Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:12 am BST

PDB ID	:	1EFL
Title	:	HUMAN MALIC ENZYME IN A QUATERNARY COMPLEX WITH NAD, MG, AND TARTRONATE
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.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

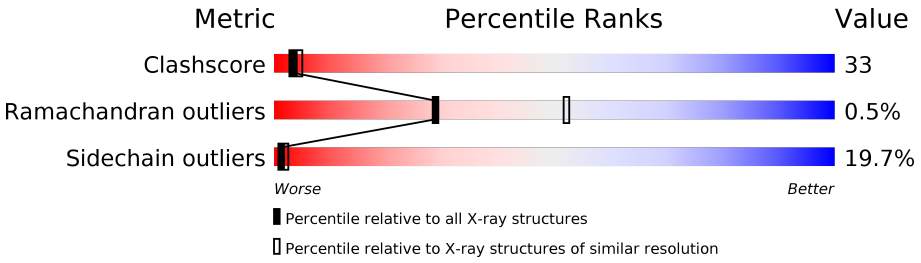
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	45% 38% 12% 5%
1	B	584	39% 44% 11% 5%
1	C	584	45% 40% 10% 5%
1	D	584	43% 42% 9% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17947 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 (three-letter code: MG) (formula: Mg).

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

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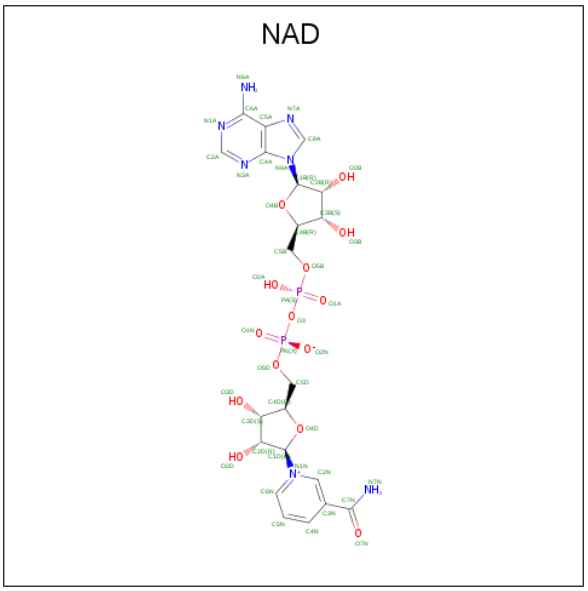
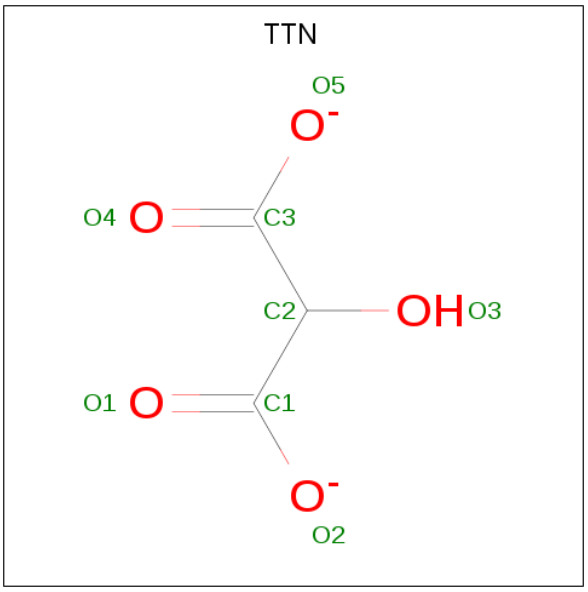
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is TARTRONATE (three-letter code: TTN) (formula: $C_3H_2O_5$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	24	Total O 24 24	0	0
5	B	17	Total O 17 17	0	0
5	C	23	Total O 23 23	0	0
5	D	27	Total O 27 27	0	0

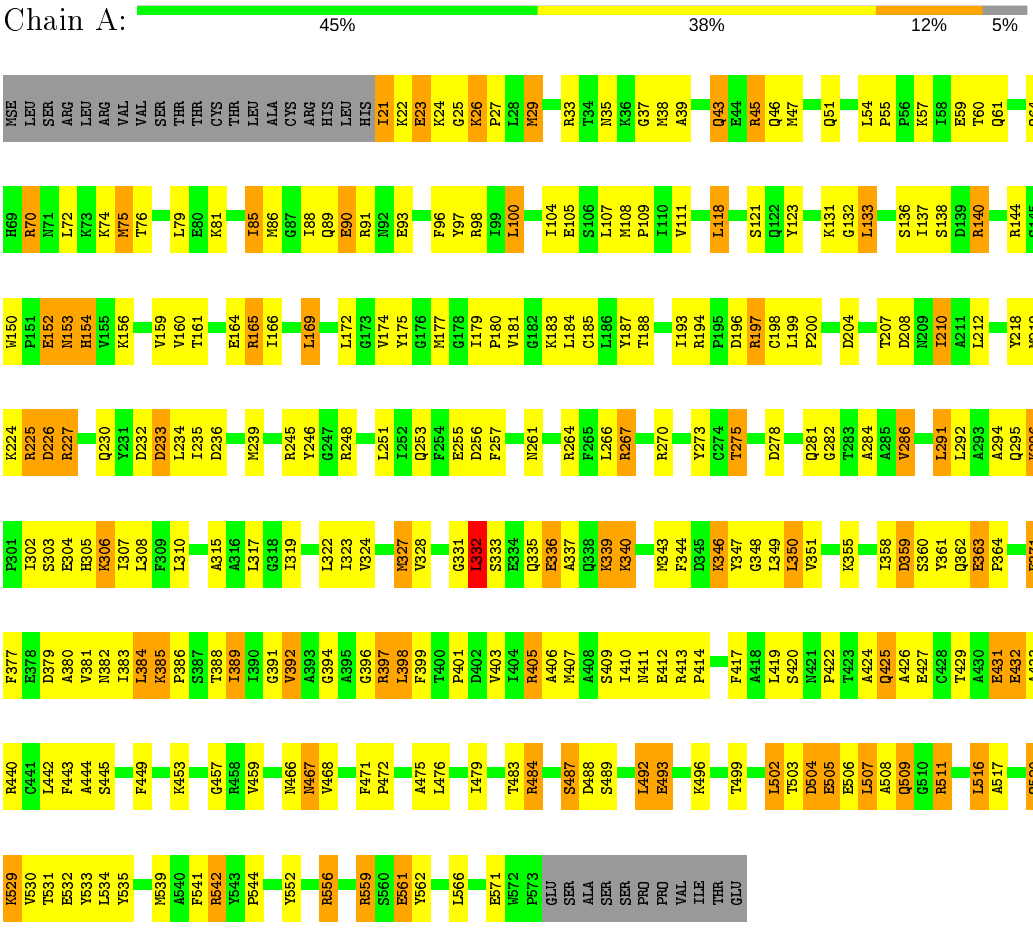
3 Residue-property plots (i)

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

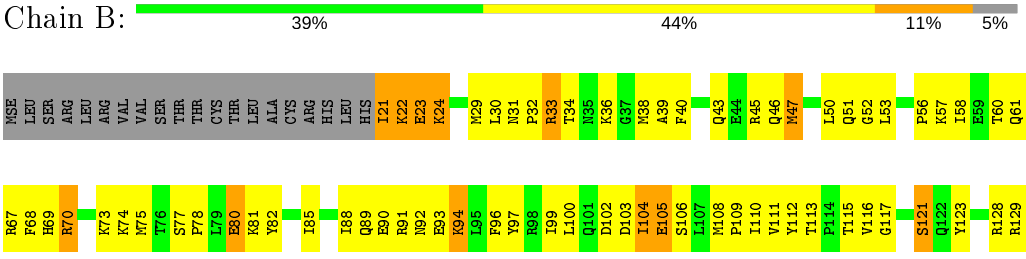
- Molecule 1: MALIC ENZYME

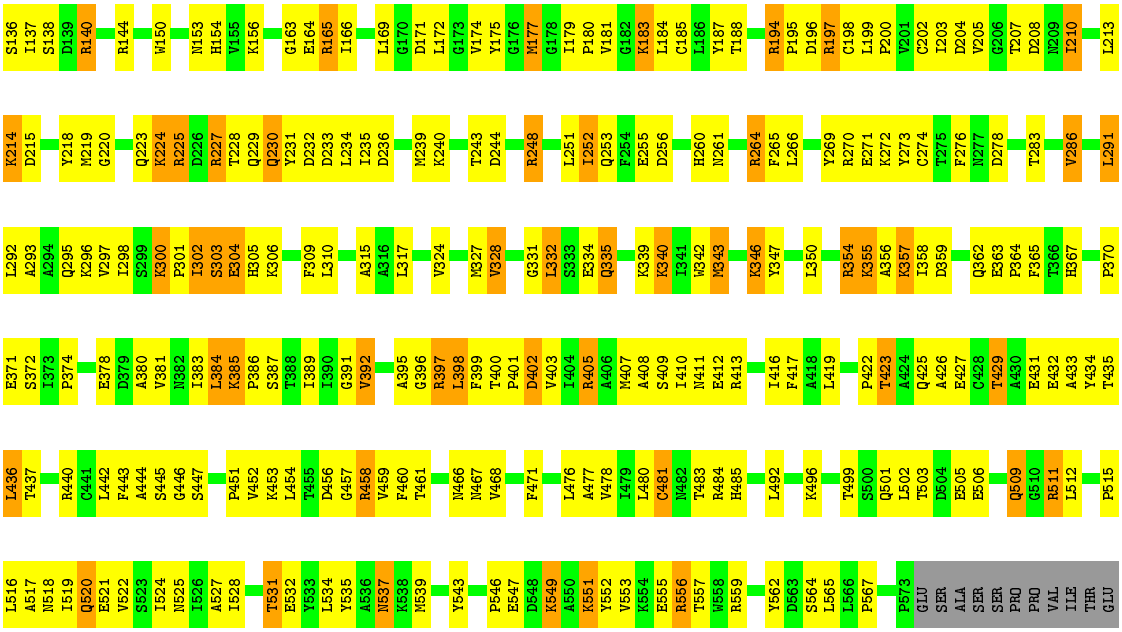
Chain A:



- Molecule 1: MALIC ENZYME

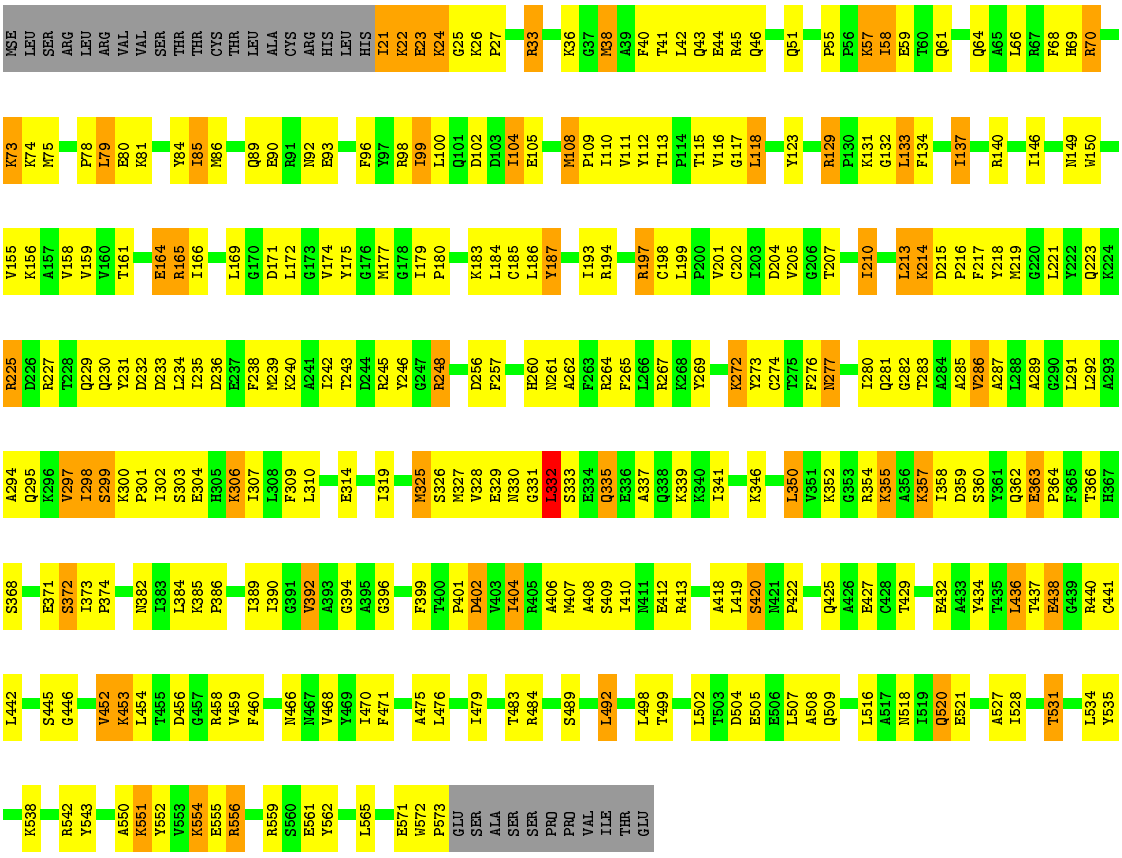
Chain B:





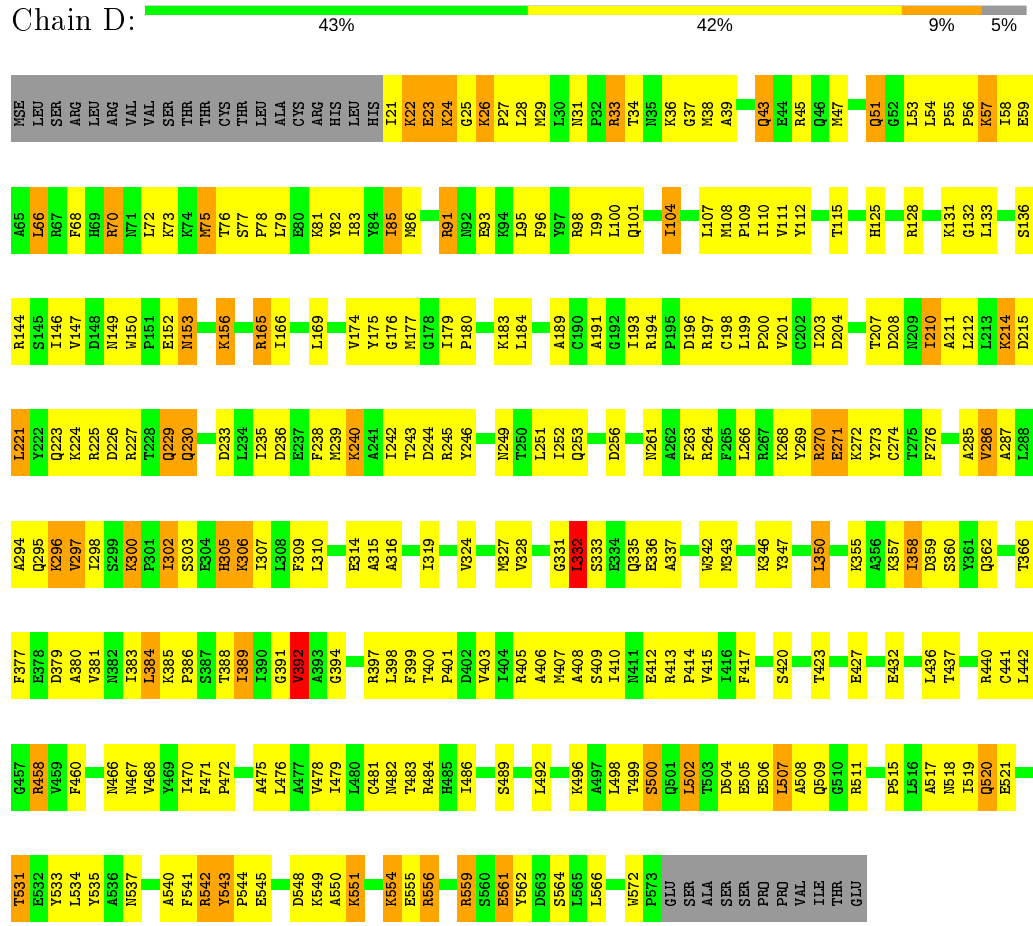
• Molecule 1: MALIC ENZYME

Chain C:



• Molecule 1: MALIC ENZYME

Chain D:



