



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 1DO8 / pdb_00001do8
Title : CRYSTAL STRUCTURE OF A CLOSED FORM OF HUMAN MITOCHONDRIAL NAD(P)⁺-DEPENDENT MALIC ENZYME
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on : 1999-12-19
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

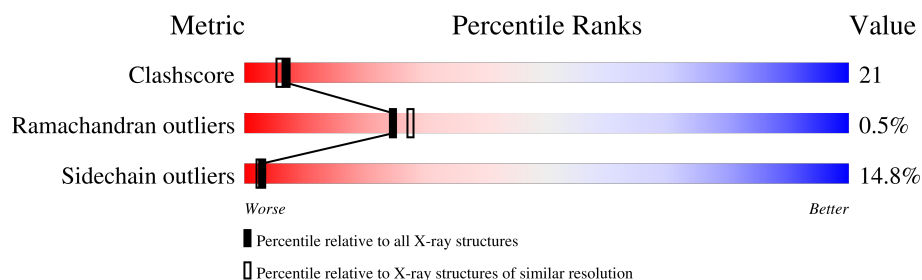
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	564	 57% 32% 9% .
1	B	564	 53% 37% 7% .
1	C	564	 60% 31% 7% .
1	D	564	 60% 30% 8% .

2 Entry composition [i](#)

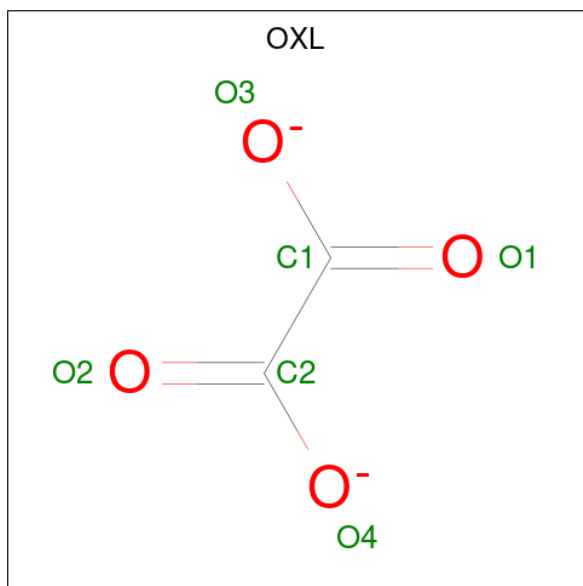
There are 5 unique types of molecules in this entry. The entry contains 18807 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MALIC ENZYME.

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

- Molecule 2 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		
2	B	1	Total	C	O	0	0
			6	2	4		

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

- Molecule 5 is water.

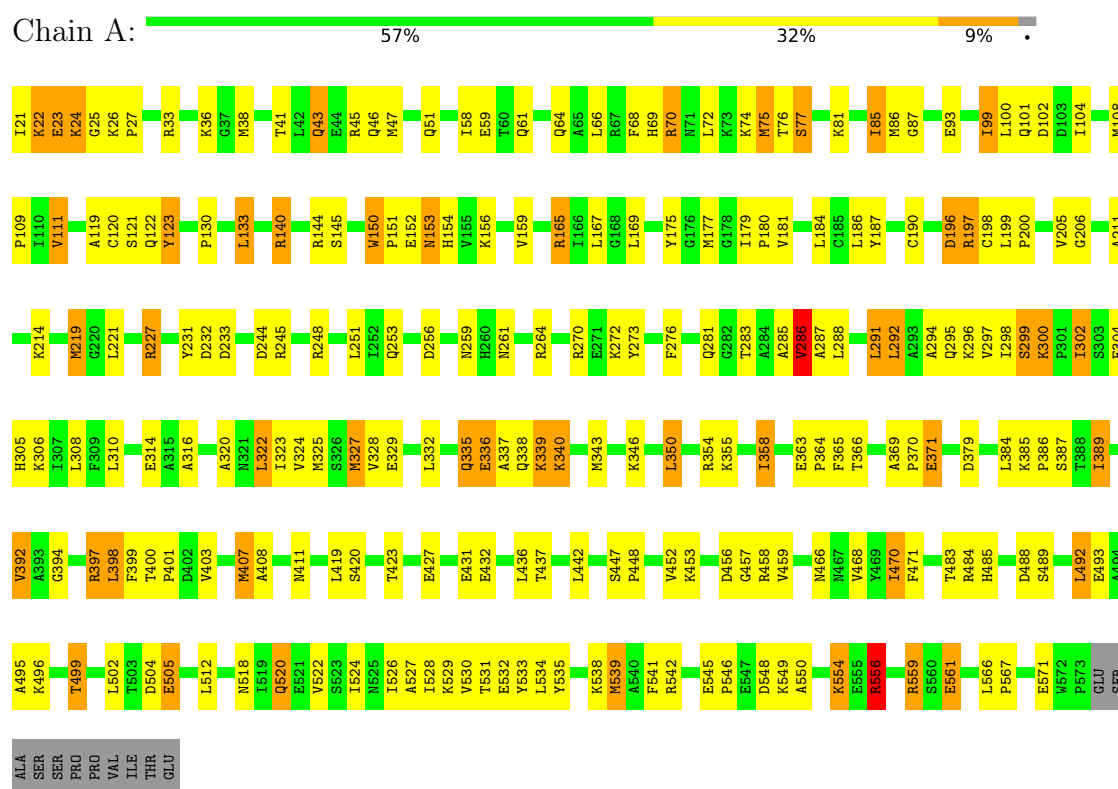
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		
5	B	199	Total	O	0	0
			199	199		
5	C	275	Total	O	0	0
			275	275		
5	D	246	Total	O	0	0
			246	246		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

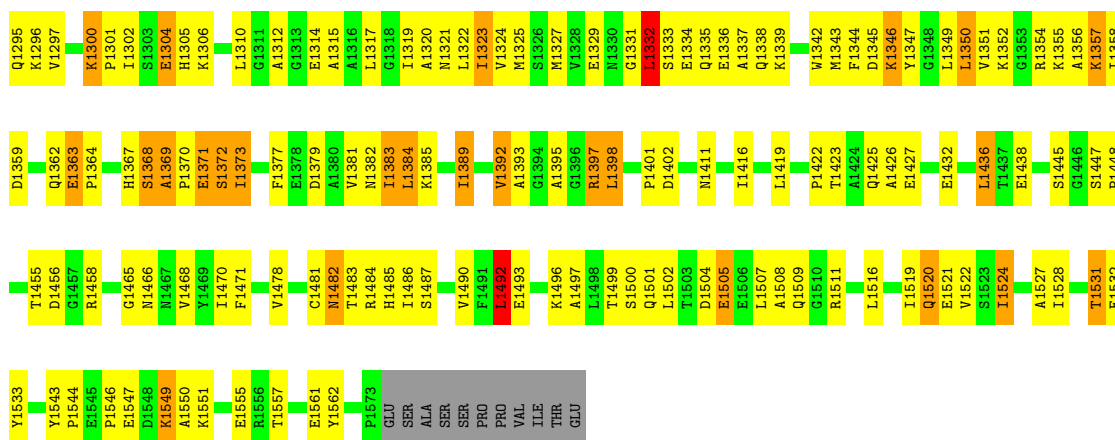
Note EDS was not executed.

