Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:21 PM EDT

PDB ID	:	1EFK
Title	:	STRUCTURE OF HUMAN MALIC ENZYME IN COMPLEX WITH KETOMALONATE
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 (i) 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 (1)) were used in the production of this report:

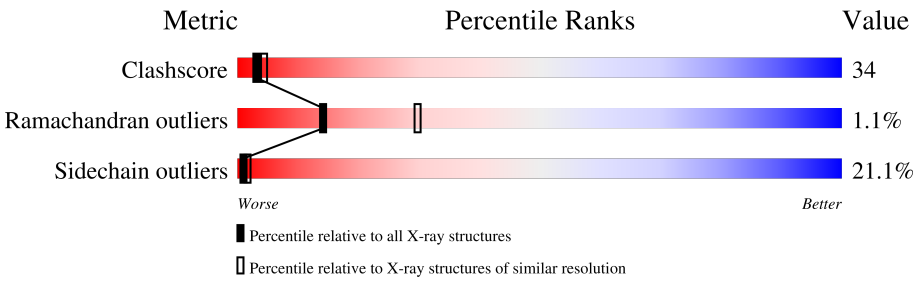
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	38% 44% 13% 5%
1	B	584	42% 41% 12% 5%
1	C	584	47% 38% 9% 5%
1	D	584	41% 39% 14% • 5%

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 (i)

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
			Total	C	N	O	S	Se			
1	A	553	4367	2796	744	804	9	14	0	0	0
1	B	553	4367	2796	744	804	9	14	0	0	0
1	C	553	4367	2796	744	804	9	14	0	0	0
1	D	553	4367	2796	744	804	9	14	0	0	0

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	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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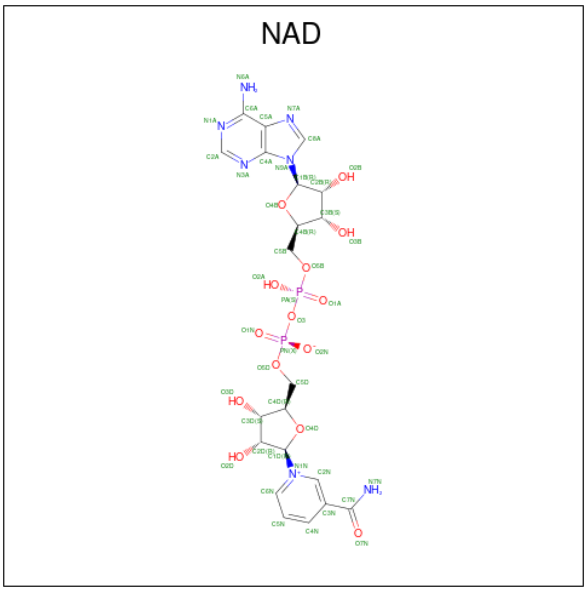
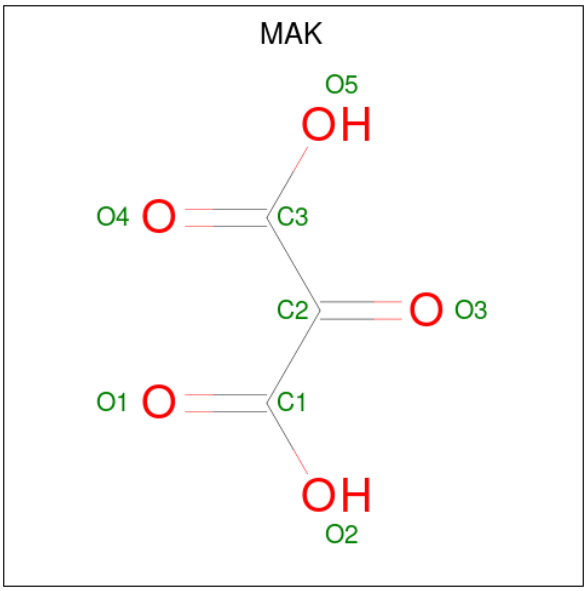
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	C	1	1	1	0	0
			Total	Mg		
2	D	1	1	1	0	0

- 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
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	9	0
			Total	C	N	O	P		
3	B	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	B	1	44	21	7	14	2	9	0
			Total	C	N	O	P		
3	C	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	C	1	44	21	7	14	2	9	0
			Total	C	N	O	P		
3	D	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	D	1	44	21	7	14	2	9	0

- Molecule 4 is ALPHA-KETOMALONIC ACID (three-letter code: MAK) (formula: $C_3H_2O_5$).



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

- Molecule 5 is water.

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

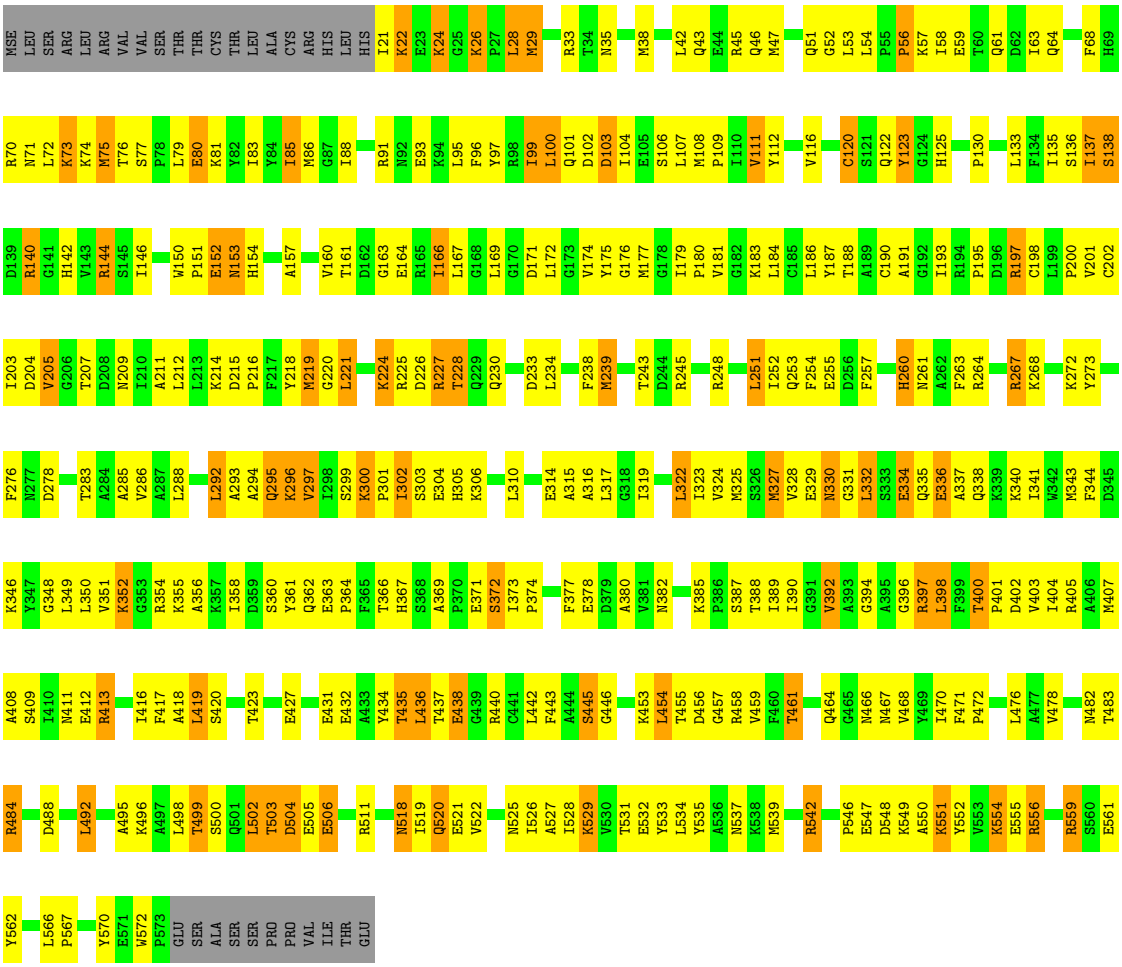
3 Residue-property plots (i)

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.