4 Data and refinement statistics (i)

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	228.80Å 117.00Å 114.30Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17947	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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: MG, TTN, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.46	0/4447	0.65	0/5998
1	B	0.46	0/4447	0.66	0/5998
1	C	0.45	0/4447	0.65	1/5998 (0.0%)
1	D	0.46	0/4447	0.65	0/5998
All	All	0.46	0/17788	0.65	1/23992 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	310	LEU	N-CA-C	-5.09	97.27	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4407	333	0
1	B	4367	0	4407	331	0
1	C	4367	0	4407	252	0
1	D	4367	0	4407	314	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	88	0	52	6	0
3	B	88	0	52	2	0
3	C	88	0	52	5	0
3	D	88	0	52	4	0
4	A	8	0	1	0	0
4	B	8	0	1	1	0
4	C	8	0	1	2	0
4	D	8	0	2	1	0
5	A	24	0	0	5	0
5	B	17	0	0	9	0
5	C	23	0	0	5	0
5	D	27	0	0	3	0
All	All	17947	0	17841	1185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.03	1.11
1:D:520:GLN:HE22	1:D:521:GLU:HG2	1.13	1.07
1:A:511:ARG:HB3	1:A:511:ARG:HH11	1.20	1.02
1:C:355:LYS:HA	1:C:355:LYS:HE2	1.42	1.01
1:B:227:ARG:HH11	1:B:227:ARG:HG2	1.24	1.00
1:D:520:GLN:NE2	1:D:521:GLU:HG2	1.75	1.00
1:D:298:ILE:HG22	1:D:300:LYS:H	1.27	0.99
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.45	0.97
1:A:108:MSE:HE3	1:A:516:LEU:HD11	1.46	0.97
1:C:327:MSE:HE3	1:C:337:ALA:HB1	1.45	0.96
3:B:1602:NAD:H51N	5:C:4090:HOH:O	1.64	0.96
1:A:324:VAL:HA	1:A:327:MSE:HE2	1.48	0.95
1:D:520:GLN:NE2	1:D:521:GLU:H	1.66	0.94
1:D:481:CYS:SG	1:D:531:THR:HB	2.08	0.94
1:B:527:ALA:O	1:B:531:THR:HG22	1.66	0.94
1:D:211:ALA:HA	1:D:214:LYS:HE2	1.51	0.93
1:B:300:LYS:HZ2	1:B:300:LYS:HB3	1.33	0.93
1:C:184:LEU:HD13	1:C:198:CYS:HB3	1.50	0.92
1:C:197:ARG:HH11	1:C:197:ARG:HG3	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:MSE:HE3	1:D:337:ALA:HB1	1.52	0.92
1:A:425:GLN:HE21	1:A:425:GLN:N	1.67	0.91
1:C:325:MSE:HE2	1:C:492:LEU:HD12	1.53	0.91
1:C:194:ARG:HB2	1:C:197:ARG:HG2	1.51	0.91
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.06	0.91
1:D:47:MSE:HE3	1:D:566:LEU:HD22	1.53	0.91
1:D:286:VAL:HG21	1:D:467:ASN:HA	1.53	0.90
1:A:405:ARG:HH11	1:A:405:ARG:HB2	1.34	0.90
1:B:184:LEU:HD22	1:B:198:CYS:HB3	1.53	0.90
1:A:397:ARG:HH11	1:A:397:ARG:HG3	1.36	0.89
1:A:371:GLU:H	1:A:371:GLU:CD	1.75	0.87
1:B:47:MSE:HE2	1:B:567:PRO:HG2	1.54	0.87
1:B:61:GLN:HA	1:B:64:GLN:HE21	1.38	0.87
1:A:227:ARG:NH1	1:A:227:ARG:HG2	1.82	0.86
1:C:85:ILE:HD12	1:C:96:PHE:HE1	1.39	0.86
1:B:453:LYS:HG2	1:B:459:VAL:HG12	1.57	0.86
1:D:381:VAL:HG13	1:D:407:MSE:HE1	1.58	0.86
1:D:300:LYS:HB3	1:D:300:LYS:HZ2	1.39	0.85
1:A:220:GLY:HA2	1:B:56:PRO:HG2	1.58	0.85
1:A:520:GLN:H	1:A:520:GLN:HE21	1.24	0.85
1:D:315:ALA:O	1:D:319:ILE:HG13	1.77	0.85
1:B:453:LYS:HE3	1:B:457:GLY:HA2	1.58	0.84
1:A:23:GLU:HA	1:A:23:GLU:OE1	1.76	0.83
1:B:378:GLU:O	1:B:381:VAL:HG12	1.77	0.83
1:A:108:MSE:HB3	1:A:109:PRO:HD3	1.58	0.83
1:A:286:VAL:HG21	1:A:467:ASN:HA	1.59	0.83
1:B:29:MSE:HE1	1:B:53:LEU:HB2	1.59	0.83
1:B:422:PRO:HD2	1:B:425:GLN:CG	2.09	0.83
1:A:166:ILE:HD12	1:A:179:ILE:HG13	1.61	0.82
1:B:397:ARG:NH2	1:B:423:THR:O	2.12	0.82
1:B:300:LYS:NZ	1:B:300:LYS:HB3	1.93	0.82
1:A:47:MSE:HE3	1:A:566:LEU:HD22	1.62	0.82
1:B:532:GLU:HG2	1:B:549:LYS:HG2	1.62	0.82
1:D:23:GLU:OE2	1:D:23:GLU:HA	1.80	0.82
1:D:107:LEU:O	1:D:111:VAL:HG12	1.78	0.81
1:D:286:VAL:HG22	1:D:470:ILE:HG13	1.61	0.81
1:D:509:GLN:HB2	5:D:4058:HOH:O	1.80	0.81
1:A:381:VAL:HG13	1:A:407:MSE:HE3	1.60	0.81
1:D:261:ASN:ND2	1:D:264:ARG:HH21	1.78	0.81
1:B:77:SER:O	1:B:81:LYS:HG3	1.80	0.81
1:D:144:ARG:HD2	1:D:147:VAL:CG2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LYS:HE3	1:D:305:HIS:ND1	1.95	0.81
1:B:67:ARG:HD2	5:B:4079:HOH:O	1.80	0.80
1:D:22:LYS:HD2	1:D:22:LYS:O	1.81	0.80
1:A:487:SER:HB3	1:A:539:MSE:HE1	1.61	0.80
1:D:559:ARG:HG3	1:D:561:GLU:OE1	1.80	0.80
1:A:425:GLN:HE21	1:A:425:GLN:H	1.27	0.80
1:D:184:LEU:HD22	1:D:198:CYS:HB3	1.64	0.80
1:B:306:LYS:HG2	1:B:386:PRO:HA	1.64	0.80
1:A:407:MSE:HE2	1:A:407:MSE:HA	1.63	0.79
1:A:425:GLN:NE2	1:A:425:GLN:N	2.31	0.79
1:A:335:GLN:O	1:A:339:LYS:HD2	1.83	0.79
1:D:328:VAL:HA	1:D:332:LEU:O	1.83	0.79
1:D:43:GLN:HG2	1:D:566:LEU:HD11	1.64	0.79
1:B:108:MSE:HE3	1:B:516:LEU:HD11	1.64	0.78
1:B:371:GLU:H	1:B:371:GLU:CD	1.87	0.78
1:B:422:PRO:HD2	1:B:425:GLN:HG3	1.65	0.78
1:A:511:ARG:NH1	1:A:511:ARG:HB3	1.98	0.78
1:D:177:MSE:HE1	1:D:180:PRO:HB2	1.66	0.78
1:D:194:ARG:HE	1:D:197:ARG:NE	1.82	0.78
1:B:343:MSE:HE3	1:B:350:LEU:HD12	1.66	0.77
1:A:21:ILE:HD13	1:A:21:ILE:N	1.99	0.77
1:B:483:THR:HG21	1:B:534:LEU:HD13	1.67	0.77
1:B:29:MSE:HE2	1:B:50:LEU:HD22	1.64	0.77
1:D:324:VAL:HA	1:D:327:MSE:HE2	1.67	0.77
1:D:310:LEU:HB3	1:D:391:GLY:HA2	1.65	0.77
1:B:431:GLU:O	1:B:435:THR:HG23	1.85	0.77
1:A:24:LYS:HE2	1:C:22:LYS:HD2	1.67	0.77
1:C:179:ILE:HB	1:C:180:PRO:HD3	1.66	0.76
1:D:466:ASN:HB3	1:D:468:VAL:HG12	1.68	0.76
1:B:29:MSE:HE2	1:B:50:LEU:HB3	1.65	0.76
1:A:175:TYR:CD2	1:A:219:MSE:HE2	2.19	0.76
1:A:511:ARG:HH11	1:A:511:ARG:CB	1.99	0.76
1:B:335:GLN:O	1:B:339:LYS:HG3	1.85	0.76
1:C:85:ILE:HG13	1:C:86:MSE:N	1.98	0.76
1:A:38:MSE:HE3	1:A:59:GLU:CD	2.07	0.76
1:B:395:ALA:HB3	1:B:398:LEU:HD21	1.68	0.76
1:D:359:ASP:OD2	1:D:362:GLN:HG3	1.85	0.76
1:B:401:PRO:O	1:B:405:ARG:HG3	1.86	0.75
1:D:298:ILE:CG2	1:D:300:LYS:HB2	2.16	0.75
1:A:154:HIS:O	1:A:197:ARG:HG3	1.87	0.75
1:B:227:ARG:CG	1:B:227:ARG:HH11	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ILE:HG22	1:D:384:LEU:HD13	1.69	0.74
1:B:47:MSE:HE3	1:D:47:MSE:SE	2.38	0.74
1:B:177:MSE:O	1:B:180:PRO:HD2	1.87	0.74
1:D:207:THR:O	1:D:224:LYS:HA	1.87	0.74
1:A:405:ARG:NH1	1:A:405:ARG:HB2	2.02	0.73
1:D:33:ARG:HD3	1:D:196:ASP:HB3	1.71	0.73
1:A:47:MSE:CE	1:A:566:LEU:HD22	2.19	0.73
1:C:551:LYS:O	1:C:555:GLU:HB2	1.88	0.73
1:D:400:THR:OG1	1:D:403:VAL:HG23	1.89	0.72
1:A:227:ARG:CG	1:A:227:ARG:HH11	1.90	0.72
1:B:105:GLU:HB2	5:B:4016:HOH:O	1.89	0.72
1:D:548:ASP:OD1	1:D:551:LYS:HB2	1.90	0.72
1:B:137:ILE:O	1:B:140:ARG:HG2	1.89	0.72
1:B:332:LEU:HD21	1:B:340:LYS:HE3	1.71	0.72
1:D:392:VAL:O	1:D:392:VAL:HG13	1.89	0.72
1:B:385:LYS:HA	1:B:410:ILE:HD13	1.70	0.72
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.53	0.71
1:C:432:GLU:O	1:C:436:LEU:HB2	1.90	0.71
1:D:240:LYS:HE3	1:D:273:TYR:OH	1.90	0.71
1:D:468:VAL:HA	1:D:471:PHE:CE2	2.26	0.71
1:B:22:LYS:NZ	1:D:27:PRO:HG2	2.05	0.71
1:B:408:ALA:HB1	1:B:440:ARG:NH2	2.06	0.71
1:B:324:VAL:O	1:B:328:VAL:HG13	1.91	0.71
1:C:306:LYS:HG2	1:C:386:PRO:HA	1.72	0.71
1:B:22:LYS:HZ3	1:D:27:PRO:HG2	1.54	0.71
1:C:289:ALA:CB	1:C:498:LEU:HD23	2.21	0.70
1:D:381:VAL:CG1	1:D:407:MSE:HE1	2.20	0.70
1:C:355:LYS:CA	1:C:355:LYS:HE2	2.19	0.70
1:D:194:ARG:HB2	1:D:197:ARG:HG3	1.72	0.70
1:A:392:VAL:HG13	1:A:392:VAL:O	1.89	0.70
1:A:81:LYS:O	1:A:85:ILE:HG23	1.91	0.70
1:D:177:MSE:CE	1:D:180:PRO:HB2	2.22	0.70
1:A:177:MSE:HE1	1:A:180:PRO:HB2	1.72	0.70
1:B:166:ILE:HG21	1:B:172:LEU:HD12	1.73	0.70
1:B:354:ARG:HE	1:B:358:ILE:HD11	1.55	0.70
1:B:90:GLU:OE1	1:B:131:LYS:HG3	1.92	0.70
1:D:253:GLN:HB2	1:D:276:PHE:CE2	2.26	0.70
1:D:520:GLN:HE22	1:D:521:GLU:CG	1.99	0.70
1:B:335:GLN:HG3	1:B:339:LYS:HE3	1.74	0.70
1:D:194:ARG:HG2	1:D:194:ARG:HH11	1.55	0.70
1:B:302:ILE:HA	1:B:305:HIS:ND1	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASN:ND2	1:B:264:ARG:CZ	2.55	0.70
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.72	0.69
1:A:520:GLN:H	1:A:520:GLN:NE2	1.88	0.69
1:B:433:ALA:O	1:B:437:THR:HG23	1.92	0.69
1:C:197:ARG:HG3	1:C:197:ARG:NH1	1.98	0.69
1:B:24:LYS:O	1:D:22:LYS:HE3	1.91	0.69
1:C:520:GLN:H	1:C:520:GLN:HE21	1.40	0.69
1:D:415:VAL:HG22	1:D:442:LEU:HD12	1.74	0.69
1:C:434:TYR:CD1	1:C:452:VAL:HG11	2.28	0.69
1:C:81:LYS:O	1:C:85:ILE:HG23	1.92	0.69
1:A:405:ARG:HH11	1:A:405:ARG:CB	2.06	0.69
1:B:537:ASN:HD22	1:B:537:ASN:N	1.91	0.68
1:D:551:LYS:O	1:D:555:GLU:HB2	1.93	0.68
1:B:305:HIS:HB2	1:B:340:LYS:HZ1	1.58	0.68
1:A:91:ARG:NE	5:A:4055:HOH:O	2.26	0.68
1:B:347:TYR:HB2	1:B:354:ARG:HH12	1.58	0.68
1:C:133:LEU:HB2	1:C:199:LEU:HD11	1.75	0.68
1:D:211:ALA:HA	1:D:214:LYS:CE	2.22	0.68
1:D:43:GLN:OE1	1:D:47:MSE:HE2	1.93	0.68
1:C:357:LYS:HD2	1:C:357:LYS:H	1.59	0.68
1:B:328:VAL:HA	1:B:332:LEU:O	1.93	0.68
1:B:60:THR:OG1	1:B:63:ILE:HG13	1.93	0.68
1:B:528:ILE:O	1:B:532:GLU:HG3	1.94	0.68
1:A:79:LEU:HB2	1:A:118:LEU:HD21	1.76	0.67
1:B:205:VAL:HG11	1:B:231:TYR:HD1	1.59	0.67
1:D:64:GLN:NE2	1:D:562:TYR:OH	2.25	0.67
1:D:306:LYS:CG	1:D:386:PRO:HA	2.23	0.67
1:A:398:LEU:HD23	1:A:398:LEU:N	2.09	0.67
1:C:23:GLU:OE1	1:C:23:GLU:HA	1.93	0.67
1:D:550:ALA:O	1:D:554:LYS:HG2	1.95	0.67
1:A:45:ARG:HB3	1:A:51:GLN:HG2	1.76	0.67
1:D:31:ASN:ND2	1:D:34:THR:HG23	2.09	0.67
1:B:291:LEU:HD13	1:B:417:PHE:CE2	2.29	0.67
1:B:75:MSE:HG2	1:B:80:GLU:CD	2.15	0.67
1:B:81:LYS:O	1:B:85:ILE:HG13	1.94	0.67
1:A:108:MSE:CE	1:A:516:LEU:HD11	2.24	0.67
1:A:137:ILE:HD12	1:A:234:LEU:HD22	1.77	0.67
1:B:91:ARG:HH11	1:B:91:ARG:HG2	1.60	0.67
1:B:253:GLN:HB2	1:B:276:PHE:CE2	2.30	0.67
1:C:85:ILE:HD11	1:C:111:VAL:HG23	1.76	0.67
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HH22	1:A:233:ASP:HB3	1.57	0.66
1:A:453:LYS:CG	1:A:459:VAL:HG22	2.24	0.66
1:A:401:PRO:HB2	1:A:405:ARG:HH22	1.59	0.66
1:B:422:PRO:HD2	1:B:425:GLN:HG2	1.77	0.66
1:C:75:MSE:HG2	1:C:80:GLU:CD	2.15	0.66
1:A:397:ARG:HG3	1:A:397:ARG:NH1	2.09	0.66
1:C:298:ILE:HD13	1:C:413:ARG:HB2	1.76	0.66
1:A:453:LYS:HG3	1:A:459:VAL:HG22	1.77	0.66
1:B:240:LYS:HE3	1:B:244:ASP:OD2	1.94	0.66
1:B:503:THR:HB	1:B:505:GLU:OE2	1.94	0.66
1:B:51:GLN:NE2	5:B:4050:HOH:O	2.28	0.66
1:D:327:MSE:CE	1:D:337:ALA:HB1	2.24	0.66
1:D:51:GLN:HA	1:D:51:GLN:HE21	1.61	0.66
1:C:79:LEU:HD22	1:C:118:LEU:HG	1.78	0.66
1:A:335:GLN:CD	1:A:339:LYS:HZ3	1.99	0.66
1:B:60:THR:H	1:B:63:ILE:HD12	1.60	0.66
1:D:137:ILE:O	1:D:140:ARG:HG2	1.95	0.66
1:C:357:LYS:HD2	1:C:357:LYS:N	2.11	0.66
1:A:324:VAL:HA	1:A:327:MSE:CE	2.22	0.66
1:A:156:LYS:HE3	1:A:479:ILE:HG23	1.77	0.66
1:B:395:ALA:HB3	1:B:398:LEU:CD2	2.26	0.66
1:A:140:ARG:NH2	1:A:230:GLN:O	2.29	0.65
1:D:437:THR:O	1:D:440:ARG:HG3	1.95	0.65
1:D:505:GLU:O	1:D:508:ALA:HB3	1.96	0.65
1:D:85:ILE:HD11	1:D:100:LEU:HD11	1.78	0.65
1:B:22:LYS:O	1:D:24:LYS:HE3	1.97	0.65
1:D:166:ILE:HD12	1:D:179:ILE:HG13	1.77	0.65
1:A:371:GLU:CD	1:A:371:GLU:N	2.47	0.65
1:A:392:VAL:CG1	1:A:392:VAL:O	2.44	0.65
1:B:492:LEU:CD2	1:B:496:LYS:HE3	2.27	0.65
1:C:314:GLU:HB2	3:C:2601:NAD:O1N	1.96	0.65
1:D:327:MSE:HE3	1:D:337:ALA:CB	2.25	0.65
1:D:346:LYS:HE2	1:D:347:TYR:CZ	2.31	0.65
1:D:350:LEU:HD23	1:D:350:LEU:N	2.11	0.65
1:B:518:ASN:O	1:B:522:VAL:HG23	1.96	0.65
1:D:502:LEU:HD13	1:D:507:LEU:CD1	2.27	0.65
1:B:309:PHE:HB2	1:B:343:MSE:HG3	1.79	0.65
1:B:81:LYS:HD2	5:B:4051:HOH:O	1.97	0.65
1:D:407:MSE:CA	1:D:407:MSE:HE2	2.27	0.65
1:D:509:GLN:HG3	1:D:511:ARG:HG3	1.77	0.65
1:D:520:GLN:NE2	1:D:521:GLU:N	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ASN:H	1:A:467:ASN:ND2	1.94	0.64
1:B:374:PRO:HG3	1:B:383:ILE:HD12	1.78	0.64
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.79	0.64
1:B:423:THR:HG23	1:B:447:SER:HB3	1.79	0.64
1:A:358:ILE:HG23	1:A:362:GLN:HB2	1.79	0.64
1:B:61:GLN:HG3	1:B:562:TYR:CE1	2.32	0.64
1:A:328:VAL:HA	1:A:332:LEU:O	1.96	0.64
1:D:385:LYS:HA	1:D:410:ILE:HD13	1.80	0.64
1:D:300:LYS:CB	1:D:300:LYS:HZ2	2.11	0.64
1:D:286:VAL:HG11	1:D:466:ASN:O	1.98	0.64
1:D:68:PHE:CE2	1:D:99:ILE:HG21	2.33	0.64
1:A:487:SER:HB3	1:A:539:MSE:CE	2.26	0.64
1:A:177:MSE:HE3	1:A:180:PRO:HD2	1.80	0.64
1:B:305:HIS:HB2	1:B:340:LYS:NZ	2.12	0.64
1:B:492:LEU:HD21	1:B:496:LYS:HE3	1.80	0.63
1:A:204:ASP:OD2	1:B:56:PRO:HG3	1.98	0.63
1:B:273:TYR:O	1:B:485:HIS:HD2	1.81	0.63
1:C:159:VAL:HG23	1:C:184:LEU:HD21	1.79	0.63
1:D:210:ILE:HG12	1:D:211:ALA:N	2.14	0.63
1:A:111:VAL:O	5:A:4046:HOH:O	2.15	0.63
1:B:110:ILE:O	1:B:115:THR:HB	1.98	0.63
1:B:116:VAL:HG13	1:B:117:GLY:N	2.14	0.63
1:A:504:ASP:OD2	1:A:504:ASP:N	2.31	0.63
1:C:70:ARG:HH11	1:C:70:ARG:HG2	1.64	0.63
1:A:298:ILE:HG22	1:A:300:LYS:HB2	1.81	0.63
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.64	0.63
1:A:88:ILE:HD13	1:A:91:ARG:HH21	1.64	0.63
1:B:261:ASN:ND2	1:B:264:ARG:NH1	2.47	0.63
1:B:501:GLN:HE22	1:B:525:ASN:HB3	1.63	0.63
1:D:153:ASN:ND2	1:D:153:ASN:H	1.97	0.63
1:B:197:ARG:NH1	1:B:197:ARG:HG3	2.12	0.63
1:C:550:ALA:O	1:C:554:LYS:HG2	1.98	0.63
1:C:90:GLU:OE1	1:C:131:LYS:HG3	1.98	0.63
1:B:346:LYS:HB2	1:B:346:LYS:NZ	2.14	0.63
1:B:468:VAL:HA	1:B:471:PHE:CE2	2.34	0.63
1:B:517:ALA:O	1:B:520:GLN:OE1	2.16	0.63
1:A:310:LEU:HB3	1:A:391:GLY:HA2	1.81	0.62
1:C:172:LEU:O	1:C:175:TYR:HB2	1.98	0.62
1:B:197:ARG:HG3	1:B:197:ARG:HH11	1.64	0.62
1:D:300:LYS:HB3	1:D:300:LYS:NZ	2.04	0.62
1:C:110:ILE:O	1:C:115:THR:HB	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:LYS:HG2	1:D:386:PRO:HA	1.82	0.62
1:D:481:CYS:HB3	1:D:540:ALA:HB1	1.79	0.62
1:A:233:ASP:OD2	1:A:233:ASP:C	2.38	0.62
1:A:483:THR:OG1	1:A:534:LEU:HD13	1.99	0.62
1:D:95:LEU:O	1:D:99:ILE:HG12	1.99	0.62
1:A:177:MSE:CE	1:A:180:PRO:HB2	2.29	0.62
1:B:23:GLU:HA	1:B:23:GLU:OE1	1.99	0.62
1:C:302:ILE:CD1	1:C:332:LEU:HD22	2.30	0.62
1:B:515:PRO:HB2	1:B:518:ASN:HD22	1.65	0.62
1:D:270:ARG:HG3	1:D:271:GLU:OE2	2.00	0.62
1:A:29:MSE:HA	1:A:35:ASN:OD1	2.00	0.62
1:D:286:VAL:HG21	1:D:467:ASN:CA	2.29	0.62
1:B:295:GLN:HA	1:B:295:GLN:OE1	1.99	0.61
1:D:108:MSE:HB3	1:D:109:PRO:HD3	1.80	0.61
1:A:307:ILE:HG13	1:A:388:THR:HB	1.81	0.61