• Molecule 1: MALIC ENZYME

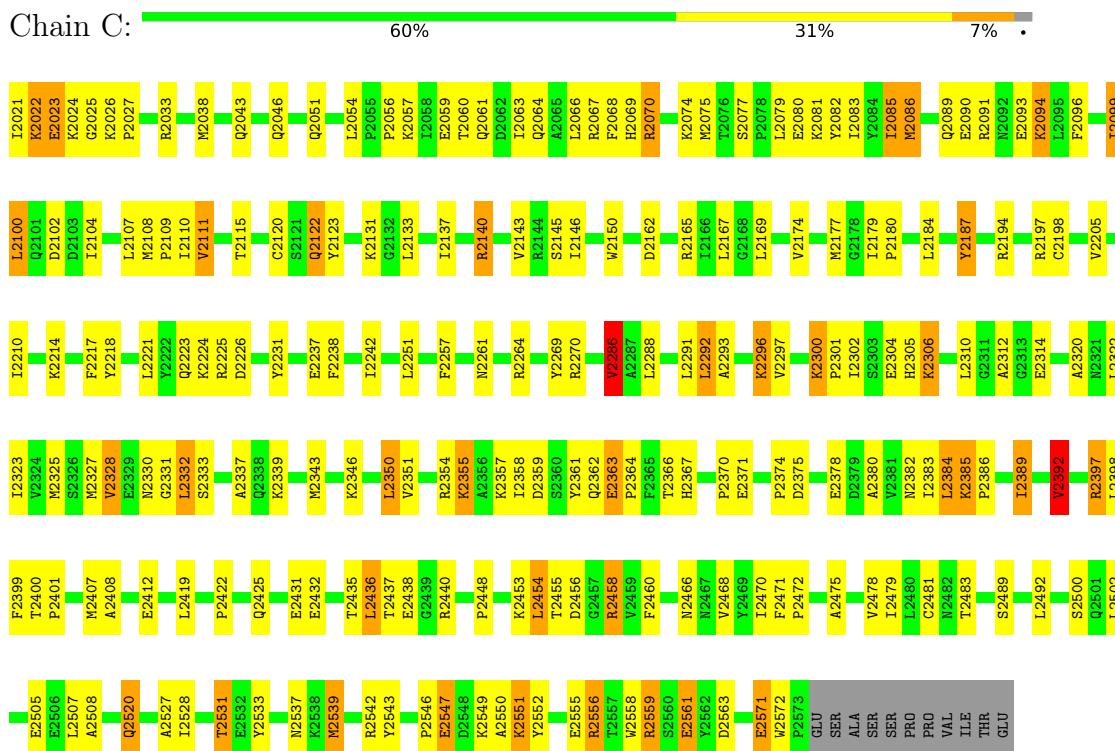


• Molecule 1: MALIC ENZYME

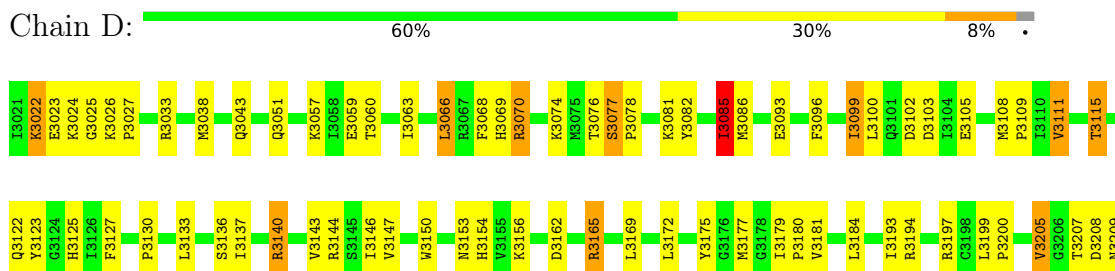




• Molecule 1: MALIC ENZYME



• Molecule 1: MALIC ENZYME



K3496	R3397	F3309	L3221
L3502	L3398	L3310	K3224
L3507	F3399	A3315	
R3511	T3400		R3227
L3512	P3401	A3320	T3228
Y3513	R3402	M3321	Q3229
P3514	V3403	L3322	Q3230
P3515		I3323	Y3231
L3516	M3407	V3324	D3232
A3517			D3233
N3518	E3412	M3327	
I3519	R3413	V3328	R3245
Q3520	P3414	E3329	Y3246
E3521			G3247
	F3417	L3332	R3248
	A3418	S3333	
	L3419	E3334	L3251
		Q3335	
I3526	E3427	E3336	
A3527		A3337	D3256
I3528	E3431	Q3338	
K3529		K3339	N3259
V3530	L3436	K3340	R3260
T3531	T3437		K3261
E3532	E3438	M3343	A3262
	G3439		F3263
	R3440	K3346	R3264
N3537	C3441		F3265
K3538	L3442	L3350	L3266
M3539		V3351	
A3540	P3448	K3352	Y3269
		G3353	
E3545	V3452	R3354	K3272
P3546	K3453	K3355	
E3547			Q3281
D3548	R3458	I3358	
K3549			A3284
A3550	T3461	E3363	A3285
K3551		P3364	V3286
	N3467	F3365	A3287
E3555	V3468	T3366	L3288
R3556	Y3469		
T3557	I3470	A3369	L3291
K3558	F3471	P3370	L3292
R3559	P3472	E3371	A3293
	G3473	S3372	A3294
E3571	V3474	I3373	Q3295
W3572			K3296
P3573	V3478	A3380	V3297
GLU			I3298
SER	C3481	L3384	S3299
ALA	N3482	K3385	K3300
SER	T3483	P3386	P3301
SER	R3484	S3387	I3302
PRO	H3485	T3388	S3303
PRO		I3389	
VAL	S3489	I3390	K3306
ILE		G3391	I3307
THR		V3392	L3308
GLU	L3492		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.00Å 118.70Å 113.00Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18807	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.45	0/4447	0.95	14/5998 (0.2%)
1	B	0.45	0/4447	0.94	16/5998 (0.3%)
1	C	0.47	0/4447	0.92	13/5998 (0.2%)
1	D	0.48	1/4447 (0.0%)	0.94	15/5998 (0.3%)
All	All	0.47	1/17788 (0.0%)	0.94	58/23992 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3514	PRO	CA-C	6.08	1.55	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3470	ILE	N-CA-C	10.53	119.94	111.62
1	B	1470	ILE	N-CA-C	9.42	119.06	111.62
1	C	2470	ILE	N-CA-C	8.97	119.27	111.56
1	A	470	ILE	N-CA-C	8.81	118.58	111.62
1	A	387	SER	N-CA-C	-7.30	104.53	113.50
1	A	419	LEU	N-CA-C	6.82	121.76	113.17
1	B	1269	TYR	N-CA-C	6.65	121.68	113.50
1	B	1419	LEU	N-CA-C	6.47	121.18	113.28
1	B	1167	LEU	CB-CA-C	-6.47	109.12	116.63
1	A	150	TRP	CA-C-N	6.42	126.18	119.05
1	A	150	TRP	C-N-CA	6.42	126.18	119.05
1	A	556	ARG	N-CA-C	6.14	119.72	112.72
1	B	1185	CYS	N-CA-C	-6.12	104.52	111.07
1	D	3077	SER	CA-C-N	6.12	125.52	118.85
1	D	3077	SER	C-N-CA	6.12	125.52	118.85
1	B	1359	ASP	N-CA-C	6.11	118.41	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	LEU	CB-CA-C	-6.02	109.61	116.54
1	B	1492	LEU	N-CA-C	-5.92	104.90	111.36
1	A	281	GLN	N-CA-C	5.88	117.77	111.36
1	D	3281	GLN	N-CA-C	5.86	117.75	111.36
1	C	2162	ASP	N-CA-C	-5.85	105.46	113.30
1	A	512	LEU	N-CA-C	-5.82	105.38	112.88
1	B	1486	ILE	N-CA-C	5.80	115.96	107.37
1	C	2448	PRO	N-CA-C	5.75	120.11	111.14
1	D	3556	ARG	N-CA-C	5.72	119.25	112.72
1	C	2310	LEU	N-CA-C	-5.72	97.87	107.99
1	A	77	SER	CA-C-N	5.71	125.56	119.28
1	A	77	SER	C-N-CA	5.71	125.56	119.28
1	D	3419	LEU	N-CA-C	5.70	120.24	113.28
1	D	3448	PRO	N-CA-C	5.69	120.02	111.14
1	C	2269	TYR	N-CA-C	5.69	120.50	113.50
1	C	2187	TYR	N-CA-C	-5.66	105.01	111.07
1	B	1162	ASP	N-CA-C	-5.62	105.18	113.61
1	D	3272	LYS	N-CA-C	-5.62	106.47	113.55
1	B	1150	TRP	CA-C-N	5.60	125.96	119.47
1	B	1150	TRP	C-N-CA	5.60	125.96	119.47
1	C	2167	LEU	CB-CA-C	-5.54	110.17	116.54
1	C	2150	TRP	CA-C-N	5.53	125.19	119.05
1	C	2150	TRP	C-N-CA	5.53	125.19	119.05
1	C	2257	PHE	N-CA-C	-5.50	102.38	110.52
1	B	1205	VAL	N-CA-C	-5.50	106.05	111.88
1	D	3323	ILE	N-CA-C	-5.46	105.18	110.42
1	A	286	VAL	CB-CA-C	-5.45	105.00	111.97
1	B	1159	VAL	N-CA-C	-5.41	99.76	107.77
1	B	1098	ARG	N-CA-C	-5.39	105.48	111.36
1	C	2419	LEU	N-CA-C	5.37	119.84	113.28
1	B	1482	ASN	N-CA-C	-5.36	104.50	111.74
1	D	3387	SER	N-CA-C	-5.29	105.97	112.90
1	A	256	ASP	N-CA-C	5.29	118.69	111.39
1	D	3256	ASP	N-CA-C	5.24	118.62	111.39
1	A	259	ASN	N-CA-C	5.19	117.34	111.11
1	C	2270	ARG	N-CA-C	5.17	118.37	111.75
1	B	1411	ASN	N-CA-C	5.12	117.92	109.72
1	D	3269	TYR	N-CA-C	5.11	120.17	113.88
1	D	3077	SER	N-CA-C	5.07	117.28	110.29
1	C	2286	VAL	CB-CA-C	-5.05	105.41	112.02
1	D	3115	THR	N-CA-C	5.04	118.90	112.34
1	D	3085	ILE	N-CA-C	5.01	115.78	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4407	208	0
1	B	4367	0	4407	235	0
1	C	4367	0	4407	149	0
1	D	4367	0	4407	182	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	52	2	0
4	B	88	0	52	3	0
4	C	88	0	52	2	0
4	D	88	0	52	1	0
5	A	239	0	0	15	0
5	B	199	0	0	30	0
5	C	275	0	0	18	0
5	D	246	0	0	11	0
All	All	18807	0	17836	753	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 21.