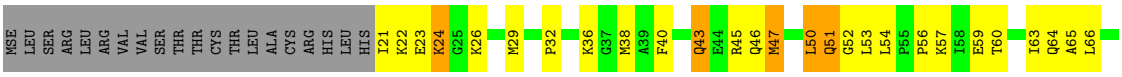
• Molecule 1: MALIC ENZYME

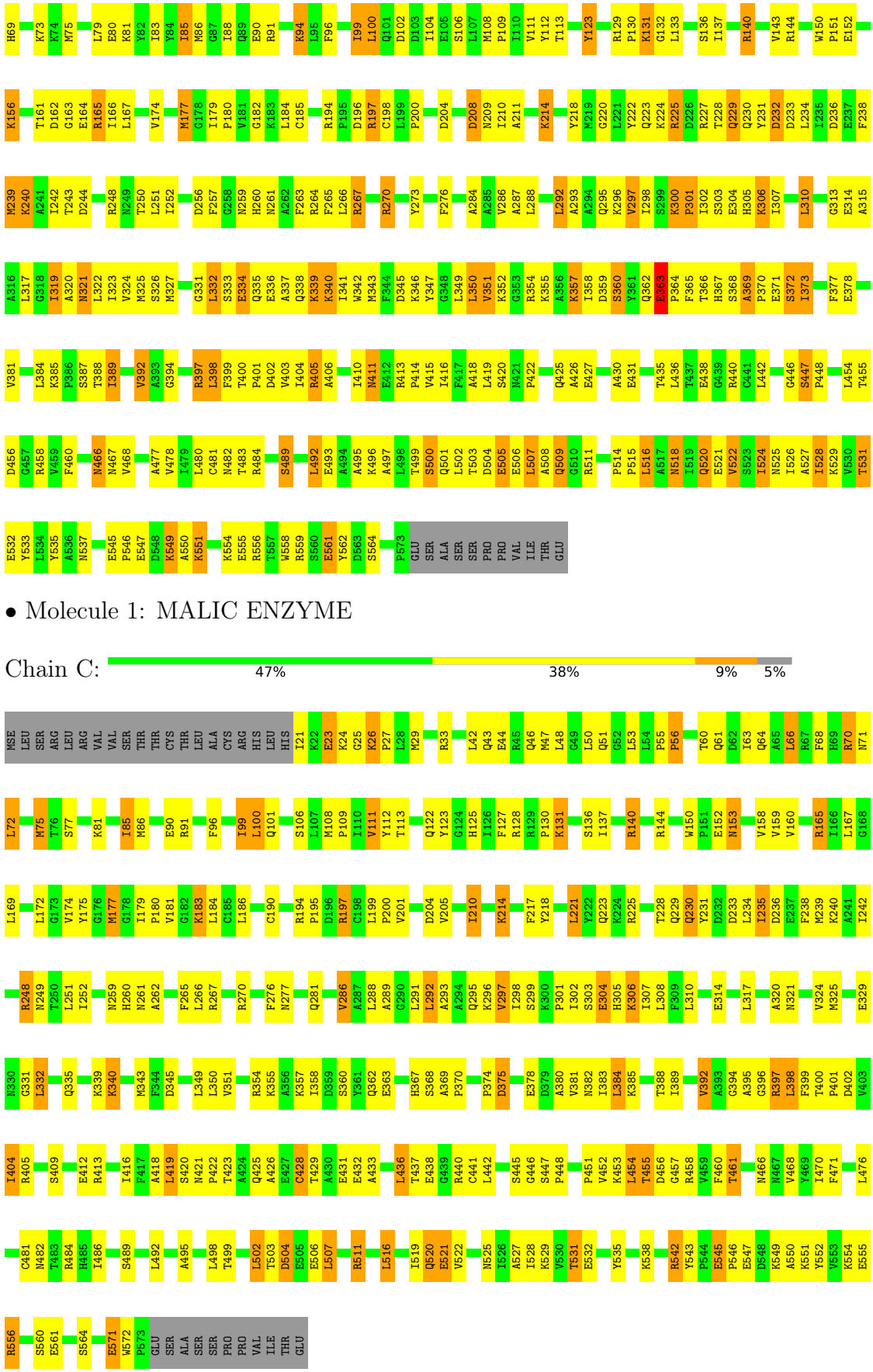
Chain A: 38% 44% 13% 5%



• Molecule 1: MALIC ENZYME

Chain B: 42% 41% 12% 5%





- Molecule 1: MALIC ENZYME

Chain C: 47% 38% 9% 5%

• Molecule 1: MALIC ENZYME

Chain D: 41% 39% 14% • 5%

MSE LEU SER ARG LEU ARG VAL VAL SER THR THR CYS THR LEU ALA CYS ARG HIS LEU HIS I21 K22 E23 K24 G25 K26 P27 L28 M29 R33 K36 G37 M38 T41 L42 Q43 E44 R45 Q46 M47 Q51 P55 P56 K57 I58 E59 T60 Q61 D62 I63 Q64 A65 L66 R67 F68

H69 R70 N71 L72 K73 K74 M75 T76 S77 K81 Y82 I83 Y84 I85 M86 Q89 E90 R91 N92 E93 K94 L95 F96 Y97 R98 I99 L100 D103 I104 E105 S106 L107 M108 P109 I110 V111 T115 C120 Y123 G124 H125 I126 K131 G132 L133 F134 I135 S136 I137 R140 V143

R144 W150 P151 E152 N153 K156 A157 T161 D162 G163 E164 R165 I166 L169 G170 D171 L172 G173 V174 Y175 G176 M177 G178 I179 P180 V181 G182 K183 L184 C185 L186 C190 A191 G192 I193 R194 R197 C198 L199 P200 V201 C202 I203 D204 V205 G206 T207 D208 N209 I210 A211 K214

F217 Y218 M219 G220 L221 K224 R225 D226 R227 T228 Q229 Q230 D233 D236 E237 F238 M239 T243 D244 R245 R248 N249 T250 L251 F254 F257 N261 R264 F265 L266 R267 K268 Y269 R270 E271 K272 I280 T283 V286 A287 L288 L291 L292 A293 A294 Q295 K296

V297 I298 S299 K300 P301 I302 S303 E304 H305 K306 I307 L308 G313 E314 A315 A316 I319 A320 N321 L322 I323 V324 M325 S326 M327 V328 E329 N330 G331 L332 S333 E334 Q335 E336 A337 Q338 K339 K340 I341 W342 M343 F344 D345 K346 Y347 G348 L349 L350 V351 K352 G353 R354 K355 I358 D359 S360 Y361

Q362 E363 P364 F365 T366 H367 S368 A369 P370 E371 P374 D375 T376 F377 E378 D379 A380 V381 N382 I383 L384 S387 T388 I389 V392 A393 G394 R397 L398 F399 T400 P401 D402 V403 I404 R405 A406 M407 A408 S409 E412 R413 P414 V415 I416 S420 T423 A426 E427 C428 T429 A430

E431 E432 T435 L436 T437 E438 G439 R440 C441 L442 F443 A444 S445 G446 S447 P448 V452 K453 L454 T455 D456 G457 R458 V459 F460 T461 Q464 G465 N466 N467 V468 F471 P472 G473 V474 A475 L476 A477 V478 I479 S489 L492 E493 S500 Q501 L502 T503 D504 E505 E506 L507 A508 Q509

G510 R511 L512 L516 A517 N518 I519 Q520 E521 V522 N525 I526 A527 I528 K529 V530 T531 E532 Y533 L534 Y535 A536 N537 K538 R542 Y543 P546 E547 D548 K549 A550 K551 Y552 V553 K554 E555 R556 T557 W558 R559 S560 E561 Y562 L566 P567 D568 E571 W572 P573 GLU SER ALA SER SER

PRO PRO VAL ILE THR GLU

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	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAK, MG, 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	0.44	0/4447	0.64	0/5998
1	B	0.45	0/4447	0.64	0/5998
1	C	0.46	0/4447	0.65	0/5998
1	D	0.45	1/4447 (0.0%)	0.64	0/5998
All	All	0.45	1/17788 (0.0%)	0.64	0/23992

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185	CYS	CB-SG	-5.57	1.72	1.81

There are no bond angle outliers.

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	359	0
1	B	4367	0	4407	313	0
1	C	4367	0	4407	217	0
1	D	4367	0	4407	334	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	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
5	C	16	0	0	3	0
5	D	16	0	0	1	0
All	All	17931	0	17836	1198	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 34.