1:C:112:TYR:CD2	1:C:113:THR:HG22	2.35	0.61
1:D:33:ARG:NH1	1:D:93:GLU:OE1	2.33	0.61
1:A:132:GLY:HA2	1:A:200:PRO:HG2	1.81	0.61
1:A:123:TYR:CD2	1:A:219:MSE:HE1	2.35	0.61
1:C:406:ALA:O	1:C:410:ILE:HG13	2.01	0.61
1:D:286:VAL:CG2	1:D:467:ASN:HA	2.27	0.61
1:C:221:LEU:HB3	1:C:223:GLN:HG2	1.82	0.61
1:D:391:GLY:HA3	1:D:427:GLU:HG2	1.82	0.61
1:A:475:ALA:O	1:A:479:ILE:HD12	2.00	0.61
1:D:298:ILE:HD11	1:D:442:LEU:CD1	2.30	0.61
1:D:70:ARG:HG2	1:D:70:ARG:NH1	2.14	0.61
1:A:55:PRO:HG3	1:B:219:MSE:HE3	1.83	0.61
1:B:47:MSE:HE2	1:B:567:PRO:CG	2.29	0.61
1:A:29:MSE:HE1	1:A:54:LEU:HD21	1.83	0.61
1:C:21:ILE:HD12	1:C:22:LYS:N	2.16	0.61
1:A:210:ILE:H	1:A:210:ILE:HD13	1.66	0.61
1:C:61:GLN:HA	1:C:64:GLN:HE21	1.66	0.61
1:D:298:ILE:HG22	1:D:300:LYS:HB2	1.81	0.61
1:C:434:TYR:HD1	1:C:452:VAL:HG11	1.64	0.60
1:C:454:LEU:HD11	1:C:460:PHE:HE2	1.64	0.60
1:D:179:ILE:HB	1:D:180:PRO:HD3	1.82	0.60
1:D:70:ARG:CG	1:D:70:ARG:HH11	2.15	0.60
1:B:177:MSE:O	1:B:181:VAL:HG23	2.00	0.60
1:D:243:THR:HG21	1:D:273:TYR:CD2	2.36	0.60
1:D:407:MSE:HA	1:D:407:MSE:HE2	1.82	0.60
1:A:443:PHE:CZ	1:A:445:SER:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ILE:HD13	1:D:235:ILE:CD1	2.31	0.60
1:C:70:ARG:HH11	1:C:70:ARG:CG	2.14	0.60
1:D:306:LYS:HE2	1:D:342:TRP:NE1	2.17	0.60
1:A:535:TYR:OH	1:A:542:ARG:HB3	2.01	0.60
1:B:532:GLU:HG2	1:B:549:LYS:CG	2.31	0.60
1:C:326:SER:O	1:C:329:GLU:HG2	2.02	0.60
1:C:483:THR:OG1	1:C:534:LEU:HD13	2.01	0.60
1:B:506:GLU:O	1:B:511:ARG:HB2	2.02	0.59
1:C:165:ARG:NH2	1:C:256:ASP:OD1	2.34	0.59
1:B:297:VAL:HG22	1:B:298:ILE:N	2.16	0.59
1:C:68:PHE:CD2	1:C:99:ILE:HG13	2.37	0.59
1:A:225:ARG:CG	1:A:225:ARG:HH11	2.16	0.59
1:A:233:ASP:OD2	1:A:234:LEU:N	2.35	0.59
1:C:248:ARG:HH22	1:C:272:LYS:HZ2	1.49	0.59
1:B:24:LYS:NZ	1:D:22:LYS:HD3	2.17	0.59
1:D:243:THR:HG21	1:D:273:TYR:CE2	2.37	0.59
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.83	0.59
1:C:21:ILE:HD12	1:C:22:LYS:H	1.67	0.59
1:D:397:ARG:NH2	1:D:423:THR:O	2.35	0.59
1:A:333:SER:OG	1:A:336:GLU:HG3	2.02	0.59
1:B:397:ARG:NH2	1:B:426:ALA:HB3	2.17	0.59
1:A:286:VAL:CG2	1:A:467:ASN:HA	2.32	0.59
1:B:543:TYR:CZ	1:C:484:ARG:HG2	2.38	0.59
1:A:57:LYS:HD3	1:B:218:TYR:O	2.02	0.59
1:B:205:VAL:HG11	1:B:231:TYR:CD1	2.38	0.59
1:C:307:ILE:N	1:C:307:ILE:HD12	2.18	0.59
1:A:150:TRP:NE1	1:A:152:GLU:HB2	2.18	0.59
1:A:132:GLY:CA	1:A:200:PRO:HG2	2.33	0.59
1:A:221:LEU:HB3	1:A:223:GLN:HG2	1.84	0.59
1:D:140:ARG:NH2	1:D:230:GLN:HG2	2.17	0.58
1:D:36:LYS:HE2	1:D:562:TYR:HB3	1.85	0.58
1:B:346:LYS:HB2	1:B:346:LYS:HZ3	1.68	0.58
1:B:46:GLN:HG3	1:B:51:GLN:HG3	1.84	0.58
1:C:552:TYR:O	1:C:556:ARG:HG2	2.02	0.58
1:A:105:GLU:HG3	1:A:516:LEU:HB3	1.86	0.58
1:C:453:LYS:HB2	1:C:459:VAL:HG22	1.85	0.58
1:D:389:ILE:HG23	1:D:399:PHE:CZ	2.38	0.58
1:A:350:LEU:HD11	1:A:362:GLN:NE2	2.17	0.58
1:A:476:LEU:HD23	1:A:527:ALA:CB	2.34	0.58
1:C:328:VAL:HA	1:C:332:LEU:O	2.02	0.58
1:D:293:ALA:O	1:D:296:LYS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:THR:O	1:A:224:LYS:HA	2.04	0.58
1:A:493:GLU:HG2	1:A:533:TYR:CD1	2.39	0.58
1:B:33:ARG:HD2	1:B:93:GLU:OE1	2.04	0.58
1:B:301:PRO:HG2	1:B:304:GLU:OE2	2.03	0.58
1:B:389:ILE:HG23	1:B:399:PHE:CZ	2.38	0.58
1:D:518:ASN:HA	1:D:520:GLN:OE1	2.02	0.58
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.86	0.58
1:C:85:ILE:HD12	1:C:96:PHE:CE1	2.31	0.58
1:D:38:MSE:SE	1:D:55:PRO:HG2	2.54	0.58
1:A:397:ARG:HD2	1:A:426:ALA:O	2.03	0.58
1:D:285:ALA:HB1	1:D:470:ILE:HD12	1.84	0.58
1:A:152:GLU:N	1:A:152:GLU:OE1	2.36	0.57
1:A:57:LYS:HZ3	1:A:59:GLU:HG2	1.68	0.57
1:B:128:ARG:HH11	1:B:128:ARG:HG3	1.69	0.57
1:A:424:ALA:HB3	1:A:425:GLN:HE22	1.68	0.57
1:B:515:PRO:HB2	1:B:518:ASN:ND2	2.19	0.57
1:B:128:ARG:NE	5:B:4056:HOH:O	2.20	0.57
1:C:420:SER:HA	3:C:2601:NAD:H1D	1.86	0.57
1:A:350:LEU:HD13	1:A:358:ILE:CD1	2.34	0.57
1:A:55:PRO:CG	1:B:219:MSE:HE3	2.34	0.57
1:B:128:ARG:NH1	1:B:128:ARG:HG3	2.18	0.57
1:B:354:ARG:HE	1:B:358:ILE:CD1	2.17	0.57
1:C:231:TYR:CE2	1:C:265:PHE:HZ	2.23	0.57
1:D:306:LYS:HG3	1:D:386:PRO:HA	1.85	0.57
1:D:535:TYR:OH	1:D:542:ARG:HB3	2.05	0.57
1:B:552:TYR:O	1:B:556:ARG:HG3	2.05	0.57
1:D:43:GLN:HG2	1:D:566:LEU:CD1	2.32	0.57
1:B:227:ARG:HG2	1:B:227:ARG:NH1	2.04	0.57
1:B:22:LYS:HZ3	1:D:27:PRO:CG	2.18	0.57
1:D:481:CYS:HB3	1:D:540:ALA:CB	2.34	0.57
1:D:86:MSE:HG3	1:D:131:LYS:HZ1	1.69	0.57
1:B:29:MSE:CE	1:B:50:LEU:HD22	2.35	0.57
1:B:343:MSE:HB3	1:B:350:LEU:HG	1.85	0.57
1:D:456:ASP:OD2	1:D:458:ARG:NH1	2.37	0.57
1:B:183:LYS:NZ	1:B:255:GLU:OE1	2.38	0.57
1:B:456:ASP:OD2	1:B:458:ARG:NH1	2.37	0.57
1:C:261:ASN:HD21	1:C:264:ARG:HH21	1.52	0.57
1:C:446:GLY:N	5:C:4012:HOH:O	2.24	0.57
1:D:526:ILE:O	1:D:530:VAL:HG23	2.05	0.57
1:B:551:LYS:O	1:B:555:GLU:HB2	2.05	0.57
1:C:412:GLU:O	1:C:440:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:GLY:HA2	1:D:420:SER:HB3	1.87	0.57
1:B:274:CYS:HB2	1:B:484:ARG:O	2.04	0.57
1:C:41:THR:OG1	1:C:44:GLU:HG3	2.04	0.57
1:A:503:THR:OG1	1:A:505:GLU:HG2	2.04	0.56
1:C:437:THR:C	1:C:438:GLU:HG2	2.25	0.56
1:D:381:VAL:CG2	1:D:389:ILE:HD11	2.35	0.56
1:A:467:ASN:HD22	1:A:467:ASN:H	1.52	0.56
1:B:227:ARG:CG	1:B:227:ARG:NH1	2.61	0.56
1:C:392:VAL:HG13	1:C:392:VAL:O	2.05	0.56
1:C:40:PHE:HE2	1:C:565:LEU:CD1	2.17	0.56
1:A:61:GLN:OE1	1:A:98:ARG:HD3	2.05	0.56
1:A:91:ARG:HD2	5:A:4055:HOH:O	2.04	0.56
1:B:184:LEU:HD12	1:B:200:PRO:HB3	1.88	0.56
1:C:350:LEU:HD22	1:C:354:ARG:CZ	2.35	0.56
1:D:81:LYS:O	1:D:85:ILE:HG22	2.06	0.56
1:B:396:GLY:O	1:B:427:GLU:HA	2.06	0.56
1:B:552:TYR:CD1	1:B:556:ARG:NH1	2.73	0.56
1:A:144:ARG:NE	1:A:148:ASP:OD1	2.38	0.56
1:A:520:GLN:HE21	1:A:520:GLN:N	1.99	0.56
1:A:527:ALA:O	1:A:531:THR:HG23	2.05	0.56
1:B:478:VAL:HG13	1:B:483:THR:OG1	2.05	0.56
1:D:86:MSE:HG3	1:D:131:LYS:NZ	2.20	0.56
1:D:432:GLU:OE2	5:D:4048:HOH:O	2.17	0.56
1:D:85:ILE:HG23	1:D:86:MSE:HE2	1.88	0.56
1:A:306:LYS:HG2	1:A:386:PRO:HA	1.87	0.56
1:A:398:LEU:CD2	1:A:398:LEU:N	2.68	0.56
1:A:484:ARG:HG2	1:D:543:TYR:CE1	2.40	0.56
1:C:79:LEU:HB2	1:C:118:LEU:HD21	1.88	0.56
1:C:61:GLN:OE1	1:C:98:ARG:HD3	2.06	0.56
1:D:72:LEU:HA	1:D:75:MSE:HG3	1.87	0.56
1:B:286:VAL:HG21	1:B:467:ASN:HA	1.87	0.56
1:C:248:ARG:NH1	1:C:273:TYR:CD2	2.74	0.56
1:C:535:TYR:OH	1:C:542:ARG:HB3	2.06	0.56
1:D:201:VAL:HG11	1:D:238:PHE:CE1	2.41	0.56
1:D:441:CYS:O	1:D:442:LEU:HD23	2.06	0.56
1:A:212:LEU:HD22	1:A:218:TYR:CD2	2.41	0.56
1:B:297:VAL:CG2	1:B:298:ILE:N	2.68	0.56
1:D:309:PHE:HB2	1:D:343:MSE:HG2	1.88	0.56
1:A:91:ARG:CD	5:A:4055:HOH:O	2.53	0.55
1:B:347:TYR:HB2	1:B:354:ARG:NH1	2.21	0.55
1:C:371:GLU:HG2	1:C:372:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:N	1:A:153:ASN:HD22	2.03	0.55
1:A:177:MSE:O	1:A:177:MSE:HG3	2.06	0.55
1:A:38:MSE:HE3	1:A:59:GLU:CG	2.36	0.55
1:C:85:ILE:HG13	1:C:86:MSE:H	1.71	0.55
1:A:225:ARG:O	1:A:227:ARG:HD2	2.06	0.55
1:B:29:MSE:HE2	1:B:50:LEU:CD2	2.33	0.55
1:C:42:LEU:O	1:C:46:GLN:HG3	2.05	0.55
1:A:66:LEU:HD22	1:A:70:ARG:CD	2.37	0.55
1:B:357:LYS:HD3	1:B:357:LYS:N	2.22	0.55
1:D:36:LYS:HB3	1:D:39:ALA:HB3	1.88	0.55
1:A:502:LEU:HD13	1:A:507:LEU:HD13	1.87	0.55
1:B:556:ARG:HH11	1:B:556:ARG:CG	2.19	0.55
1:C:302:ILE:HG23	1:C:303:SER:N	2.22	0.55
1:D:261:ASN:HD21	1:D:264:ARG:HH21	1.53	0.55
1:A:64:GLN:NE2	1:A:562:TYR:OH	2.37	0.55
1:B:476:LEU:HD23	1:B:527:ALA:CB	2.37	0.55
1:C:205:VAL:HG11	1:C:231:TYR:HD1	1.72	0.55
1:C:242:ILE:CG2	1:C:243:THR:N	2.69	0.55
1:B:105:GLU:HG2	1:B:516:LEU:HB3	1.89	0.55
1:B:154:HIS:O	1:B:197:ARG:HD2	2.07	0.55
1:B:350:LEU:HD22	1:B:354:ARG:NH2	2.22	0.55
1:B:75:MSE:HG2	1:B:80:GLU:OE1	2.07	0.55
1:C:45:ARG:HB3	1:C:51:GLN:HG2	1.89	0.55
1:A:104:ILE:HG13	1:A:108:MSE:HE2	1.89	0.55
1:A:305:HIS:O	1:A:340:LYS:HD3	2.07	0.55
1:A:331:GLY:O	1:A:332:LEU:C	2.45	0.55
1:A:431:GLU:OE2	1:A:431:GLU:HA	2.07	0.55
1:B:446:GLY:O	1:B:466:ASN:ND2	2.38	0.55
1:C:108:MSE:HB3	1:C:109:PRO:HD3	1.89	0.55
1:A:146:ILE:O	1:A:149:ASN:HB2	2.08	0.54
1:A:315:ALA:O	1:A:319:ILE:HG13	2.07	0.54
1:B:179:ILE:HB	1:B:180:PRO:HD3	1.89	0.54
1:B:432:GLU:O	1:B:436:LEU:HB2	2.07	0.54
1:C:264:ARG:HG2	1:C:264:ARG:HH11	1.72	0.54
1:C:389:ILE:HB	1:C:407:MSE:HE2	1.88	0.54
1:D:144:ARG:HA	1:D:147:VAL:HG22	1.89	0.54
1:D:287:ALA:CB	1:D:319:ILE:HD13	2.37	0.54
1:A:140:ARG:NH2	1:A:233:ASP:HB3	2.22	0.54
1:C:325:MSE:HE1	1:C:489:SER:HA	1.88	0.54
1:D:68:PHE:CE2	1:D:72:LEU:HD22	2.42	0.54
1:A:153:ASN:ND2	1:A:153:ASN:N	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:CE2	1:A:219:MSE:HE2	2.42	0.54
1:A:298:ILE:CG2	1:A:300:LYS:HB2	2.37	0.54
1:B:300:LYS:NZ	1:B:300:LYS:CB	2.62	0.54
1:C:112:TYR:CD1	1:C:186:LEU:HD11	2.43	0.54
1:D:194:ARG:HE	1:D:197:ARG:CZ	2.20	0.54
1:D:300:LYS:CB	1:D:300:LYS:NZ	2.65	0.54
1:A:261:ASN:ND2	1:A:264:ARG:HE	2.06	0.54
1:D:379:ASP:O	1:D:383:ILE:HD13	2.07	0.54
1:D:401:PRO:O	1:D:405:ARG:HG3	2.07	0.54
1:A:137:ILE:HA	1:A:234:LEU:HD22	1.89	0.54
1:A:177:MSE:CE	1:A:200:PRO:HB2	2.37	0.54
1:C:300:LYS:HG3	1:C:301:PRO:HD2	1.90	0.54
1:C:46:GLN:HG2	1:C:51:GLN:HG3	1.90	0.54
1:D:475:ALA:O	1:D:479:ILE:HD12	2.08	0.54
1:A:24:LYS:HG3	1:C:22:LYS:HE2	1.89	0.54
1:A:22:LYS:NZ	1:C:27:PRO:HG2	2.23	0.54
1:C:287:ALA:O	1:C:291:LEU:HD13	2.06	0.54
1:D:242:ILE:HG22	1:D:243:THR:N	2.23	0.54
1:D:307:ILE:HG13	1:D:388:THR:HB	1.90	0.54
1:B:29:MSE:HE1	1:B:53:LEU:CB	2.34	0.54
1:B:29:MSE:HE3	1:B:53:LEU:HD12	1.90	0.54
1:C:552:TYR:CD1	1:C:556:ARG:NH1	2.75	0.54
1:D:460:PHE:CD2	1:D:460:PHE:N	2.76	0.54
1:D:486:ILE:HD12	1:D:486:ILE:N	2.22	0.54
1:A:282:GLY:O	1:A:286:VAL:HG23	2.07	0.54
1:B:331:GLY:O	1:B:332:LEU:O	2.26	0.54
1:A:219:MSE:HG2	1:B:38:MSE:HE1	1.88	0.54
1:B:91:ARG:NH1	1:B:91:ARG:HG2	2.23	0.54
1:C:358:ILE:HG23	1:C:362:GLN:HB2	1.88	0.54
1:C:354:ARG:HG2	1:C:358:ILE:HD11	1.90	0.54
1:D:298:ILE:HG22	1:D:300:LYS:N	2.10	0.54
1:A:68:PHE:HZ	1:A:85:ILE:HG22	1.71	0.53
1:B:374:PRO:HB3	1:B:380:ALA:N	2.22	0.53
1:B:431:GLU:OE2	1:B:452:VAL:HG13	2.07	0.53
1:C:286:VAL:HG11	1:C:466:ASN:O	2.08	0.53
1:C:335:GLN:NE2	1:C:339:LYS:NZ	2.56	0.53
1:B:310:LEU:HB3	1:B:391:GLY:HA2	1.90	0.53
1:D:21:ILE:HD12	1:D:21:ILE:N	2.24	0.53
1:A:25:GLY:HA3	1:C:22:LYS:HE3	1.90	0.53
1:A:397:ARG:HD3	1:A:397:ARG:N	2.24	0.53
1:B:22:LYS:HD2	1:D:24:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:PRO:HB3	1:B:436:LEU:HD21	1.90	0.53
1:B:58:ILE:HG22	1:B:58:ILE:O	2.07	0.53
1:B:77:SER:OG	1:B:80:GLU:HB3	2.08	0.53
1:C:227:ARG:HG2	1:C:227:ARG:NH1	2.23	0.53
1:C:527:ALA:O	1:C:531:THR:CG2	2.56	0.53
1:D:414:PRO:HD2	1:D:441:CYS:HA	1.89	0.53
1:D:70:ARG:CG	1:D:70:ARG:NH1	2.71	0.53
1:A:210:ILE:CD1	1:A:210:ILE:H	2.22	0.53
1:A:434:TYR:CZ	1:A:443:PHE:HB3	2.44	0.53
1:A:505:GLU:O	1:A:508:ALA:HB3	2.08	0.53
1:B:546:PRO:HG2	1:B:549:LYS:HD2	1.90	0.53
1:B:133:LEU:HB2	1:B:199:LEU:HD11	1.90	0.53
1:B:24:LYS:HZ3	1:D:22:LYS:HD3	1.74	0.53
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.72	0.53
1:D:245:ARG:HD3	1:D:246:TYR:CZ	2.44	0.53
1:D:294:ALA:O	1:D:297:VAL:HG22	2.09	0.53
1:D:556:ARG:HG2	1:D:556:ARG:NH1	2.24	0.53
1:A:300:LYS:HZ2	1:A:300:LYS:HB3	1.73	0.53
1:B:137:ILE:HA	1:B:234:LEU:HD22	1.90	0.53
1:B:261:ASN:HA	1:B:264:ARG:HG2	1.91	0.53
1:B:363:GLU:HB3	1:B:364:PRO:HD3	1.91	0.53
1:B:453:LYS:CG	1:B:459:VAL:HG12	2.36	0.53
1:C:331:GLY:O	1:C:332:LEU:O	2.27	0.53
1:D:412:GLU:HG3	1:D:413:ARG:CD	2.38	0.53
1:D:427:GLU:N	1:D:427:GLU:OE1	2.41	0.53
1:C:194:ARG:CB	1:C:197:ARG:HG2	2.32	0.53
1:D:274:CYS:SG	1:D:486:ILE:HD11	2.49	0.53
1:D:37:GLY:C	1:D:39:ALA:H	2.12	0.53
1:A:411:ASN:HB2	1:A:414:PRO:HG3	1.90	0.53
1:B:177:MSE:HG2	1:B:202:CYS:HB2	1.91	0.53
1:B:30:LEU:O	1:B:32:PRO:HD3	2.09	0.53
1:B:402:ASP:OD2	1:B:402:ASP:N	2.42	0.53
1:B:45:ARG:HB3	1:B:51:GLN:HG2	1.91	0.53
1:C:116:VAL:HG13	1:C:117:GLY:N	2.23	0.53
1:C:505:GLU:H	1:C:505:GLU:CD	2.11	0.53
1:A:300:LYS:NZ	1:A:305:HIS:HD2	2.07	0.52
1:B:184:LEU:O	1:B:187:TYR:HB2	2.09	0.52
1:B:239:MSE:CE	1:B:252:ILE:HD12	2.39	0.52
1:C:527:ALA:O	1:C:531:THR:HG23	2.09	0.52
1:B:400:THR:OG1	1:B:403:VAL:HG23	2.09	0.52
1:D:70:ARG:HH11	1:D:70:ARG:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ARG:NH1	1:B:356:ALA:HB3	2.24	0.52
1:B:484:ARG:HG2	1:C:543:TYR:CZ	2.44	0.52
1:A:359:ASP:OD2	1:A:361:TYR:N	2.41	0.52
1:A:382:ASN:O	1:A:385:LYS:HD2	2.09	0.52
1:B:197:ARG:CG	1:B:197:ARG:HH11	2.22	0.52
1:B:466:ASN:HB3	1:B:468:VAL:HG12	1.92	0.52
1:C:89:GLN:NE2	1:C:185:CYS:SG	2.82	0.52
1:B:239:MSE:HE1	1:B:252:ILE:HD12	1.92	0.52
1:B:261:ASN:HD21	1:B:264:ARG:CZ	2.21	0.52
1:B:358:ILE:HG23	1:B:362:GLN:HB2	1.92	0.52
1:B:88:ILE:HD13	1:B:99:ILE:HD13	1.91	0.52
1:B:293:ALA:O	1:B:296:LYS:HB2	2.10	0.52
1:D:194:ARG:HE	1:D:197:ARG:HE	1.57	0.52
1:D:295:GLN:OE1	1:D:295:GLN:HA	2.10	0.52
1:C:454:LEU:CD1	1:C:460:PHE:HE2	2.22	0.52
1:B:215:ASP:OD2	1:B:218:TYR:N	2.42	0.52
1:B:343:MSE:HE3	1:B:350:LEU:CD1	2.39	0.52
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.91	0.52
1:C:248:ARG:HH22	1:C:272:LYS:NZ	2.08	0.52
1:D:165:ARG:NH2	4:D:3603:TTN:O1	2.43	0.52
1:D:350:LEU:CD2	1:D:350:LEU:N	2.72	0.52
1:D:194:ARG:NH1	1:D:194:ARG:HG2	2.25	0.52
1:A:96:PHE:O	1:A:100:LEU:HD22	2.10	0.51
1:C:221:LEU:HD23	1:C:223:GLN:CD	2.30	0.51
1:C:298:ILE:HD11	1:C:442:LEU:HD12	1.91	0.51
1:A:261:ASN:HA	1:A:264:ARG:HG2	1.92	0.51
1:B:260:HIS:CD2	1:B:264:ARG:HH11	2.28	0.51
1:B:528:ILE:O	1:B:531:THR:HG23	2.10	0.51
1:D:184:LEU:HD12	1:D:200:PRO:HB3	1.91	0.51
1:D:300:LYS:HE3	1:D:305:HIS:CE1	2.45	0.51
1:C:429:THR:HG23	1:C:432:GLU:OE2	2.10	0.51
1:D:191:ALA:HB3	1:D:193:ILE:HD12	1.93	0.51
1:B:116:VAL:CG1	1:B:117:GLY:N	2.73	0.51
1:B:31:ASN:HB3	1:B:34:THR:OG1	2.10	0.51
