:HD11	1:B:460:PHE:HE2	1.86	0.40
1:C:137:ILE:HD12	1:C:234:LEU:HD22	2.02	0.40
1:A:68:PHE:CG	1:A:99:ILE:HG13	2.55	0.40
1:A:71:ASN:ND2	1:A:74:LYS:HZ1	2.20	0.40
1:B:112:TYR:CG	1:B:113:THR:N	2.90	0.40
1:B:298:ILE:HD11	1:B:442:LEU:HD13	2.03	0.40
1:B:319:ILE:O	1:B:320:ALA:C	2.64	0.40
1:B:466:ASN:C	1:B:468:VAL:N	2.78	0.40
1:D:91:ARG:CG	1:D:91:ARG:NH1	2.82	0.40
1:D:366:THR:HG22	1:D:366:THR:O	2.21	0.40
1:A:153:ASN:ND2	1:A:153:ASN:N	2.70	0.40
1:A:534:LEU:HD23	1:A:539:MSE:HE2	2.04	0.40
1:C:186:LEU:HD13	1:C:468:VAL:HG23	2.03	0.40
1:C:399:PHE:HB2	1:C:428:CYS:HB3	2.04	0.40
1:D:134:PHE:CE2	1:D:177:MSE:HG3	2.56	0.40
1:D:144:ARG:HD2	1:D:144:ARG:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:MSE:HE2	1:D:219:MSE:HB2	1.88	0.40
1:D:329:GLU:CG	1:D:330:ASN:HD22	2.32	0.40
1:D:339:LYS:HA	1:D:339:LYS:HD3	1.79	0.40
1:D:552:TYR:CD1	1:D:556:ARG:CZ	3.04	0.40
1:A:38:MSE:CB	1:A:59:GLU:HG3	2.51	0.40
1:A:329:GLU:O	1:A:329:GLU:HG3	2.20	0.40
1:A:397:ARG:HG3	1:A:427:GLU:O	2.20	0.40
1:B:520:GLN:HE21	1:B:520:GLN:N	2.03	0.40
1:B:561:GLU:CD	1:B:561:GLU:N	2.78	0.40
1:C:301:PRO:HD2	1:C:304:GLU:OE1	2.21	0.40
1:C:511:ARG:HH11	1:C:511:ARG:HB3	1.86	0.40
1:D:194:ARG:HH21	1:D:197:ARG:NE	2.20	0.40
1:D:359:ASP:OD2	1:D:362:GLN:HG3	2.22	0.40
1:D:537:ASN:C	1:D:538:LYS:CG	2.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/584 (94%)	512 (93%)	34 (6%)	5 (1%)	14	30
1	B	551/584 (94%)	512 (93%)	32 (6%)	7 (1%)	9	21
1	C	551/584 (94%)	513 (93%)	34 (6%)	4 (1%)	18	38
1	D	551/584 (94%)	499 (91%)	43 (8%)	9 (2%)	7	16
All	All	2204/2336 (94%)	2036 (92%)	143 (6%)	25 (1%)	11	25

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	LEU

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Mol	Chain	Res	Type
1	B	332	LEU
1	C	332	LEU
1	D	270	ARG
1	D	332	LEU
1	B	360	SER
1	D	397	ARG
1	A	103	ASP
1	B	123	TYR
1	B	209	ASN
1	C	392	VAL
1	D	56	PRO
1	D	103	ASP
1	A	56	PRO
1	B	369	ALA
1	D	218	TYR
1	D	335	GLN
1	C	56	PRO
1	C	360	SER
1	A	302	ILE
1	B	392	VAL
1	D	302	ILE
1	A	166	ILE
1	B	363	GLU
1	D	392	VAL

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	469/483 (97%)	356 (76%)	113 (24%)	1	1
1	B	469/483 (97%)	359 (76%)	110 (24%)	1	1
1	C	469/483 (97%)	371 (79%)	98 (21%)	1	2
1	D	469/483 (97%)	344 (73%)	125 (27%)	0	1
All	All	1876/1932 (97%)	1430 (76%)	446 (24%)	1	1

All (446) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	24	LYS
1	A	26	LYS
1	A	28	LEU
1	A	29	MSE
1	A	47	MSE
1	A	57	LYS
1	A	63	ILE
1	A	70	ARG
1	A	73	LYS
1	A	75	MSE
1	A	76	THR
1	A	80	GLU
1	A	85	ILE
1	A	99	ILE
1	A	100	LEU
1	A	101	GLN
1	A	102	ASP
1	A	111	VAL
1	A	120	CYS
1	A	121	SER
1	A	123	TYR
1	A	133	LEU
1	A	137	ILE
1	A	138	SER
1	A	140	ARG
1	A	144	ARG
1	A	152	GLU
1	A	153	ASN
1	A	164	GLU
1	A	169	LEU
1	A	181	VAL
1	A	183	LYS
1	A	193	ILE
1	A	197	ARG
1	A	205	VAL
1	A	212	LEU
1	A	219	MSE
1	A	221	LEU
1	A	227	ARG
1	A	228	THR
1	A	240	LYS

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Mol	Chain	Res	Type
1	A	245	ARG
1	A	248	ARG
1	A	251	LEU
1	A	267	ARG
1	A	271	GLU
1	A	272	LYS
1	A	283	THR
1	A	286	VAL
1	A	291	LEU
1	A	292	LEU
1	A	295	GLN
1	A	296	LYS
1	A	297	VAL
1	A	300	LYS
1	A	304	GLU
1	A	306	LYS
1	A	322	LEU
1	A	327	MSE
1	A	329	GLU
1	A	334	GLU
1	A	335	GLN
1	A	336	GLU
1	A	340	LYS
1	A	341	ILE
1	A	346	LYS
1	A	352	LYS
1	A	355	LYS
1	A	360	SER
1	A	372	SER
1	A	378	GLU
1	A	384	LEU
1	A	385	LYS
1	A	387	SER
1	A	392	VAL
1	A	397	ARG
1	A	398	LEU
1	A	400	THR
1	A	402	ASP
1	A	404	ILE
1	A	409	SER
1	A	413	ARG
1	A	419	LEU

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Mol	Chain	Res	Type
1	A	423	THR
1	A	431	GLU
1	A	435	THR
1	A	436	LEU
1	A	438	GLU
1	A	445	SER
1	A	454	LEU
1	A	455	THR
1	A	461	THR
1	A	470	ILE
1	A	484	ARG
1	A	486	ILE
1	A	489	SER
1	A	492	LEU
1	A	499	THR
1	A	502	LEU
1	A	503	THR
1	A	504	ASP
1	A	505	GLU
1	A	506	GLU
1	A	511	ARG
1	A	518	ASN
1	A	520	GLN
1	A	529	LYS
1	A	547	GLU
1	A	551	LYS
1	A	554	LYS
1	A	556	ARG
1	A	559	ARG
1	B	22	LYS
1	B	24	LYS
1	B	26	LYS
1	B	43	GLN
1	B	47	MSE
1	B	50	LEU
1	B	51	GLN
1	B	57	LYS
1	B	63	ILE
1	B	66	LEU
1	B	73	LYS
1	B	74	LYS
1	B	75	MSE

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Mol	Chain	Res	Type
1	B	83	ILE
1	B	85	ILE
1	B	94	LYS
1	B	99	ILE
1	B	100	LEU
1	B	104	ILE
1	B	106	SER
1	B	123	TYR
1	B	129	ARG
1	B	131	LYS
1	B	140	ARG
1	B	156	LYS
1	B	164	GLU
1	B	165	ARG
1	B	169	LEU
1	B	193	ILE
1	B	208	ASP
1	B	214	LYS
1	B	219	MSE
1	B	221	LEU
1	B	223	GLN
1	B	224	LYS
1	B	225	ARG
1	B	229	GLN
1	B	232	ASP
1	B	233	ASP
1	B	239	MSE
1	B	240	LYS
1	B	252	ILE
1	B	267	ARG
1	B	270	ARG
1	B	286	VAL
1	B	292	LEU
1	B	297	VAL
1	B	298	ILE
1	B	300	LYS
1	B	303	SER
1	B	306	LYS
1	B	307	ILE
1	B	310	LEU
1	B	319	ILE
1	B	321	ASN