All (1198) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:371:GLU:CD	1:D:371:GLU:H	1.73	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
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:C:453:LYS:HE3	1:C:457:GLY:HA2	1.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:371:GLU:CD	1:B:371:GLU:H	1.84	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:A:38:MSE:HE3	1:A:59:GLU:CD	2.02	0.80
1:D:437:THR:O	1:D:440:ARG:HG3	1.82	0.79
1:B:505:GLU:CD	1:B:505:GLU:H	1.85	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:505:GLU:CD	1:B:505:GLU:N	2.40	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
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:D:249:ASN:C	1:D:249:ASN:HD22	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:300:LYS:HZ1	1:A:304:GLU:C	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:537:ASN:C	1:D:538:LYS:HG2	2.20	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
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: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:301:PRO:HG2	1:B:304:GLU:CD	2.21	0.61
1:B:64:GLN:NE2	1:B:562:TYR:OH	2.34	0.61
1:A:150:TRP:HE1	1:A:152:GLU:CD	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:36:LYS:HE3	1:D:562:TYR:HB3	1.84	0.59
1:D:89:GLN:HG2	1:D:131:LYS:HZ3	1.67	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:346:LYS:HZ3	1:B:346:LYS:HB2	1.66	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:B:315:ALA:HB3	1:B:392:VAL:HG21	1.82	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:85:ILE:HG13	1:C:86:MSE:N	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:175:TYR:HE2	1:D:218:TYR:HA	1.67	0.58
1:A:38:MSE:HE3	1:A:59:GLU:OE1	2.03	0.58
1:C:66:LEU:HD22	1:C:70:ARG:NH1	2.18	0.58
1:C:481:CYS:O	1:C:482:ASN:HB2	2.02	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:301:PRO:O	1:C:304:GLU:HG2	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HG	1:B:492:LEU:HD23	1.86	0.57
1:D:300:LYS:HE3	1:D:304:GLU:CB	2.24	0.57
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:413:ARG:HH21	1:A:440:ARG:C	2.08	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:24:LYS:O	1:D:22:LYS:NZ	2.36	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: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:D:363:GLU:OE1	1:D:363:GLU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:HZ3	1:B:562:TYR:HB3	1.72	0.55
1:B:75:MSE:HG2	1:B:80:GLU:CD	2.26	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:332:LEU:HG	1:A:336:GLU:CD	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:371:GLU:CD	1:D:371:GLU:N	2.51	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:D:166:ILE:HG13	1:D:172:LEU:HB2	1.89	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:C:127:PHE:CD2	1:D:38:MSE:HE2	2.43	0.54
1:B:516:LEU:HD12	1:B:516:LEU:O	2.08	0.54
1:C:153:ASN:C	1:C:153:ASN:HD22	2.11	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:A:456:ASP:CG	1:A:458:ARG:HH11	2.10	0.53
1:B:373:ILE:O	1:B:373:ILE:HG22	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:503:THR:OG1	1:C:506:GLU:HG3	2.09	0.53
1:D:38:MSE:HE3	1:D:59:GLU:CD	2.28	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:504:ASP:OD2	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:B:177:MSE:C	1:B:180:PRO:HD2	2.28	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:226:ASP:C	1:D:226:ASP:OD1	2.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:437:THR:O	1:D:438:GLU:HB2	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:C:456:ASP:OD1	1:C:456:ASP:C	2.50	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:226:ASP:OD1	1:A:226:ASP:C	2.48	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:A:551:LYS:HB3	1:A:551:LYS:HZ2	1.76	0.49
1:D:186:LEU:HD13	1:D:468:VAL:CG2	2.42	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:332:LEU:CD2	1:A:340:LYS:NZ	2.75	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: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:D:329:GLU:C	1:D:330:ASN:HD22	2.16	0.49
1:A:478:VAL:HG13	1:A:483:THR:HB	1.95	0.49
1:C:47:MSE:C	1:C:48:LEU:HD23	2.33	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:306:LYS:HZ3	1:C:306:LYS:HB2	1.77	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:D:174:VAL:C	1:D:176:GLY:H	2.17	0.48
1:A:174:VAL:C	1:A:176:GLY:H	2.16	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: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:C:441:CYS:C	1:C:442:LEU:HD23	2.34	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: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:A:332:LEU:CD2	1:A:340:LYS:HZ3	2.26	0.48
1:B:276:PHE:CD1	1:B:276:PHE:C	2.87	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:404:ILE:HG21	1:D:436:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:533:TYR:CE1	1:B:537:ASN:ND2	2.80	0.48
1:C:447:SER:HB3	1:C:448:PRO:HD2	1.96	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:295:GLN:HE22	1:A:299:SER:C	2.17	0.47
1:B:415:VAL:C	1:B:416:ILE:HD12	2.34	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: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:249:ASN:C	1:D:249:ASN:ND2	2.65	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:267:ARG:CZ	1:D:267:ARG:HB2	2.46	0.46
1:D:330:ASN:HD22	1:D:330:ASN:N	2.13	0.46
1:B:211:ALA:O	1:B:214:LYS:HG3	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:C	1:A:330:ASN:H	2.19	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:57:LYS:HZ3	1:B:59:GLU:HG2	1.81	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:B:401:PRO:HA	1:B:436:LEU:HD23	1.97	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: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
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:A:522:VAL:O	1:A:526:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:359:ASP:O	1:B:360:SER:C	2.54	0.45
1:B:524:ILE:O	1:B:528:ILE:CG1	2.64	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:ILE:HD12	1:C:85:ILE:C	2.38	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:130:PRO:C	1:C:131:LYS:HG2	2.38	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:A:174:VAL:C	1:A:176:GLY:N	2.71	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: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:C:286:VAL:HG11	1:C:466:ASN:C	2.38	0.43
1:D:197:ARG:NH1	1:D:197:ARG:HG2	2.33	0.43
1:A:332:LEU:HD23	1:A:340:LYS:HZ3	1.84	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
1:B:357:LYS:H	1:B:357:LYS:HG2	1.36	0.43
1:D:328:VAL:HA	1:D:332:LEU:O	2.18	0.43
1:D:359:ASP:O	1:D:360:SER:C	2.56	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: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:260:HIS:C	1:C:260:HIS:CD2	2.92	0.43
1:C:288:LEU:HG	1:C:292:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:503:THR:HG23	1:A:506:GLU:CD	2.39	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:298:ILE:O	1:D:299:SER:C	2.57	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: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:B:410:ILE:HG22	1:B:411:ASN:CG	2.39	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
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:D:301:PRO:O	1:D:302:ILE:C	2.57	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: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:174:VAL:C	1:D:176:GLY:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:137:ILE:HG13	1:A:137:ILE:O	2.18	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:528:ILE:HG23	1:B:550:ALA:HA	2.01	0.42
1:C:23:GLU:CD	1:C:24:LYS:H	2.22	0.42
1:C:25:GLY:C	1:C:27:PRO:HD2	2.40	0.42
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: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:253:GLN:NE2	1:A:278:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:344:PHE:C	1:D:344:PHE:CD2	2.92	0.42
1:A:53:LEU:N	1:A:53:LEU:HD23	2.34	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: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:209:ASN:OD1	1:A:209:ASN:C	2.58	0.42
1:A:434:TYR:CZ	1:A:443:PHE:HB3	2.55	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: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
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: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: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:D:217:PHE:O	1:D:218:TYR:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:HB3	1:A:300:LYS:NZ	2.28	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:D:22:LYS:HD3	1:D:22:LYS:C	2.40	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: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: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
1:A:268:LYS:O	1:A:268:LYS:HG2	2.20	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: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:150:TRP:NE1	1:A:152:GLU:CD	2.74	0.41
1:A:301:PRO:O	1:A:302:ILE:C	2.56	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:B:456:ASP:OD1	1:B:456:ASP:C	2.59	0.41
1:B:503:THR:OG1	1:B:506:GLU:OE1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:332:LEU:HD23	1:A:340:LYS:HZ1	1.86	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:502:LEU:HD21	1:A:506:GLU:HB2	2.03	0.41
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:329:GLU:O	1:A:329:GLU:HG3	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:346:LYS:HB2	1:B:346:LYS:NZ	2.32	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:D:533:TYR:C	1:D:533:TYR:CD2	2.95	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
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: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:C:217:PHE:O	1:C:218:TYR:C	2.59	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

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%)	17	35
1	B	551/584 (94%)	512 (93%)	32 (6%)	7 (1%)	12	24
1	C	551/584 (94%)	513 (93%)	34 (6%)	4 (1%)	22	43
1	D	551/584 (94%)	499 (91%)	43 (8%)	9 (2%)	9	19
All	All	2204/2336 (94%)	2036 (92%)	143 (6%)	25 (1%)	14	30

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	LEU
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 (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%)	374 (80%)	95 (20%)	1 2
1	C	469/483 (97%)	380 (81%)	89 (19%)	1 2
1	D	469/483 (97%)	356 (76%)	113 (24%)	0 1
All	All	1876/1932 (97%)	1481 (79%)	395 (21%)	1 2

All (395) 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	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	91	ARG
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	123	TYR
1	A	133	LEU
1	A	137	ILE
1	A	138	SER
1	A	140	ARG

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Mol	Chain	Res	Type
1	A	144	ARG
1	A	152	GLU
1	A	153	ASN
1	A	169	LEU
1	A	197	ARG
1	A	205	VAL
1	A	212	LEU
1	A	219	MSE
1	A	221	LEU
1	A	224	LYS
1	A	227	ARG
1	A	228	THR
1	A	238	PHE
1	A	239	MSE
1	A	248	ARG
1	A	251	LEU
1	A	260	HIS
1	A	267	ARG
1	A	272	LYS
1	A	283	THR
1	A	286	VAL
1	A	292	LEU
1	A	295	GLN
1	A	296	LYS
1	A	297	VAL
1	A	300	LYS
1	A	306	LYS
1	A	322	LEU
1	A	327	MSE
1	A	330	ASN
1	A	334	GLU
1	A	335	GLN
1	A	336	GLU
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	392	VAL
1	A	397	ARG
1	A	398	LEU

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Mol	Chain	Res	Type
1	A	400	THR
1	A	402	ASP
1	A	409	SER
1	A	413	ARG
1	A	419	LEU
1	A	423	THR
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	464	GLN
1	A	484	ARG
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	518	ASN
1	A	520	GLN
1	A	529	LYS
1	A	542	ARG
1	A	547	GLU
1	A	551	LYS
1	A	554	LYS
1	A	556	ARG
1	A	559	ARG
1	A	561	GLU
1	B	22	LYS
1	B	24	LYS
1	B	43	GLN
1	B	47	MSE
1	B	50	LEU
1	B	51	GLN
1	B	66	LEU
1	B	73	LYS
1	B	85	ILE
1	B	94	LYS

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Mol	Chain	Res	Type
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	165	ARG
1	B	177	MSE
1	B	197	ARG
1	B	208	ASP
1	B	214	LYS
1	B	223	GLN
1	B	224	LYS
1	B	225	ARG
1	B	227	ARG
1	B	229	GLN
1	B	232	ASP
1	B	233	ASP
1	B	236	ASP
1	B	239	MSE
1	B	240	LYS
1	B	248	ARG
1	B	267	ARG
1	B	270	ARG
1	B	292	LEU
1	B	297	VAL
1	B	300	LYS
1	B	301	PRO
1	B	303	SER
1	B	306	LYS
1	B	310	LEU
1	B	319	ILE
1	B	321	ASN
1	B	326	SER
1	B	334	GLU
1	B	339	LYS
1	B	340	LYS
1	B	350	LEU
1	B	351	VAL

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Mol	Chain	Res	Type
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	397	ARG
1	B	398	LEU
1	B	402	ASP
1	B	405	ARG
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	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	514	PRO
1	B	516	LEU
1	B	518	ASN
1	B	520	GLN
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	561	GLU

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Mol	Chain	Res	Type
1	B	564	SER
1	C	21	ILE
1	C	23	GLU
1	C	26	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	125	HIS
1	C	131	LYS
1	C	140	ARG
1	C	153	ASN
1	C	165	ARG
1	C	169	LEU
1	C	177	MSE
1	C	183	LYS
1	C	197	ARG
1	C	210	ILE
1	C	214	LYS
1	C	221	LEU
1	C	223	GLN
1	C	225	ARG
1	C	230	GLN
1	C	235	ILE
1	C	236	ASP
1	C	240	LYS
1	C	248	ARG
1	C	249	ASN
1	C	251	LEU
1	C	267	ARG
1	C	286	VAL
1	C	291	LEU
1	C	292	LEU