1:B:452:VAL:O	1:B:459:VAL:HA	2.11	0.51
1:C:150:TRP:CE2	1:C:199:LEU:HD13	2.46	0.51
1:C:357:LYS:CD	1:C:357:LYS:N	2.73	0.51
1:B:228:THR:OG1	1:B:230:GLN:HB2	2.10	0.51
1:C:132:GLY:HA3	1:C:177:MSE:HE3	1.92	0.51
1:C:327:MSE:HE3	1:C:337:ALA:CB	2.29	0.51
1:D:306:LYS:HE2	1:D:342:TRP:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:CE2	1:A:218:TYR:HA	2.45	0.51
1:A:307:ILE:HD12	1:A:307:ILE:N	2.25	0.51
1:B:88:ILE:HG22	1:B:96:PHE:HB2	1.92	0.51
1:A:61:GLN:HG3	1:A:562:TYR:CE1	2.46	0.51
1:D:309:PHE:CE1	1:D:316:ALA:HA	2.46	0.51
1:C:137:ILE:HA	1:C:234:LEU:HD22	1.93	0.51
1:A:300:LYS:NZ	1:A:305:HIS:CD2	2.79	0.50
1:B:194:ARG:NH2	1:B:196:ASP:OD2	2.44	0.50
1:B:150:TRP:CE2	1:B:199:LEU:HD13	2.45	0.50
1:B:374:PRO:HG3	1:B:383:ILE:CD1	2.40	0.50
1:C:164:GLU:HG3	1:C:225:ARG:NE	2.26	0.50
1:C:454:LEU:HD11	1:C:460:PHE:CE2	2.45	0.50
1:C:520:GLN:H	1:C:520:GLN:NE2	2.05	0.50
1:D:397:ARG:HA	1:D:427:GLU:O	2.11	0.50
1:A:184:LEU:HD13	1:A:198:CYS:HB3	1.94	0.50
1:A:267:ARG:HG3	1:A:267:ARG:O	2.11	0.50
1:B:261:ASN:CG	1:B:264:ARG:NH1	2.64	0.50
1:C:207:THR:CG2	1:C:213:LEU:HD13	2.41	0.50
1:C:57:LYS:HG3	1:C:58:ILE:N	2.25	0.50
1:D:208:ASP:CG	1:D:227:ARG:HH22	2.14	0.50
1:C:401:PRO:HA	1:C:404:ILE:HG13	1.92	0.50
1:A:346:LYS:HD3	1:A:347:TYR:CE1	2.47	0.50
1:A:506:GLU:O	1:A:511:ARG:HG3	2.11	0.50
1:D:291:LEU:HD13	1:D:417:PHE:CE2	2.45	0.50
1:D:86:MSE:N	1:D:86:MSE:HE2	2.26	0.50
1:D:68:PHE:CD2	1:D:99:ILE:HG21	2.47	0.50
1:B:505:GLU:O	1:B:509:GLN:HG2	2.12	0.50
1:B:534:LEU:CD2	1:B:539:MSE:HE2	2.42	0.50
1:D:144:ARG:HG2	1:D:144:ARG:HH11	1.76	0.50
1:D:392:VAL:O	1:D:392:VAL:CG1	2.58	0.50
1:D:61:GLN:HG3	1:D:562:TYR:CE1	2.47	0.50
1:A:319:ILE:O	1:A:323:ILE:HG13	2.12	0.50
1:D:482:ASN:HD21	3:D:3602:NAD:H4B	1.76	0.50
1:A:43:GLN:O	1:A:47:MSE:HB2	2.11	0.50
1:B:327:MSE:HG2	1:B:332:LEU:HD22	1.94	0.50
1:A:59:GLU:CD	1:A:67:ARG:HH12	2.14	0.50
1:B:315:ALA:HB3	1:B:392:VAL:HG21	1.94	0.50
1:D:25:GLY:C	1:D:27:PRO:HD2	2.32	0.50
1:A:57:LYS:NZ	1:A:59:GLU:HG2	2.26	0.50
1:B:239:MSE:HE2	1:B:273:TYR:CD1	2.47	0.50
1:B:68:PHE:CD2	1:B:99:ILE:HG12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:MSE:CE	1:A:407:MSE:HA	2.38	0.49
1:A:472:PRO:HD2	5:A:4029:HOH:O	2.10	0.49
1:B:286:VAL:CG2	1:B:467:ASN:HA	2.42	0.49
1:C:350:LEU:HD22	1:C:354:ARG:NH2	2.27	0.49
1:D:210:ILE:O	1:D:214:LYS:HG3	2.12	0.49
1:D:346:LYS:HE2	1:D:347:TYR:OH	2.12	0.49
1:A:412:GLU:HG3	1:A:413:ARG:HG2	1.93	0.49
1:B:297:VAL:HG21	1:B:442:LEU:HD21	1.94	0.49
1:C:217:PHE:HZ	1:D:66:LEU:HD13	1.76	0.49
1:C:286:VAL:HG13	1:C:470:ILE:HG12	1.93	0.49
1:D:177:MSE:HE3	1:D:180:PRO:HD2	1.94	0.49
1:D:527:ALA:O	1:D:531:THR:CG2	2.60	0.49
1:A:273:TYR:HB2	1:A:275:THR:CG2	2.42	0.49
1:A:376:THR:O	1:A:379:ASP:HB2	2.11	0.49
1:A:38:MSE:HE3	1:A:59:GLU:HG3	1.94	0.49
1:B:93:GLU:OE1	1:B:195:PRO:HB2	2.12	0.49
1:C:276:PHE:HB2	1:C:281:GLN:OE1	2.12	0.49
1:C:146:ILE:O	1:C:149:ASN:HB2	2.13	0.49
1:B:248:ARG:HB3	1:C:543:TYR:CZ	2.48	0.49
1:C:36:LYS:HE2	1:C:562:TYR:HB3	1.93	0.49
1:D:212:LEU:HD22	1:D:218:TYR:CD2	2.48	0.49
1:A:140:ARG:NH2	1:A:230:GLN:HA	2.27	0.49
1:C:408:ALA:HB1	1:C:440:ARG:NH2	2.28	0.49
1:C:298:ILE:HD11	1:C:442:LEU:CD1	2.43	0.49
1:C:79:LEU:HD22	1:C:118:LEU:CG	2.41	0.49
1:A:184:LEU:O	1:A:187:TYR:HB2	2.12	0.49
1:B:140:ARG:CZ	1:B:230:GLN:HG3	2.43	0.49
1:A:24:LYS:O	1:C:22:LYS:HE2	2.12	0.49
1:D:502:LEU:HD13	1:D:507:LEU:HD12	1.95	0.49
1:D:556:ARG:NE	3:D:3602:NAD:O2A	2.46	0.49
1:C:418:ALA:O	5:C:4012:HOH:O	2.18	0.49
1:D:208:ASP:OD2	1:D:227:ARG:NH2	2.34	0.49
1:D:239:MSE:O	1:D:243:THR:HG23	2.13	0.49
1:D:405:ARG:HH11	1:D:405:ARG:HG3	1.78	0.49
1:A:310:LEU:HD22	1:A:399:PHE:CE2	2.48	0.49
1:A:89:GLN:HB2	1:A:96:PHE:CD2	2.48	0.49
1:A:397:ARG:NH1	1:A:397:ARG:CG	2.75	0.49
1:A:396:GLY:C	1:A:398:LEU:HD23	2.34	0.49
1:A:467:ASN:O	1:A:471:PHE:HD2	1.95	0.49
1:B:207:THR:O	1:B:224:LYS:HA	2.13	0.49
1:B:521:GLU:HG2	1:B:525:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:MSE:CE	1:A:337:ALA:HB1	2.30	0.48
1:B:451:PRO:HG3	1:B:461:THR:HG23	1.94	0.48
1:B:518:ASN:HA	1:B:520:GLN:OE1	2.13	0.48
1:C:197:ARG:HH11	1:C:197:ARG:CG	2.13	0.48
1:C:165:ARG:NH2	4:C:2603:TTN:O1	2.46	0.48
1:A:245:ARG:HD3	1:A:246:TYR:CE1	2.48	0.48
1:A:37:GLY:C	1:A:39:ALA:H	2.17	0.48
1:A:385:LYS:HA	1:A:410:ILE:HD13	1.95	0.48
1:A:72:LEU:HA	1:A:75:MSE:HG3	1.94	0.48
1:B:266:LEU:O	1:B:270:ARG:HB3	2.12	0.48
1:C:116:VAL:CG1	1:C:117:GLY:N	2.75	0.48
1:D:144:ARG:HD2	1:D:147:VAL:HG21	1.91	0.48
1:A:194:ARG:HG3	3:A:602:NAD:C6A	2.43	0.48
1:B:29:MSE:CE	1:B:50:LEU:HB3	2.40	0.48
1:D:333:SER:H	1:D:336:GLU:CG	2.26	0.48
1:D:314:GLU:HB2	3:D:3601:NAD:O1N	2.12	0.48
1:A:29:MSE:HE1	1:A:54:LEU:CD2	2.43	0.48
1:B:235:ILE:O	1:B:239:MSE:HG2	2.14	0.48
1:B:453:LYS:HG2	1:B:459:VAL:CG1	2.34	0.48
1:D:45:ARG:CZ	1:D:58:ILE:HD13	2.43	0.48
1:D:156:LYS:HD3	1:D:479:ILE:HG23	1.94	0.48
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.79	0.48
1:A:248:ARG:HG2	1:A:248:ARG:HH11	1.79	0.48
1:A:377:PHE:CZ	1:A:389:ILE:HD12	2.49	0.48
1:B:339:LYS:HA	1:B:367:HIS:CE1	2.49	0.48
1:C:309:PHE:HE2	1:C:341:ILE:HG23	1.79	0.48
1:D:371:GLU:HG3	1:D:371:GLU:H	1.39	0.48
1:A:300:LYS:NZ	1:A:300:LYS:HB3	2.29	0.48
1:D:381:VAL:CG1	1:D:407:MSE:CE	2.91	0.48
1:B:389:ILE:HG22	1:B:416:ILE:HA	1.95	0.48
1:D:140:ARG:CZ	1:D:230:GLN:HG2	2.44	0.48
1:D:506:GLU:O	1:D:509:GLN:HG2	2.12	0.48
1:A:294:ALA:O	1:A:297:VAL:HG22	2.13	0.48
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.96	0.48
1:A:502:LEU:CD1	1:A:507:LEU:HD13	2.44	0.48
1:B:412:GLU:O	1:B:440:ARG:NH1	2.46	0.48
1:B:501:GLN:NE2	1:B:525:ASN:HB3	2.28	0.48
1:C:468:VAL:HA	1:C:471:PHE:CE2	2.49	0.48
1:D:306:LYS:HZ2	1:D:306:LYS:HB2	1.79	0.48
1:A:542:ARG:HH12	1:A:544:PRO:HD2	1.78	0.48
1:A:559:ARG:HB3	1:A:561:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:TYR:HE2	1:B:261:ASN:ND2	2.12	0.48
1:B:255:GLU:OE2	1:B:278:ASP:CB	2.62	0.48
1:B:520:GLN:O	1:B:524:ILE:HD12	2.13	0.48
1:C:235:ILE:HG13	1:C:265:PHE:CZ	2.49	0.48
1:A:26:LYS:N	1:A:27:PRO:CD	2.77	0.48
1:A:397:ARG:HA	1:A:427:GLU:O	2.14	0.48
1:C:166:ILE:HD12	1:C:179:ILE:HG13	1.95	0.48
1:C:301:PRO:HG2	1:C:304:GLU:CD	2.34	0.48
1:C:396:GLY:O	1:C:427:GLU:HA	2.14	0.48
1:D:520:GLN:CD	1:D:520:GLN:H	2.17	0.48
1:A:137:ILE:HG13	1:A:137:ILE:O	2.13	0.47
1:A:194:ARG:HG3	3:A:602:NAD:N1A	2.29	0.47
1:B:537:ASN:ND2	1:B:537:ASN:N	2.59	0.47
1:B:556:ARG:NH1	1:B:556:ARG:CG	2.74	0.47
1:B:169:LEU:HD13	1:B:422:PRO:HD3	1.95	0.47
3:C:2602:NAD:O3B	5:C:4060:HOH:O	2.10	0.47
1:D:177:MSE:CE	1:D:200:PRO:HB2	2.44	0.47
1:D:24:LYS:HA	1:D:28:LEU:CD1	2.44	0.47
1:D:415:VAL:CG2	1:D:442:LEU:HD12	2.44	0.47
1:C:335:GLN:NE2	1:C:339:LYS:HZ1	2.12	0.47
1:A:150:TRP:CD1	1:A:152:GLU:HB2	2.49	0.47
1:A:159:VAL:HG13	1:A:253:GLN:NE2	2.29	0.47
1:A:468:VAL:HA	1:A:471:PHE:HE2	1.72	0.47
1:B:163:GLY:HA2	1:B:166:ILE:HD11	1.96	0.47
1:B:92:ASN:HB2	5:B:4003:HOH:O	2.14	0.47
1:C:294:ALA:O	1:C:297:VAL:HG13	2.13	0.47
1:D:174:VAL:C	1:D:176:GLY:H	2.18	0.47
1:D:239:MSE:HE3	1:D:252:ILE:HD13	1.96	0.47
1:D:377:PHE:CE2	1:D:399:PHE:CE2	3.02	0.47
1:A:150:TRP:HE1	1:A:152:GLU:HB2	1.78	0.47
1:A:417:PHE:CD1	1:A:444:ALA:HB3	2.50	0.47
1:B:165:ARG:NH2	4:B:1603:TTN:O1	2.48	0.47
1:B:443:PHE:CZ	1:B:445:SER:HB3	2.50	0.47
1:A:25:GLY:HA3	1:C:22:LYS:CE	2.45	0.47
1:A:137:ILE:HA	1:A:234:LEU:CD2	2.45	0.47
1:A:363:GLU:HB3	1:A:364:PRO:CD	2.44	0.47
1:A:484:ARG:HD2	1:A:541:PHE:CD1	2.48	0.47
1:C:264:ARG:NH1	1:C:264:ARG:HG2	2.29	0.47
1:D:152:GLU:HG2	1:D:196:ASP:O	2.14	0.47
1:D:405:ARG:HG3	1:D:405:ARG:NH1	2.30	0.47
1:A:208:ASP:O	1:A:210:ILE:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ARG:HG3	1:A:561:GLU:OE1	2.15	0.47
1:B:140:ARG:NH2	1:B:230:GLN:HG3	2.30	0.47
1:B:194:ARG:HB2	1:B:197:ARG:CG	2.44	0.47
1:D:23:GLU:O	1:D:28:LEU:HD11	2.15	0.47
1:D:389:ILE:HG23	1:D:399:PHE:CE1	2.50	0.47
1:D:527:ALA:O	1:D:531:THR:HG23	2.15	0.47
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.95	0.47
1:A:85:ILE:CG1	1:A:86:MSE:N	2.77	0.47
1:A:225:ARG:NH1	1:A:225:ARG:CG	2.73	0.47
1:C:210:ILE:O	1:C:214:LYS:HG3	2.15	0.47
1:D:542:ARG:NH1	1:D:544:PRO:HD2	2.30	0.47
1:B:208:ASP:OD1	1:B:224:LYS:HD3	2.15	0.47
1:B:434:TYR:HD1	1:B:452:VAL:HG21	1.78	0.47
1:A:221:LEU:HD13	1:B:56:PRO:HB2	1.97	0.47
1:B:75:MSE:HG2	1:B:80:GLU:CG	2.45	0.47
1:A:174:VAL:HG21	1:A:220:GLY:CA	2.45	0.46
1:A:381:VAL:CG1	1:A:407:MSE:HE3	2.41	0.46
1:A:484:ARG:HD2	1:A:541:PHE:CE1	2.51	0.46
1:B:166:ILE:O	1:B:169:LEU:HB2	2.15	0.46
1:B:57:LYS:HG3	1:B:58:ILE:N	2.30	0.46
1:C:137:ILE:HG13	1:C:137:ILE:O	2.15	0.46
1:C:61:GLN:HG3	1:C:562:TYR:CE1	2.50	0.46
1:C:70:ARG:NH1	1:C:70:ARG:CG	2.76	0.46
1:D:165:ARG:NH2	1:D:256:ASP:OD1	2.48	0.46
1:C:422:PRO:HD2	1:C:425:GLN:HE21	1.81	0.46
1:D:298:ILE:HG21	1:D:300:LYS:HB2	1.94	0.46
1:D:406:ALA:O	1:D:410:ILE:HG13	2.16	0.46
1:D:520:GLN:HE21	1:D:521:GLU:N	2.12	0.46
1:A:487:SER:CB	1:A:539:MSE:HE1	2.41	0.46
1:C:302:ILE:CG2	1:C:303:SER:N	2.78	0.46
1:C:363:GLU:N	1:C:364:PRO:CD	2.77	0.46
1:A:24:LYS:C	1:C:22:LYS:HE2	2.35	0.46
1:A:286:VAL:HG21	1:A:467:ASN:CA	2.39	0.46
1:D:407:MSE:HG3	1:D:414:PRO:CB	2.45	0.46
1:D:385:LYS:HG3	1:D:410:ILE:HD13	1.98	0.46
1:D:79:LEU:O	1:D:83:ILE:HG13	2.14	0.46
1:A:29:MSE:HE2	1:A:29:MSE:HB3	1.89	0.46
1:B:549:LYS:O	1:B:553:VAL:HG23	2.16	0.46
1:D:112:TYR:OH	1:D:183:LYS:HE2	2.15	0.46
1:D:289:ALA:CB	1:D:498:LEU:HD23	2.45	0.46
1:A:484:ARG:HG2	1:D:543:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:NH2	1:D:91:ARG:HB2	2.31	0.46
1:A:306:LYS:C	1:A:307:ILE:HD12	2.36	0.46
1:A:424:ALA:HB3	1:A:425:GLN:NE2	2.30	0.46
1:A:46:GLN:CG	1:A:51:GLN:HG3	2.46	0.46
1:B:29:MSE:HE2	1:B:50:LEU:CB	2.40	0.46
1:B:387:SER:HA	1:B:411:ASN:OD1	2.16	0.46
1:C:61:GLN:HA	1:C:64:GLN:NE2	2.29	0.46
1:D:100:LEU:HD23	1:D:189:ALA:HB2	1.98	0.46
1:D:401:PRO:HA	1:D:436:LEU:HD13	1.98	0.46
1:A:152:GLU:HG3	1:A:196:ASP:O	2.16	0.46
1:A:363:GLU:N	1:A:364:PRO:HD2	2.31	0.46
1:D:331:GLY:O	1:D:332:LEU:C	2.53	0.46
1:D:476:LEU:HD23	1:D:527:ALA:CB	2.46	0.46
1:A:144:ARG:HE	1:A:148:ASP:CG	2.19	0.46
1:B:109:PRO:HA	1:B:113:THR:O	2.15	0.46
1:B:335:GLN:O	1:B:339:LYS:CG	2.59	0.46
1:C:355:LYS:HZ3	1:C:357:LYS:NZ	2.14	0.46
1:D:78:PRO:HB3	1:D:110:ILE:HD12	1.97	0.46
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.76	0.46
1:D:398:LEU:N	1:D:398:LEU:HD12	2.29	0.46
1:D:484:ARG:HG3	1:D:541:PHE:CE1	2.50	0.46
1:D:533:TYR:CZ	1:D:537:ASN:ND2	2.84	0.46
1:A:96:PHE:CZ	1:A:100:LEU:HD21	2.50	0.46
1:B:298:ILE:HG22	1:B:300:LYS:H	1.80	0.46
1:C:394:GLY:HA2	1:C:420:SER:HB3	1.98	0.46
1:D:204:ASP:OD2	1:D:221:LEU:N	2.44	0.46
1:D:144:ARG:NH1	1:D:244:ASP:HB3	2.31	0.46
1:A:136:SER:HB2	1:A:221:LEU:CD2	2.46	0.45
1:A:210:ILE:N	1:A:210:ILE:HD13	2.30	0.45
1:A:343:MSE:HB2	1:A:350:LEU:HG	1.98	0.45
1:C:155:VAL:HB	1:C:246:TYR:CD1	2.51	0.45
1:D:253:GLN:HG2	1:D:253:GLN:O	2.16	0.45
1:A:21:ILE:N	1:A:21:ILE:CD1	2.68	0.45
1:A:266:LEU:O	1:A:270:ARG:HB3	2.16	0.45
1:A:397:ARG:CD	1:A:397:ARG:N	2.80	0.45
1:A:403:VAL:O	1:A:406:ALA:HB3	2.16	0.45
1:B:22:LYS:HA	1:D:24:LYS:CE	2.46	0.45
1:B:85:ILE:CD1	1:B:110:ILE:HG21	2.46	0.45
1:D:21:ILE:HG21	1:D:28:LEU:HD21	1.98	0.45
1:A:105:GLU:OE2	1:A:517:ALA:HB2	2.15	0.45
1:A:492:LEU:HD22	1:A:496:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD21	1:B:398:LEU:CB	2.46	0.45
1:C:69:HIS:HE1	1:C:102:ASP:OD2	1.98	0.45
1:D:359:ASP:OD2	1:D:359:ASP:C	2.55	0.45
1:B:24:LYS:NZ	1:D:22:LYS:CD	2.79	0.45
1:D:175:TYR:CD1	1:D:212:LEU:HD21	2.52	0.45
1:D:412:GLU:HG3	1:D:413:ARG:HD2	1.99	0.45
1:D:496:LYS:HA	1:D:499:THR:HG22	1.99	0.45
1:A:26:LYS:HA	1:A:29:MSE:HG3	1.98	0.45
1:A:327:MSE:HG2	1:A:332:LEU:HD23	1.98	0.45
1:C:229:GLN:HG3	1:C:233:ASP:OD2	2.16	0.45
1:C:297:VAL:HG22	1:C:298:ILE:HG12	1.97	0.45
1:C:289:ALA:HB2	1:C:498:LEU:HD23	1.98	0.45
1:D:36:LYS:O	1:D:39:ALA:HB3	2.16	0.45
1:A:23:GLU:CA	1:A:23:GLU:OE1	2.57	0.45
1:A:327:MSE:HE3	1:A:337:ALA:CB	2.32	0.45
1:A:509:GLN:HG2	1:A:511:ARG:HG3	1.99	0.45
1:B:177:MSE:C	1:B:180:PRO:HD2	2.36	0.45
1:C:194:ARG:HB2	1:C:197:ARG:CG	2.36	0.45
1:C:26:LYS:N	1:C:27:PRO:CD	2.80	0.45
1:D:545:GLU:OE2	1:D:549:LYS:NZ	2.37	0.45
1:A:156:LYS:HB3	1:A:156:LYS:HE3	1.73	0.45
1:A:529:LYS:HE3	1:A:529:LYS:HA	1.99	0.45
1:C:104:ILE:HG12	1:C:108:MSE:CE	2.46	0.45
1:C:184:LEU:O	1:C:187:TYR:HB2	2.17	0.45
1:C:392:VAL:O	3:C:2601:NAD:H51N	2.15	0.45
1:C:78:PRO:HB3	1:C:110:ILE:CD1	2.47	0.45
1:D:61:GLN:OE1	1:D:98:ARG:HD3	2.17	0.45
1:A:227:ARG:CG	1:A:227:ARG:NH1	2.56	0.45
1:A:359:ASP:OD2	1:A:361:TYR:HD1	2.00	0.45
1:B:343:MSE:HE1	1:B:365:PHE:HB2	1.99	0.45
1:B:343:MSE:HE2	1:B:343:MSE:HB2	1.81	0.45
1:C:25:GLY:C	1:C:27:PRO:HD2	2.37	0.45
1:D:517:ALA:O	1:D:520:GLN:OE1	2.35	0.45
1:A:226:ASP:OD1	1:A:226:ASP:C	2.55	0.45
1:C:373:ILE:O	1:C:373:ILE:CG2	2.65	0.45
1:C:285:ALA:HB3	1:C:470:ILE:HG13	1.99	0.45
1:A:46:GLN:HG3	1:A:51:GLN:HG3	1.99	0.45
1:B:535:TYR:CZ	1:B:546:PRO:HD2	2.52	0.45
1:A:194:ARG:HD3	1:A:197:ARG:NE	2.32	0.44
1:A:165:ARG:O	1:A:256:ASP:HB3	2.17	0.44
1:B:172:LEU:O	1:B:175:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:TYR:CE1	1:C:556:ARG:NH1	2.85	0.44
1:D:298:ILE:HD11	1:D:442:LEU:HD12	1.99	0.44
1:A:297:VAL:CG2	1:A:442:LEU:HD11	2.47	0.44
1:B:342:TRP:CH2	1:B:370:PRO:HD3	2.52	0.44
1:B:36:LYS:HB3	1:B:39:ALA:HB3	1.98	0.44
1:B:444:ALA:HB2	1:B:512:LEU:HD12	2.00	0.44
1:D:150:TRP:CE2	1:D:199:LEU:HD13	2.52	0.44
1:A:33:ARG:HD2	1:A:93:GLU:OE1	2.18	0.44
1:B:255:GLU:OE2	1:B:278:ASP:HB3	2.17	0.44
1:B:261:ASN:ND2	1:B:265:PHE:CE1	2.86	0.44
1:C:217:PHE:CZ	1:D:66:LEU:HD13	2.52	0.44