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Mol	Chain	Res	Type
1	B	323	ILE
1	B	326	SER
1	B	334	GLU
1	B	339	LYS
1	B	340	LYS
1	B	350	LEU
1	B	351	VAL
1	B	355	LYS
1	B	357	LYS
1	B	363	GLU
1	B	368	SER
1	B	372	SER
1	B	373	ILE
1	B	378	GLU
1	B	385	LYS
1	B	389	ILE
1	B	390	ILE
1	B	397	ARG
1	B	398	LEU
1	B	402	ASP
1	B	405	ARG
1	B	410	ILE
1	B	411	ASN
1	B	413	ARG
1	B	438	GLU
1	B	440	ARG
1	B	447	SER
1	B	455	THR
1	B	458	ARG
1	B	466	ASN
1	B	489	SER
1	B	492	LEU
1	B	499	THR
1	B	500	SER
1	B	502	LEU
1	B	505	GLU
1	B	507	LEU
1	B	509	GLN
1	B	511	ARG
1	B	516	LEU
1	B	518	ASN
1	B	519	ILE

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Mol	Chain	Res	Type
1	B	520	GLN
1	B	521	GLU
1	B	522	VAL
1	B	524	ILE
1	B	528	ILE
1	B	529	LYS
1	B	531	THR
1	B	547	GLU
1	B	549	LYS
1	B	551	LYS
1	B	555	GLU
1	B	561	GLU
1	B	564	SER
1	C	21	ILE
1	C	23	GLU
1	C	26	LYS
1	C	28	LEU
1	C	57	LYS
1	C	66	LEU
1	C	70	ARG
1	C	71	ASN
1	C	72	LEU
1	C	75	MSE
1	C	77	SER
1	C	85	ILE
1	C	99	ILE
1	C	100	LEU
1	C	101	GLN
1	C	111	VAL
1	C	122	GLN
1	C	123	TYR
1	C	126	ILE
1	C	131	LYS
1	C	140	ARG
1	C	146	ILE
1	C	153	ASN
1	C	169	LEU
1	C	183	LYS
1	C	210	ILE
1	C	214	LYS
1	C	221	LEU
1	C	225	ARG

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Mol	Chain	Res	Type
1	C	228	THR
1	C	230	GLN
1	C	235	ILE
1	C	239	MSE
1	C	240	LYS
1	C	248	ARG
1	C	251	LEU
1	C	252	ILE
1	C	267	ARG
1	C	286	VAL
1	C	291	LEU
1	C	292	LEU
1	C	297	VAL
1	C	300	LYS
1	C	302	ILE
1	C	304	GLU
1	C	305	HIS
1	C	306	LYS
1	C	314	GLU
1	C	325	MSE
1	C	335	GLN
1	C	339	LYS
1	C	340	LYS
1	C	355	LYS
1	C	357	LYS
1	C	363	GLU
1	C	368	SER
1	C	371	GLU
1	C	375	ASP
1	C	384	LEU
1	C	389	ILE
1	C	390	ILE
1	C	397	ARG
1	C	398	LEU
1	C	404	ILE
1	C	409	SER
1	C	415	VAL
1	C	419	LEU
1	C	436	LEU
1	C	438	GLU
1	C	442	LEU
1	C	452	VAL

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Mol	Chain	Res	Type
1	C	454	LEU
1	C	455	THR
1	C	458	ARG
1	C	461	THR
1	C	482	ASN
1	C	483	THR
1	C	484	ARG
1	C	492	LEU
1	C	502	LEU
1	C	504	ASP
1	C	507	LEU
1	C	511	ARG
1	C	516	LEU
1	C	519	ILE
1	C	520	GLN
1	C	521	GLU
1	C	531	THR
1	C	542	ARG
1	C	543	TYR
1	C	545	GLU
1	C	547	GLU
1	C	554	LYS
1	C	556	ARG
1	C	560	SER
1	C	561	GLU
1	C	564	SER
1	C	571	GLU
1	D	21	ILE
1	D	22	LYS
1	D	24	LYS
1	D	29	MSE
1	D	36	LYS
1	D	43	GLN
1	D	47	MSE
1	D	51	GLN
1	D	57	LYS
1	D	58	ILE
1	D	60	THR
1	D	66	LEU
1	D	70	ARG
1	D	74	LYS
1	D	75	MSE

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Mol	Chain	Res	Type
1	D	76	THR
1	D	85	ILE
1	D	89	GLN
1	D	91	ARG
1	D	94	LYS
1	D	99	ILE
1	D	100	LEU
1	D	120	CYS
1	D	123	TYR
1	D	133	LEU
1	D	140	ARG
1	D	144	ARG
1	D	146	ILE
1	D	152	GLU
1	D	153	ASN
1	D	156	LYS
1	D	158	VAL
1	D	169	LEU
1	D	177	MSE
1	D	181	VAL
1	D	183	LYS
1	D	197	ARG
1	D	205	VAL
1	D	210	ILE
1	D	214	LYS
1	D	221	LEU
1	D	225	ARG
1	D	227	ARG
1	D	229	GLN
1	D	237	GLU
1	D	239	MSE
1	D	245	ARG
1	D	249	ASN
1	D	251	LEU
1	D	261	ASN
1	D	266	LEU
1	D	267	ARG
1	D	270	ARG
1	D	283	THR
1	D	286	VAL
1	D	291	LEU
1	D	292	LEU

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Mol	Chain	Res	Type
1	D	298	ILE
1	D	299	SER
1	D	300	LYS
1	D	303	SER
1	D	305	HIS
1	D	322	LEU
1	D	323	ILE
1	D	327	MSE
1	D	329	GLU
1	D	332	LEU
1	D	333	SER
1	D	335	GLN
1	D	336	GLU
1	D	339	LYS
1	D	341	ILE
1	D	350	LEU
1	D	355	LYS
1	D	358	ILE
1	D	360	SER
1	D	363	GLU
1	D	371	GLU
1	D	376	THR
1	D	383	ILE
1	D	384	LEU
1	D	387	SER
1	D	388	THR
1	D	389	ILE
1	D	392	VAL
1	D	397	ARG
1	D	405	ARG
1	D	409	SER
1	D	412	GLU
1	D	428	CYS
1	D	431	GLU
1	D	436	LEU
1	D	440	ARG
1	D	445	SER
1	D	452	VAL
1	D	455	THR
1	D	456	ASP
1	D	464	GLN
1	D	489	SER

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Mol	Chain	Res	Type
1	D	492	LEU
1	D	496	LYS
1	D	500	SER
1	D	502	LEU
1	D	504	ASP
1	D	507	LEU
1	D	509	GLN
1	D	512	LEU
1	D	518	ASN
1	D	520	GLN
1	D	521	GLU
1	D	526	ILE
1	D	529	LYS
1	D	531	THR
1	D	534	LEU
1	D	538	LYS
1	D	547	GLU
1	D	549	LYS
1	D	551	LYS
1	D	554	LYS
1	D	555	GLU
1	D	556	ARG
1	D	557	THR
1	D	559	ARG
1	D	561	GLU
1	D	571	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	71	ASN
1	A	122	GLN
1	A	153	ASN
1	A	261	ASN
1	A	295	GLN
1	A	305	HIS
1	A	330	ASN
1	A	482	ASN
1	A	520	GLN
1	B	51	GLN

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Mol	Chain	Res	Type
1	B	64	GLN
1	B	69	HIS
1	B	154	HIS
1	B	229	GLN
1	B	261	ASN
1	B	338	GLN
1	B	362	GLN
1	B	367	HIS
1	B	425	GLN
1	B	467	ASN
1	B	482	ASN
1	B	501	GLN
1	B	518	ASN
1	B	520	GLN
1	C	51	GLN
1	C	64	GLN
1	C	69	HIS
1	C	71	ASN
1	C	122	GLN
1	C	153	ASN
1	C	154	HIS
1	C	223	GLN
1	C	229	GLN
1	C	305	HIS
1	C	335	GLN
1	C	362	GLN
1	C	425	GLN
1	C	467	ASN
1	C	482	ASN
1	C	509	GLN
1	C	520	GLN
1	D	35	ASN
1	D	51	GLN
1	D	64	GLN
1	D	69	HIS
1	D	122	GLN
1	D	125	HIS
1	D	153	ASN
1	D	154	HIS
1	D	249	ASN
1	D	260	HIS
1	D	261	ASN

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Mol	Chain	Res	Type
1	D	305	HIS
1	D	321	ASN
1	D	330	ASN
1	D	425	GLN
1	D	482	ASN
1	D	485	HIS
1	D	520	GLN