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Mol	Chain	Res	Type
1	C	297	VAL
1	C	304	GLU
1	C	306	LYS
1	C	314	GLU
1	C	321	ASN
1	C	335	GLN
1	C	339	LYS
1	C	340	LYS
1	C	345	ASP
1	C	355	LYS
1	C	357	LYS
1	C	363	GLU
1	C	368	SER
1	C	375	ASP
1	C	384	LEU
1	C	397	ARG
1	C	398	LEU
1	C	404	ILE
1	C	409	SER
1	C	419	LEU
1	C	428	CYS
1	C	436	LEU
1	C	438	GLU
1	C	454	LEU
1	C	455	THR
1	C	461	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	538	LYS
1	C	542	ARG
1	C	543	TYR
1	C	545	GLU
1	C	547	GLU

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Mol	Chain	Res	Type
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	22	LYS
1	D	23	GLU
1	D	24	LYS
1	D	29	MSE
1	D	36	LYS
1	D	51	GLN
1	D	60	THR
1	D	62	ASP
1	D	66	LEU
1	D	70	ARG
1	D	74	LYS
1	D	75	MSE
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	125	HIS
1	D	133	LEU
1	D	140	ARG
1	D	144	ARG
1	D	152	GLU
1	D	153	ASN
1	D	156	LYS
1	D	165	ARG
1	D	169	LEU
1	D	177	MSE
1	D	183	LYS
1	D	197	ARG
1	D	205	VAL
1	D	210	ILE
1	D	214	LYS
1	D	221	LEU

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Mol	Chain	Res	Type
1	D	227	ARG
1	D	229	GLN
1	D	236	ASP
1	D	237	GLU
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
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	327	MSE
1	D	329	GLU
1	D	333	SER
1	D	335	GLN
1	D	336	GLU
1	D	339	LYS
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	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

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Mol	Chain	Res	Type
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
1	D	492	LEU
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	529	LYS
1	D	531	THR
1	D	534	LEU
1	D	535	TYR
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 (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	71	ASN

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Mol	Chain	Res	Type
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	43	GLN
1	B	51	GLN
1	B	64	GLN
1	B	69	HIS
1	B	154	HIS
1	B	229	GLN
1	B	338	GLN
1	B	362	GLN
1	B	367	HIS
1	B	425	GLN
1	B	482	ASN
1	B	501	GLN
1	B	518	ASN
1	B	520	GLN
1	C	64	GLN
1	C	69	HIS
1	C	71	ASN
1	C	153	ASN
1	C	229	GLN
1	C	261	ASN
1	C	321	ASN
1	C	335	GLN
1	C	362	GLN
1	C	425	GLN
1	C	482	ASN
1	C	520	GLN
1	D	51	GLN
1	D	64	GLN
1	D	69	HIS
1	D	122	GLN
1	D	153	ASN
1	D	154	HIS
1	D	230	GLN
1	D	249	ASN

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Mol	Chain	Res	Type
1	D	261	ASN
1	D	305	HIS
1	D	330	ASN
1	D	425	GLN
1	D	482	ASN
1	D	518	ASN
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 monosaccharides 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	-	42,48,48	2.03	11 (26%)	50,73,73	1.26	4 (8%)
3	NAD	B	1601	-	42,48,48	1.89	10 (23%)	50,73,73	1.38	5 (10%)
3	NAD	C	2602	-	42,48,48	2.19	10 (23%)	50,73,73	1.43	6 (12%)
4	MAK	D	3603	2	7,7,7	2.13	5 (71%)	8,9,9	1.88	4 (50%)
3	NAD	A	602	-	42,48,48	2.12	10 (23%)	50,73,73	1.46	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	D	3601	-	42,48,48	2.15	11 (26%)	50,73,73	1.30	3 (6%)
3	NAD	C	2601	-	42,48,48	2.05	11 (26%)	50,73,73	1.32	6 (12%)
4	MAK	A	603	2	7,7,7	1.77	3 (42%)	8,9,9	1.87	4 (50%)
4	MAK	B	1603	2	7,7,7	2.35	5 (71%)	8,9,9	1.85	3 (37%)
3	NAD	B	1602	-	42,48,48	2.15	10 (23%)	50,73,73	1.45	6 (12%)
4	MAK	C	2603	2	7,7,7	1.99	4 (57%)	8,9,9	1.88	3 (37%)
3	NAD	D	3602	-	42,48,48	2.07	9 (21%)	50,73,73	1.46	6 (12%)

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	-	-	2/26/62/62	0/5/5/5
3	NAD	B	1601	-	-	5/26/62/62	0/5/5/5
3	NAD	C	2602	-	-	5/26/62/62	0/5/5/5
4	MAK	D	3603	2	-	1/8/8/8	-
3	NAD	A	602	-	-	4/26/62/62	0/5/5/5
3	NAD	D	3601	-	-	3/26/62/62	0/5/5/5
3	NAD	C	2601	-	-	8/26/62/62	0/5/5/5
4	MAK	A	603	2	-	4/8/8/8	-
4	MAK	B	1603	2	-	1/8/8/8	-
3	NAD	B	1602	-	-	5/26/62/62	0/5/5/5
4	MAK	C	2603	2	-	4/8/8/8	-
3	NAD	D	3602	-	-	5/26/62/62	0/5/5/5