1:A:166:ILE:HG21	1:A:172:LEU:HD12	2.00	0.44
1:A:156:LYS:CE	1:A:479:ILE:HG23	2.47	0.44
1:B:229:GLN:HG3	1:B:229:GLN:O	2.16	0.44
1:B:395:ALA:CB	1:B:398:LEU:HD21	2.43	0.44
1:B:408:ALA:HB1	1:B:440:ARG:HH22	1.78	0.44
1:C:282:GLY:O	1:C:286:VAL:HG22	2.18	0.44
1:D:212:LEU:HD13	1:D:218:TYR:CE2	2.52	0.44
1:A:235:ILE:O	1:A:239:MSE:HG2	2.18	0.44
1:A:412:GLU:O	1:A:440:ARG:HD2	2.18	0.44
1:B:332:LEU:HD21	1:B:340:LYS:CE	2.46	0.44
1:A:429:THR:OG1	1:A:432:GLU:HG2	2.17	0.44
1:A:552:TYR:O	1:A:556:ARG:NH1	2.51	0.44
1:A:346:LYS:HD2	3:A:601:NAD:O2B	2.18	0.44
1:B:346:LYS:CB	1:B:346:LYS:NZ	2.74	0.44
1:B:359:ASP:OD1	1:B:362:GLN:HG3	2.17	0.44
1:C:205:VAL:HG11	1:C:231:TYR:CD1	2.53	0.44
1:A:24:LYS:HE2	1:C:22:LYS:HA	1.99	0.44
1:C:352:LYS:N	1:C:366:THR:HG22	2.32	0.44
1:C:505:GLU:O	1:C:508:ALA:HB3	2.18	0.44
1:C:92:ASN:HB2	5:C:4011:HOH:O	2.16	0.44
1:D:226:ASP:C	1:D:226:ASP:OD1	2.55	0.44
1:A:333:SER:H	1:A:336:GLU:CD	2.21	0.44
1:B:481:CYS:HB3	1:B:483:THR:CG2	2.47	0.44
1:C:231:TYR:HE2	1:C:265:PHE:HZ	1.65	0.44
1:D:174:VAL:C	1:D:176:GLY:N	2.71	0.44
1:D:43:GLN:O	1:D:47:MSE:HG3	2.16	0.44
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.65	0.44
1:A:317:LEU:HD21	1:A:343:MSE:HE1	2.00	0.44
1:A:429:THR:HA	1:A:449:PHE:CE1	2.53	0.44
1:A:453:LYS:HG2	1:A:459:VAL:HG22	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASN:HD21	1:B:264:ARG:NH2	2.14	0.44
1:B:343:MSE:CE	1:B:350:LEU:HD12	2.41	0.44
1:C:57:LYS:HD3	1:D:218:TYR:O	2.17	0.44
1:A:384:LEU:O	1:A:385:LYS:HB2	2.18	0.44
1:A:391:GLY:HA3	1:A:427:GLU:HG2	2.00	0.44
1:A:401:PRO:HB2	1:A:405:ARG:NH2	2.31	0.44
1:B:108:MSE:HB3	1:B:109:PRO:CD	2.48	0.44
1:B:174:VAL:HG12	1:B:174:VAL:O	2.18	0.44
1:B:317:LEU:HD21	1:B:362:GLN:HG2	2.00	0.44
1:C:174:VAL:CG1	1:C:174:VAL:O	2.65	0.44
1:C:164:GLU:HG3	1:C:225:ARG:CZ	2.47	0.44
1:C:420:SER:OG	1:C:427:GLU:OE2	2.36	0.44
1:C:75:MSE:HG2	1:C:80:GLU:CG	2.48	0.44
1:D:310:LEU:HD21	1:D:398:LEU:HB2	2.00	0.44
1:B:397:ARG:HA	1:B:427:GLU:O	2.18	0.43
1:C:382:ASN:O	1:C:385:LYS:NZ	2.48	0.43
1:C:559:ARG:HG2	1:C:561:GLU:HG2	2.00	0.43
1:D:215:ASP:OD1	1:D:216:PRO:HD2	2.18	0.43
1:D:85:ILE:HD11	1:D:100:LEU:CD1	2.46	0.43
1:B:97:TYR:CE2	1:B:188:THR:HB	2.53	0.43
1:B:306:LYS:HD3	1:B:384:LEU:O	2.18	0.43
1:C:335:GLN:HB3	1:C:335:GLN:HE21	1.57	0.43
1:C:73:LYS:HE2	1:C:73:LYS:HA	2.00	0.43
1:D:253:GLN:HB2	1:D:276:PHE:HE2	1.81	0.43
1:D:358:ILE:HG12	1:D:366:THR:OG1	2.18	0.43
1:B:298:ILE:HG22	1:B:300:LYS:HB2	2.00	0.43
1:B:370:PRO:O	1:B:371:GLU:C	2.57	0.43
1:B:392:VAL:HG13	1:B:392:VAL:O	2.18	0.43
1:B:423:THR:HG23	1:B:447:SER:CB	2.48	0.43
1:D:556:ARG:HG2	1:D:556:ARG:HH11	1.82	0.43
1:A:350:LEU:N	1:A:350:LEU:HD23	2.33	0.43
1:A:468:VAL:HA	1:A:471:PHE:CD2	2.51	0.43
1:C:164:GLU:HG3	1:C:225:ARG:CD	2.48	0.43
1:C:174:VAL:CG2	1:C:204:ASP:HB2	2.49	0.43
1:C:218:TYR:O	1:D:57:LYS:HE3	2.17	0.43
1:C:382:ASN:OD1	1:C:382:ASN:N	2.51	0.43
1:D:136:SER:HA	1:D:204:ASP:O	2.18	0.43
1:D:554:LYS:HG2	1:D:554:LYS:H	1.50	0.43
1:A:308:LEU:HB3	1:A:389:ILE:HD13	1.99	0.43
1:A:419:LEU:O	3:A:601:NAD:H2N	2.18	0.43
1:B:128:ARG:CD	5:B:4056:HOH:O	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:HD12	1:B:21:ILE:HA	1.77	0.43
1:B:525:ASN:HA	1:B:528:ILE:HD12	2.00	0.43
1:D:298:ILE:HD11	1:D:442:LEU:HD11	1.99	0.43
1:D:556:ARG:CG	1:D:556:ARG:HH11	2.32	0.43
1:D:60:THR:OG1	1:D:63:ILE:HG12	2.17	0.43
1:A:164:GLU:OE1	1:A:225:ARG:HD3	2.17	0.43
1:A:284:ALA:CB	1:A:322:LEU:HD12	2.48	0.43
1:C:248:ARG:NH2	1:C:272:LYS:NZ	2.66	0.43
1:D:110:ILE:O	1:D:115:THR:HB	2.18	0.43
1:B:24:LYS:HZ2	1:D:22:LYS:CD	2.32	0.43
1:B:174:VAL:HG21	1:B:220:GLY:HA3	2.00	0.43
1:B:429:THR:HG23	1:B:432:GLU:OE2	2.19	0.43
1:C:75:MSE:HG2	1:C:80:GLU:HG2	2.01	0.43
1:D:306:LYS:HG3	1:D:306:LYS:O	2.18	0.43
1:C:134:PHE:HB3	1:D:56:PRO:HD3	2.01	0.43
1:A:401:PRO:HA	1:A:436:LEU:HD23	2.01	0.43
1:A:420:SER:HA	3:A:601:NAD:H1D	2.01	0.43
1:B:165:ARG:NH2	1:B:256:ASP:OD1	2.52	0.43
1:B:359:ASP:C	1:B:359:ASP:OD1	2.57	0.43
1:D:146:ILE:O	1:D:149:ASN:HB2	2.19	0.43
1:B:213:LEU:CD1	1:B:224:LYS:HZ2	2.31	0.43
1:B:243:THR:HG21	1:B:273:TYR:CD2	2.54	0.43
1:B:343:MSE:CE	1:B:365:PHE:HB2	2.49	0.43
1:B:477:ALA:O	1:B:481:CYS:HB2	2.18	0.43
1:C:528:ILE:HA	1:C:531:THR:HG23	2.00	0.43
1:C:55:PRO:CG	1:D:219:MSE:HE3	2.49	0.43
1:D:23:GLU:CA	1:D:23:GLU:OE2	2.61	0.43
1:D:26:LYS:N	1:D:27:PRO:CD	2.82	0.43
1:C:133:LEU:HD23	1:D:53:LEU:HD23	2.01	0.43
1:D:61:GLN:HG3	1:D:562:TYR:CZ	2.54	0.43
1:A:153:ASN:H	1:A:153:ASN:HD22	1.66	0.43
1:A:302:ILE:HG23	1:A:332:LEU:HD22	2.01	0.43
1:A:362:GLN:O	1:A:363:GLU:C	2.57	0.43
1:B:40:PHE:HE2	1:B:565:LEU:CD1	2.31	0.43
1:B:77:SER:HA	1:B:78:PRO:HD3	1.86	0.43
1:C:329:GLU:HG3	1:C:330:ASN:ND2	2.34	0.43
1:C:38:MSE:HB3	1:C:59:GLU:HG3	2.01	0.43
1:D:373:ILE:O	1:D:373:ILE:HG22	2.18	0.43
1:D:502:LEU:HD13	1:D:507:LEU:HD11	2.01	0.43
1:A:160:VAL:HG22	1:A:161:THR:N	2.34	0.42
1:B:260:HIS:CD2	1:B:264:ARG:NH1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:CG2	1:B:359:ASP:N	2.81	0.42
1:D:177:MSE:HE1	1:D:200:PRO:HB2	2.00	0.42
1:D:305:HIS:HD2	1:D:307:ILE:HD11	1.84	0.42
1:A:300:LYS:HZ1	1:A:304:GLU:C	2.22	0.42
1:A:429:THR:HG22	1:A:449:PHE:CZ	2.54	0.42
1:B:302:ILE:CG2	1:B:303:SER:N	2.82	0.42
1:C:108:MSE:HE3	1:C:108:MSE:HB2	1.77	0.42
1:C:164:GLU:HG3	1:C:225:ARG:HD3	2.01	0.42
1:C:238:PHE:CE1	1:C:242:ILE:HD13	2.55	0.42
1:C:242:ILE:HG22	1:C:243:THR:N	2.33	0.42
1:C:161:THR:HA	1:C:257:PHE:CE1	2.54	0.42
1:C:295:GLN:OE1	1:C:295:GLN:HA	2.18	0.42
1:C:373:ILE:HA	1:C:374:PRO:HD2	1.90	0.42
1:C:402:ASP:OD1	1:C:402:ASP:N	2.52	0.42
1:C:38:MSE:HG2	1:C:57:LYS:O	2.18	0.42
1:C:99:ILE:HA	1:C:99:ILE:HD13	1.69	0.42
1:C:171:ASP:OD2	1:C:225:ARG:NE	2.36	0.42
1:B:22:LYS:HA	1:D:24:LYS:HE2	2.01	0.42
1:D:377:PHE:CE2	1:D:399:PHE:HE2	2.37	0.42
1:A:529:LYS:HA	1:A:532:GLU:HG3	2.01	0.42
1:A:467:ASN:ND2	3:A:601:NAD:O7N	2.45	0.42
1:B:297:VAL:HG22	1:B:298:ILE:H	1.83	0.42
1:D:483:THR:OG1	1:D:534:LEU:HD13	2.19	0.42
1:B:354:ARG:CZ	1:B:356:ALA:HB3	2.49	0.42
1:B:419:LEU:O	3:B:1601:NAD:H2N	2.19	0.42
1:C:239:MSE:HE2	1:C:269:TYR:CD1	2.55	0.42
1:C:452:VAL:HG22	1:C:452:VAL:O	2.18	0.42
1:C:528:ILE:HG12	1:C:550:ALA:HA	2.01	0.42
1:C:572:TRP:HA	1:C:573:PRO:HD3	1.90	0.42
1:D:59:GLU:HB3	1:D:63:ILE:HG13	2.01	0.42
1:B:300:LYS:HE2	1:B:304:GLU:O	2.19	0.42
1:C:104:ILE:HG12	1:C:108:MSE:HE1	2.02	0.42
1:C:104:ILE:CG2	1:C:105:GLU:N	2.83	0.42
1:C:158:VAL:HA	1:C:199:LEU:O	2.20	0.42
1:C:475:ALA:O	1:C:479:ILE:HD12	2.20	0.42
1:A:165:ARG:NH2	1:A:256:ASP:OD1	2.52	0.42
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.55	0.42
1:A:509:GLN:HE21	1:A:509:GLN:HB3	1.64	0.42
1:A:85:ILE:HG12	1:A:86:MSE:N	2.34	0.42
1:C:283:THR:O	1:C:286:VAL:HG23	2.20	0.42
1:D:443:PHE:O	5:D:4062:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:VAL:HG12	1:D:507:LEU:HD23	2.00	0.42
1:A:286:VAL:HG11	1:A:466:ASN:O	2.18	0.42
1:A:453:LYS:NZ	1:A:457:GLY:HA2	2.34	0.42
1:B:389:ILE:HB	1:B:407:MSE:HE2	2.02	0.42
1:C:534:LEU:HA	1:C:534:LEU:HD23	1.80	0.42
1:D:64:GLN:HB3	1:D:95:LEU:CD2	2.50	0.42
1:D:82:TYR:C	1:D:82:TYR:CD2	2.93	0.42
1:A:174:VAL:HG21	1:A:220:GLY:HA3	2.02	0.42
1:A:349:LEU:HD23	1:A:351:VAL:CG1	2.50	0.42
1:C:335:GLN:O	1:C:339:LYS:HE3	2.19	0.42
1:C:453:LYS:CB	1:C:459:VAL:HG22	2.49	0.42
1:C:108:MSE:SE	1:C:516:LEU:HD21	2.69	0.42
1:A:218:TYR:O	1:B:57:LYS:HD3	2.20	0.42
1:A:255:GLU:OE2	1:A:278:ASP:HB3	2.20	0.42
1:A:432:GLU:O	1:A:436:LEU:HB2	2.19	0.42
1:B:492:LEU:HD23	1:B:496:LYS:HE3	2.00	0.42
1:C:213:LEU:HA	1:C:213:LEU:HD12	1.83	0.42
1:C:277:ASN:HD22	1:C:277:ASN:C	2.24	0.42
1:D:197:ARG:NH1	3:D:3602:NAD:O2B	2.53	0.42
1:D:229:GLN:NE2	1:D:229:GLN:HA	2.34	0.42
1:D:515:PRO:HG2	1:D:518:ASN:OD1	2.20	0.42
1:A:291:LEU:HA	1:A:291:LEU:HD12	1.81	0.41
1:A:344:PHE:CE2	1:A:348:GLY:HA2	2.55	0.41
1:A:399:PHE:CG	1:A:427:GLU:HB3	2.54	0.41
1:C:133:LEU:HD11	1:C:146:ILE:HG22	2.01	0.41
1:D:144:ARG:O	1:D:147:VAL:CG2	2.68	0.41
1:D:263:PHE:CZ	1:D:314:GLU:HA	2.55	0.41
1:D:85:ILE:HG12	1:D:96:PHE:HE1	1.85	0.41
1:A:174:VAL:CG2	1:A:220:GLY:HA3	2.50	0.41
1:A:161:THR:HA	1:A:257:PHE:CE1	2.56	0.41
1:A:561:GLU:CD	1:A:561:GLU:H	2.24	0.41
1:B:144:ARG:HD2	1:B:144:ARG:HA	1.94	0.41
1:B:210:ILE:O	1:B:214:LYS:HG2	2.20	0.41
1:C:174:VAL:HG12	1:C:174:VAL:O	2.20	0.41
1:C:171:ASP:CG	1:C:225:ARG:HH21	2.23	0.41
1:C:359:ASP:OD1	1:C:362:GLN:CD	2.59	0.41
1:D:132:GLY:CA	1:D:200:PRO:HG2	2.50	0.41
1:D:239:MSE:HE1	1:D:252:ILE:HG21	2.02	0.41
1:D:269:TYR:O	1:D:271:GLU:N	2.53	0.41
1:D:26:LYS:HD3	1:D:26:LYS:O	2.20	0.41
1:A:108:MSE:HB3	1:A:109:PRO:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:OD2	1:B:106:SER:HB3	2.20	0.41
1:B:194:ARG:NH2	1:B:196:ASP:CG	2.74	0.41
1:B:331:GLY:O	1:B:332:LEU:C	2.57	0.41
1:D:381:VAL:HG22	1:D:389:ILE:HD11	2.02	0.41
1:D:407:MSE:HG3	1:D:414:PRO:HB2	2.02	0.41
1:D:478:VAL:HG13	1:D:483:THR:HB	2.01	0.41
1:A:401:PRO:HB3	1:A:436:LEU:CD2	2.47	0.41
1:B:105:GLU:HG3	1:B:517:ALA:N	2.36	0.41
1:B:225:ARG:HG2	1:B:225:ARG:HH11	1.85	0.41
1:B:521:GLU:HG2	1:B:525:ASN:HD22	1.84	0.41
1:D:389:ILE:HD12	1:D:407:MSE:SE	2.70	0.41
1:B:128:ARG:HD3	5:B:4056:HOH:O	2.20	0.41
1:B:520:GLN:CD	1:B:520:GLN:H	2.23	0.41
1:B:68:PHE:CD1	1:B:88:ILE:HD11	2.55	0.41
1:C:287:ALA:HB3	1:C:319:ILE:HG12	2.02	0.41
1:C:389:ILE:HG23	1:C:399:PHE:CZ	2.55	0.41
1:D:496:LYS:O	1:D:500:SER:HB3	2.20	0.41
1:A:296:LYS:HE2	1:A:296:LYS:HB2	1.75	0.41
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.77	0.41
1:A:429:THR:H	1:A:432:GLU:CG	2.32	0.41
1:B:174:VAL:HG22	1:B:204:ASP:HB2	2.02	0.41
1:B:454:LEU:CD1	1:B:460:PHE:HE2	2.34	0.41
1:B:82:TYR:HA	1:B:85:ILE:HD12	2.03	0.41
1:B:94:LYS:HB3	1:B:562:TYR:CE2	2.56	0.41
1:C:183:LYS:NZ	4:C:2603:TTN:C3	2.83	0.41
1:D:261:ASN:HD22	1:D:264:ARG:HE	1.68	0.41
1:A:90:GLU:OE2	1:A:131:LYS:HD2	2.21	0.41
1:A:219:MSE:HB2	1:A:219:MSE:HE3	1.86	0.41
1:A:284:ALA:HB1	1:A:322:LEU:HD12	2.02	0.41
1:A:401:PRO:O	1:A:405:ARG:NH1	2.53	0.41
1:B:235:ILE:HG22	1:B:269:TYR:OH	2.21	0.41
1:C:215:ASP:HA	1:C:216:PRO:HD3	1.83	0.41
1:C:274:CYS:HB2	1:C:484:ARG:O	2.20	0.41
1:D:29:MSE:HE3	1:D:54:LEU:HG	2.02	0.41
1:A:66:LEU:HD22	1:A:70:ARG:NE	2.36	0.41
1:C:260:HIS:CD2	1:C:264:ARG:HE	2.39	0.41
1:D:383:ILE:HG22	1:D:384:LEU:N	2.35	0.41
1:D:104:ILE:HG21	1:D:519:ILE:HG22	2.03	0.41
1:A:26:LYS:HD3	1:A:29:MSE:HG3	2.03	0.41
1:A:372:SER:O	1:A:383:ILE:HD13	2.21	0.41
1:A:169:LEU:HD22	1:A:422:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TYR:OH	1:A:443:PHE:HB3	2.21	0.41
1:C:418:ALA:O	1:C:445:SER:HA	2.21	0.41
1:D:456:ASP:OD1	1:D:458:ARG:HB2	2.20	0.41
1:A:308:LEU:HB3	1:A:389:ILE:CD1	2.51	0.41
1:A:396:GLY:O	1:A:398:LEU:HD23	2.21	0.41
1:B:112:TYR:CD2	1:B:113:THR:HG22	2.56	0.41
1:C:33:ARG:HD2	1:C:93:GLU:OE2	2.21	0.41
1:D:77:SER:O	1:D:81:LYS:HG3	2.21	0.41
1:A:133:LEU:HB2	1:A:199:LEU:HD11	2.03	0.41
1:A:22:LYS:HE3	1:C:24:LYS:O	2.20	0.41
1:B:104:ILE:HG23	1:B:105:GLU:N	2.35	0.41
1:B:194:ARG:NH2	1:B:196:ASP:OD1	2.54	0.41
1:B:315:ALA:CB	1:B:392:VAL:HG21	2.51	0.41
1:C:419:LEU:O	3:C:2601:NAD:H2N	2.21	0.41
1:C:262:ALA:HB1	1:C:280:ILE:HD11	2.03	0.41
1:D:380:ALA:O	1:D:384:LEU:HB2	2.21	0.41
1:D:407:MSE:CA	1:D:407:MSE:CE	2.98	0.41
1:D:408:ALA:HB2	1:D:437:THR:HG22	2.02	0.41
1:B:194:ARG:HB3	1:B:194:ARG:HE	1.34	0.40
1:B:355:LYS:HE2	1:B:355:LYS:HB2	1.97	0.40
1:C:295:GLN:O	1:C:299:SER:N	2.43	0.40
1:B:543:TYR:CE1	1:C:484:ARG:HG2	2.55	0.40
1:C:550:ALA:O	1:C:554:LYS:CG	2.69	0.40
1:C:79:LEU:O	1:C:79:LEU:HD12	2.21	0.40
1:D:174:VAL:HG12	1:D:174:VAL:O	2.21	0.40
1:D:302:ILE:HG22	1:D:303:SER:N	2.37	0.40
1:A:380:ALA:O	1:A:384:LEU:HB2	2.21	0.40
1:A:526:ILE:O	1:A:530:VAL:HG23	2.22	0.40
1:B:89:GLN:NE2	1:B:185:CYS:SG	2.95	0.40
1:B:380:ALA:O	1:B:384:LEU:HB2	2.21	0.40
1:B:60:THR:O	1:B:64:GLN:HG3	2.22	0.40
1:B:66:LEU:O	1:B:70:ARG:HB2	2.21	0.40
1:C:193:ILE:HD11	1:C:476:LEU:HB2	2.03	0.40
1:C:201:VAL:HG12	1:C:202:CYS:N	2.35	0.40
1:C:235:ILE:O	1:C:239:MSE:HG2	2.21	0.40
1:A:123:TYR:HB3	1:A:219:MSE:HE1	2.02	0.40
1:A:97:TYR:CE2	1:A:188:THR:HB	2.56	0.40
1:A:24:LYS:O	1:C:22:LYS:CE	2.69	0.40
1:A:297:VAL:CG2	1:A:298:ILE:N	2.84	0.40
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.83	0.40
1:A:559:ARG:HD3	1:A:559:ARG:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ARG:HH11	1:B:128:ARG:CG	2.29	0.40
1:B:171:ASP:CG	1:B:225:ARG:HE	2.23	0.40
1:B:298:ILE:CG2	1:B:300:LYS:HB2	2.51	0.40
1:D:177:MSE:O	1:D:180:PRO:HD2	2.21	0.40
1:D:221:LEU:HB3	1:D:223:GLN:HG2	2.03	0.40
1:B:69:HIS:HE1	1:B:102:ASP:OD2	2.05	0.40
1:B:174:VAL:CG2	1:B:220:GLY:HA3	2.50	0.40
1:B:358:ILE:HG22	1:B:359:ASP:N	2.36	0.40
1:B:552:TYR:CE1	1:B:556:ARG:CZ	3.05	0.40
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.89	0.40
1:C:399:PHE:CG	1:C:427:GLU:HB3	2.56	0.40
1:D:441:CYS:C	1:D:442:LEU:HD23	2.42	0.40
1:A:177:MSE:CE	1:A:177:MSE:O	2.70	0.40
1:B:248:ARG:HB3	1:C:543:TYR:OH	2.22	0.40
5:B:4078:HOH:O	1:C:543:TYR:HD1	2.05	0.40
1:C:75:MSE:HE1	1:C:84:TYR:CG	2.56	0.40
1:D:33:ARG:HG3	1:D:33:ARG:NH1	2.36	0.40
1:D:398:LEU:N	1:D:398:LEU:CD1	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/584 (94%)	516 (94%)	33 (6%)	2 (0%)	34	57
1	B	551/584 (94%)	513 (93%)	35 (6%)	3 (0%)	29	52
1	C	551/584 (94%)	525 (95%)	23 (4%)	3 (0%)	29	52
1	D	551/584 (94%)	515 (94%)	32 (6%)	4 (1%)	22	43
All	All	2204/2336 (94%)	2069 (94%)	123 (6%)	12 (0%)	29	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	LEU
1	C	332	LEU
1	C	392	VAL
1	A	332	LEU
1	D	270	ARG
1	D	332	LEU
1	A	433	ALA
1	B	121	SER
1	C	441	CYS
1	D	392	VAL
1	B	392	VAL
1	D	472	PRO