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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	A	601	-	46,48,48	2.11	14 (30%)	64,73,73	1.83	9 (14%)
3	NAD	D	3602	-	46,48,48	2.16	14 (30%)	64,73,73	1.84	11 (17%)
4	MAK	C	2603	2	7,7,7	2.08	5 (71%)	9,9,9	1.93	3 (33%)
4	MAK	A	603	2	7,7,7	1.85	3 (42%)	9,9,9	1.92	4 (44%)
4	MAK	B	1603	2	7,7,7	2.47	5 (71%)	9,9,9	1.92	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	B	1602	-	46,48,48	2.23	14 (30%)	64,73,73	1.83	11 (17%)
3	NAD	D	3601	-	46,48,48	2.12	12 (26%)	64,73,73	1.89	9 (14%)
3	NAD	C	2601	-	46,48,48	2.02	11 (23%)	64,73,73	1.90	12 (18%)
3	NAD	B	1601	-	46,48,48	1.86	10 (21%)	64,73,73	1.86	11 (17%)
4	MAK	D	3603	2	7,7,7	2.23	5 (71%)	9,9,9	1.96	4 (44%)
3	NAD	C	2602	-	46,48,48	2.19	12 (26%)	64,73,73	1.83	11 (17%)
3	NAD	A	602	-	46,48,48	2.18	12 (26%)	64,73,73	1.85	11 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	601	-	-	3/30/62/62	0/5/5/5
3	NAD	D	3602	-	-	5/30/62/62	0/5/5/5
4	MAK	C	2603	2	-	4/8/8/8	-
4	MAK	A	603	2	-	4/8/8/8	-
4	MAK	B	1603	2	-	1/8/8/8	-
3	NAD	B	1602	-	-	6/30/62/62	0/5/5/5
3	NAD	D	3601	-	-	2/30/62/62	0/5/5/5
3	NAD	C	2601	-	-	7/30/62/62	0/5/5/5
3	NAD	B	1601	-	-	5/30/62/62	0/5/5/5
4	MAK	D	3603	2	-	1/8/8/8	-
3	NAD	C	2602	-	-	5/30/62/62	0/5/5/5
3	NAD	A	602	-	-	6/30/62/62	0/5/5/5

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3602	NAD	C2N-N1N	8.31	1.44	1.35
3	A	602	NAD	C2N-N1N	8.30	1.44	1.35
3	B	1602	NAD	C2N-N1N	8.30	1.44	1.35
3	C	2602	NAD	C2N-N1N	7.91	1.43	1.35
3	C	2601	NAD	C2N-N1N	7.11	1.42	1.35
3	A	601	NAD	C2N-N1N	7.10	1.42	1.35
3	D	3601	NAD	C2N-N1N	6.70	1.42	1.35
3	B	1602	NAD	O4D-C1D	5.80	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2602	NAD	O4D-C1D	5.61	1.48	1.40
3	D	3601	NAD	O4D-C1D	5.32	1.47	1.40
3	C	2601	NAD	C3N-C7N	5.06	1.58	1.50
3	B	1601	NAD	C2N-N1N	4.99	1.40	1.35
3	D	3601	NAD	C3N-C7N	4.81	1.57	1.50
3	D	3601	NAD	C5A-N7A	-4.68	1.30	1.39
3	A	602	NAD	C5A-N7A	-4.67	1.30	1.39
3	A	601	NAD	O4D-C1D	4.60	1.46	1.40
3	D	3602	NAD	O4D-C1D	4.47	1.46	1.40
3	C	2601	NAD	C5A-N7A	-4.44	1.31	1.39
3	A	602	NAD	O4D-C1D	4.34	1.46	1.40
3	D	3602	NAD	C5A-N7A	-4.28	1.31	1.39
3	D	3601	NAD	C6N-N1N	4.27	1.45	1.35
4	B	1603	MAK	C3-C2	-4.21	1.50	1.54
3	A	602	NAD	C6N-N1N	4.15	1.44	1.35
3	C	2602	NAD	C6N-N1N	4.14	1.44	1.35
3	B	1601	NAD	C5A-N7A	-4.09	1.31	1.39
3	B	1602	NAD	C6N-N1N	4.08	1.44	1.35
3	D	3602	NAD	C6N-N1N	4.04	1.44	1.35
3	C	2602	NAD	C5A-N7A	-4.00	1.31	1.39
3	B	1601	NAD	C3N-C7N	3.99	1.56	1.50
3	A	601	NAD	C6N-N1N	3.98	1.44	1.35
3	A	601	NAD	C5A-N7A	-3.92	1.31	1.39
3	A	601	NAD	PN-O3	-3.75	1.55	1.59
3	B	1601	NAD	C6N-N1N	3.65	1.43	1.35
3	A	601	NAD	C3N-C7N	3.63	1.56	1.50
3	C	2601	NAD	C6N-N1N	3.55	1.43	1.35
3	D	3601	NAD	C4N-C3N	3.52	1.44	1.39
3	B	1601	NAD	O4D-C1D	3.45	1.45	1.40
3	B	1602	NAD	C5A-N7A	-3.45	1.32	1.39
3	D	3601	NAD	C5A-C4A	-3.42	1.33	1.39
4	D	3603	MAK	C3-C2	-3.39	1.51	1.54
3	B	1602	NAD	C3N-C7N	3.32	1.55	1.50
3	D	3602	NAD	C3N-C7N	3.30	1.55	1.50
3	A	602	NAD	C3N-C7N	3.28	1.55	1.50
3	C	2602	NAD	C3N-C7N	3.25	1.55	1.50
3	B	1601	NAD	C5A-C4A	-3.23	1.33	1.39
3	C	2601	NAD	C5A-C4A	-3.23	1.33	1.39
3	C	2602	NAD	O4B-C1B	3.00	1.48	1.42
3	A	601	NAD	C5A-C4A	-2.97	1.33	1.39
3	D	3602	NAD	C5A-C4A	-2.84	1.34	1.39
3	C	2601	NAD	O4D-C1D	2.78	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	NAD	C8A-N7A	2.77	1.37	1.31
3	A	601	NAD	C4N-C3N	2.76	1.43	1.39
4	C	2603	MAK	C3-C2	-2.69	1.52	1.54
3	A	602	NAD	C5A-C4A	-2.65	1.34	1.39
3	A	602	NAD	C8A-N7A	2.64	1.36	1.31
4	B	1603	MAK	O5-C3	-2.63	1.23	1.30
3	A	601	NAD	C2A-N3A	2.63	1.38	1.33
4	D	3603	MAK	O5-C3	-2.60	1.23	1.30
4	C	2603	MAK	O2-C1	-2.60	1.23	1.30
3	B	1601	NAD	C4A-N9A	-2.58	1.32	1.37
3	C	2602	NAD	C8A-N7A	2.58	1.36	1.31
3	D	3602	NAD	PN-O3	2.58	1.62	1.59
3	A	602	NAD	C2A-N3A	2.57	1.38	1.33
3	C	2602	NAD	C2A-N3A	2.56	1.38	1.33
3	B	1602	NAD	PN-O3	2.55	1.62	1.59
3	C	2601	NAD	C5N-C4N	2.54	1.43	1.38
3	D	3602	NAD	C8A-N7A	2.52	1.36	1.31
4	B	1603	MAK	O2-C1	-2.49	1.23	1.30
3	A	602	NAD	C4N-C3N	2.48	1.43	1.39
4	D	3603	MAK	O2-C1	-2.45	1.23	1.30
4	A	603	MAK	O3-C2	2.44	1.28	1.23
4	A	603	MAK	O2-C1	-2.44	1.23	1.30
4	B	1603	MAK	C1-C2	-2.43	1.52	1.54
3	A	601	NAD	PA-O3	-2.38	1.56	1.59
4	C	2603	MAK	O5-C3	-2.37	1.24	1.30
3	B	1602	NAD	C4N-C3N	2.37	1.43	1.39
4	A	603	MAK	O5-C3	-2.37	1.24	1.30
3	C	2602	NAD	C4N-C3N	2.36	1.43	1.39
4	C	2603	MAK	O3-C2	2.33	1.28	1.23
4	B	1603	MAK	O3-C2	2.32	1.28	1.23
3	B	1602	NAD	O4B-C1B	2.29	1.47	1.42
3	D	3601	NAD	O4B-C1B	2.29	1.47	1.42
3	A	602	NAD	O4B-C1B	2.29	1.47	1.42
4	D	3603	MAK	O3-C2	2.28	1.28	1.23
3	A	601	NAD	C2A-N1A	2.28	1.38	1.33
3	C	2602	NAD	C2A-N1A	2.27	1.38	1.33
3	B	1602	NAD	C5A-C4A	-2.27	1.35	1.39
3	A	601	NAD	C5N-C4N	2.26	1.42	1.38
3	D	3602	NAD	C4N-C3N	2.26	1.42	1.39
3	B	1602	NAD	O4D-C4D	2.26	1.50	1.45
3	D	3602	NAD	O4B-C1B	2.24	1.47	1.42
3	B	1602	NAD	C2A-N1A	2.24	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2601	NAD	C4A-N9A	-2.23	1.33	1.37
3	B	1601	NAD	C8A-N7A	2.23	1.36	1.31
3	D	3601	NAD	C4A-N9A	-2.22	1.33	1.37
4	D	3603	MAK	C1-C2	-2.21	1.52	1.54
3	C	2601	NAD	C2A-N3A	2.20	1.37	1.33
3	C	2602	NAD	C5A-C4A	-2.20	1.35	1.39
3	B	1602	NAD	C2A-N3A	2.15	1.37	1.33
3	B	1601	NAD	PA-O3	2.10	1.61	1.59
3	A	601	NAD	C8A-N7A	2.10	1.35	1.31
3	C	2601	NAD	C8A-N7A	2.10	1.35	1.31
3	A	602	NAD	C2A-N1A	2.09	1.37	1.33
4	C	2603	MAK	C1-C2	-2.08	1.52	1.54
3	C	2602	NAD	C5N-C4N	2.07	1.42	1.38
3	D	3601	NAD	C5N-C4N	2.07	1.42	1.38
3	D	3601	NAD	C2A-N1A	2.05	1.37	1.33
3	C	2601	NAD	C2A-N1A	2.05	1.37	1.33
3	B	1602	NAD	C5N-C4N	2.05	1.42	1.38
3	D	3602	NAD	C2A-N3A	2.04	1.37	1.33
3	D	3602	NAD	C5N-C4N	2.03	1.42	1.38
3	A	602	NAD	C1B-N9A	2.02	1.51	1.46
3	D	3602	NAD	C4A-N9A	-2.02	1.33	1.37
3	D	3601	NAD	C2A-N3A	2.01	1.37	1.33
3	D	3602	NAD	C2A-N1A	2.01	1.37	1.33
3	B	1601	NAD	O4B-C4B	2.01	1.49	1.45
3	A	601	NAD	O4B-C1B	2.01	1.46	1.42