All (753) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:HE2	1:A:181:VAL:HG23	1.29	1.14
1:D:3177:MSE:HE2	1:D:3181:VAL:HG23	1.35	1.08
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.18	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1358:ILE:HG22	5:B:4650:HOH:O	1.54	1.06
1:A:140:ARG:HH22	1:A:233:ASP:HB3	1.14	1.05
1:D:3389:ILE:HG21	5:D:4639:HOH:O	1.58	1.03
1:B:1302:ILE:HG12	1:B:1332:LEU:HD11	1.41	0.99
1:B:1332:LEU:HD12	1:B:1332:LEU:H	1.28	0.96
1:D:3140:ARG:HH22	1:D:3233:ASP:HB3	1.26	0.96
1:C:2422:PRO:HD2	1:C:2425:GLN:HE21	1.31	0.95
1:D:3327:MSE:HE3	1:D:3337:ALA:HB1	1.44	0.95
1:B:1371:GLU:CD	1:B:1371:GLU:H	1.71	0.94
1:C:2300:LYS:HB3	1:C:2300:LYS:HZ2	1.29	0.94
1:A:300:LYS:HZ3	1:A:304:GLU:HB2	1.33	0.92
1:B:1342:TRP:HE3	1:B:1349:LEU:HD11	1.32	0.91
1:D:3520:GLN:H	1:D:3520:GLN:HE21	1.19	0.91
1:D:3086:MSE:HE1	1:D:3111:VAL:HG22	1.53	0.90
1:D:3261:ASN:HD22	1:D:3264:ARG:HE	1.16	0.90
1:C:2210:ILE:HG22	1:C:2214:LYS:HE2	1.53	0.89
1:B:1022:LYS:HE2	1:D:3025:GLY:HA3	1.52	0.89
1:B:1422:PRO:HD2	1:B:1425:GLN:HE21	1.37	0.89
1:B:1024:LYS:HZ2	1:D:3022:LYS:HD2	1.34	0.89
1:A:177:MSE:HE1	1:A:180:PRO:HB2	1.54	0.89
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.19	0.88
1:A:371:GLU:H	1:A:371:GLU:CD	1.82	0.88
1:B:1315:ALA:HB3	1:B:1392:VAL:HG21	1.55	0.87
1:B:1261:ASN:HD22	1:B:1264:ARG:HD3	1.40	0.87
1:D:3343:MSE:HE2	1:D:3365:PHE:HB2	1.56	0.87
1:C:2302:ILE:HD13	1:C:2332:LEU:HD13	1.56	0.87
1:D:3527:ALA:O	1:D:3531:THR:HG22	1.75	0.86
1:B:1029:MSE:HE2	1:B:1050:LEU:HD22	1.57	0.86
1:D:3369:ALA:HB1	1:D:3373:ILE:HD11	1.58	0.85
1:A:66:LEU:HD21	1:A:70:ARG:NH1	1.91	0.85
1:A:154:HIS:HB2	5:A:4947:HOH:O	1.76	0.84
1:B:1327:MSE:HE3	1:B:1337:ALA:HB1	1.59	0.84
1:A:140:ARG:NH2	1:A:233:ASP:HB3	1.92	0.83
1:C:2527:ALA:O	1:C:2531:THR:HG23	1.78	0.83
1:C:2520:GLN:H	1:C:2520:GLN:HE21	1.22	0.83
1:C:2300:LYS:HB3	1:C:2300:LYS:NZ	1.92	0.83
1:B:1377:PHE:O	1:B:1381:VAL:HG23	1.79	0.82
1:B:1389:ILE:HG21	5:B:4275:HOH:O	1.80	0.82
1:D:3177:MSE:HE1	1:D:3180:PRO:HB2	1.62	0.81
1:A:294:ALA:O	1:A:297:VAL:HG22	1.79	0.81
1:B:1060:THR:H	1:B:1063:ILE:HD12	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3332:LEU:HD21	1:D:3340:LYS:HE2	1.63	0.81
1:A:123:TYR:CD2	1:A:219:MSE:HE1	2.11	0.81
1:D:3085:ILE:HD11	1:D:3111:VAL:CG2	2.10	0.80
1:A:66:LEU:HD22	1:B:1217:PHE:HZ	1.47	0.80
1:B:1363:GLU:HB3	1:B:1364:PRO:HD3	1.64	0.80
1:B:1081:LYS:O	1:B:1085:ILE:HG23	1.82	0.80
1:A:343:MSE:HE2	1:A:365:PHE:HB2	1.63	0.80
1:B:1335:GLN:HB2	5:B:4934:HOH:O	1.82	0.80
1:C:2090:GLU:OE1	1:C:2131:LYS:HE3	1.82	0.80
1:C:2081:LYS:O	1:C:2085:ILE:HG23	1.82	0.80
1:B:1029:MSE:CE	1:B:1050:LEU:HD22	2.12	0.79
1:B:1395:ALA:HB3	5:B:4720:HOH:O	1.80	0.79
1:D:3261:ASN:ND2	1:D:3264:ARG:HE	1.80	0.79
1:C:2371:GLU:CD	1:C:2371:GLU:H	1.91	0.79
1:B:1021:ILE:HD11	5:B:4943:HOH:O	1.82	0.78
1:A:407:MSE:HA	1:A:407:MSE:CE	2.14	0.78
1:A:33:ARG:HD3	1:A:93:GLU:OE2	1.82	0.78
1:A:527:ALA:O	1:A:531:THR:HG23	1.83	0.77
1:C:2327:MSE:HE3	1:C:2337:ALA:HB1	1.66	0.77
1:A:300:LYS:HB3	1:A:300:LYS:HZ2	1.50	0.77
1:B:1343:MSE:HE1	5:B:4327:HOH:O	1.84	0.77
1:C:2085:ILE:HG13	1:C:2086:MSE:N	2.00	0.77
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.67	0.76
1:D:3300:LYS:HB3	1:D:3300:LYS:HZ2	1.48	0.76
1:B:1261:ASN:ND2	1:B:1264:ARG:HH11	1.84	0.76
1:C:2392:VAL:O	1:C:2392:VAL:HG13	1.86	0.76
1:C:2454:LEU:HD11	1:C:2460:PHE:HE2	1.50	0.76
1:A:177:MSE:HE3	1:A:180:PRO:HD2	1.68	0.75
1:A:534:LEU:HA	1:A:539:MSE:HG3	1.69	0.75
1:A:550:ALA:O	1:A:554:LYS:HG2	1.86	0.75
1:C:2293:ALA:HA	1:C:2296:LYS:HE2	1.68	0.75
1:C:2389:ILE:HG21	5:C:4314:HOH:O	1.86	0.75
1:D:3177:MSE:HE3	1:D:3177:MSE:O	1.86	0.75
1:A:156:LYS:HG2	1:A:197:ARG:HG2	1.69	0.74
1:B:1263:PHE:HE1	5:B:4936:HOH:O	1.69	0.74
1:B:1370:PRO:HD2	1:B:1373:ILE:HD12	1.69	0.74
1:D:3081:LYS:O	1:D:3085:ILE:HG23	1.87	0.74
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.67	0.74
1:D:3286:VAL:HG21	1:D:3467:ASN:HA	1.70	0.74
1:A:261:ASN:ND2	1:A:264:ARG:HE	1.86	0.74
1:B:1393:ALA:HB3	5:B:4720:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:MSE:HG2	1:B:1038:MSE:HE1	1.70	0.73
1:D:3338:GLN:HB2	1:D:3339:LYS:NZ	2.03	0.73
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.54	0.73
1:C:2323:ILE:HG22	1:C:2327:MSE:HE2	1.69	0.73
1:B:1397:ARG:HH21	1:B:1426:ALA:HB3	1.54	0.72
1:A:22:LYS:HE2	1:C:2024:LYS:O	1.89	0.72
1:A:495:ALA:O	1:A:499:THR:HG22	1.90	0.72
1:B:1024:LYS:NZ	1:D:3022:LYS:HA	2.04	0.72
1:C:2086:MSE:HE1	1:C:2111:VAL:HG22	1.70	0.72
1:A:407:MSE:HE2	1:A:411:ASN:HD22	1.56	0.71
1:A:493:GLU:HG3	1:A:533:TYR:CD1	2.26	0.71
1:D:3323:ILE:HG22	1:D:3327:MSE:HE2	1.71	0.71
1:D:3571:GLU:HG3	5:D:4551:HOH:O	1.90	0.71
1:C:2301:PRO:HB2	1:C:2304:GLU:HG3	1.70	0.71
1:A:77:SER:C	5:A:4952:HOH:O	2.34	0.71
1:D:3300:LYS:HB3	1:D:3300:LYS:NZ	2.04	0.71
1:D:3520:GLN:H	1:D:3520:GLN:NE2	1.88	0.70
1:B:1085:ILE:HD12	1:B:1096:PHE:HE1	1.56	0.70
1:D:3137:ILE:HB	1:D:3205:VAL:HG12	1.73	0.70
1:C:2094:LYS:HE2	1:C:2558:TRP:CZ2	2.27	0.70
1:C:2306:LYS:HG2	1:C:2386:PRO:HA	1.74	0.70
1:B:1075:MSE:HG2	1:B:1080:GLU:CD	2.17	0.70
1:B:1363:GLU:N	5:B:4650:HOH:O	2.24	0.70
1:B:1546:PRO:HG2	1:B:1549:LYS:HD2	1.73	0.69
1:A:392:VAL:CG1	1:A:392:VAL:O	2.40	0.69
1:A:493:GLU:HG2	5:A:4484:HOH:O	1.92	0.69
1:B:1069:HIS:HE1	1:B:1102:ASP:OD2	1.74	0.69
1:D:3272:LYS:NZ	1:D:3272:LYS:HB3	2.08	0.69
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.75	0.69
1:B:1371:GLU:CD	1:B:1371:GLU:N	2.50	0.69
1:C:2520:GLN:HG2	5:C:4086:HOH:O	1.92	0.69
1:C:2551:LYS:O	1:C:2555:GLU:HB2	1.91	0.69