5.3.2 Protein sidechains (i)

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%)	371 (79%)	98 (21%)	1 2
1	B	469/483 (97%)	373 (80%)	96 (20%)	1 2
1	C	469/483 (97%)	379 (81%)	90 (19%)	1 2
1	D	469/483 (97%)	384 (82%)	85 (18%)	1 2
All	All	1876/1932 (97%)	1507 (80%)	369 (20%)	1 2

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	23	GLU
1	A	26	LYS
1	A	29	MSE
1	A	43	GLN
1	A	45	ARG
1	A	60	THR
1	A	66	LEU
1	A	70	ARG
1	A	74	LYS

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Mol	Chain	Res	Type
1	A	75	MSE
1	A	76	THR
1	A	85	ILE
1	A	90	GLU
1	A	100	LEU
1	A	107	LEU
1	A	118	LEU
1	A	121	SER
1	A	133	LEU
1	A	138	SER
1	A	140	ARG
1	A	152	GLU
1	A	153	ASN
1	A	154	HIS
1	A	165	ARG
1	A	169	LEU
1	A	183	LYS
1	A	185	CYS
1	A	193	ILE
1	A	197	ARG
1	A	210	ILE
1	A	221	LEU
1	A	225	ARG
1	A	226	ASP
1	A	227	ARG
1	A	232	ASP
1	A	233	ASP
1	A	236	ASP
1	A	251	LEU
1	A	267	ARG
1	A	275	THR
1	A	281	GLN
1	A	286	VAL
1	A	291	LEU
1	A	292	LEU
1	A	295	GLN
1	A	296	LYS
1	A	299	SER
1	A	300	LYS
1	A	303	SER
1	A	306	LYS
1	A	327	MSE

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Mol	Chain	Res	Type
1	A	332	LEU
1	A	336	GLU
1	A	339	LYS
1	A	340	LYS
1	A	346	LYS
1	A	350	LEU
1	A	355	LYS
1	A	359	ASP
1	A	360	SER
1	A	363	GLU
1	A	371	GLU
1	A	375	ASP
1	A	384	LEU
1	A	385	LYS
1	A	389	ILE
1	A	392	VAL
1	A	397	ARG
1	A	398	LEU
1	A	405	ARG
1	A	409	SER
1	A	425	GLN
1	A	431	GLU
1	A	432	GLU
1	A	436	LEU
1	A	467	ASN
1	A	484	ARG
1	A	487	SER
1	A	488	ASP
1	A	489	SER
1	A	492	LEU
1	A	493	GLU
1	A	499	THR
1	A	502	LEU
1	A	504	ASP
1	A	505	GLU
1	A	507	LEU
1	A	509	GLN
1	A	511	ARG
1	A	516	LEU
1	A	520	GLN
1	A	529	LYS
1	A	542	ARG

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Mol	Chain	Res	Type
1	A	556	ARG
1	A	559	ARG
1	A	561	GLU
1	A	571	GLU
1	B	21	ILE
1	B	22	LYS
1	B	23	GLU
1	B	24	LYS
1	B	33	ARG
1	B	43	GLN
1	B	47	MSE
1	B	66	LEU
1	B	70	ARG
1	B	73	LYS
1	B	74	LYS
1	B	80	GLU
1	B	94	LYS
1	B	100	LEU
1	B	104	ILE
1	B	105	GLU
1	B	111	VAL
1	B	121	SER
1	B	123	TYR
1	B	129	ARG
1	B	133	LEU
1	B	136	SER
1	B	138	SER
1	B	140	ARG
1	B	153	ASN
1	B	156	LYS
1	B	164	GLU
1	B	165	ARG
1	B	177	MSE
1	B	183	LYS
1	B	194	ARG
1	B	197	ARG
1	B	203	ILE
1	B	210	ILE
1	B	214	LYS
1	B	223	GLN
1	B	224	LYS
1	B	225	ARG

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Mol	Chain	Res	Type
1	B	227	ARG
1	B	230	GLN
1	B	232	ASP
1	B	233	ASP
1	B	236	ASP
1	B	248	ARG
1	B	251	LEU
1	B	252	ILE
1	B	264	ARG
1	B	271	GLU
1	B	272	LYS
1	B	283	THR
1	B	286	VAL
1	B	291	LEU
1	B	292	LEU
1	B	300	LYS
1	B	302	ILE
1	B	303	SER
1	B	304	GLU
1	B	328	VAL
1	B	334	GLU
1	B	335	GLN
1	B	340	LYS
1	B	343	MSE
1	B	346	LYS
1	B	354	ARG
1	B	355	LYS
1	B	357	LYS
1	B	372	SER
1	B	384	LEU
1	B	385	LYS
1	B	397	ARG
1	B	398	LEU
1	B	402	ASP
1	B	405	ARG
1	B	409	SER
1	B	413	ARG
1	B	423	THR
1	B	429	THR
1	B	436	LEU
1	B	458	ARG
1	B	480	LEU

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Mol	Chain	Res	Type
1	B	481	CYS
1	B	499	THR
1	B	502	LEU
1	B	509	GLN
1	B	511	ARG
1	B	519	ILE
1	B	520	GLN
1	B	531	THR
1	B	537	ASN
1	B	547	GLU
1	B	549	LYS
1	B	551	LYS
1	B	556	ARG
1	B	557	THR
1	B	559	ARG
1	B	564	SER
1	C	21	ILE
1	C	22	LYS
1	C	23	GLU
1	C	24	LYS
1	C	33	ARG
1	C	38	MSE
1	C	43	GLN
1	C	57	LYS
1	C	58	ILE
1	C	66	LEU
1	C	70	ARG
1	C	73	LYS
1	C	74	LYS
1	C	79	LEU
1	C	85	ILE
1	C	99	ILE
1	C	100	LEU
1	C	104	ILE
1	C	108	MSE
1	C	118	LEU
1	C	123	TYR
1	C	129	ARG
1	C	133	LEU
1	C	137	ILE
1	C	140	ARG
1	C	156	LYS

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Mol	Chain	Res	Type
1	C	164	GLU
1	C	165	ARG
1	C	169	LEU
1	C	187	TYR
1	C	197	ARG
1	C	210	ILE
1	C	213	LEU
1	C	214	LYS
1	C	219	MSE
1	C	225	ARG
1	C	230	GLN
1	C	232	ASP
1	C	236	ASP
1	C	240	LYS
1	C	245	ARG
1	C	248	ARG
1	C	267	ARG
1	C	272	LYS
1	C	277	ASN
1	C	286	VAL
1	C	292	LEU
1	C	297	VAL
1	C	298	ILE
1	C	299	SER
1	C	306	LYS
1	C	325	MSE
1	C	332	LEU
1	C	333	SER
1	C	335	GLN
1	C	346	LYS
1	C	350	LEU
1	C	355	LYS
1	C	357	LYS
1	C	360	SER
1	C	363	GLU
1	C	368	SER
1	C	372	SER
1	C	384	LEU
1	C	390	ILE
1	C	402	ASP
1	C	404	ILE
1	C	409	SER

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Mol	Chain	Res	Type
1	C	420	SER
1	C	436	LEU
1	C	438	GLU
1	C	452	VAL
1	C	453	LYS
1	C	456	ASP
1	C	458	ARG
1	C	492	LEU
1	C	499	THR
1	C	502	LEU
1	C	504	ASP
1	C	507	LEU
1	C	509	GLN
1	C	518	ASN
1	C	520	GLN
1	C	521	GLU
1	C	531	THR
1	C	538	LYS
1	C	551	LYS
1	C	554	LYS
1	C	556	ARG
1	C	571	GLU
1	D	22	LYS
1	D	23	GLU
1	D	24	LYS
1	D	26	LYS
1	D	33	ARG
1	D	43	GLN
1	D	51	GLN
1	D	57	LYS
1	D	62	ASP
1	D	63	ILE
1	D	66	LEU
1	D	70	ARG
1	D	73	LYS
1	D	75	MSE
1	D	76	THR
1	D	85	ILE
1	D	91	ARG
1	D	101	GLN
1	D	104	ILE
1	D	125	HIS

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Mol	Chain	Res	Type
1	D	128	ARG
1	D	133	LEU
1	D	138	SER
1	D	140	ARG
1	D	153	ASN
1	D	156	LYS
1	D	165	ARG
1	D	169	LEU
1	D	210	ILE
1	D	214	LYS
1	D	221	LEU
1	D	225	ARG
1	D	229	GLN
1	D	230	GLN
1	D	233	ASP
1	D	236	ASP
1	D	240	LYS
1	D	249	ASN
1	D	251	LEU
1	D	266	LEU
1	D	268	LYS
1	D	271	GLU
1	D	272	LYS
1	D	286	VAL
1	D	291	LEU
1	D	292	LEU
1	D	296	LYS
1	D	297	VAL
1	D	300	LYS
1	D	302	ILE
1	D	305	HIS
1	D	306	LYS
1	D	332	LEU
1	D	335	GLN
1	D	350	LEU
1	D	355	LYS
1	D	357	LYS
1	D	358	ILE
1	D	360	SER
1	D	371	GLU
1	D	373	ILE
1	D	384	LEU

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Mol	Chain	Res	Type
1	D	389	ILE
1	D	392	VAL
1	D	409	SER
1	D	447	SER
1	D	458	ARG
1	D	489	SER
1	D	492	LEU
1	D	500	SER
1	D	502	LEU
1	D	504	ASP
1	D	507	LEU
1	D	520	GLN
1	D	529	LYS
1	D	531	THR
1	D	542	ARG
1	D	543	TYR
1	D	551	LYS
1	D	554	LYS
1	D	556	ARG
1	D	559	ARG
1	D	561	GLU
1	D	564	SER
1	D	572	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	89	GLN
1	A	101	GLN
1	A	153	ASN
1	A	261	ASN
1	A	281	GLN
1	A	305	HIS
1	A	425	GLN
1	A	482	ASN
1	A	520	GLN
1	B	43	GLN
1	B	64	GLN
1	B	69	HIS
1	B	229	GLN

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Mol	Chain	Res	Type
1	B	260	HIS
1	B	261	ASN
1	B	330	ASN
1	B	335	GLN
1	B	482	ASN
1	B	485	HIS
1	B	501	GLN
1	B	518	ASN
1	B	525	ASN
1	B	537	ASN
1	C	43	GLN
1	C	64	GLN
1	C	69	HIS
1	C	229	GLN
1	C	230	GLN
1	C	261	ASN
1	C	277	ASN
1	C	321	ASN
1	C	330	ASN
1	C	335	GLN
1	C	425	GLN
1	C	482	ASN
1	C	509	GLN
1	C	520	GLN
1	D	51	GLN
1	D	64	GLN
1	D	153	ASN
1	D	154	HIS
1	D	223	GLN
1	D	229	GLN
1	D	230	GLN
1	D	261	ASN
1	D	330	ASN
1	D	482	ASN
1	D	485	HIS
1	D	520	GLN
1	D	537	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	B	1601	-	42,48,48	2.11	12 (28%)	50,73,73	1.35	5 (10%)
4	TTN	D	3603	2	1,7,7	0.38	0	0,9,9	0.00	-
3	NAD	C	2601	-	42,48,48	2.08	12 (28%)	50,73,73	1.34	3 (6%)
4	TTN	B	1603	2	1,7,7	0.35	0	0,9,9	0.00	-
3	NAD	C	2602	-	42,48,48	2.29	14 (33%)	50,73,73	1.39	6 (12%)
3	NAD	D	3602	-	42,48,48	2.23	11 (26%)	50,73,73	1.44	6 (12%)
4	TTN	A	603	2	1,7,7	0.32	0	0,9,9	0.00	-
3	NAD	A	602	-	42,48,48	2.19	11 (26%)	50,73,73	1.46	6 (12%)
3	NAD	B	1602	-	42,48,48	2.15	12 (28%)	50,73,73	1.35	6 (12%)
3	NAD	A	601	-	42,48,48	2.01	11 (26%)	50,73,73	1.37	5 (10%)
3	NAD	D	3601	-	42,48,48	2.10	12 (28%)	50,73,73	1.32	4 (8%)
4	TTN	C	2603	2	1,7,7	0.12	0	0,9,9	0.00	-