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2602	NAD	C5A-C4A-N3A	-6.22	118.16	126.72
3	A	602	NAD	C5A-C4A-N3A	-6.12	118.28	126.72
3	B	1602	NAD	C5A-C4A-N3A	-6.10	118.32	126.72
3	C	2601	NAD	C5A-C4A-N3A	-6.09	118.33	126.72
3	D	3602	NAD	C5A-C4A-N3A	-5.97	118.49	126.72
3	A	601	NAD	C5A-C4A-N3A	-5.92	118.57	126.72
3	D	3601	NAD	C5A-C4A-N3A	-5.89	118.61	126.72
3	B	1601	NAD	C5A-C4A-N3A	-5.71	118.86	126.72
3	B	1601	NAD	N3A-C2A-N1A	-5.44	120.34	128.58
3	C	2601	NAD	C6A-C5A-C4A	5.35	124.48	117.18
3	C	2601	NAD	C6A-C5A-N7A	-5.33	121.82	132.09
3	D	3601	NAD	C6A-C5A-N7A	-5.33	121.82	132.09
3	D	3601	NAD	C6A-C5A-C4A	5.21	124.29	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAD	C6A-C5A-N7A	-5.20	122.06	132.09
3	D	3602	NAD	N3A-C2A-N1A	-5.20	120.71	128.58
3	B	1601	NAD	C6A-C5A-N7A	-5.19	122.08	132.09
3	D	3601	NAD	N3A-C2A-N1A	-5.17	120.76	128.58
3	A	601	NAD	C6A-C5A-N7A	-5.15	122.16	132.09
3	C	2601	NAD	N3A-C4A-N9A	5.15	135.92	127.17
3	A	601	NAD	N3A-C4A-N9A	5.10	135.85	127.17
3	A	602	NAD	C6A-C5A-C4A	5.07	124.10	117.18
3	D	3601	NAD	N3A-C4A-N9A	5.06	135.78	127.17
3	C	2601	NAD	N3A-C2A-N1A	-5.05	120.94	128.58
3	B	1602	NAD	C6A-C5A-N7A	-5.04	122.37	132.09
3	A	602	NAD	N3A-C2A-N1A	-5.03	120.96	128.58
3	A	601	NAD	C6A-C5A-C4A	5.03	124.05	117.18
3	C	2602	NAD	N3A-C4A-N9A	4.99	135.66	127.17
3	D	3602	NAD	C6A-C5A-N7A	-4.99	122.47	132.09
3	B	1601	NAD	C6A-C5A-C4A	4.99	123.99	117.18
3	C	2602	NAD	C6A-C5A-C4A	4.98	123.97	117.18
3	C	2602	NAD	C6A-C5A-N7A	-4.97	122.50	132.09
3	A	602	NAD	N3A-C4A-N9A	4.97	135.63	127.17
3	B	1602	NAD	N3A-C4A-N9A	4.97	135.63	127.17
3	B	1602	NAD	C6A-C5A-C4A	4.96	123.94	117.18
3	A	601	NAD	N3A-C2A-N1A	-4.95	121.09	128.58
3	C	2602	NAD	N3A-C2A-N1A	-4.94	121.11	128.58
3	D	3602	NAD	C6A-C5A-C4A	4.88	123.84	117.18
3	B	1602	NAD	N3A-C2A-N1A	-4.87	121.21	128.58
3	D	3602	NAD	N3A-C4A-N9A	4.81	135.35	127.17
3	B	1601	NAD	N3A-C4A-N9A	4.72	135.19	127.17
3	D	3601	NAD	N9A-C8A-N7A	-3.83	108.51	113.94
3	B	1601	NAD	N9A-C8A-N7A	-3.76	108.60	113.94
3	A	601	NAD	N9A-C8A-N7A	-3.73	108.65	113.94
3	C	2601	NAD	N9A-C8A-N7A	-3.68	108.72	113.94
3	D	3602	NAD	N9A-C8A-N7A	-3.56	108.89	113.94
3	A	602	NAD	N9A-C8A-N7A	-3.52	108.94	113.94
3	B	1602	NAD	N9A-C8A-N7A	-3.49	108.99	113.94
3	C	2602	NAD	N9A-C8A-N7A	-3.39	109.13	113.94
3	C	2602	NAD	C2A-N3A-C4A	3.31	119.92	111.83
3	B	1602	NAD	C2A-N3A-C4A	3.26	119.78	111.83
3	C	2601	NAD	C2A-N3A-C4A	3.24	119.75	111.83
3	D	3602	NAD	C2A-N3A-C4A	3.23	119.71	111.83
3	B	1601	NAD	C2A-N3A-C4A	3.22	119.69	111.83
3	A	602	NAD	C2A-N3A-C4A	3.20	119.65	111.83
3	D	3601	NAD	C4D-O4D-C1D	-3.18	107.01	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3601	NAD	C2A-N3A-C4A	3.14	119.50	111.83
3	A	601	NAD	C2A-N3A-C4A	3.08	119.36	111.83
4	C	2603	MAK	O2-C1-C2	2.99	121.33	112.94
3	A	602	NAD	C6N-N1N-C2N	-2.95	119.37	121.88
3	B	1601	NAD	C4A-C5A-N7A	2.93	113.93	110.58
3	D	3601	NAD	C4A-C5A-N7A	2.90	113.89	110.58
4	B	1603	MAK	O2-C1-C2	2.85	120.93	112.94
3	A	602	NAD	C4A-C5A-N7A	2.84	113.83	110.58
3	A	601	NAD	C4A-C5A-N7A	2.81	113.80	110.58
3	D	3602	NAD	C6N-N1N-C2N	-2.81	119.49	121.88
4	A	603	MAK	O2-C1-C2	2.79	120.77	112.94
3	A	601	NAD	C4D-O4D-C1D	-2.76	107.40	109.92
3	C	2601	NAD	C4D-O4D-C1D	-2.75	107.41	109.92
3	B	1602	NAD	C6N-N1N-C2N	-2.74	119.54	121.88
3	D	3602	NAD	C4A-C5A-N7A	2.72	113.69	110.58
3	C	2601	NAD	C4A-C5A-N7A	2.72	113.69	110.58
3	B	1602	NAD	C4A-C5A-N7A	2.71	113.68	110.58
4	D	3603	MAK	O2-C1-C2	2.65	120.36	112.94
3	C	2602	NAD	C4A-C5A-N7A	2.58	113.53	110.58
3	C	2602	NAD	C6N-N1N-C2N	-2.57	119.69	121.88
4	D	3603	MAK	O5-C3-C2	2.51	119.97	112.94
3	B	1601	NAD	C3N-C7N-N7N	-2.46	114.71	117.74
4	D	3603	MAK	O3-C2-C1	2.45	123.78	117.79
4	B	1603	MAK	O3-C2-C1	2.45	123.77	117.79
3	B	1601	NAD	C4D-O4D-C1D	-2.43	107.70	109.92
4	A	603	MAK	O5-C3-C2	2.42	119.72	112.94
3	B	1601	NAD	O4B-C1B-N9A	2.38	112.66	108.09
3	C	2601	NAD	C3N-C7N-N7N	-2.33	114.87	117.74
4	C	2603	MAK	O5-C3-C2	2.33	119.47	112.94
3	C	2601	NAD	O4B-C1B-N9A	2.31	112.53	108.09
4	B	1603	MAK	O5-C3-C2	2.30	119.39	112.94
4	A	603	MAK	O3-C2-C1	2.27	123.32	117.79
4	C	2603	MAK	O3-C2-C1	2.27	123.32	117.79
3	B	1602	NAD	C2D-C3D-C4D	2.26	106.98	102.61
3	D	3602	NAD	C3B-C2B-C1B	2.26	105.74	101.46
3	A	602	NAD	C3B-C2B-C1B	2.23	105.67	101.46
3	B	1602	NAD	C3B-C2B-C1B	2.19	105.60	101.46
3	C	2602	NAD	C3B-C2B-C1B	2.17	105.57	101.46
3	A	602	NAD	C2D-C3D-C4D	2.16	106.79	102.61
3	C	2601	NAD	O7N-C7N-C3N	2.16	122.24	119.60
3	C	2602	NAD	C2D-C3D-C4D	2.16	106.78	102.61
4	D	3603	MAK	O3-C2-C3	2.13	123.00	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3602	NAD	C2D-C3D-C4D	2.07	106.60	102.61
4	A	603	MAK	O3-C2-C3	2.02	122.73	117.79