1:D:3400:THR:OG1	1:D:3403:VAL:HG23	1.93	0.69
1:A:177:MSE:HE3	1:A:177:MSE:O	1.92	0.69
1:A:320:ALA:HB2	5:A:4862:HOH:O	1.93	0.69
1:B:1029:MSE:HE1	1:B:1053:LEU:HD12	1.73	0.69
1:B:1397:ARG:NH2	1:B:1426:ALA:HB3	2.08	0.68
1:B:1333:SER:OG	1:B:1336:GLU:HG2	1.93	0.68
1:B:1342:TRP:CE3	1:B:1349:LEU:HD11	2.23	0.68
1:A:302:ILE:HD11	1:A:327:MSE:HG2	1.74	0.68
1:C:2422:PRO:HD2	1:C:2425:GLN:NE2	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1393:ALA:CB	5:B:4720:HOH:O	2.41	0.67
1:B:1370:PRO:HG2	1:B:1372:SER:O	1.95	0.67
1:B:1501:GLN:NE2	1:B:1522:VAL:HG13	2.08	0.67
1:D:3548:ASP:OD2	1:D:3551:LYS:HG3	1.95	0.67
1:A:130:PRO:HG3	1:B:1054:LEU:HD23	1.76	0.67
1:B:1268:LYS:HD3	1:B:1269:TYR:CZ	2.30	0.67
1:B:1233:ASP:HB2	5:B:4649:HOH:O	1.95	0.67
1:D:3086:MSE:HE1	1:D:3111:VAL:CG2	2.25	0.66
1:A:300:LYS:NZ	1:A:304:GLU:HB2	2.07	0.66
1:A:324:VAL:HA	1:A:327:MSE:CE	2.25	0.66
1:D:3338:GLN:HB2	1:D:3339:LYS:HZ3	1.60	0.66
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.59	0.66
1:B:1524:ILE:O	1:B:1528:ILE:HG13	1.96	0.66
1:C:2061:GLN:HA	1:C:2064:GLN:HE21	1.61	0.66
1:A:175:TYR:HD2	1:A:219:MSE:HE2	1.61	0.66
1:B:1177:MSE:O	1:B:1180:PRO:HD2	1.95	0.66
1:B:1261:ASN:HA	1:B:1264:ARG:HG2	1.75	0.66
1:B:1505:GLU:CD	1:B:1505:GLU:H	2.04	0.66
1:B:1302:ILE:HA	1:B:1305:HIS:ND1	2.11	0.66
1:B:1369:ALA:HB1	1:B:1373:ILE:HD11	1.77	0.66
1:C:2468:VAL:HA	1:C:2471:PHE:CE2	2.31	0.66
1:B:1354:ARG:HD3	1:B:1358:ILE:HD11	1.78	0.65
1:D:3177:MSE:O	1:D:3180:PRO:HD2	1.97	0.65
1:D:3551:LYS:NZ	1:D:3551:LYS:HB3	2.11	0.65
1:B:1332:LEU:H	1:B:1332:LEU:CD1	2.08	0.65
1:D:3261:ASN:HD22	1:D:3264:ARG:NE	1.91	0.65
1:A:38:MSE:HE3	1:A:59:GLU:CD	2.22	0.65
1:A:559:ARG:HG3	1:A:561:GLU:OE1	1.97	0.65
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.77	0.65
1:C:2261:ASN:ND2	1:C:2264:ARG:HH21	1.95	0.65
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.79	0.64
1:B:1342:TRP:CZ3	1:B:1349:LEU:HD21	2.32	0.64
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.80	0.64
1:D:3334:GLU:O	1:D:3338:GLN:HG3	1.97	0.64
1:A:505:GLU:N	1:A:505:GLU:CD	2.54	0.64
1:D:3184:LEU:HD12	1:D:3200:PRO:HG3	1.80	0.64
1:A:350:LEU:HD22	1:A:354:ARG:NH1	2.13	0.63
1:B:1181:VAL:HG11	5:B:4503:HOH:O	1.97	0.63
1:D:3431:GLU:OE1	1:D:3452:VAL:HG13	1.97	0.63
1:A:24:LYS:O	1:C:2022:LYS:HE2	1.98	0.63
1:A:505:GLU:CD	1:A:505:GLU:H	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1528:ILE:HD13	1:B:1550:ALA:HA	1.80	0.63
1:D:3528:ILE:O	1:D:3531:THR:HG23	1.99	0.63
1:D:3286:VAL:HG22	1:D:3470:ILE:HG13	1.81	0.63
1:A:85:ILE:HD11	1:A:111:VAL:CG2	2.29	0.62
1:A:177:MSE:O	1:A:180:PRO:HD2	1.99	0.62
1:A:211:ALA:HA	1:A:214:LYS:HE2	1.81	0.62
1:B:1075:MSE:HG2	1:B:1080:GLU:OE1	1.98	0.62
1:B:1389:ILE:HG12	5:B:4275:HOH:O	1.99	0.62
1:D:3327:MSE:CE	1:D:3337:ALA:HB1	2.25	0.62
1:A:153:ASN:HD22	1:A:153:ASN:H	1.45	0.62
1:A:23:GLU:HG3	1:A:27:PRO:HB2	1.81	0.62
1:D:3272:LYS:HB3	1:D:3272:LYS:HZ3	1.63	0.62
1:A:177:MSE:CE	1:A:180:PRO:HB2	2.28	0.62
1:B:1312:ALA:CB	1:B:1343:MSE:HE3	2.29	0.62
1:B:1368:SER:HA	5:B:4846:HOH:O	1.99	0.62
1:C:2425:GLN:HG3	5:C:4790:HOH:O	1.99	0.62
1:B:1323:ILE:HG22	1:B:1327:MSE:HE2	1.82	0.61
1:A:456:ASP:OD1	1:A:458:ARG:HD3	2.00	0.61
1:D:3125:HIS:CE1	5:D:4912:HOH:O	2.52	0.61
1:D:3284:ALA:HB1	1:D:3322:LEU:HD13	1.81	0.61
1:A:175:TYR:CD2	1:A:219:MSE:HE2	2.35	0.61
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.82	0.61
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.35	0.61
1:B:1367:HIS:CB	5:B:4824:HOH:O	2.48	0.61
1:A:153:ASN:H	1:A:153:ASN:ND2	1.97	0.61
1:A:153:ASN:ND2	1:A:153:ASN:N	2.49	0.61
1:A:407:MSE:HA	1:A:407:MSE:HE3	1.81	0.61
1:B:1133:LEU:HB2	1:B:1199:LEU:HD11	1.83	0.61
1:A:144:ARG:HH12	1:A:244:ASP:HB3	1.64	0.60
1:C:2520:GLN:H	1:C:2520:GLN:NE2	1.96	0.60
1:C:2179:ILE:HB	1:C:2180:PRO:HD3	1.83	0.60
1:B:1352:LYS:HB2	5:B:4846:HOH:O	1.99	0.60
1:B:1079:LEU:O	1:B:1083:ILE:HG13	2.02	0.60
1:C:2552:TYR:O	1:C:2556:ARG:HG3	2.01	0.60
1:D:3335:GLN:HG2	1:D:3339:LYS:HE2	1.82	0.60
1:A:25:GLY:HA3	1:C:2022:LYS:HE2	1.83	0.60
1:B:1085:ILE:HD12	1:B:1096:PHE:CE1	2.37	0.60
1:B:1140:ARG:HB2	1:B:1140:ARG:CZ	2.32	0.60
1:B:1261:ASN:HA	1:B:1264:ARG:HD3	1.83	0.60
1:A:305:HIS:O	1:A:340:LYS:HG2	2.01	0.60
1:B:1312:ALA:HB1	1:B:1343:MSE:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:4632:HOH:O	4:C:2602:NAD:H51N	2.01	0.60
1:D:3085:ILE:HG13	1:D:3086:MSE:HE2	1.84	0.60
1:B:1085:ILE:HG13	1:B:1086:MSE:N	2.15	0.60
1:B:1025:GLY:C	1:B:1027:PRO:HD2	2.26	0.59
1:C:2361:TYR:O	1:C:2364:PRO:HD2	2.02	0.59
1:A:407:MSE:CE	1:A:411:ASN:ND2	2.64	0.59
1:C:2075:MSE:HE2	5:C:4558:HOH:O	2.03	0.59
1:D:3315:ALA:HB3	1:D:3392:VAL:HG21	1.84	0.59
1:D:3371:GLU:CD	1:D:3371:GLU:H	2.07	0.59
1:D:3528:ILE:O	1:D:3532:GLU:HG3	2.01	0.59
1:B:1357:LYS:O	1:B:1358:ILE:HD13	2.03	0.59
1:D:3154:HIS:HB2	5:D:4342:HOH:O	2.02	0.59
1:D:3179:ILE:HB	1:D:3180:PRO:HD3	1.85	0.59
1:D:3298:ILE:HD11	1:D:3442:LEU:HD12	1.85	0.59
1:B:1370:PRO:HD2	1:B:1373:ILE:CD1	2.32	0.59
1:D:3060:THR:H	1:D:3063:ILE:HD12	1.68	0.59
1:C:2300:LYS:NZ	1:C:2304:GLU:HB2	2.17	0.59
1:C:2184:LEU:HD22	1:C:2198:CYS:HB3	1.85	0.58
1:B:1140:ARG:HH22	1:B:1233:ASP:HB3	1.66	0.58
1:A:324:VAL:HA	1:A:327:MSE:HE3	1.85	0.58
1:B:1261:ASN:HB3	1:B:1265:PHE:CE1	2.38	0.58
1:C:2094:LYS:HE2	1:C:2558:TRP:HZ2	1.67	0.58
1:A:407:MSE:HE2	1:A:411:ASN:ND2	2.17	0.58
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.67	0.58
1:B:1300:LYS:HZ3	1:B:1304:GLU:C	2.12	0.58
1:D:3140:ARG:NH2	1:D:3233:ASP:HB3	2.09	0.58
1:D:3177:MSE:CE	1:D:3180:PRO:HB2	2.32	0.58
1:D:3293:ALA:HA	1:D:3296:LYS:HE2	1.86	0.58