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3602	NAD	C2N-N1N	7.51	1.44	1.35
3	A	602	NAD	C2N-N1N	7.51	1.44	1.35
3	B	1602	NAD	C2N-N1N	7.50	1.44	1.35
3	C	2602	NAD	C2N-N1N	7.15	1.43	1.35
3	C	2601	NAD	C2N-N1N	6.43	1.42	1.35
3	A	601	NAD	C2N-N1N	6.42	1.42	1.35
3	D	3601	NAD	C2N-N1N	6.06	1.42	1.35
3	C	2602	NAD	O4B-C1B	5.62	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	NAD	O4D-C1D	5.32	1.48	1.41
3	C	2602	NAD	O4D-C1D	5.14	1.48	1.41
3	C	2601	NAD	C3N-C7N	5.03	1.58	1.50
3	D	3601	NAD	O4D-C1D	4.86	1.47	1.41
3	D	3601	NAD	C3N-C7N	4.78	1.57	1.50
3	B	1601	NAD	C2N-N1N	4.52	1.40	1.35
3	B	1602	NAD	O4B-C1B	4.46	1.47	1.41
3	D	3601	NAD	O4B-C1B	4.45	1.47	1.41
3	A	602	NAD	O4B-C1B	4.45	1.47	1.41
3	D	3602	NAD	O4B-C1B	4.38	1.47	1.41
3	A	601	NAD	O4D-C1D	4.19	1.46	1.41
3	D	3602	NAD	O4D-C1D	4.07	1.46	1.41
3	A	601	NAD	C2A-N3A	4.03	1.38	1.32
4	B	1603	MAK	C3-C2	-4.00	1.50	1.54
3	A	601	NAD	O4B-C1B	3.98	1.46	1.41
3	A	602	NAD	C2A-N3A	3.98	1.38	1.32
3	B	1601	NAD	C3N-C7N	3.97	1.56	1.50
3	C	2602	NAD	C2A-N3A	3.97	1.38	1.32
3	D	3601	NAD	C6N-N1N	3.95	1.45	1.35
3	A	602	NAD	O4D-C1D	3.95	1.46	1.41
3	A	602	NAD	C6N-N1N	3.84	1.44	1.35
3	C	2602	NAD	C6N-N1N	3.83	1.44	1.35
3	B	1602	NAD	C6N-N1N	3.78	1.44	1.35
3	D	3602	NAD	C6N-N1N	3.74	1.44	1.35
3	A	601	NAD	C6N-N1N	3.68	1.44	1.35
3	B	1601	NAD	C2D-C1D	-3.67	1.48	1.53
3	A	601	NAD	C3N-C7N	3.61	1.56	1.50
3	B	1601	NAD	O4B-C1B	3.61	1.46	1.41
3	C	2601	NAD	C2A-N3A	3.56	1.37	1.32
3	C	2601	NAD	C2B-C1B	-3.54	1.48	1.53
3	B	1602	NAD	C2A-N3A	3.51	1.37	1.32
3	D	3602	NAD	C2A-N3A	3.39	1.37	1.32
3	B	1601	NAD	C6N-N1N	3.37	1.43	1.35
3	D	3601	NAD	C2A-N3A	3.36	1.37	1.32
3	B	1602	NAD	C3N-C7N	3.30	1.55	1.50
3	D	3602	NAD	C3N-C7N	3.28	1.55	1.50
3	C	2601	NAD	C6N-N1N	3.28	1.43	1.35
3	A	602	NAD	C3N-C7N	3.27	1.55	1.50
3	C	2601	NAD	C2D-C1D	-3.26	1.48	1.53
3	C	2602	NAD	C3N-C7N	3.24	1.55	1.50
4	D	3603	MAK	C3-C2	-3.22	1.51	1.54
3	B	1601	NAD	C2A-N3A	3.20	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3601	NAD	C4N-C3N	3.18	1.44	1.39
3	B	1601	NAD	O4D-C1D	3.11	1.45	1.41
3	D	3601	NAD	C5A-C4A	-3.00	1.33	1.40
3	B	1601	NAD	C5A-C4A	-2.88	1.33	1.40
3	C	2601	NAD	C5A-C4A	-2.88	1.33	1.40
3	D	3601	NAD	C2D-C1D	-2.80	1.49	1.53
3	C	2601	NAD	O4B-C1B	2.73	1.44	1.41
3	A	601	NAD	C5A-C4A	-2.70	1.33	1.40
3	D	3602	NAD	C5A-C4A	-2.61	1.34	1.40
3	B	1601	NAD	C2B-C1B	-2.56	1.49	1.53
4	C	2603	MAK	C3-C2	-2.54	1.52	1.54
3	D	3601	NAD	C5A-N7A	-2.53	1.30	1.39
3	A	602	NAD	C5A-N7A	-2.53	1.30	1.39
4	A	603	MAK	O3-C2	2.51	1.28	1.23
3	A	601	NAD	C4N-C3N	2.51	1.43	1.39
3	A	602	NAD	C5A-C4A	-2.48	1.34	1.40
3	C	2601	NAD	O4D-C1D	2.48	1.44	1.41
4	B	1603	MAK	O5-C3	-2.46	1.23	1.30
3	D	3601	NAD	C2B-C1B	-2.45	1.50	1.53
4	D	3603	MAK	O5-C3	-2.43	1.23	1.30
4	C	2603	MAK	O2-C1	-2.43	1.23	1.30
3	A	601	NAD	C2D-C1D	-2.42	1.50	1.53
3	C	2601	NAD	C5A-N7A	-2.41	1.31	1.39
4	C	2603	MAK	O3-C2	2.41	1.28	1.23
4	B	1603	MAK	O3-C2	2.39	1.28	1.23
4	D	3603	MAK	O3-C2	2.36	1.28	1.23
3	D	3602	NAD	C5A-N7A	-2.33	1.31	1.39
4	B	1603	MAK	O2-C1	-2.32	1.23	1.30
4	D	3603	MAK	O2-C1	-2.29	1.23	1.30
4	B	1603	MAK	C1-C2	-2.29	1.52	1.54
4	A	603	MAK	O2-C1	-2.28	1.23	1.30
3	A	602	NAD	C4N-C3N	2.26	1.43	1.39
3	B	1602	NAD	O4D-C4D	2.24	1.50	1.45
3	B	1601	NAD	C5A-N7A	-2.24	1.31	1.39
3	B	1602	NAD	C5A-C4A	-2.22	1.35	1.40
4	C	2603	MAK	O5-C3	-2.22	1.24	1.30
4	A	603	MAK	O5-C3	-2.21	1.24	1.30
3	A	601	NAD	C2A-N1A	2.19	1.38	1.33
3	C	2602	NAD	C5A-N7A	-2.19	1.31	1.39
3	C	2602	NAD	C2A-N1A	2.19	1.38	1.33
3	C	2602	NAD	C5A-C4A	-2.18	1.35	1.40
3	B	1602	NAD	C4N-C3N	2.17	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	NAD	C2A-N1A	2.16	1.37	1.33
3	C	2602	NAD	C4N-C3N	2.15	1.43	1.39
3	A	601	NAD	C5A-N7A	-2.15	1.31	1.39
4	D	3603	MAK	C1-C2	-2.07	1.52	1.54
3	D	3602	NAD	C4N-C3N	2.07	1.42	1.39
3	C	2601	NAD	C5N-C4N	2.05	1.43	1.38
3	A	602	NAD	C2A-N1A	2.02	1.37	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1601	NAD	N3A-C2A-N1A	-5.33	120.34	128.68
3	D	3602	NAD	N3A-C2A-N1A	-5.10	120.71	128.68
3	D	3601	NAD	N3A-C2A-N1A	-5.07	120.76	128.68
3	C	2601	NAD	N3A-C2A-N1A	-4.95	120.94	128.68
3	A	602	NAD	N3A-C2A-N1A	-4.94	120.96	128.68
3	A	601	NAD	N3A-C2A-N1A	-4.86	121.09	128.68
3	C	2602	NAD	N3A-C2A-N1A	-4.84	121.11	128.68
3	B	1602	NAD	N3A-C2A-N1A	-4.78	121.21	128.68
3	B	1601	NAD	C4A-C5A-N7A	4.35	113.93	109.40
3	D	3601	NAD	C4A-C5A-N7A	4.31	113.89	109.40
3	A	602	NAD	C4A-C5A-N7A	4.25	113.83	109.40
3	A	601	NAD	C4A-C5A-N7A	4.22	113.80	109.40
3	D	3602	NAD	C4A-C5A-N7A	4.12	113.69	109.40
3	C	2601	NAD	C4A-C5A-N7A	4.12	113.69	109.40
3	B	1602	NAD	C4A-C5A-N7A	4.11	113.68	109.40
3	C	2602	NAD	C4A-C5A-N7A	3.96	113.53	109.40
3	B	1602	NAD	C3D-C2D-C1D	3.77	106.65	100.98
3	C	2602	NAD	C3D-C2D-C1D	3.75	106.63	100.98
3	A	602	NAD	C3D-C2D-C1D	3.70	106.55	100.98
3	D	3602	NAD	C3D-C2D-C1D	3.44	106.16	100.98
3	D	3602	NAD	C3B-C2B-C1B	3.16	105.74	100.98
3	A	602	NAD	C3B-C2B-C1B	3.12	105.67	100.98
3	B	1602	NAD	C3B-C2B-C1B	3.07	105.60	100.98
3	C	2602	NAD	C3B-C2B-C1B	3.05	105.57	100.98
3	A	602	NAD	C6N-N1N-C2N	-2.86	119.37	121.97
4	C	2603	MAK	O2-C1-C2	2.82	121.33	113.22
3	D	3602	NAD	C6N-N1N-C2N	-2.73	119.49	121.97
4	B	1603	MAK	O2-C1-C2	2.68	120.93	113.22
3	B	1602	NAD	C6N-N1N-C2N	-2.67	119.54	121.97
4	A	603	MAK	O2-C1-C2	2.62	120.77	113.22
3	B	1601	NAD	C3N-C7N-N7N	-2.53	114.71	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2602	NAD	C6N-N1N-C2N	-2.50	119.69	121.97
4	D	3603	MAK	O2-C1-C2	2.48	120.36	113.22
4	D	3603	MAK	O3-C2-C1	2.43	123.78	117.81
4	B	1603	MAK	O3-C2-C1	2.43	123.77	117.81
3	C	2601	NAD	C3N-C7N-N7N	-2.40	114.87	117.75
4	D	3603	MAK	O5-C3-C2	2.35	119.97	113.22
3	D	3601	NAD	C3D-C2D-C1D	2.27	104.40	100.98
4	A	603	MAK	O5-C3-C2	2.26	119.72	113.22
4	A	603	MAK	O3-C2-C1	2.25	123.32	117.81
4	C	2603	MAK	O3-C2-C1	2.25	123.32	117.81
3	A	601	NAD	C3B-C2B-C1B	2.25	104.36	100.98
3	B	1602	NAD	C2D-C3D-C4D	2.23	106.98	102.64
3	B	1601	NAD	C3D-C2D-C1D	2.20	104.28	100.98
3	C	2601	NAD	C3D-C2D-C1D	2.18	104.25	100.98
3	C	2601	NAD	O7N-C7N-C3N	2.18	122.24	119.63
4	C	2603	MAK	O5-C3-C2	2.17	119.47	113.22
4	B	1603	MAK	O5-C3-C2	2.14	119.39	113.22
3	A	601	NAD	C3D-C2D-C1D	2.14	104.20	100.98
3	A	602	NAD	C2D-C3D-C4D	2.13	106.79	102.64
3	C	2602	NAD	C2D-C3D-C4D	2.13	106.78	102.64
3	B	1601	NAD	C3B-C2B-C1B	2.13	104.18	100.98
4	D	3603	MAK	O3-C2-C3	2.12	123.00	117.81
3	C	2601	NAD	C3B-C2B-C1B	2.04	104.05	100.98
3	D	3602	NAD	C2D-C3D-C4D	2.04	106.60	102.64
4	A	603	MAK	O3-C2-C3	2.00	122.73	117.81

There are no chirality outliers.

All (47) 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

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Mol	Chain	Res	Type	Atoms
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
4	B	1603	MAK	O1-C1-C2-O3
4	D	3603	MAK	O1-C1-C2-O3
3	B	1602	NAD	C4D-C5D-O5D-PN
3	B	1602	NAD	PA-O3-PN-O5D
3	C	2602	NAD	PA-O3-PN-O5D
3	A	602	NAD	C4D-C5D-O5D-PN
3	C	2602	NAD	C4D-C5D-O5D-PN
3	D	3602	NAD	C4D-C5D-O5D-PN
3	C	2602	NAD	C5B-O5B-PA-O2A
4	A	603	MAK	O1-C1-C2-C3
4	C	2603	MAK	O1-C1-C2-C3
4	A	603	MAK	O2-C1-C2-O3
4	C	2603	MAK	O2-C1-C2-O3
3	C	2601	NAD	O4B-C4B-C5B-O5B
4	A	603	MAK	O2-C1-C2-C3
4	C	2603	MAK	O2-C1-C2-C3
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	B	1601	NAD	C2D-C1D-N1N-C2N
3	D	3601	NAD	O4B-C4B-C5B-O5B
3	C	2601	NAD	PN-O3-PA-O2A
3	B	1602	NAD	C5D-O5D-PN-O1N
3	D	3602	NAD	C5D-O5D-PN-O1N
3	A	601	NAD	O4B-C4B-C5B-O5B
3	C	2601	NAD	C3B-C4B-C5B-O5B