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAD	O4D-C1D-N1N-C6N
3	A	602	NAD	C5B-O5B-PA-O2A
3	A	602	NAD	C5B-O5B-PA-O3
3	A	602	NAD	PA-O3-PN-O5D
3	B	1601	NAD	O4D-C1D-N1N-C2N
3	B	1601	NAD	O4D-C1D-N1N-C6N
3	B	1602	NAD	C5B-O5B-PA-O2A
3	B	1602	NAD	C5B-O5B-PA-O3
3	C	2601	NAD	O4D-C1D-N1N-C2N
3	C	2601	NAD	O4D-C1D-N1N-C6N
3	C	2601	NAD	C2D-C1D-N1N-C2N
3	C	2601	NAD	C2D-C1D-N1N-C6N
3	C	2602	NAD	C5B-O5B-PA-O2A
3	C	2602	NAD	C5B-O5B-PA-O3
3	C	2602	NAD	C5D-O5D-PN-O1N
3	D	3601	NAD	O4D-C1D-N1N-C2N
3	D	3601	NAD	O4D-C1D-N1N-C6N
3	D	3602	NAD	C5B-O5B-PA-O2A
3	D	3602	NAD	C5B-O5B-PA-O3
3	D	3602	NAD	PA-O3-PN-O5D
3	B	1601	NAD	O4B-C4B-C5B-O5B
3	B	1601	NAD	C3B-C4B-C5B-O5B
3	B	1602	NAD	C4D-C5D-O5D-PN
3	B	1602	NAD	PA-O3-PN-O5D
3	C	2602	NAD	PA-O3-PN-O5D
4	A	603	MAK	O1-C1-C2-C3
4	C	2603	MAK	O1-C1-C2-C3
3	B	1602	NAD	C5D-O5D-PN-O1N
3	D	3602	NAD	C5D-O5D-PN-O1N
3	A	602	NAD	C4D-C5D-O5D-PN
3	C	2602	NAD	C4D-C5D-O5D-PN
3	D	3602	NAD	C4D-C5D-O5D-PN
4	A	603	MAK	O2-C1-C2-O3
4	C	2603	MAK	O2-C1-C2-O3
4	A	603	MAK	O2-C1-C2-C3

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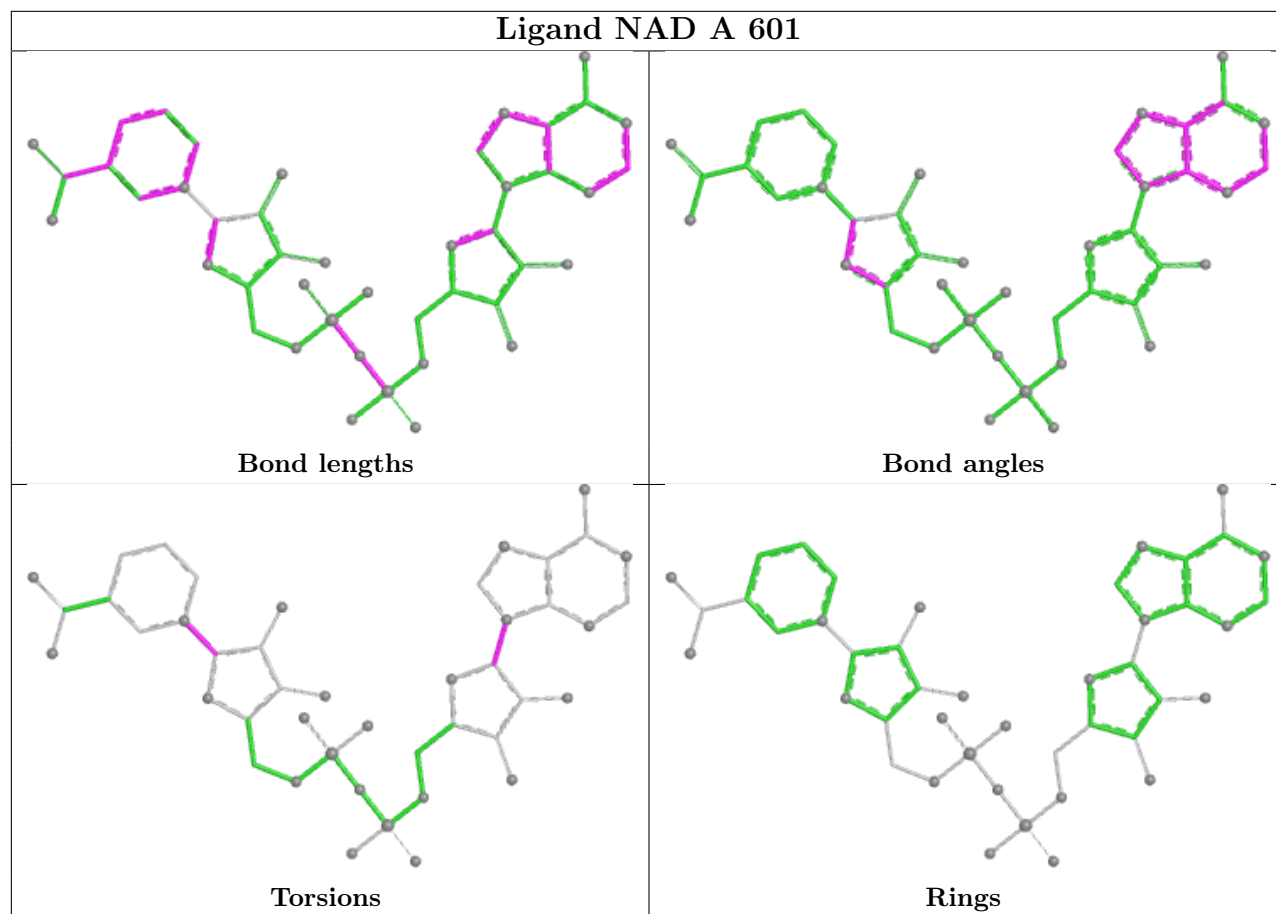
Mol	Chain	Res	Type	Atoms
4	C	2603	MAK	O2-C1-C2-C3
3	B	1601	NAD	C2D-C1D-N1N-C2N
4	B	1603	MAK	O1-C1-C2-O3
4	D	3603	MAK	O1-C1-C2-O3
3	A	601	NAD	O4D-C1D-N1N-C2N
3	C	2601	NAD	PN-O3-PA-O1A
4	A	603	MAK	O1-C1-C2-O3
4	C	2603	MAK	O1-C1-C2-O3
3	C	2601	NAD	O4B-C4B-C5B-O5B
3	C	2601	NAD	PN-O3-PA-O2A
3	A	601	NAD	C2B-C1B-N9A-C8A
3	A	602	NAD	PN-O3-PA-O2A
3	A	602	NAD	PA-O3-PN-O2N
3	B	1602	NAD	PA-O3-PN-O2N