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	B	1601	-	-	3/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TTN	D	3603	2	-	0/0/8/8	-
3	NAD	C	2601	-	-	2/26/62/62	0/5/5/5
4	TTN	B	1603	2	-	0/0/8/8	-
3	NAD	C	2602	-	-	9/26/62/62	0/5/5/5
3	NAD	D	3602	-	-	12/26/62/62	0/5/5/5
4	TTN	A	603	2	-	0/0/8/8	-
3	NAD	A	602	-	-	11/26/62/62	0/5/5/5
3	NAD	B	1602	-	-	11/26/62/62	0/5/5/5
3	NAD	A	601	-	-	2/26/62/62	0/5/5/5
3	NAD	D	3601	-	-	2/26/62/62	0/5/5/5
4	TTN	C	2603	2	-	0/0/8/8	-

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3602	NAD	C2N-N1N	7.58	1.44	1.35
3	C	2602	NAD	C2N-N1N	7.51	1.44	1.35
3	B	1602	NAD	C2N-N1N	7.40	1.44	1.35
3	A	602	NAD	C2N-N1N	7.35	1.43	1.35
3	C	2602	NAD	O4D-C1D	6.80	1.50	1.41
3	D	3602	NAD	O4D-C1D	6.54	1.50	1.41
3	A	601	NAD	C2N-N1N	6.34	1.42	1.35
3	C	2601	NAD	C2N-N1N	6.04	1.42	1.35
3	D	3601	NAD	C2N-N1N	6.03	1.42	1.35
3	B	1602	NAD	O4D-C1D	5.89	1.49	1.41
3	A	602	NAD	O4D-C1D	5.72	1.49	1.41
3	B	1601	NAD	C2N-N1N	5.61	1.41	1.35
3	B	1601	NAD	C2B-C1B	-5.28	1.45	1.53
3	A	601	NAD	O4B-C1B	4.60	1.47	1.41
3	D	3601	NAD	O4B-C1B	4.52	1.47	1.41
3	C	2601	NAD	C3N-C7N	4.29	1.57	1.50
3	B	1601	NAD	O4B-C1B	4.17	1.46	1.41
3	D	3601	NAD	C6N-N1N	4.15	1.45	1.35
3	A	602	NAD	O4B-C1B	4.11	1.46	1.41
3	C	2601	NAD	C2B-C1B	-4.07	1.47	1.53
3	C	2602	NAD	O4B-C1B	4.05	1.46	1.41
3	A	602	NAD	C6N-N1N	3.86	1.44	1.35
3	C	2601	NAD	C6N-N1N	3.86	1.44	1.35
3	D	3602	NAD	C6N-N1N	3.82	1.44	1.35
3	D	3602	NAD	O4B-C1B	3.76	1.46	1.41
3	D	3601	NAD	C2B-C1B	-3.76	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3601	NAD	C2A-N3A	3.75	1.38	1.32
3	C	2602	NAD	C6N-N1N	3.72	1.44	1.35
3	D	3602	NAD	C2A-N3A	3.71	1.38	1.32
3	C	2601	NAD	O4B-C1B	3.67	1.46	1.41
3	A	601	NAD	C2A-N3A	3.65	1.38	1.32
3	B	1602	NAD	C6N-N1N	3.63	1.44	1.35
3	B	1601	NAD	C6N-N1N	3.61	1.44	1.35
3	D	3601	NAD	C3N-C7N	3.60	1.56	1.50
3	D	3601	NAD	O4D-C1D	3.59	1.46	1.41
3	B	1601	NAD	O4D-C1D	3.57	1.46	1.41
3	C	2601	NAD	C2A-N3A	3.52	1.37	1.32
3	B	1602	NAD	C2A-N3A	3.50	1.37	1.32
3	A	602	NAD	C2A-N3A	3.41	1.37	1.32
3	A	601	NAD	C2B-C1B	-3.41	1.48	1.53
3	B	1602	NAD	O4B-C1B	3.40	1.45	1.41
3	B	1601	NAD	C3N-C7N	3.38	1.55	1.50
3	B	1601	NAD	C2D-C1D	-3.35	1.48	1.53
3	B	1602	NAD	C3N-C7N	3.31	1.55	1.50
3	A	601	NAD	C6N-N1N	3.30	1.43	1.35
3	C	2602	NAD	O4D-C4D	3.23	1.52	1.45
3	C	2601	NAD	C2D-C1D	-3.21	1.48	1.53
3	C	2602	NAD	C3N-C7N	3.16	1.55	1.50
3	A	602	NAD	C3N-C7N	3.16	1.55	1.50
3	C	2601	NAD	C5A-C4A	-3.15	1.32	1.40
3	C	2602	NAD	C2A-N3A	3.12	1.37	1.32
3	A	601	NAD	C3N-C7N	3.05	1.55	1.50
3	A	601	NAD	C5A-C4A	-2.97	1.33	1.40
3	A	601	NAD	C2D-C1D	-2.95	1.49	1.53
3	B	1601	NAD	C2A-N3A	2.89	1.36	1.32
3	D	3602	NAD	C3N-C7N	2.83	1.54	1.50
3	A	602	NAD	C5A-C4A	-2.80	1.33	1.40
3	B	1602	NAD	C5A-C4A	-2.74	1.33	1.40
3	D	3601	NAD	C2A-N1A	2.72	1.39	1.33
3	B	1601	NAD	C5A-C4A	-2.65	1.33	1.40
3	B	1601	NAD	C2A-N1A	2.64	1.38	1.33
3	B	1602	NAD	C2B-C1B	-2.62	1.49	1.53
3	C	2602	NAD	C5A-C4A	-2.61	1.34	1.40
3	D	3601	NAD	C5A-C4A	-2.54	1.34	1.40
3	D	3601	NAD	C4N-C3N	2.54	1.43	1.39
3	B	1601	NAD	C5A-N7A	-2.46	1.30	1.39
3	A	601	NAD	O4D-C1D	2.46	1.44	1.41
3	D	3601	NAD	C2D-C1D	-2.45	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3602	NAD	O4D-C4D	2.40	1.50	1.45
3	D	3602	NAD	C5A-C4A	-2.40	1.34	1.40
3	C	2602	NAD	PN-O5D	2.37	1.68	1.59
3	D	3602	NAD	C5A-N7A	-2.36	1.31	1.39
3	C	2601	NAD	O4D-C1D	2.25	1.44	1.41
3	C	2601	NAD	C5A-N7A	-2.24	1.31	1.39
3	D	3601	NAD	C5A-N7A	-2.23	1.31	1.39
3	A	601	NAD	C2A-N1A	2.21	1.38	1.33
3	A	601	NAD	C5A-N7A	-2.20	1.31	1.39
3	C	2601	NAD	C5N-C4N	2.20	1.43	1.38
3	A	602	NAD	O4D-C4D	2.20	1.49	1.45
3	C	2602	NAD	C5A-N7A	-2.18	1.31	1.39
3	A	602	NAD	C5A-N7A	-2.16	1.31	1.39
3	D	3602	NAD	C4N-C3N	2.16	1.43	1.39
3	B	1602	NAD	C4N-C3N	2.15	1.43	1.39
3	B	1602	NAD	C2A-N1A	2.14	1.37	1.33
3	B	1602	NAD	C5A-N7A	-2.13	1.32	1.39
3	C	2601	NAD	C4N-C3N	2.12	1.42	1.39
3	A	602	NAD	C4N-C3N	2.12	1.42	1.39
3	A	602	NAD	C2B-C1B	-2.11	1.50	1.53
3	C	2602	NAD	C4N-C3N	2.10	1.42	1.39
3	D	3602	NAD	C2A-N1A	2.09	1.37	1.33
3	B	1602	NAD	O4D-C4D	2.08	1.49	1.45
3	B	1601	NAD	C4N-C3N	2.07	1.42	1.39
3	C	2602	NAD	C2B-C1B	-2.07	1.50	1.53
3	C	2602	NAD	C2A-N1A	2.03	1.37	1.33
3	C	2602	NAD	C2N-C3N	2.00	1.42	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2601	NAD	N3A-C2A-N1A	-5.35	120.32	128.68
3	A	602	NAD	N3A-C2A-N1A	-5.19	120.57	128.68
3	A	601	NAD	N3A-C2A-N1A	-5.15	120.64	128.68
3	B	1601	NAD	N3A-C2A-N1A	-5.07	120.75	128.68
3	D	3601	NAD	N3A-C2A-N1A	-5.06	120.78	128.68
3	D	3602	NAD	N3A-C2A-N1A	-4.99	120.88	128.68
3	B	1602	NAD	N3A-C2A-N1A	-4.89	121.04	128.68
3	C	2602	NAD	N3A-C2A-N1A	-4.76	121.24	128.68
3	A	601	NAD	C4A-C5A-N7A	4.27	113.85	109.40
3	B	1601	NAD	C4A-C5A-N7A	4.26	113.84	109.40
3	C	2601	NAD	C4A-C5A-N7A	4.25	113.83	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3601	NAD	C4A-C5A-N7A	4.24	113.82	109.40
3	A	602	NAD	C4A-C5A-N7A	4.06	113.64	109.40
3	D	3602	NAD	C4A-C5A-N7A	3.74	113.30	109.40
3	C	2602	NAD	C4A-C5A-N7A	3.71	113.26	109.40
3	B	1602	NAD	C4A-C5A-N7A	3.50	113.05	109.40
3	A	602	NAD	C3D-C2D-C1D	3.37	106.05	100.98
3	C	2602	NAD	C3D-C2D-C1D	3.36	106.03	100.98
3	D	3602	NAD	C3D-C2D-C1D	3.35	106.03	100.98
3	D	3602	NAD	C3B-C2B-C1B	3.17	105.75	100.98
3	B	1602	NAD	C3D-C2D-C1D	3.09	105.62	100.98
3	D	3602	NAD	C6N-N1N-C2N	-2.96	119.28	121.97
3	A	602	NAD	C6N-N1N-C2N	-2.95	119.28	121.97
3	A	602	NAD	C3B-C2B-C1B	2.80	105.19	100.98
3	A	601	NAD	C3D-C2D-C1D	2.80	105.19	100.98
3	C	2602	NAD	C6N-N1N-C2N	-2.70	119.52	121.97
3	C	2602	NAD	C3B-C2B-C1B	2.62	104.92	100.98
3	B	1601	NAD	C3D-C2D-C1D	2.60	104.90	100.98
3	C	2601	NAD	C3D-C2D-C1D	2.57	104.84	100.98
3	B	1602	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
3	D	3601	NAD	C3D-C2D-C1D	2.33	104.49	100.98
3	B	1601	NAD	C3N-C7N-N7N	-2.30	114.98	117.75
3	B	1602	NAD	C3B-C2B-C1B	2.24	104.36	100.98
3	D	3602	NAD	C2D-C3D-C4D	2.23	106.97	102.64
3	A	602	NAD	C2D-C3D-C4D	2.19	106.91	102.64
3	B	1601	NAD	C6N-N1N-C2N	-2.16	120.00	121.97
3	C	2602	NAD	C2D-C3D-C4D	2.14	106.81	102.64
3	B	1602	NAD	C2D-C3D-C4D	2.13	106.79	102.64
3	A	601	NAD	C6N-N1N-C2N	-2.09	120.07	121.97
3	D	3601	NAD	C3N-C7N-N7N	-2.06	115.28	117.75
3	A	601	NAD	C3N-C7N-N7N	-2.05	115.29	117.75

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3602	NAD	C5B-O5B-PA-O1A
3	D	3602	NAD	PA-O3-PN-O5D
3	D	3602	NAD	C5D-O5D-PN-O1N
3	D	3602	NAD	C5D-O5D-PN-O2N
3	D	3602	NAD	C3D-C4D-C5D-O5D
3	C	2601	NAD	O4D-C1D-N1N-C6N
3	C	2602	NAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	2602	NAD	C5D-O5D-PN-O1N
3	C	2602	NAD	C5D-O5D-PN-O2N
3	C	2602	NAD	O4D-C4D-C5D-O5D
3	C	2602	NAD	C3D-C4D-C5D-O5D
3	B	1601	NAD	O4D-C1D-N1N-C6N
3	A	602	NAD	C5B-O5B-PA-O1A
3	A	602	NAD	PA-O3-PN-O5D
3	A	602	NAD	C5D-O5D-PN-O3
3	A	602	NAD	C5D-O5D-PN-O2N
3	A	602	NAD	C3D-C4D-C5D-O5D
3	B	1602	NAD	C5B-O5B-PA-O1A
3	B	1602	NAD	C5D-O5D-PN-O3
3	B	1602	NAD	C5D-O5D-PN-O2N
3	B	1602	NAD	C3D-C4D-C5D-O5D
3	A	601	NAD	O4D-C1D-N1N-C6N
3	D	3601	NAD	O4D-C1D-N1N-C6N
3	D	3602	NAD	O4D-C4D-C5D-O5D
3	A	602	NAD	O4D-C4D-C5D-O5D
3	B	1602	NAD	O4D-C4D-C5D-O5D
3	A	602	NAD	O4B-C4B-C5B-O5B
3	B	1602	NAD	PA-O3-PN-O5D
3	A	602	NAD	C4D-C5D-O5D-PN
3	D	3602	NAD	C5D-O5D-PN-O3
3	A	602	NAD	C5B-O5B-PA-O3
3	D	3602	NAD	O4B-C4B-C5B-O5B
3	D	3602	NAD	C4D-C5D-O5D-PN
3	C	2602	NAD	C4D-C5D-O5D-PN
3	D	3602	NAD	C5B-O5B-PA-O2A
3	C	2602	NAD	C5B-O5B-PA-O2A
3	A	602	NAD	C5B-O5B-PA-O2A
3	B	1602	NAD	C5B-O5B-PA-O2A
3	B	1602	NAD	C4D-C5D-O5D-PN
3	B	1601	NAD	O4B-C4B-C5B-O5B
3	B	1602	NAD	C4B-C5B-O5B-PA
3	A	602	NAD	C3B-C4B-C5B-O5B
3	B	1602	NAD	O4B-C4B-C5B-O5B
3	D	3602	NAD	C5B-O5B-PA-O3
3	C	2602	NAD	C5B-O5B-PA-O3
3	C	2602	NAD	C5D-O5D-PN-O3
3	B	1602	NAD	C5B-O5B-PA-O3
3	D	3602	NAD	C3B-C4B-C5B-O5B
3	C	2601	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	B	1601	NAD	C3B-C4B-C5B-O5B
3	D	3601	NAD	O4B-C4B-C5B-O5B
3	A	601	NAD	O4B-C4B-C5B-O5B

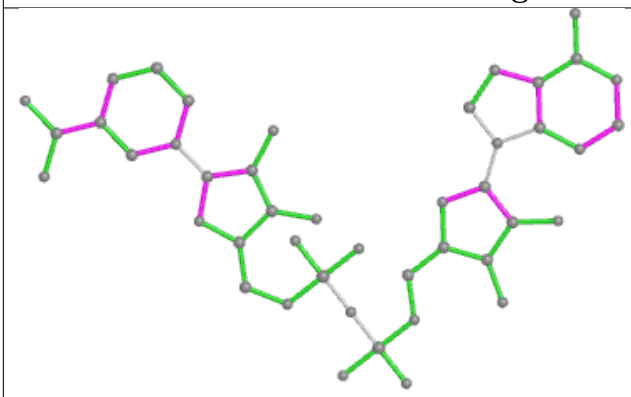
There are no ring outliers.

11 monomers are involved in 21 short contacts:

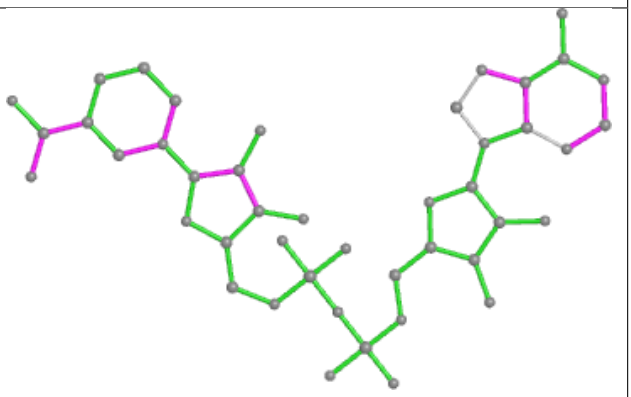
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1601	NAD	1	0
4	D	3603	TTN	1	0
3	C	2601	NAD	4	0
4	B	1603	TTN	1	0
3	C	2602	NAD	1	0
3	D	3602	NAD	3	0
3	A	602	NAD	2	0
3	B	1602	NAD	1	0
3	A	601	NAD	4	0
3	D	3601	NAD	1	0
4	C	2603	TTN	2	0

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 then 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.