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
3	B	1601	NAD	4	0

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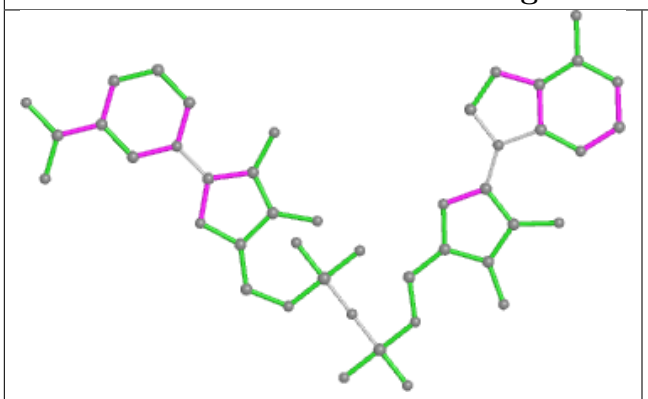
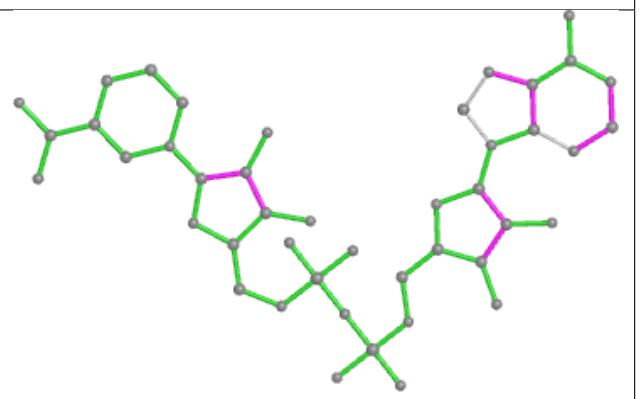
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3603	MAK	2	0
3	A	602	NAD	1	0
3	D	3601	NAD	3	0
3	C	2601	NAD	3	0
4	A	603	MAK	1	0
4	B	1603	MAK	1	0
3	B	1602	NAD	1	0
4	C	2603	MAK	1	0

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 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.