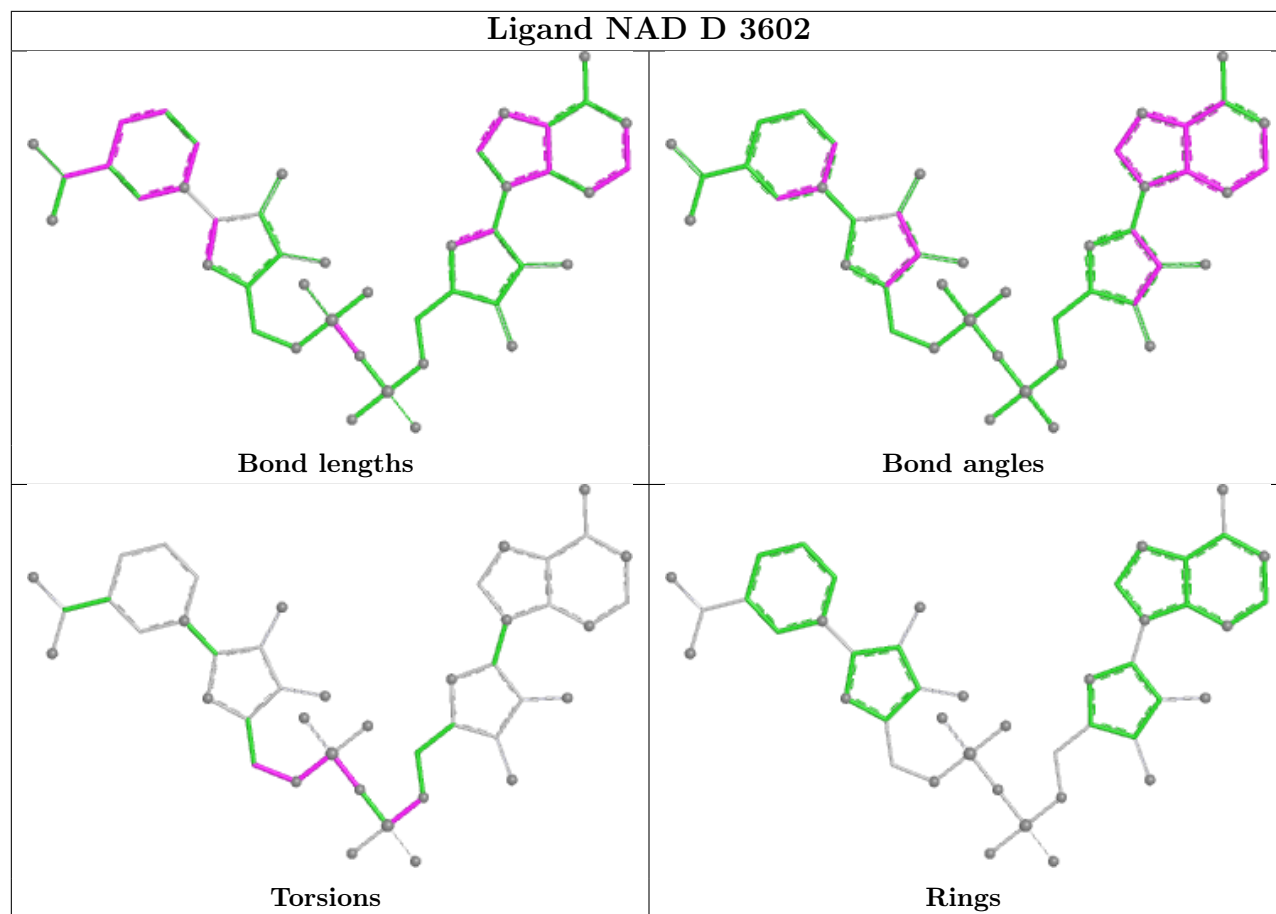
There are no ring outliers.

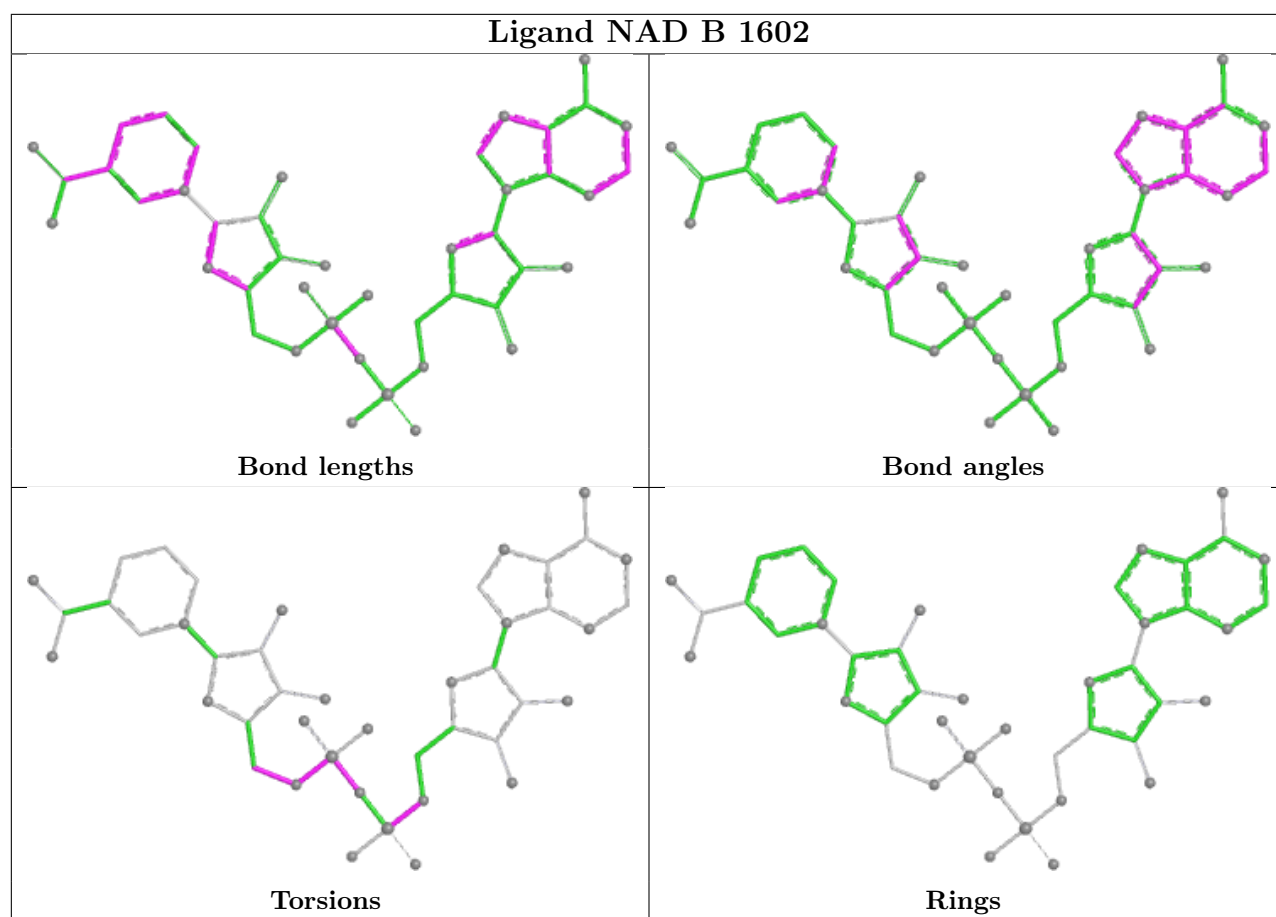
10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAD	3	0
4	C	2603	MAK	1	0
4	A	603	MAK	1	0
4	B	1603	MAK	1	0
3	B	1602	NAD	1	0
3	D	3601	NAD	3	0
3	C	2601	NAD	3	0
3	B	1601	NAD	4	0
4	D	3603	MAK	2	0
3	A	602	NAD	1	0