1:C:2323:ILE:O	1:C:2327:MSE:HG3	2.03	0.58
1:B:1392:VAL:HG22	1:B:1392:VAL:O	2.02	0.58
1:D:3144:ARG:NH2	1:D:3245:ARG:HB2	2.18	0.58
1:D:3177:MSE:HE3	1:D:3180:PRO:HD2	1.86	0.58
1:A:286:VAL:HG11	1:A:466:ASN:O	2.04	0.57
1:B:1505:GLU:N	1:B:1505:GLU:OE2	2.37	0.57
1:B:1350:LEU:HD23	1:B:1354:ARG:NH1	2.20	0.57
1:D:3302:ILE:HG12	1:D:3332:LEU:HD11	1.84	0.57
1:B:1159:VAL:HG23	1:B:1184:LEU:HD21	1.87	0.57
1:C:2312:ALA:HB1	1:C:2343:MSE:HE3	1.86	0.57
1:D:3324:VAL:HA	1:D:3327:MSE:CE	2.35	0.57
1:A:332:LEU:HD21	1:A:340:LYS:HE2	1.86	0.57
1:A:520:GLN:HE21	1:A:520:GLN:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1527:ALA:O	1:B:1531:THR:CG2	2.53	0.57
1:C:2382:ASN:O	1:C:2385:LYS:HD2	2.03	0.57
1:D:3492:LEU:HD22	1:D:3496:LYS:HE3	1.87	0.57
1:C:2210:ILE:O	1:C:2214:LYS:HG3	2.04	0.57
1:B:1024:LYS:NZ	1:D:3022:LYS:HD2	2.16	0.57
1:C:2293:ALA:O	1:C:2296:LYS:HB2	2.05	0.57
1:C:2061:GLN:HA	1:C:2064:GLN:NE2	2.19	0.57
1:C:2320:ALA:CB	5:C:4058:HOH:O	2.52	0.57
1:C:2359:ASP:OD2	1:C:2362:GLN:HG3	2.05	0.56
1:C:2392:VAL:O	1:C:2392:VAL:CG1	2.52	0.56
1:A:47:MSE:HG2	5:C:4312:HOH:O	2.04	0.56
1:B:1261:ASN:HA	1:B:1264:ARG:CG	2.35	0.56
1:B:1334:GLU:O	1:B:1338:GLN:HG3	2.03	0.56
1:B:1354:ARG:NE	1:B:1358:ILE:HD11	2.20	0.56
1:B:1343:MSE:SE	5:B:4104:HOH:O	2.73	0.56
1:D:3085:ILE:HD11	1:D:3111:VAL:HG23	1.87	0.56
1:B:1354:ARG:CD	1:B:1358:ILE:HD11	2.35	0.56
1:C:2397:ARG:NH1	5:C:4346:HOH:O	2.38	0.56
1:A:358:ILE:HD12	1:A:366:THR:OG1	2.06	0.56
1:D:3358:ILE:HD13	1:D:3366:THR:HG21	1.88	0.56
1:A:38:MSE:HE3	1:A:59:GLU:OE1	2.05	0.56
1:D:3085:ILE:HD11	1:D:3111:VAL:HG21	1.86	0.56
1:A:68:PHE:CD2	1:A:99:ILE:HG13	2.41	0.55
1:B:1177:MSE:C	1:B:1180:PRO:HD2	2.31	0.55
1:C:2547:GLU:HB2	5:C:4930:HOH:O	2.06	0.55
1:D:3093:GLU:O	1:D:3096:PHE:HB3	2.05	0.55
1:A:408:ALA:HB2	1:A:437:THR:HG22	1.88	0.55
1:D:3060:THR:OG1	1:D:3063:ILE:HG13	2.06	0.55
1:D:3392:VAL:HG13	1:D:3392:VAL:O	2.06	0.55
1:B:1301:PRO:HD2	1:B:1304:GLU:HG3	1.88	0.55
1:C:2060:THR:H	1:C:2063:ILE:HD12	1.72	0.55
1:C:2184:LEU:O	1:C:2187:TYR:HB2	2.07	0.55
1:B:1261:ASN:HA	1:B:1264:ARG:CD	2.37	0.55
1:B:1302:ILE:CG1	1:B:1332:LEU:HD11	2.26	0.55
1:C:2343:MSE:SE	5:C:4058:HOH:O	2.74	0.55
1:C:2478:VAL:HG13	1:C:2483:THR:HB	1.87	0.55
1:D:3066:LEU:HD22	1:D:3070:ARG:HE	1.70	0.55
1:D:3412:GLU:O	1:D:3440:ARG:HD2	2.06	0.55
1:D:3538:LYS:HD2	1:D:3538:LYS:N	2.21	0.55
1:A:285:ALA:HB1	1:A:470:ILE:HD12	1.89	0.55
1:D:3023:GLU:HG3	1:D:3027:PRO:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:O	1:A:392:VAL:HG13	2.06	0.55
1:C:2054:LEU:HD23	1:D:3130:PRO:HG3	1.89	0.55
1:C:2137:ILE:O	1:C:2140:ARG:HG2	2.07	0.55
1:C:2293:ALA:HA	1:C:2296:LYS:CE	2.37	0.55
1:A:85:ILE:HD11	1:A:111:VAL:HG21	1.89	0.54
1:B:1077:SER:O	1:B:1081:LYS:HG3	2.07	0.54
1:B:1505:GLU:CD	1:B:1505:GLU:N	2.65	0.54
1:A:144:ARG:NH1	1:A:244:ASP:HB3	2.21	0.54
1:A:302:ILE:HG12	1:A:332:LEU:CD1	2.38	0.54
1:C:2177:MSE:O	1:C:2180:PRO:HD2	2.07	0.54
1:B:1432:GLU:O	1:B:1436:LEU:HB2	2.07	0.54
1:A:33:ARG:NH1	1:A:93:GLU:OE1	2.40	0.54
1:A:407:MSE:HA	1:A:407:MSE:HE2	1.87	0.54
1:A:549:LYS:HG2	5:A:4766:HOH:O	2.07	0.54
1:B:1379:ASP:O	1:B:1383:ILE:HD12	2.07	0.54
1:B:1493:GLU:HG3	1:B:1533:TYR:CD1	2.43	0.54
1:D:3315:ALA:CB	1:D:3392:VAL:HG21	2.38	0.54
1:A:546:PRO:O	1:A:549:LYS:NZ	2.40	0.54
1:B:1024:LYS:HZ2	1:D:3022:LYS:HA	1.69	0.54
1:B:1349:LEU:HG	1:B:1351:VAL:HG13	1.90	0.54
1:A:298:ILE:HD11	1:A:442:LEU:HD12	1.90	0.54
1:B:1154:HIS:O	1:B:1197:ARG:HD3	2.07	0.54
1:A:453:LYS:HZ1	1:A:457:GLY:HA2	1.73	0.54
1:B:1496:LYS:O	1:B:1500:SER:HB3	2.08	0.54
1:A:298:ILE:HD11	1:A:442:LEU:CD1	2.38	0.54
1:B:1346:LYS:H	1:B:1346:LYS:HD2	1.73	0.54
1:A:45:ARG:NH2	1:A:58:ILE:HD13	2.23	0.53
1:C:2075:MSE:HG2	1:C:2080:GLU:CD	2.33	0.53
1:D:3284:ALA:CB	1:D:3322:LEU:HD13	2.38	0.53
1:B:1315:ALA:HB3	1:B:1392:VAL:CG2	2.35	0.53
1:B:1358:ILE:CG2	5:B:4650:HOH:O	2.31	0.53
1:C:2355:LYS:HA	1:C:2355:LYS:HE2	1.90	0.53
1:C:2559:ARG:HB3	1:C:2561:GLU:HG2	1.91	0.53
1:B:1024:LYS:HZ1	1:D:3022:LYS:HA	1.73	0.53
1:C:2358:ILE:HD13	1:C:2366:THR:HG21	1.90	0.53
1:D:3537:ASN:C	1:D:3538:LYS:HD2	2.33	0.53
1:B:1312:ALA:HB1	1:B:1343:MSE:HE3	1.90	0.53
1:C:2559:ARG:HG3	1:C:2561:GLU:OE1	2.07	0.53
1:B:1320:ALA:O	1:B:1324:VAL:HG23	2.09	0.53
1:C:2131:LYS:O	1:C:2177:MSE:HE3	2.07	0.53
1:D:3177:MSE:O	1:D:3177:MSE:CE	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2325:MSE:HE1	1:C:2489:SER:HA	1.91	0.53
1:A:483:THR:OG1	1:A:534:LEU:HD13	2.08	0.53
1:C:2086:MSE:CE	1:C:2111:VAL:HG22	2.37	0.53
1:C:2328:VAL:HA	1:C:2332:LEU:O	2.08	0.53
1:A:453:LYS:NZ	1:A:457:GLY:HA2	2.24	0.53
1:D:3208:ASP:OD2	1:D:3227:ARG:NH2	2.40	0.53
1:D:3229:GLN:O	1:D:3229:GLN:HG2	2.09	0.53
1:D:3380:ALA:O	1:D:3384:LEU:HB2	2.08	0.53
1:A:81:LYS:O	1:A:85:ILE:HG23	2.09	0.52
1:C:2069:HIS:HE1	1:C:2102:ASP:OD2	1.93	0.52
1:C:2302:ILE:HA	1:C:2305:HIS:ND1	2.25	0.52
1:D:3343:MSE:CE	1:D:3365:PHE:HB2	2.34	0.52
1:A:302:ILE:HG12	1:A:332:LEU:HD11	1.92	0.52
1:B:1029:MSE:HE1	1:B:1053:LEU:CD1	2.39	0.52
1:B:1325:MSE:HE2	1:B:1492:LEU:CD1	2.39	0.52
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.90	0.52
1:A:397:ARG:HA	1:A:427:GLU:O	2.10	0.52
1:D:3038:MSE:HE3	1:D:3059:GLU:CD	2.35	0.52
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.24	0.52
1:C:2355:LYS:HA	1:C:2355:LYS:CE	2.40	0.52
1:A:548:ASP:C	1:A:548:ASP:OD1	2.52	0.51
1:B:1286:VAL:HG11	1:B:1466:ASN:O	2.10	0.51
1:B:1068:PHE:CD2	1:B:1099:ILE:HG13	2.46	0.51
1:B:1300:LYS:NZ	1:B:1304:GLU:HG3	2.25	0.51
1:C:2226:ASP:OD1	1:C:2226:ASP:C	2.53	0.51
1:D:3232:ASP:CG	1:D:3264:ARG:HH22	2.19	0.51