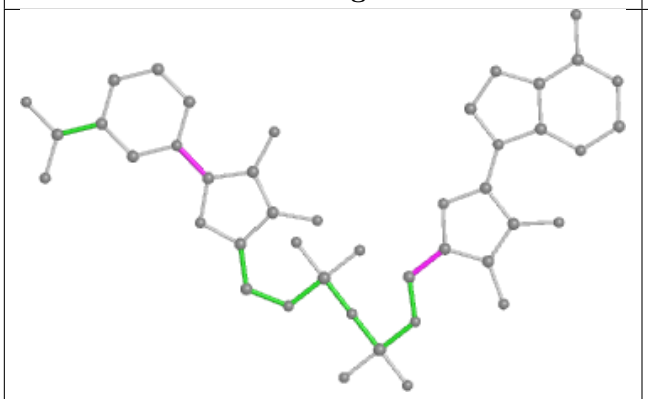
Ligand NAD A 601



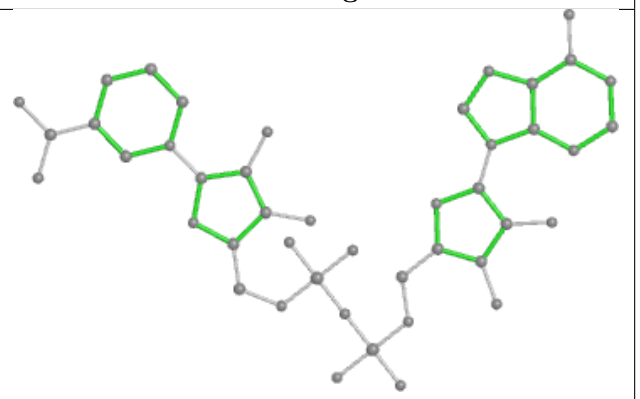
Bond lengths



Bond angles

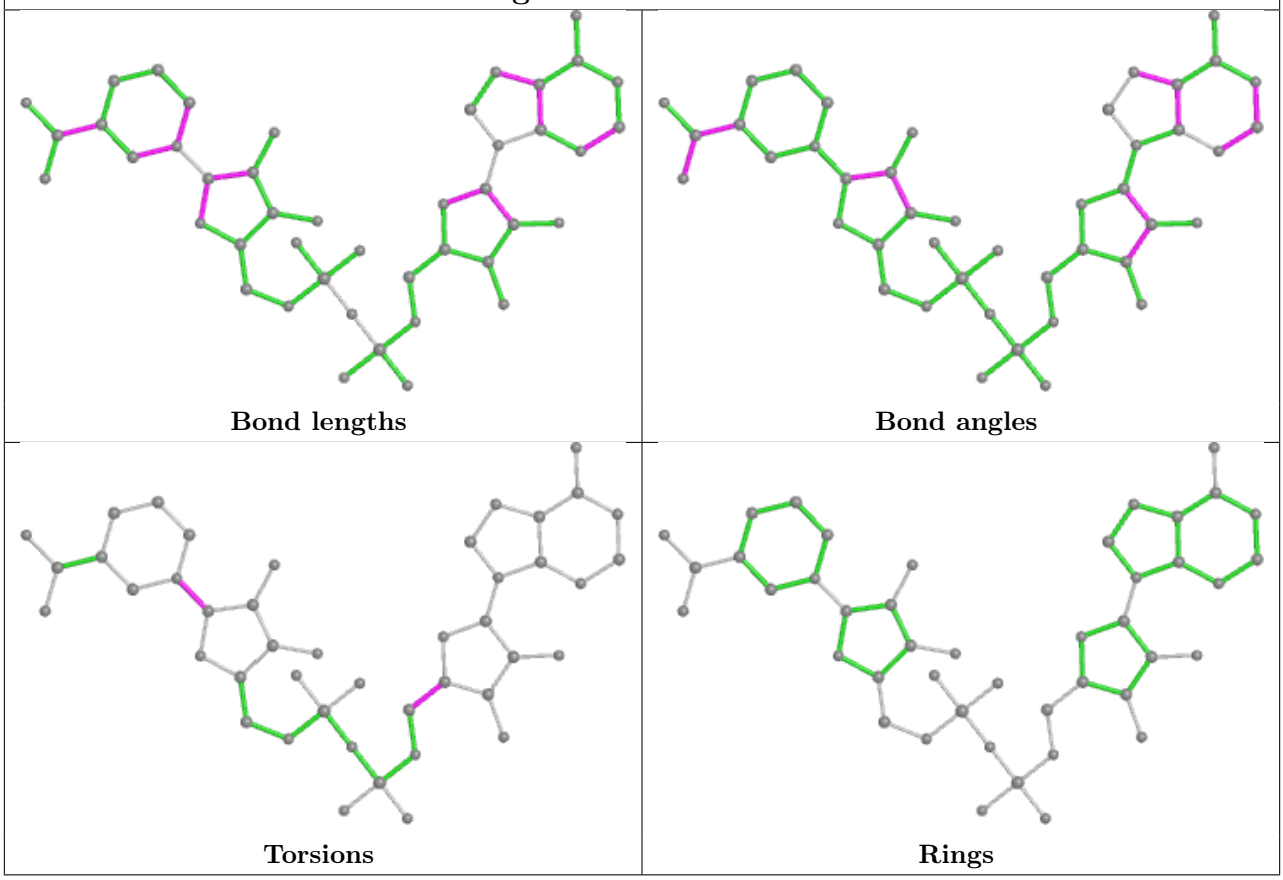


Torsions

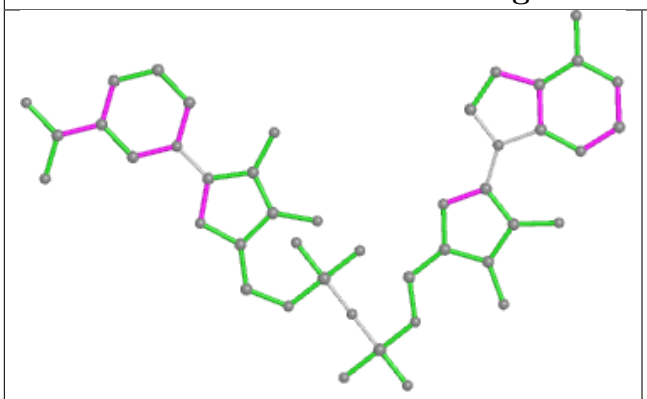


Rings

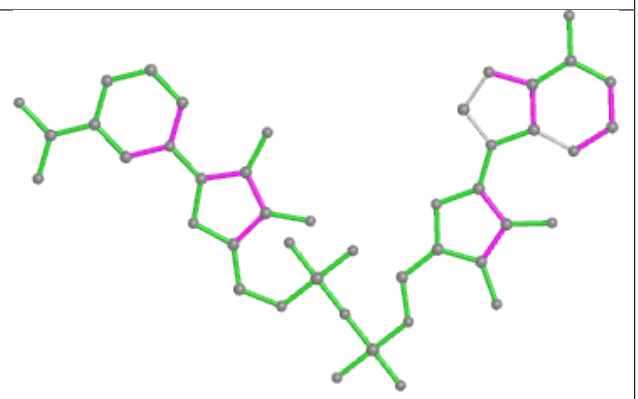
Ligand NAD B 1601



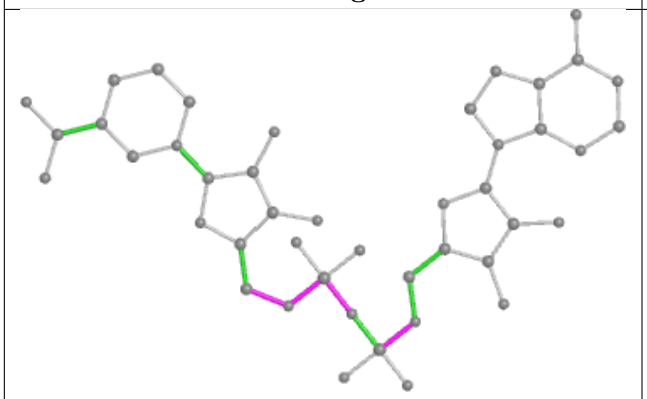
Ligand NAD C 2602



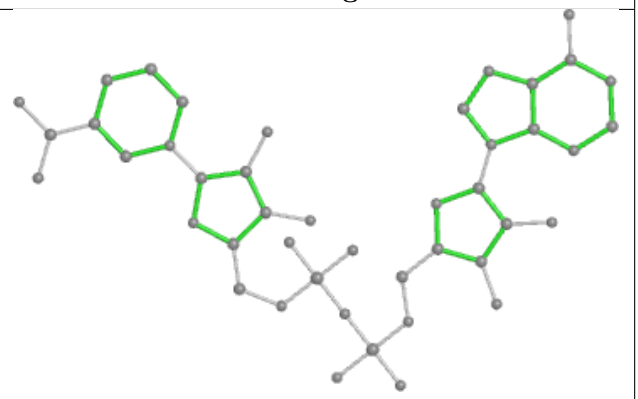
Bond lengths



Bond angles

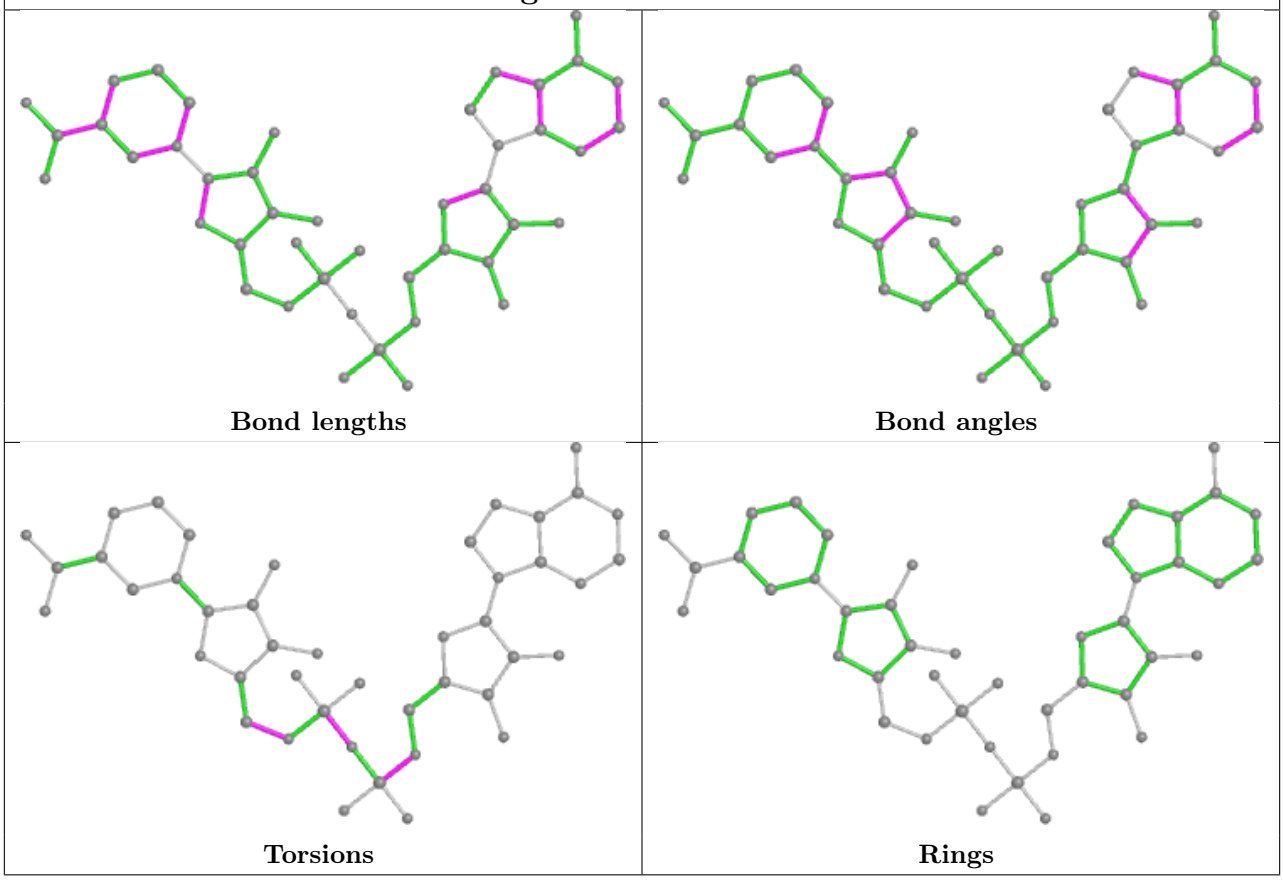


Torsions

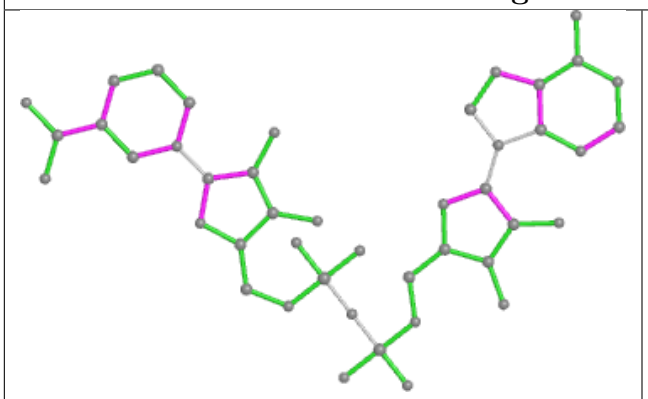


Rings

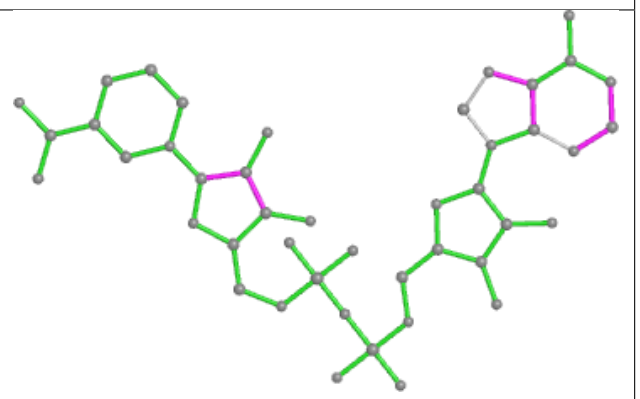
Ligand NAD A 602



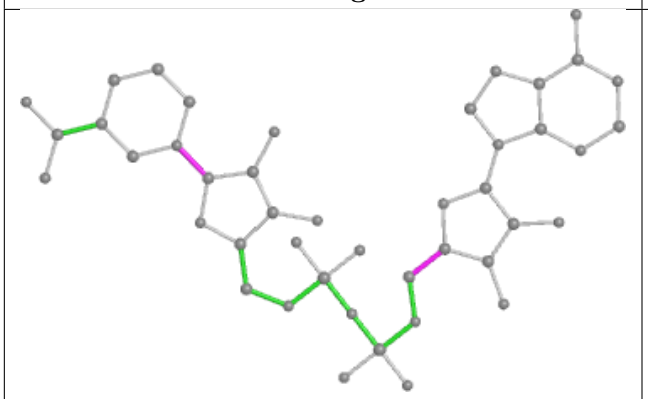
Ligand NAD D 3601