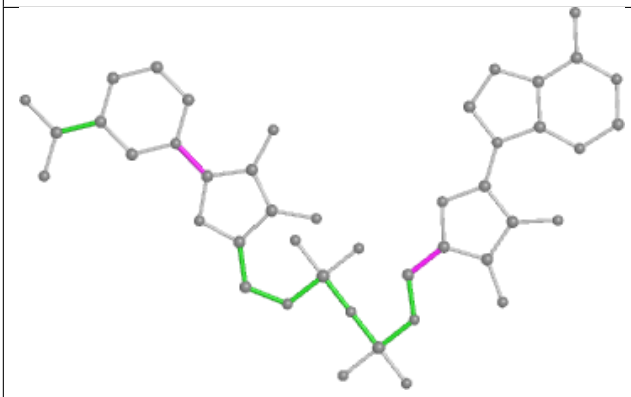
Ligand NAD B 1601



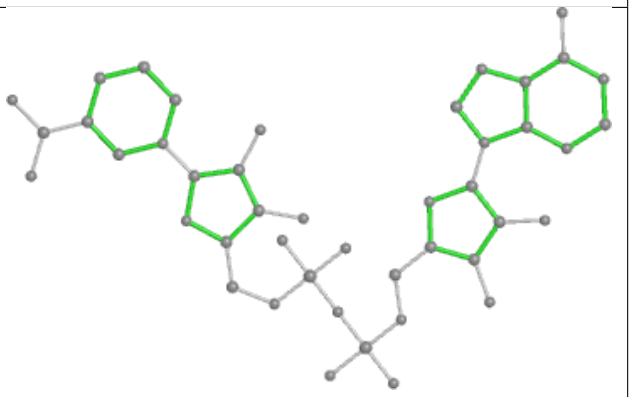
Bond lengths



Bond angles

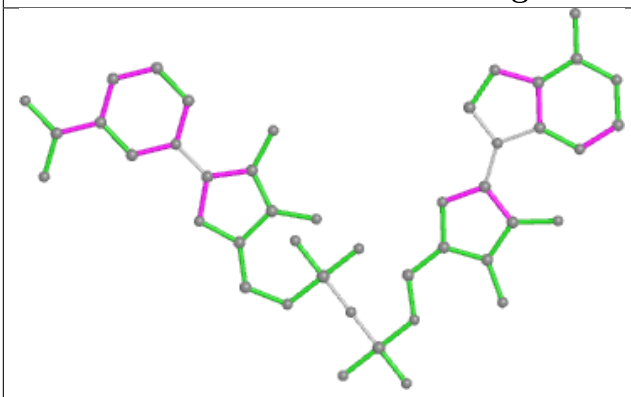


Torsions

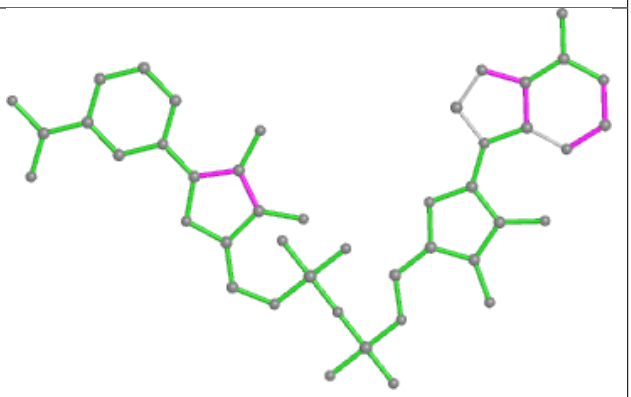


Rings

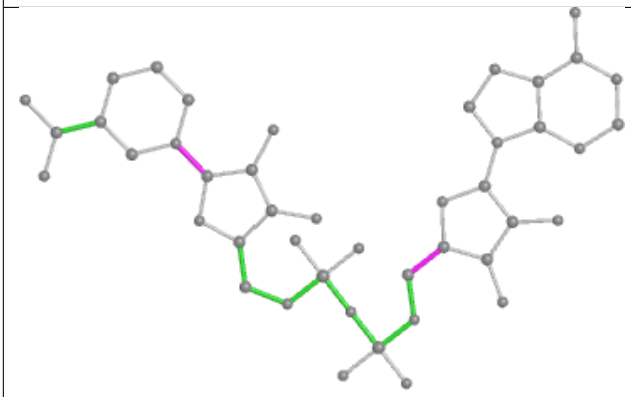
Ligand NAD C 2601



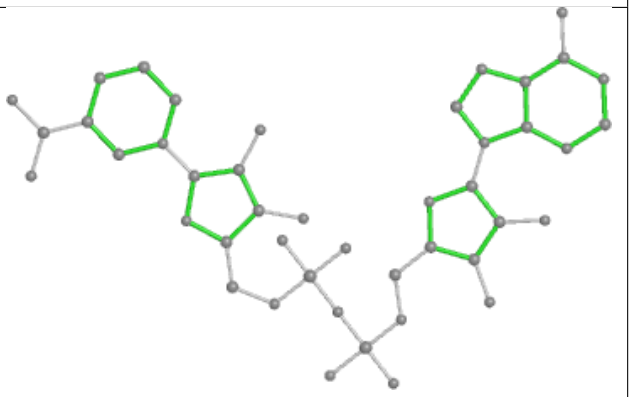
Bond lengths



Bond angles

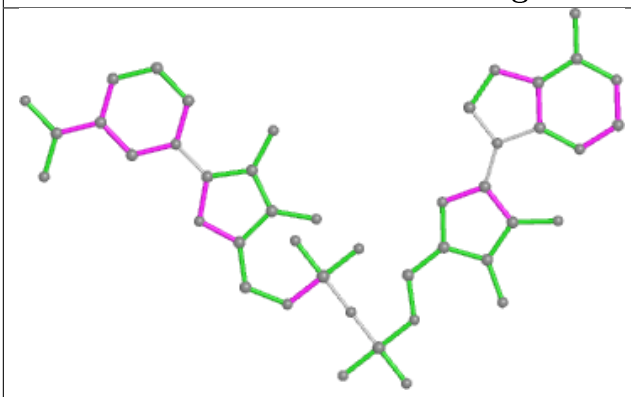


Torsions

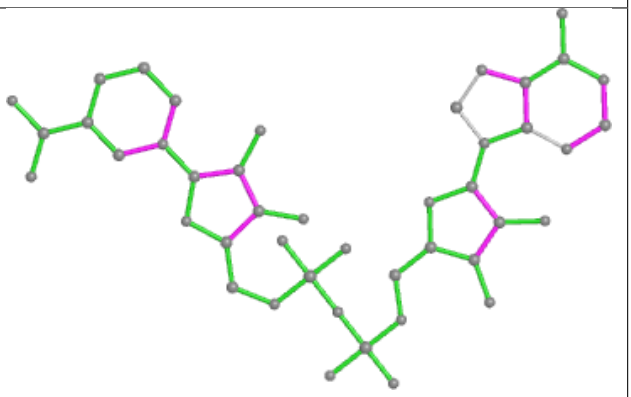


Rings

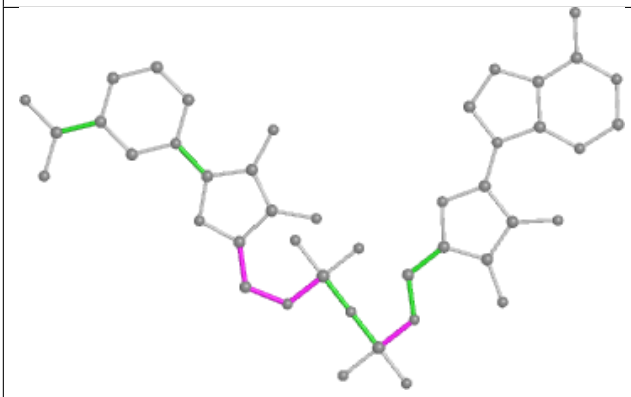
Ligand NAD C 2602



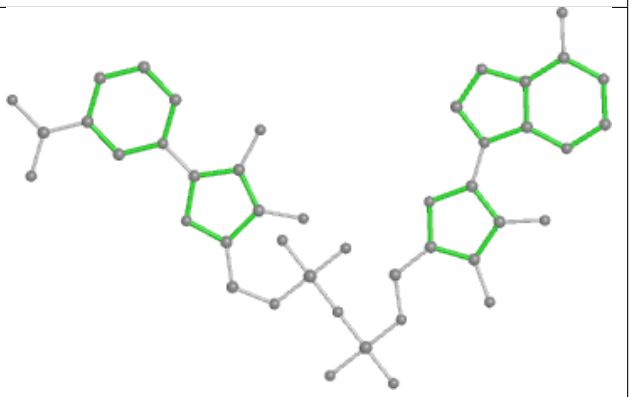
Bond lengths



Bond angles

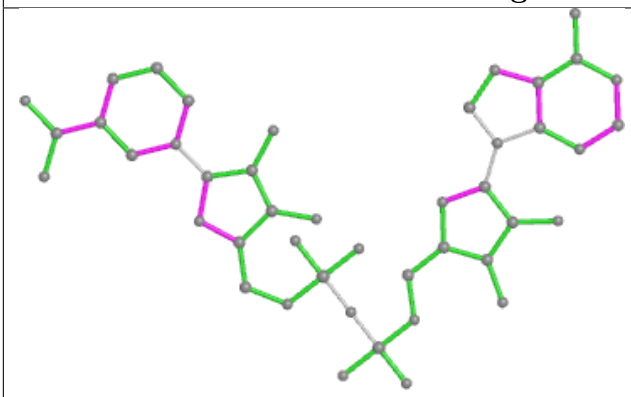


Torsions

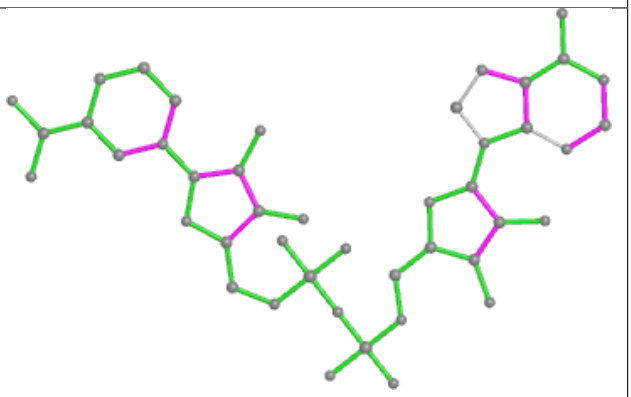


Rings

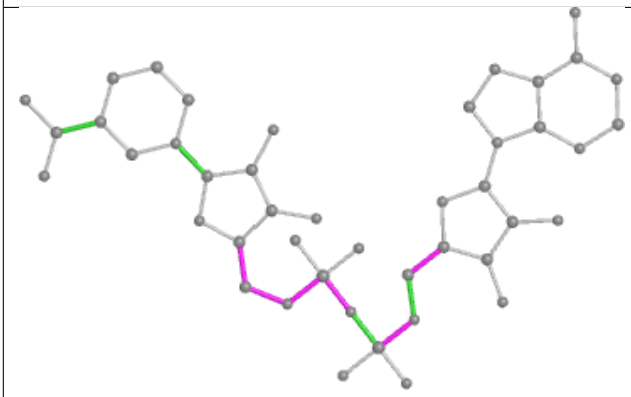
Ligand NAD D 3602



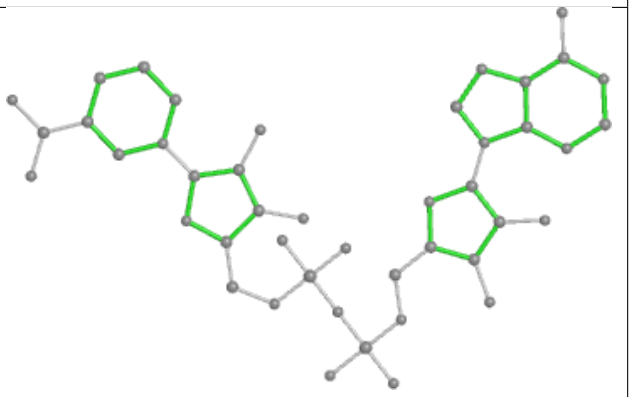
Bond lengths



Bond angles

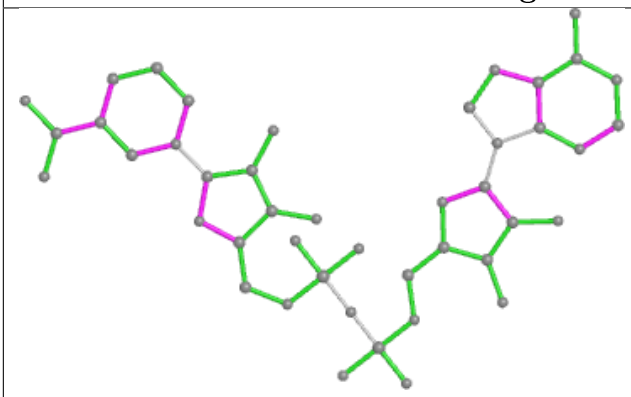


Torsions

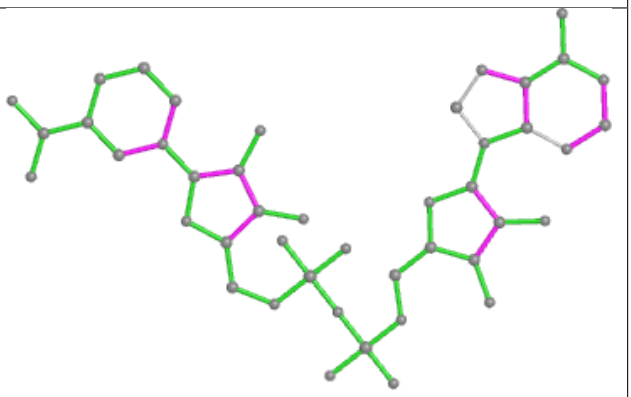


Rings

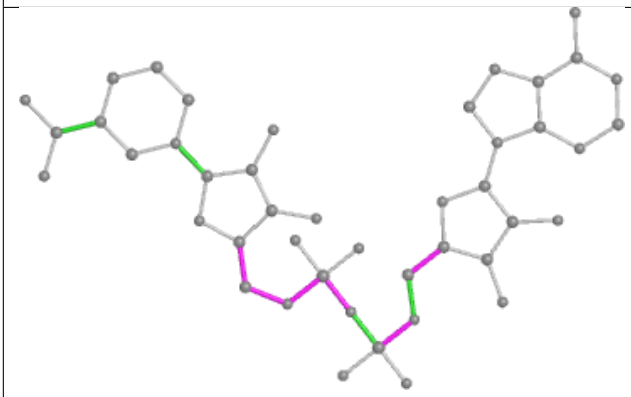
Ligand NAD A 602



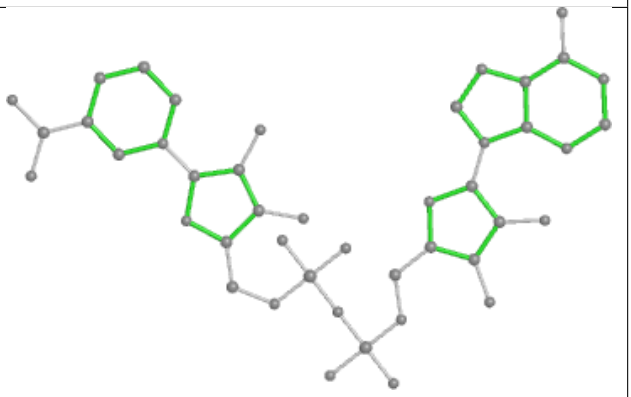
Bond lengths



Bond angles

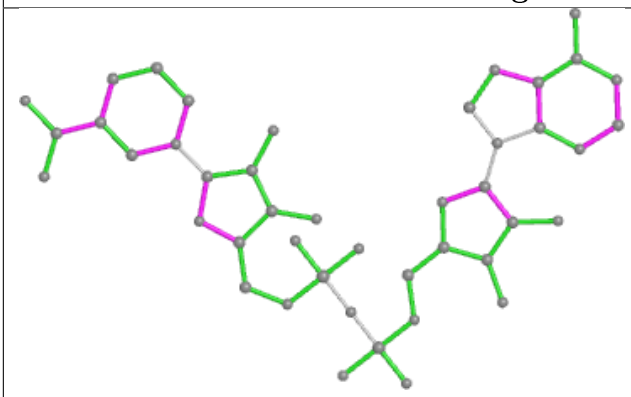


Torsions

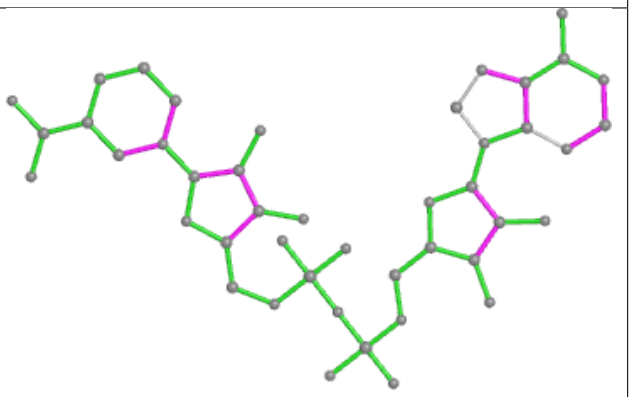


Rings

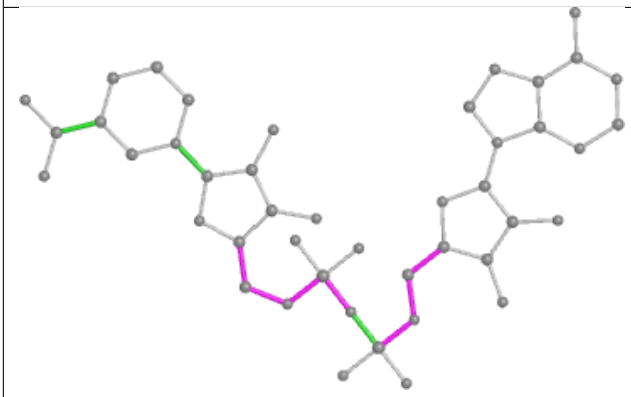
Ligand NAD B 1602



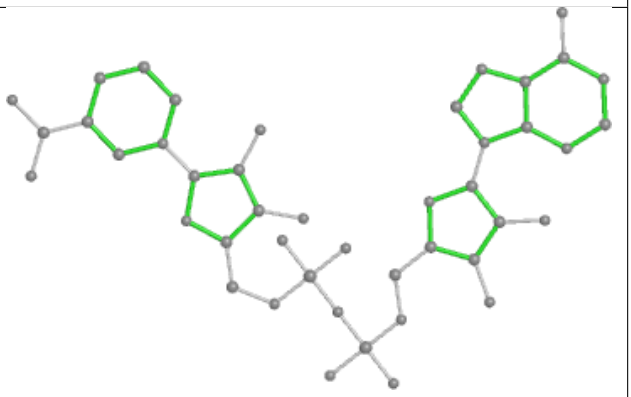
Bond lengths



Bond angles

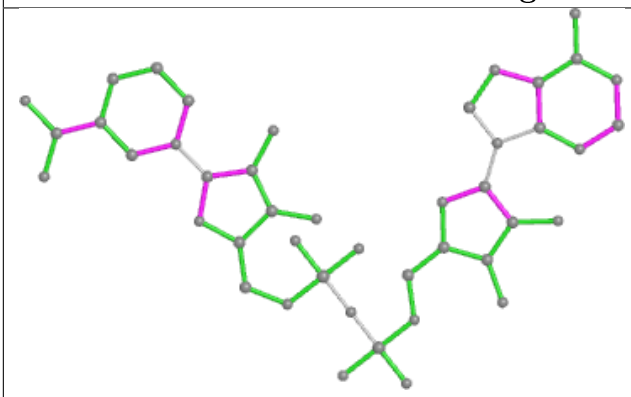


Torsions

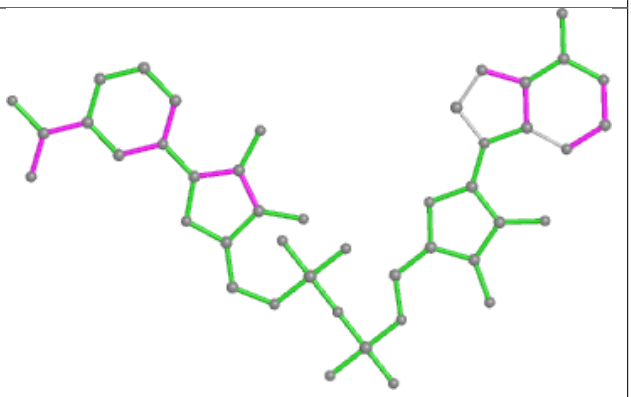


Rings

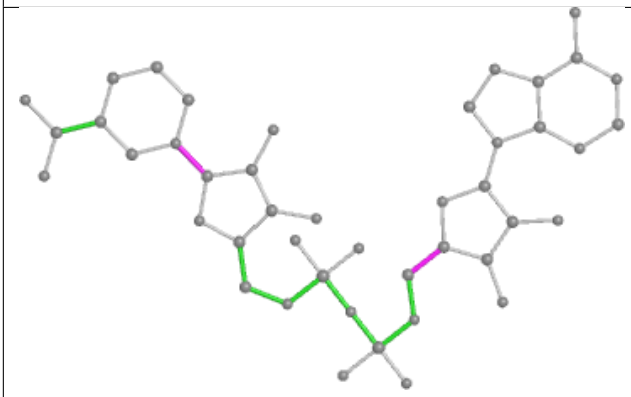
Ligand NAD A 601



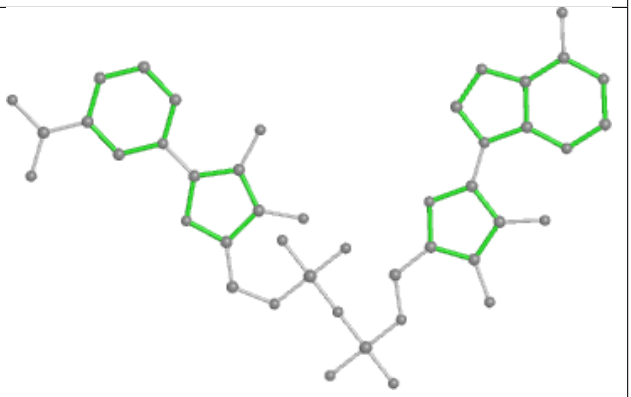
Bond lengths



Bond angles

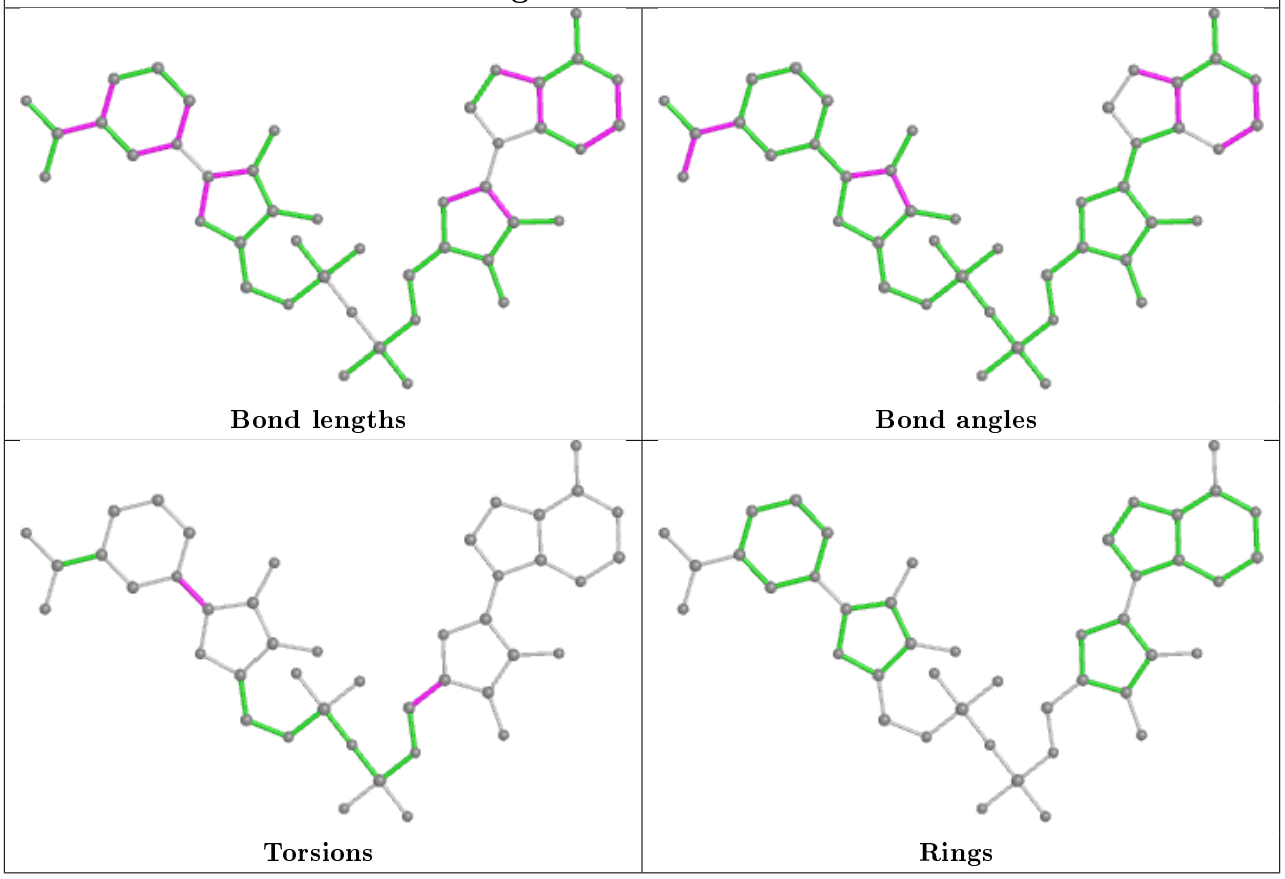


Torsions



Rings

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.