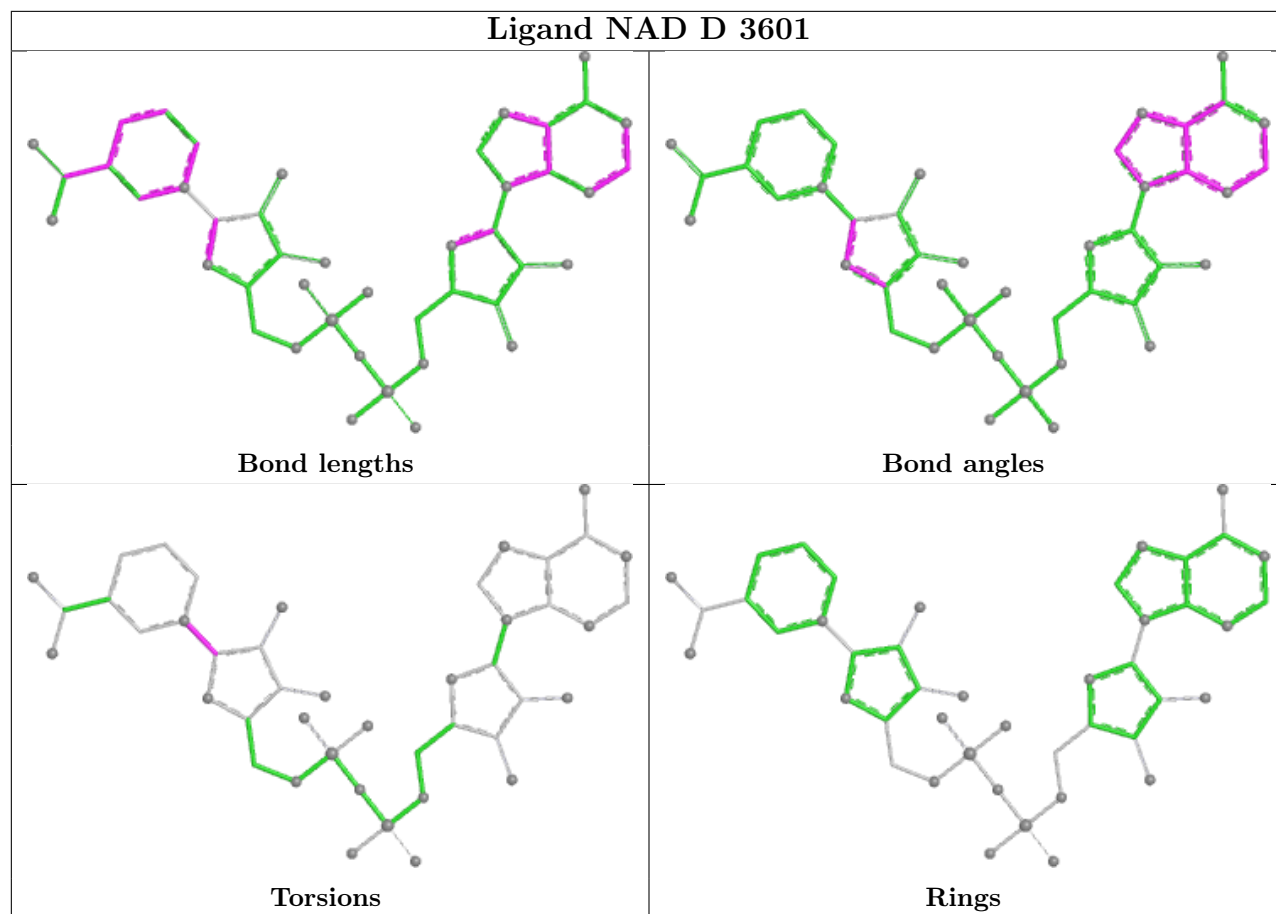
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