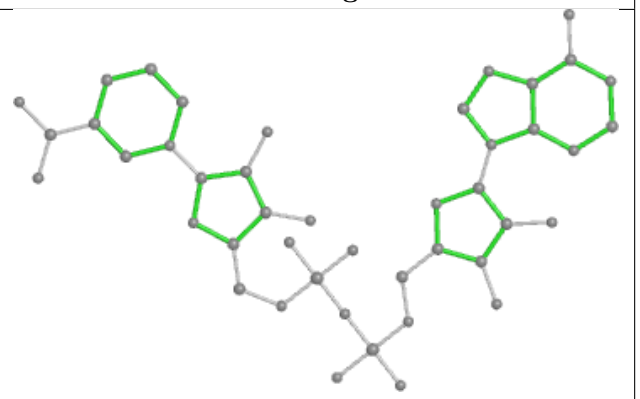
Bond lengths



Bond angles

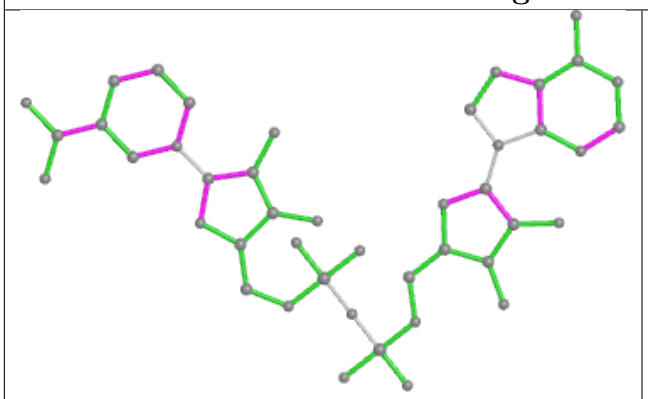


Torsions

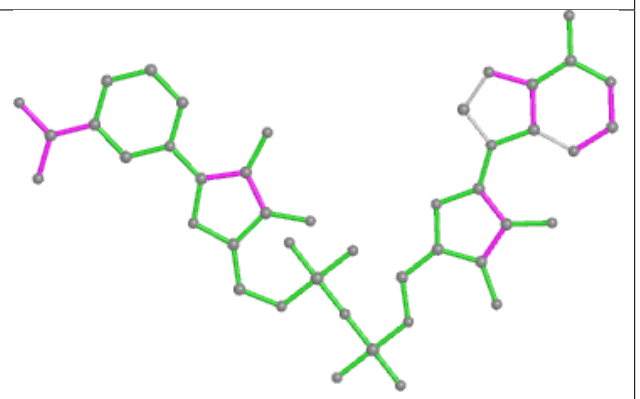


Rings

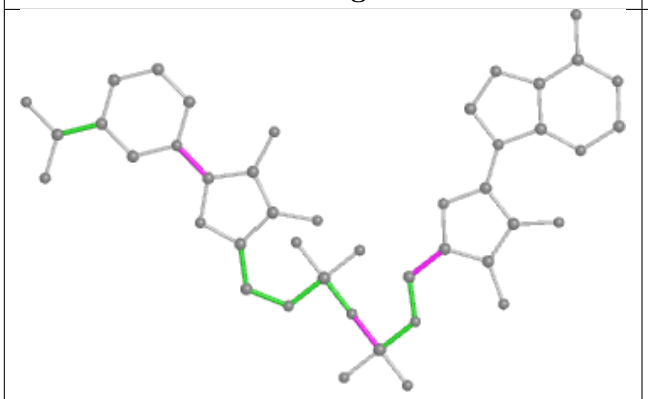
Ligand NAD C 2601



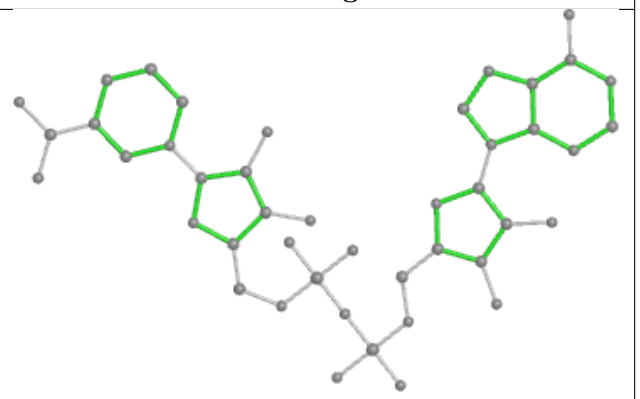
Bond lengths



Bond angles

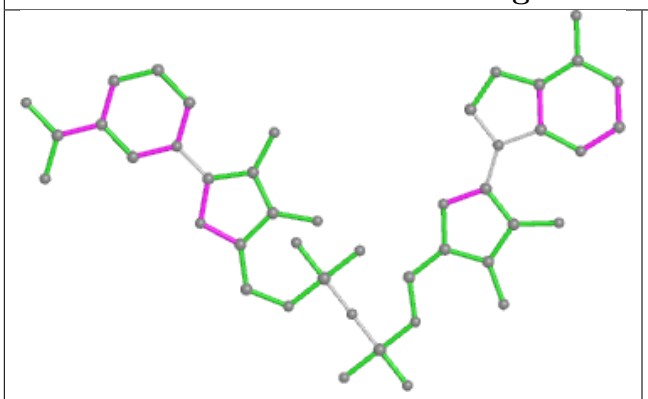


Torsions

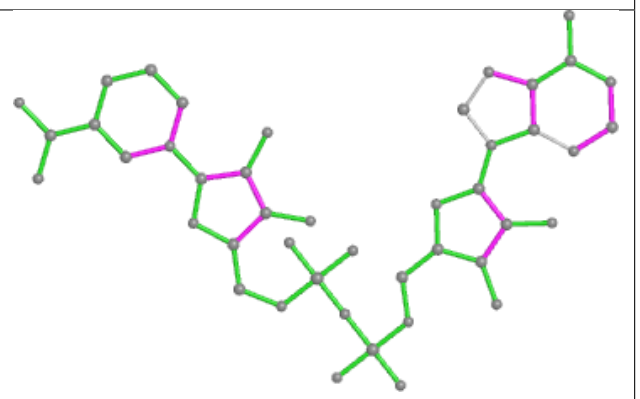


Rings

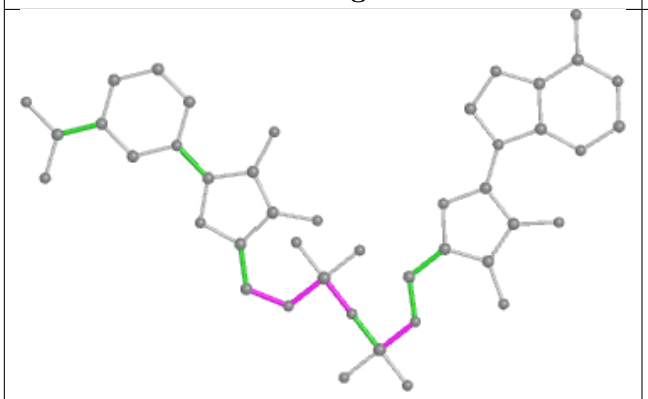
Ligand NAD B 1602



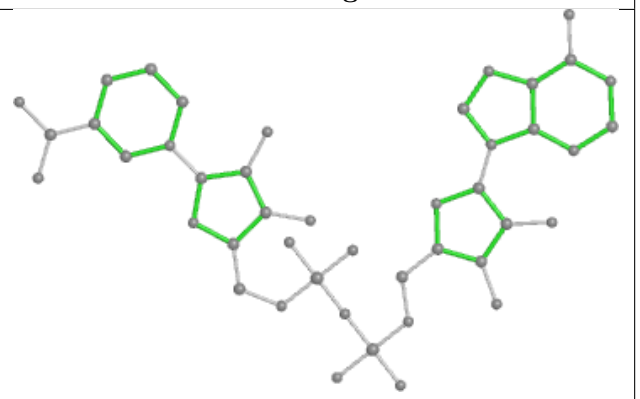
Bond lengths



Bond angles

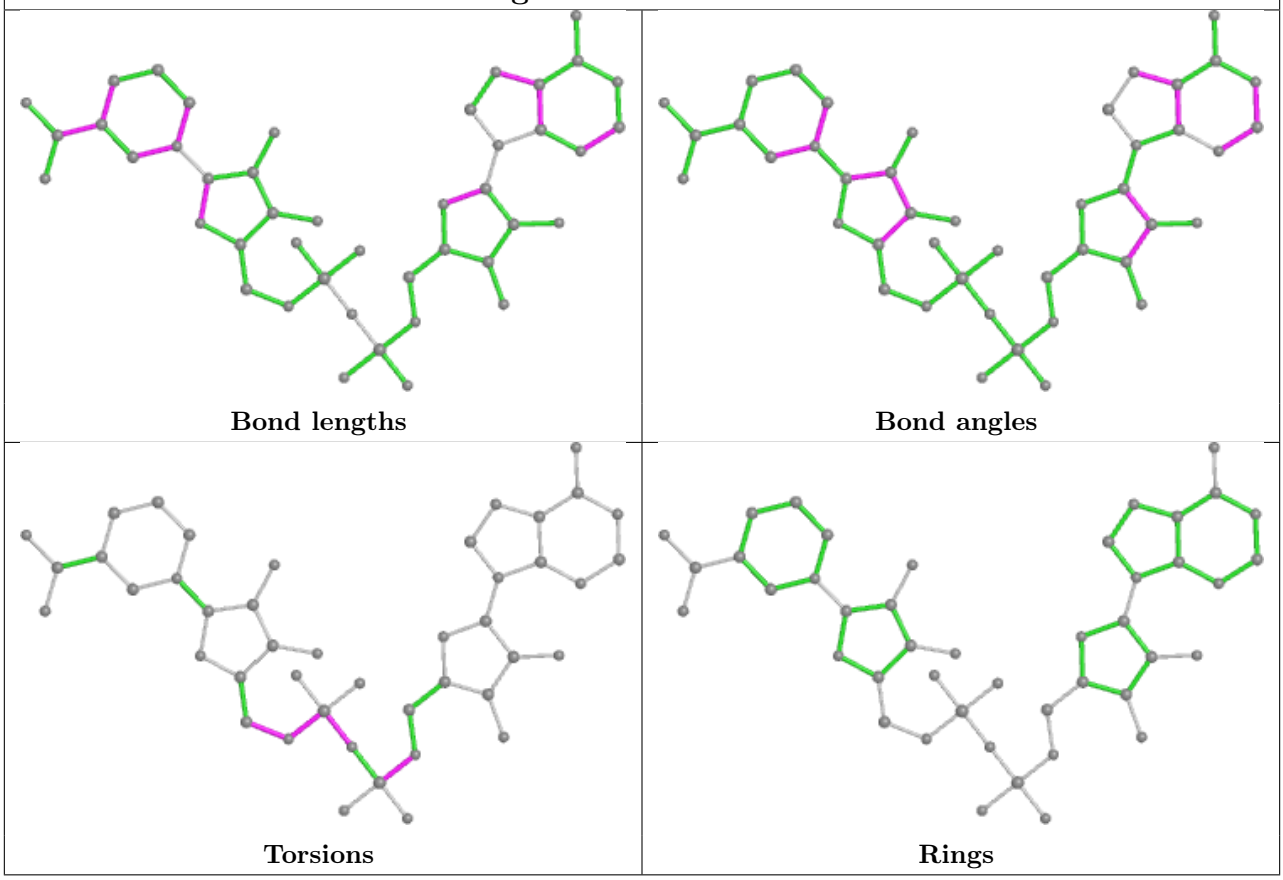


Torsions



Rings

Ligand NAD D 3602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.