1:D:3389:ILE:HG12	5:D:4639:HOH:O	2.10	0.51
1:A:386:PRO:O	1:A:407:MSE:HE1	2.10	0.51
1:D:3324:VAL:HA	1:D:3327:MSE:HE3	1.93	0.51
1:D:3068:PHE:CD2	1:D:3099:ILE:HG13	2.45	0.51
1:B:1196:ASP:OD1	1:B:1196:ASP:N	2.44	0.51
1:B:1314:GLU:HG3	4:B:1601:NAD:O2A	2.11	0.51
1:B:1505:GLU:O	1:B:1508:ALA:HB3	2.10	0.51
1:A:273:TYR:O	1:A:485:HIS:HD2	1.93	0.51
1:A:288:LEU:HG	1:A:292:LEU:HD22	1.92	0.51
1:D:3333:SER:HB3	1:D:3336:GLU:HB3	1.92	0.51
1:A:85:ILE:HD11	1:A:111:VAL:HG23	1.92	0.51
1:A:556:ARG:CG	1:A:556:ARG:HH11	2.24	0.51
1:B:1325:MSE:HE2	1:B:1492:LEU:HD12	1.92	0.51
1:B:1345:ASP:HB2	4:B:1601:NAD:O2B	2.10	0.51
1:D:3350:LEU:HD22	1:D:3354:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:HE3	1:A:180:PRO:CD	2.39	0.51
1:C:2481:CYS:SG	1:C:2531:THR:HB	2.50	0.51
1:D:3412:GLU:HG3	1:D:3413:ARG:HG2	1.93	0.51
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.93	0.51
1:B:1342:TRP:HZ3	1:B:1349:LEU:HD21	1.74	0.50
1:B:1528:ILE:O	1:B:1532:GLU:HG3	2.10	0.50
1:C:2505:GLU:O	1:C:2508:ALA:HB3	2.10	0.50
1:D:3389:ILE:HG23	1:D:3399:PHE:CE1	2.46	0.50
1:D:3502:LEU:CD1	1:D:3507:LEU:HG	2.41	0.50
1:A:350:LEU:HD13	1:A:358:ILE:CD1	2.41	0.50
1:D:3320:ALA:HB2	5:D:4695:HOH:O	2.11	0.50
1:A:119:ALA:O	1:A:123:TYR:N	2.45	0.50
1:A:397:ARG:NH2	1:A:423:THR:O	2.44	0.50
1:B:1022:LYS:HD2	1:B:1022:LYS:O	2.12	0.50
1:A:177:MSE:SE	5:A:4018:HOH:O	2.79	0.50
1:C:2350:LEU:HD22	1:C:2354:ARG:NH1	2.27	0.50
1:B:1261:ASN:HD22	1:B:1264:ARG:HH11	1.57	0.50
1:B:1445:SER:O	1:B:1465:GLY:N	2.44	0.50
1:C:2300:LYS:HE2	5:C:4931:HOH:O	2.10	0.50
1:C:2301:PRO:HD2	1:C:2304:GLU:OE1	2.11	0.50
1:C:2454:LEU:HD11	1:C:2460:PHE:CE2	2.39	0.50
1:D:3023:GLU:CG	1:D:3027:PRO:HB2	2.42	0.50
1:D:3085:ILE:HG13	1:D:3086:MSE:N	2.24	0.50
1:B:1343:MSE:HE2	1:B:1350:LEU:HD12	1.92	0.50
1:C:2312:ALA:HB1	1:C:2343:MSE:CE	2.42	0.50
1:C:2371:GLU:CD	1:C:2371:GLU:N	2.66	0.50
1:C:2412:GLU:O	1:C:2440:ARG:HD2	2.12	0.50
1:B:1346:LYS:HD2	4:B:1601:NAD:O2B	2.11	0.50
1:A:484:ARG:HG3	1:A:541:PHE:CE1	2.47	0.50
1:B:1136:SER:HA	1:B:1204:ASP:O	2.12	0.50
1:B:1481:CYS:SG	1:B:1531:THR:HB	2.52	0.50
1:C:2079:LEU:O	1:C:2083:ILE:HG13	2.11	0.50
1:B:1338:GLN:OE1	1:B:1364:PRO:HB3	2.11	0.49
1:B:1350:LEU:CD2	1:B:1354:ARG:NH1	2.75	0.49
1:B:1383:ILE:HG22	1:B:1384:LEU:HD13	1.94	0.49
1:D:3150:TRP:CE2	1:D:3199:LEU:HD13	2.47	0.49
1:B:1312:ALA:HB1	1:B:1343:MSE:HE1	1.94	0.49
1:C:2556:ARG:HH11	1:C:2556:ARG:CG	2.25	0.49
1:D:3122:GLN:HE22	1:D:3125:HIS:CD2	2.30	0.49
1:D:3343:MSE:HE2	1:D:3365:PHE:CB	2.36	0.49
1:A:407:MSE:HE1	1:A:411:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:LYS:HG2	1:B:1562:TYR:CD2	2.47	0.49
1:B:1081:LYS:HE3	5:B:4336:HOH:O	2.11	0.49
1:C:2238:PHE:CE1	1:C:2242:ILE:HG13	2.47	0.49
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.93	0.49
1:A:400:THR:OG1	1:A:403:VAL:HG23	2.13	0.49
1:B:1315:ALA:CB	1:B:1392:VAL:HG21	2.36	0.49
1:A:72:LEU:HA	1:A:75:MSE:HG3	1.94	0.49
1:B:1227:ARG:HG2	1:B:1227:ARG:NH1	2.26	0.49
1:B:1301:PRO:HG2	1:B:1304:GLU:OE2	2.13	0.49
1:D:3315:ALA:HB3	1:D:3392:VAL:CG2	2.43	0.49
1:C:2300:LYS:HZ3	1:C:2304:GLU:HB2	1.77	0.49
1:D:3302:ILE:CD1	1:D:3332:LEU:HD13	2.42	0.49
1:A:299:SER:HB3	5:A:4513:HOH:O	2.12	0.49
1:B:1527:ALA:O	1:B:1531:THR:HG22	2.13	0.49
1:C:2091:ARG:HB3	5:C:4893:HOH:O	2.12	0.49
1:C:2527:ALA:O	1:C:2531:THR:CG2	2.58	0.49
1:A:219:MSE:HG2	1:B:1038:MSE:CE	2.41	0.48
1:A:308:LEU:HD23	1:A:389:ILE:HD11	1.94	0.48
1:A:535:TYR:OH	1:A:542:ARG:HB3	2.12	0.48
1:C:2067:ARG:HD2	5:C:4187:HOH:O	2.13	0.48
1:A:85:ILE:HG13	1:A:86:MSE:N	2.28	0.48
1:A:325:MSE:HE1	1:A:488:ASP:CB	2.43	0.48
1:A:526:ILE:O	1:A:530:VAL:HG23	2.13	0.48
1:B:1456:ASP:OD1	1:B:1456:ASP:C	2.56	0.48
1:D:3520:GLN:HE21	1:D:3520:GLN:N	1.99	0.48
1:C:2363:GLU:HB3	1:C:2364:PRO:HD3	1.96	0.48
1:D:3401:PRO:HA	1:D:3436:LEU:CD1	2.44	0.48
1:A:184:LEU:O	1:A:187:TYR:HB2	2.13	0.48
1:C:2068:PHE:CD2	1:C:2099:ILE:HG13	2.47	0.48
1:D:3288:LEU:HG	1:D:3292:LEU:HD22	1.95	0.48
1:D:3306:LYS:HG2	1:D:3386:PRO:HA	1.95	0.48
1:D:3521:GLU:HG2	5:D:4042:HOH:O	2.13	0.48
1:D:3302:ILE:HG23	1:D:3303:SER:N	2.28	0.48
1:D:3551:LYS:O	1:D:3555:GLU:HB2	2.13	0.48
1:A:46:GLN:HG2	1:A:51:GLN:HG3	1.96	0.48
1:B:1029:MSE:HE2	1:B:1050:LEU:HB3	1.95	0.48
1:B:1302:ILE:HA	1:B:1305:HIS:CE1	2.49	0.48
1:B:1336:GLU:HA	1:B:1339:LYS:HG3	1.96	0.48
1:B:1343:MSE:HE2	1:B:1350:LEU:CD1	2.44	0.48
1:B:1350:LEU:HD22	1:B:1358:ILE:HD11	1.94	0.48
1:A:186:LEU:O	1:A:190:CYS:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1140:ARG:HB2	1:B:1140:ARG:NH1	2.29	0.47
1:D:3051:GLN:HE21	1:D:3051:GLN:HA	1.79	0.47
1:A:350:LEU:HB3	1:A:358:ILE:HD11	1.96	0.47
1:D:3143:VAL:O	1:D:3147:VAL:HG23	2.14	0.47
1:D:3291:LEU:HD13	1:D:3417:PHE:CE2	2.49	0.47
1:D:3528:ILE:HG12	1:D:3550:ALA:HA	1.96	0.47
1:A:66:LEU:O	1:A:66:LEU:HD23	2.14	0.47
1:B:1169:LEU:HD13	1:B:1422:PRO:HD3	1.96	0.47
1:B:1520:GLN:NE2	1:B:1520:GLN:H	2.12	0.47
1:D:3033:ARG:NH1	1:D:3093:GLU:OE2	2.39	0.47
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.96	0.47
1:C:2546:PRO:O	1:C:2549:LYS:NZ	2.44	0.47
1:D:3144:ARG:HA	1:D:3144:ARG:HD2	1.72	0.47
1:D:3302:ILE:HG12	1:D:3332:LEU:CD1	2.43	0.47
1:A:33:ARG:HH11	1:A:93:GLU:CD	2.23	0.47
1:A:165:ARG:O	1:A:165:ARG:NE	2.47	0.47
1:A:407:MSE:HE1	1:A:411:ASN:ND2	2.29	0.47
1:B:1194:ARG:HB2	1:B:1197:ARG:HG3	1.96	0.47
1:B:1288:LEU:HG	1:B:1292:LEU:HD22	1.96	0.47
1:B:1295:GLN:OE1	1:B:1295:GLN:HA	2.13	0.47
1:A:492:LEU:O	1:A:496:LYS:HG3	2.15	0.47
1:D:3245:ARG:HG2	1:D:3246:TYR:CD1	2.50	0.47
1:A:70:ARG:O	1:A:74:LYS:HE3	2.14	0.47
1:A:120:CYS:O	1:A:175:TYR:HB3	2.14	0.47