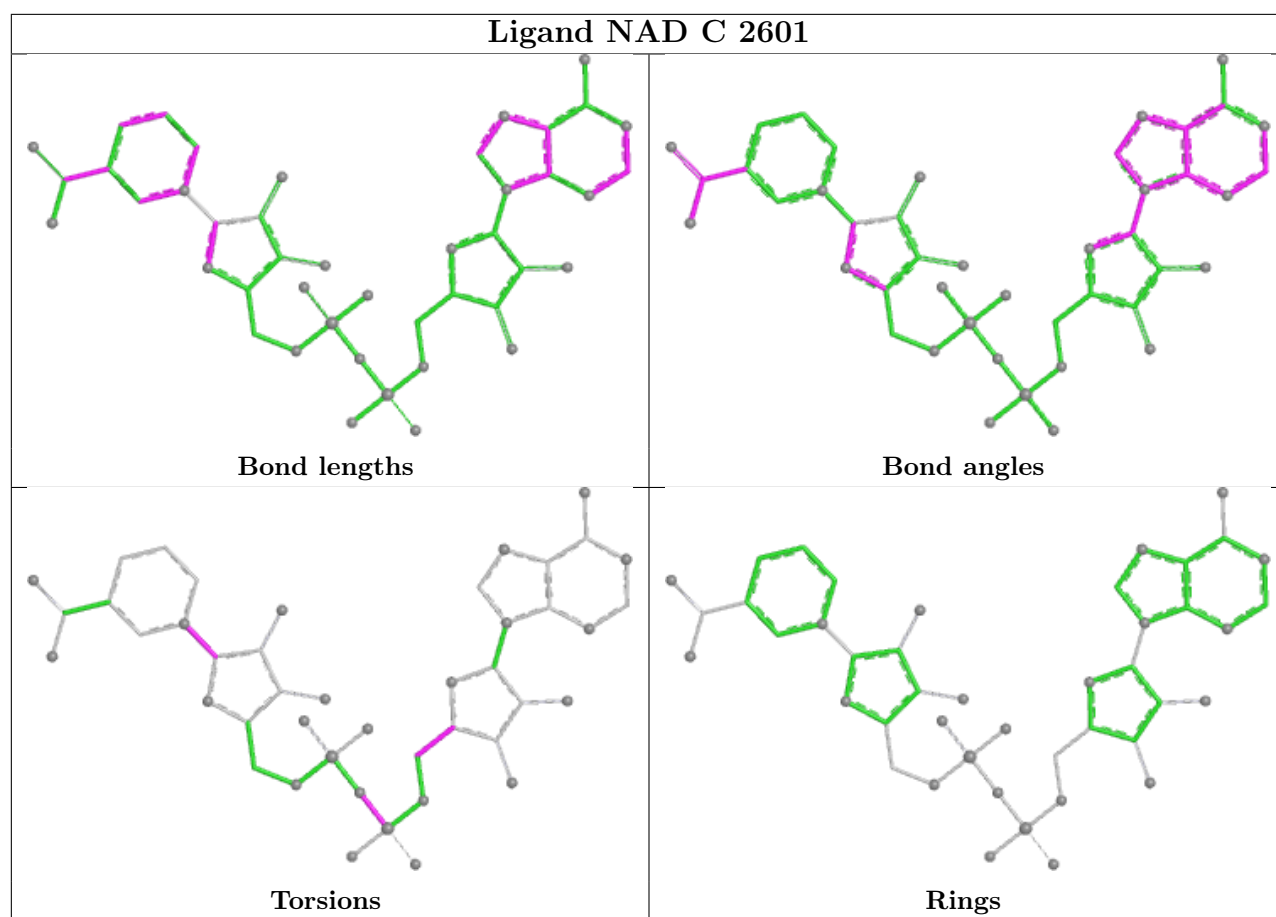


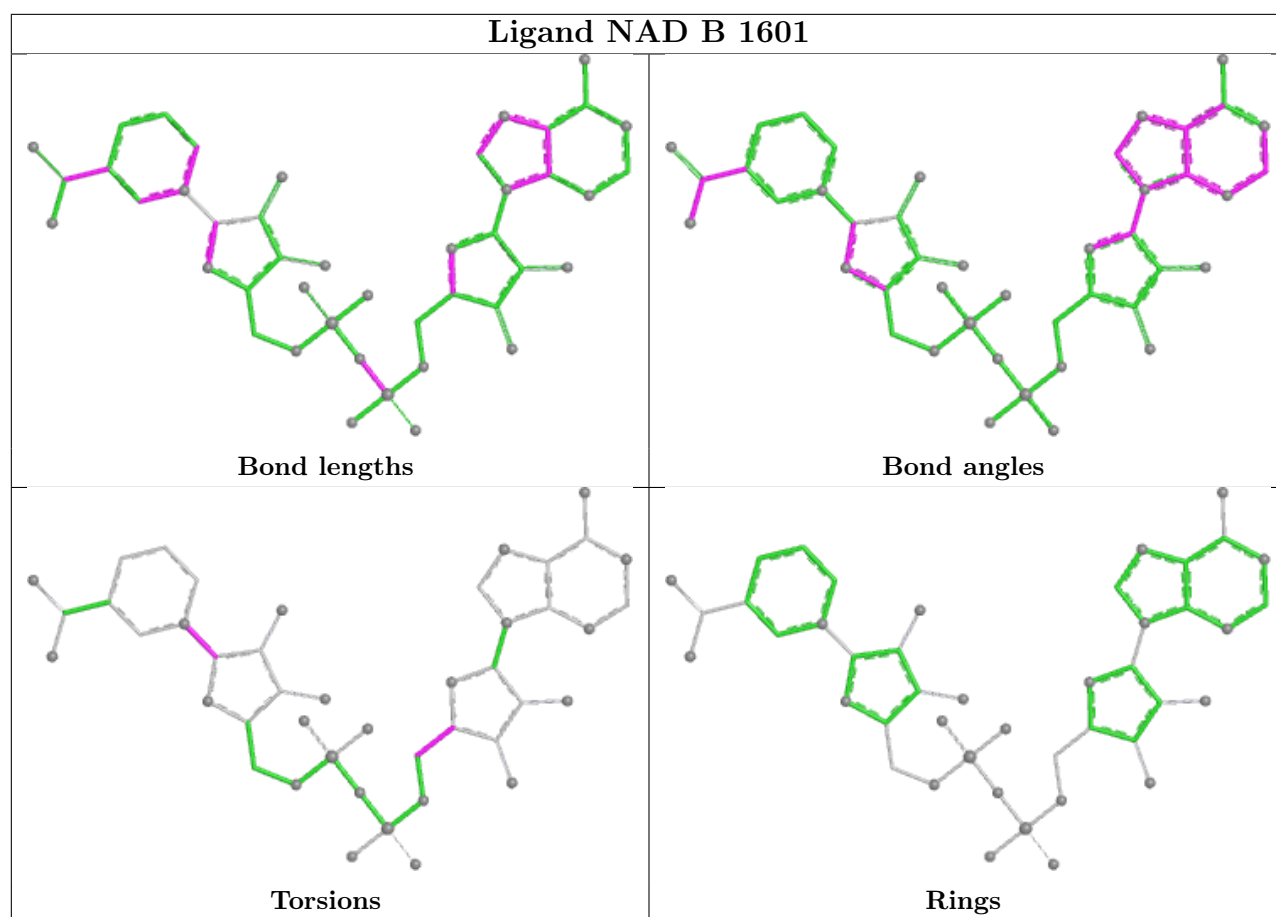


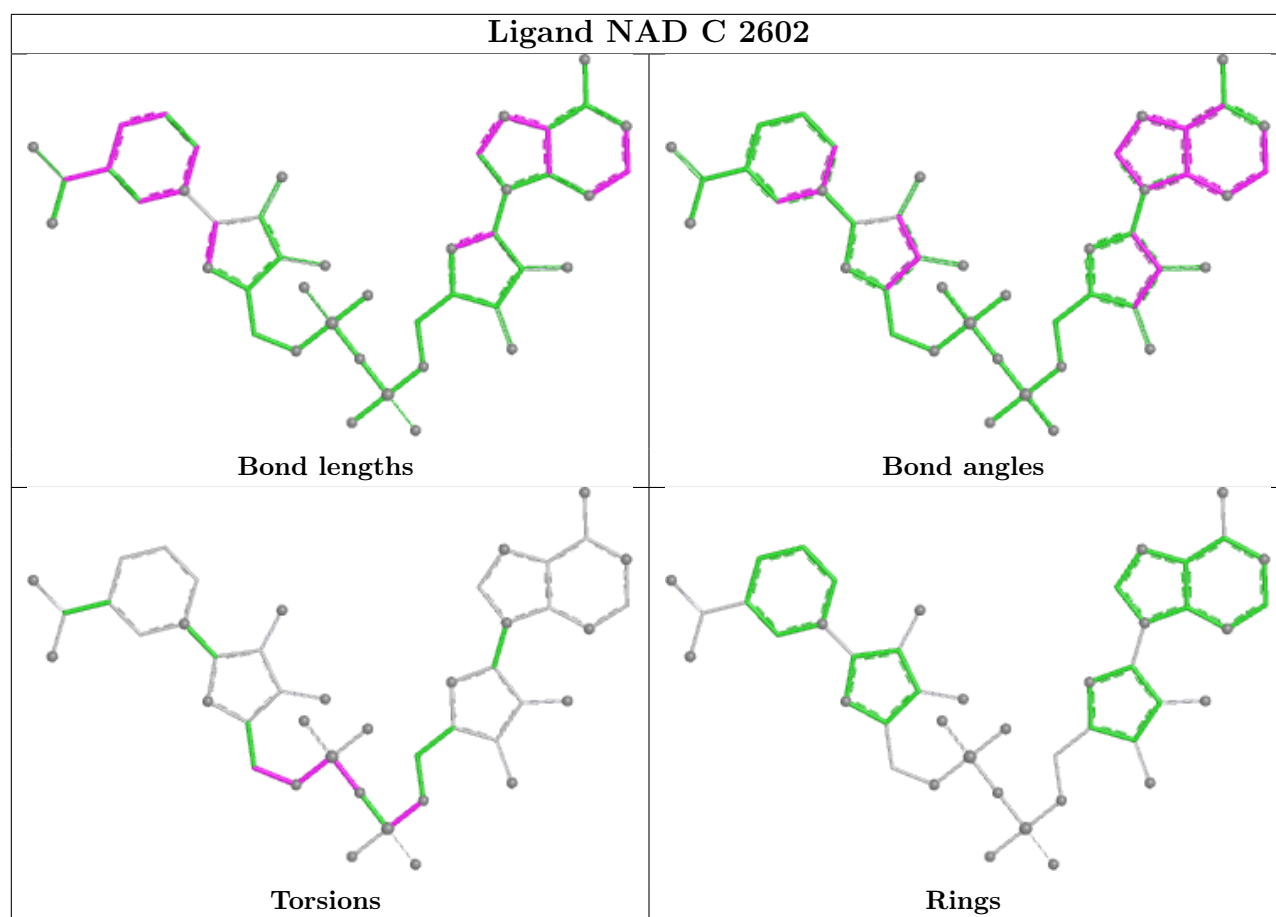


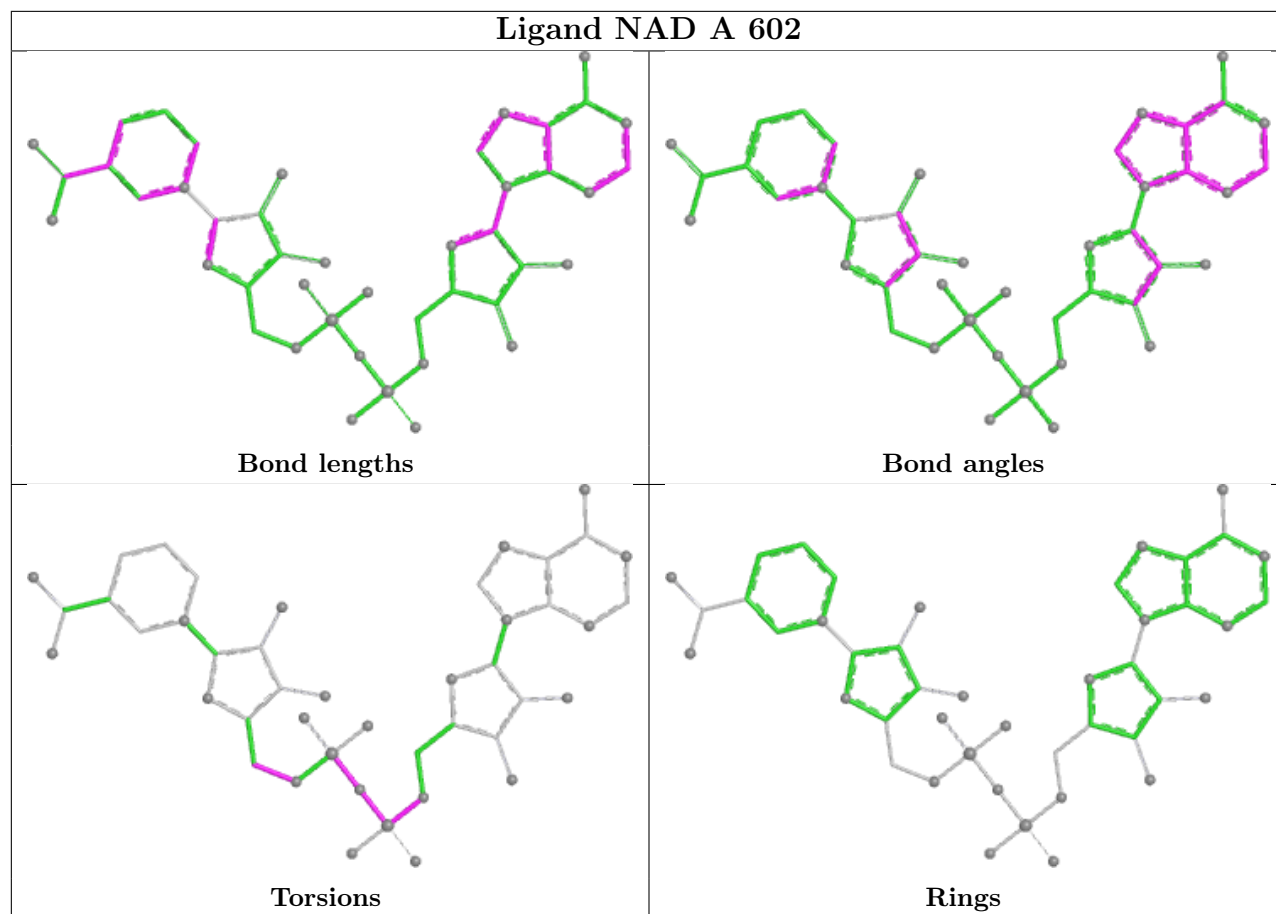
Ligand NAD D 3601











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.