1:A:232:ASP:CG	1:A:264:ARG:HH22	2.23	0.47
1:A:518:ASN:O	1:A:522:VAL:HG23	2.14	0.47
1:B:1022:LYS:HE2	1:D:3024:LYS:O	2.14	0.47
1:B:1274:CYS:HB2	1:B:1484:ARG:O	2.14	0.47
1:C:2528:ILE:HG12	1:C:2550:ALA:HA	1.95	0.47
1:D:3286:VAL:CG2	1:D:3467:ASN:HA	2.43	0.47
1:D:3154:HIS:O	1:D:3197:ARG:HD3	2.15	0.47
1:A:206:GLY:HA2	5:A:4098:HOH:O	2.14	0.47
1:A:401:PRO:HA	1:A:436:LEU:CD2	2.45	0.47
1:D:3310:LEU:HB3	1:D:3391:GLY:HA2	1.96	0.47
1:A:177:MSE:O	1:A:177:MSE:CE	2.62	0.47
1:A:314:GLU:HB2	4:A:601:NAD:O1N	2.15	0.47
1:D:3512:LEU:HG	5:D:4471:HOH:O	2.16	0.46
1:A:253:GLN:HB2	1:A:276:PHE:CE2	2.49	0.46
1:A:504:ASP:OD2	1:A:504:ASP:N	2.48	0.46
1:C:2085:ILE:HD12	1:C:2096:PHE:HE1	1.80	0.46
1:D:3400:THR:HB	1:D:3401:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3481:CYS:HB3	1:D:3540:ALA:CB	2.44	0.46
1:A:43:GLN:OE1	1:A:47:MSE:HE1	2.16	0.46
1:B:1146:ILE:O	1:B:1149:ASN:HB2	2.16	0.46
1:C:2177:MSE:C	1:C:2180:PRO:HD2	2.40	0.46
1:D:3140:ARG:NH2	1:D:3230:GLN:O	2.49	0.46
1:A:431:GLU:CD	1:A:452:VAL:HG13	2.40	0.46
1:B:1166:ILE:HA	1:B:1256:ASP:OD2	2.16	0.46
1:B:1248:ARG:HH22	1:B:1272:LYS:HG2	1.81	0.46
1:C:2025:GLY:C	1:C:2027:PRO:HD2	2.41	0.46
1:C:2300:LYS:HZ2	1:C:2300:LYS:CB	2.11	0.46
1:C:2571:GLU:HG3	1:C:2572:TRP:N	2.30	0.46
1:D:3144:ARG:HH21	1:D:3245:ARG:HB2	1.80	0.46
1:D:3468:VAL:HA	1:D:3471:PHE:CE2	2.50	0.46
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.98	0.46
1:B:1325:MSE:O	1:B:1329:GLU:HB2	2.16	0.46
1:C:2331:GLY:O	1:C:2332:LEU:O	2.33	0.46
1:D:3272:LYS:NZ	1:D:3272:LYS:CB	2.77	0.46
1:C:2288:LEU:HG	1:C:2292:LEU:HD22	1.98	0.46
1:D:3397:ARG:HA	1:D:3427:GLU:O	2.16	0.46
1:A:23:GLU:OE1	1:A:23:GLU:HA	2.14	0.46
1:A:150:TRP:CE2	1:A:199:LEU:HD13	2.51	0.46
1:A:392:VAL:O	1:A:392:VAL:HG12	2.14	0.46
1:B:1367:HIS:HB2	5:B:4824:HOH:O	2.14	0.46
1:B:1527:ALA:O	1:B:1531:THR:HG23	2.16	0.46
1:D:3099:ILE:HD12	1:D:3099:ILE:HA	1.68	0.46
1:B:1532:GLU:HG2	1:B:1549:LYS:HG2	1.98	0.46
1:A:21:ILE:N	1:A:21:ILE:HD12	2.31	0.45
1:B:1235:ILE:O	1:B:1239:MSE:HG2	2.16	0.45
1:D:3526:ILE:O	1:D:3530:VAL:HG23	2.16	0.45
1:A:156:LYS:CG	1:A:197:ARG:HG2	2.44	0.45
1:A:332:LEU:HA	1:A:336:GLU:OE2	2.16	0.45
1:C:2145:SER:HB3	5:C:4036:HOH:O	2.15	0.45
1:D:3066:LEU:HD22	1:D:3070:ARG:NE	2.32	0.45
1:A:371:GLU:CD	1:A:371:GLU:N	2.62	0.45
1:C:2022:LYS:HD2	1:C:2022:LYS:O	2.16	0.45
1:C:2194:ARG:NH1	1:C:2197:ARG:NH2	2.65	0.45
1:C:2374:PRO:HB3	1:C:2383:ILE:HD12	1.98	0.45
1:C:2471:PHE:CG	1:C:2472:PRO:HD3	2.52	0.45
5:C:4932:HOH:O	1:D:3063:ILE:HD13	2.15	0.45
1:A:177:MSE:CE	1:A:200:PRO:HB2	2.47	0.45
1:B:1172:LEU:O	1:B:1175:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1367:HIS:HB3	5:B:4824:HOH:O	2.16	0.45
1:C:2069:HIS:HD2	5:C:4306:HOH:O	1.99	0.45
1:C:2408:ALA:HB2	1:C:2437:THR:HG22	1.98	0.45
1:D:3339:LYS:N	1:D:3339:LYS:HD3	2.29	0.45
1:A:287:ALA:O	1:A:291:LEU:HD22	2.17	0.45
1:A:528:ILE:O	1:A:532:GLU:HG3	2.16	0.45
1:A:538:LYS:HA	5:A:4882:HOH:O	2.16	0.45
1:B:1232:ASP:OD1	1:B:1264:ARG:NH2	2.49	0.45
1:A:338:GLN:HB2	1:A:339:LYS:NZ	2.31	0.45
1:A:453:LYS:HD2	1:A:459:VAL:HG22	1.98	0.45
1:B:1315:ALA:O	1:B:1319:ILE:HG13	2.17	0.45
1:B:1335:GLN:O	1:B:1339:LYS:HG3	2.16	0.45
1:B:1401:PRO:HA	1:B:1436:LEU:HD23	1.97	0.45
1:A:66:LEU:HD21	1:A:70:ARG:HH11	1.75	0.45
1:A:108:MSE:N	1:A:109:PRO:CD	2.79	0.45
1:B:1259:ASN:ND2	5:B:4936:HOH:O	2.49	0.45
1:B:1350:LEU:HD22	1:B:1358:ILE:CD1	2.47	0.45
1:C:2286:VAL:HG11	1:C:2466:ASN:O	2.17	0.45
1:B:1075:MSE:HE1	1:B:1084:TYR:CD2	2.51	0.45
1:B:1456:ASP:OD1	1:B:1458:ARG:HD3	2.16	0.45
1:B:1481:CYS:O	1:B:1482:ASN:HB2	2.17	0.45
1:D:3343:MSE:SE	5:D:4695:HOH:O	2.84	0.45
1:A:133:LEU:HB2	1:A:199:LEU:HD11	1.99	0.44
1:B:1024:LYS:HZ2	1:D:3022:LYS:CD	2.18	0.44
1:B:1312:ALA:HB2	1:B:1343:MSE:HE3	1.98	0.44
1:D:3026:LYS:N	1:D:3027:PRO:CD	2.80	0.44
1:D:3184:LEU:HD12	1:D:3200:PRO:CG	2.46	0.44
1:D:3481:CYS:HB3	1:D:3540:ALA:HB1	1.99	0.44
1:C:2412:GLU:HG2	5:C:4719:HOH:O	2.17	0.44
1:C:2432:GLU:O	1:C:2436:LEU:HB2	2.17	0.44
1:C:2454:LEU:HD12	1:C:2458:ARG:HB2	1.99	0.44
1:D:3555:GLU:HB3	1:D:3556:ARG:NH1	2.31	0.44
1:A:554:LYS:HG2	1:A:554:LYS:H	1.38	0.44
1:C:2205:VAL:HG11	1:C:2231:TYR:HD1	1.82	0.44
1:D:3286:VAL:HG22	1:D:3470:ILE:CG1	2.47	0.44
1:D:3484:ARG:O	1:D:3485:HIS:CD2	2.70	0.44
1:A:66:LEU:HD22	1:B:1217:PHE:CZ	2.38	0.44
1:C:2033:ARG:HD3	1:C:2093:GLU:OE2	2.16	0.44
1:A:122:GLN:O	1:A:123:TYR:C	2.58	0.44
1:B:1208:ASP:OD1	1:B:1224:LYS:HB3	2.17	0.44
1:B:1484:ARG:HG2	1:C:2543:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3259:ASN:O	1:D:3263:PHE:HD1	2.01	0.44
1:A:297:VAL:HG23	1:A:298:ILE:HG13	1.98	0.44
1:B:1351:VAL:HA	1:B:1367:HIS:O	2.18	0.44
1:D:3078:PRO:HD2	5:D:4900:HOH:O	2.17	0.44
1:D:3338:GLN:HB2	1:D:3339:LYS:HZ2	1.79	0.44
1:A:339:LYS:NZ	1:A:339:LYS:N	2.65	0.43
1:A:545:GLU:OE2	1:A:549:LYS:NZ	2.47	0.43
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.80	0.43
1:C:2314:GLU:HB2	4:C:2601:NAD:O1N	2.18	0.43
1:B:1108:MSE:HE3	1:B:1516:LEU:HD11	2.00	0.43
1:B:1248:ARG:NH2	1:B:1272:LYS:HG2	2.33	0.43
1:C:2089:GLN:OE1	1:C:2131:LYS:HE2	2.17	0.43
1:D:3399:PHE:CG	1:D:3427:GLU:HB3	2.53	0.43
1:A:432:GLU:O	1:A:436:LEU:HB2	2.18	0.43
1:B:1060:THR:N	1:B:1063:ILE:HD12	2.25	0.43
1:D:3108:MSE:N	1:D:3109:PRO:CD	2.81	0.43
1:D:3172:LEU:O	1:D:3175:TYR:HB2	2.19	0.43
1:D:3194:ARG:HG2	1:D:3558:TRP:CD1	2.53	0.43
1:A:24:LYS:HD3	1:C:2024:LYS:HB3	2.01	0.43
1:C:2300:LYS:NZ	1:C:2300:LYS:CB	2.62	0.43
1:A:154:HIS:O	1:A:197:ARG:HG3	2.18	0.43
1:A:389:ILE:HG23	1:A:399:PHE:CZ	2.54	0.43
1:B:1036:LYS:HE2	1:B:1562:TYR:HB3	2.01	0.43
1:C:2082:TYR:O	1:C:2086:MSE:HB2	2.19	0.43
1:D:3478:VAL:HG13	1:D:3483:THR:HB	2.01	0.43
1:C:2038:MSE:HE2	1:D:3127:PHE:CE2	2.53	0.43
1:C:2431:GLU:O	1:C:2435:THR:HG23	2.18	0.43
1:D:3177:MSE:SE	5:D:4067:HOH:O	2.86	0.43
1:B:1104:ILE:HG23	1:B:1105:GLU:N	2.32	0.43
1:B:1300:LYS:NZ	1:B:1301:PRO:O	2.52	0.43
1:C:2542:ARG:HD3	1:C:2542:ARG:C	2.44	0.43
1:D:3022:LYS:HD2	1:D:3022:LYS:O	2.19	0.43
1:D:3115:THR:O	1:D:3115:THR:HG22	2.19	0.43
1:B:1335:GLN:HG3	1:B:1339:LYS:HE2	2.00	0.43
1:C:2100:LEU:HA	1:C:2107:LEU:HD12	1.99	0.43
1:A:152:GLU:HG2	1:A:196:ASP:O	2.19	0.43
1:B:1521:GLU:HG2	5:B:4059:HOH:O	2.18	0.43
1:B:1543:TYR:HA	1:B:1544:PRO:C	2.43	0.43
1:C:2070:ARG:O	1:C:2074:LYS:HD3	2.18	0.43
1:C:2556:ARG:CG	1:C:2556:ARG:NH1	2.80	0.43
1:D:3105:GLU:OE2	1:D:3516:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:N	1:A:350:LEU:HD23	2.34	0.43
1:B:1351:VAL:CG1	1:B:1369:ALA:HA	2.49	0.43
1:B:1368:SER:O	1:B:1369:ALA:C	2.62	0.43
1:B:1401:PRO:HA	1:B:1436:LEU:CD2	2.48	0.43
1:A:66:LEU:HD21	1:A:70:ARG:CZ	2.46	0.42
1:B:1273:TYR:O	1:B:1485:HIS:HD2	2.02	0.42
1:C:2539:MSE:HE2	1:C:2539:MSE:HB3	1.91	0.42
1:D:3298:ILE:O	1:D:3299:SER:C	2.60	0.42
1:A:26:LYS:O	1:A:27:PRO:C	2.61	0.42
1:A:87:GLY:HA3	5:A:4428:HOH:O	2.18	0.42
1:A:350:LEU:HD13	1:A:358:ILE:HD13	2.00	0.42
1:B:1317:LEU:CG	5:B:4327:HOH:O	2.67	0.42
1:B:1320:ALA:CB	5:B:4104:HOH:O	2.66	0.42
1:B:1505:GLU:O	1:B:1509:GLN:HG3	2.18	0.42
1:D:3025:GLY:C	1:D:3027:PRO:HD2	2.44	0.42
1:A:392:VAL:CG1	5:A:4007:HOH:O	2.67	0.42
1:A:466:ASN:HA	4:A:601:NAD:O7N	2.19	0.42
1:B:1031:ASN:HA	1:B:1032:PRO:HD2	1.87	0.42
1:D:3207:THR:O	1:D:3224:LYS:HA	2.18	0.42
1:A:447:SER:HB3	1:A:448:PRO:HD2	2.00	0.42
1:B:1140:ARG:CZ	1:B:1140:ARG:CB	2.97	0.42
1:A:41:THR:O	1:A:45:ARG:HG3	2.19	0.42
1:A:549:LYS:HG2	1:A:549:LYS:H	1.62	0.42
1:C:2454:LEU:C	1:C:2456:ASP:H	2.28	0.42
1:C:2456:ASP:OD1	1:C:2456:ASP:C	2.60	0.42
1:A:159:VAL:O	1:A:180:PRO:HB3	2.19	0.42
1:A:283:THR:HA	1:A:286:VAL:HG23	2.00	0.42
1:B:1182:GLY:HA3	5:B:4647:HOH:O	2.19	0.42
1:D:3194:ARG:HE	1:D:3197:ARG:HG3	1.84	0.42
1:C:2389:ILE:HG23	1:C:2399:PHE:CZ	2.54	0.42
1:C:2475:ALA:O	1:C:2479:ILE:HG13	2.19	0.42
1:A:297:VAL:HG21	1:A:442:LEU:CD2	2.50	0.42
1:B:1355:LYS:HD2	1:B:1355:LYS:HA	1.89	0.42
1:C:2077:SER:O	1:C:2081:LYS:HG3	2.18	0.42
1:D:3407:MSE:HG3	1:D:3414:PRO:HB3	2.02	0.42
1:A:205:VAL:HG11	1:A:231:TYR:HD1	1.85	0.42
1:A:322:LEU:HD22	1:A:322:LEU:HA	1.79	0.42
1:A:556:ARG:NH1	1:A:556:ARG:HG2	2.34	0.42
1:B:1322:LEU:HD12	1:B:1322:LEU:HA	1.91	0.42
1:B:1332:LEU:HD12	1:B:1332:LEU:N	2.13	0.42
1:C:2110:ILE:O	1:C:2115:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:CD2	1:A:151:PRO:HD2	2.55	0.42
1:A:159:VAL:HG23	1:A:184:LEU:HD21	2.02	0.42
1:C:2351:VAL:HA	1:C:2367:HIS:O	2.20	0.42
1:A:456:ASP:OD1	1:A:456:ASP:C	2.63	0.41
1:B:1184:LEU:O	1:B:1187:TYR:HB2	2.20	0.41
1:B:1345:ASP:C	1:B:1347:TYR:H	2.28	0.41
1:B:1347:TYR:HB2	1:B:1354:ARG:HH22	1.85	0.41
1:B:1487:SER:OG	1:B:1490:VAL:HG23	2.20	0.41
1:B:1497:ALA:O	1:B:1501:GLN:HG3	2.20	0.41
1:D:3162:ASP:C	1:D:3162:ASP:OD1	2.63	0.41
1:D:3301:PRO:O	1:D:3302:ILE:C	2.63	0.41
1:A:520:GLN:O	1:A:524:ILE:HG12	2.20	0.41
1:C:2370:PRO:O	1:C:2371:GLU:C	2.62	0.41
1:C:2400:THR:HB	1:C:2401:PRO:HD2	2.02	0.41
1:D:3545:GLU:HA	1:D:3546:PRO:HD3	1.92	0.41
1:A:300:LYS:HZ1	1:A:304:GLU:C	2.27	0.41
1:B:1261:ASN:CA	1:B:1264:ARG:HG2	2.49	0.41
1:B:1317:LEU:HD11	5:B:4327:HOH:O	2.21	0.41
1:D:3551:LYS:HB3	1:D:3551:LYS:HZ2	1.85	0.41
1:A:36:LYS:NZ	5:A:4588:HOH:O	2.53	0.41
1:A:69:HIS:HE1	1:A:102:ASP:OD2	2.03	0.41
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.94	0.41
1:B:1036:LYS:HB3	1:B:1039:ALA:HB3	2.02	0.41
1:B:1119:ALA:O	1:B:1123:TYR:N	2.53	0.41
1:B:1310:LEU:HD13	1:B:1377:PHE:CD1	2.56	0.41
1:C:2533:TYR:O	1:C:2537:ASN:ND2	2.47	0.41
1:C:2539:MSE:CE	5:C:4084:HOH:O	2.67	0.41
1:A:335:GLN:O	1:A:339:LYS:HD2	2.19	0.41
1:B:1310:LEU:HD21	1:B:1398:LEU:HD23	2.02	0.41
1:C:2046:GLN:HG2	1:C:2051:GLN:HG3	2.00	0.41
1:C:2322:LEU:HD12	1:C:2322:LEU:HA	1.78	0.41
1:C:2407:MSE:HG3	5:C:4314:HOH:O	2.20	0.41
1:D:3474:VAL:O	1:D:3478:VAL:HG23	2.20	0.41
1:A:379:ASP:HA	5:A:4486:HOH:O	2.19	0.41
1:B:1184:LEU:HD22	1:B:1198:CYS:HB3	2.02	0.41
1:B:1210:ILE:CD1	5:B:4445:HOH:O	2.69	0.41
1:C:2385:LYS:N	1:C:2386:PRO:CD	2.83	0.41
1:D:3069:HIS:HE1	1:D:3102:ASP:OD2	2.04	0.41
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.84	0.41
1:B:1069:HIS:CE1	1:B:1102:ASP:OD2	2.65	0.41
1:B:1331:GLY:O	1:B:1332:LEU:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2174:VAL:O	1:C:2174:VAL:HG12	2.20	0.41
1:D:3136:SER:HB2	1:D:3221:LEU:HD22	2.03	0.41
1:D:3335:GLN:O	1:D:3339:LYS:HE2	2.20	0.41
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.92	0.41
1:B:1397:ARG:HA	1:B:1427:GLU:O	2.20	0.41
1:C:2120:CYS:C	1:C:2122:GLN:H	2.28	0.41
1:D:3077:SER:O	1:D:3081:LYS:HG3	2.21	0.41
1:D:3482:ASN:HD21	4:D:3602:NAD:H4B	1.86	0.41
1:A:400:THR:HB	1:A:401:PRO:HD2	2.02	0.41
1:B:1082:TYR:CZ	1:B:1086:MSE:HG3	2.56	0.41
1:B:1183:LYS:HE3	1:B:1255:GLU:CD	2.45	0.41
1:B:1261:ASN:HD21	1:B:1264:ARG:HH11	1.62	0.41
1:B:1273:TYR:O	1:B:1485:HIS:CD2	2.74	0.41
1:B:1370:PRO:O	1:B:1371:GLU:C	2.64	0.41
1:D:3308:LEU:HD23	1:D:3389:ILE:HD11	2.03	0.41
1:D:3453:LYS:HA	1:D:3458:ARG:O	2.21	0.41
1:B:1166:ILE:HD12	1:B:1179:ILE:HG13	2.01	0.41
1:D:3082:TYR:CD2	1:D:3082:TYR:C	2.99	0.41
1:A:24:LYS:HZ2	1:C:2022:LYS:HD2	1.85	0.40
1:B:1268:LYS:NZ	5:B:4587:HOH:O	2.49	0.40
1:B:1354:ARG:HH21	1:B:1356:ALA:HB3	1.86	0.40
1:B:1382:ASN:O	1:B:1385:LYS:HG3	2.22	0.40
1:C:2380:ALA:O	1:C:2384:LEU:HB2	2.20	0.40
1:D:3209:ASN:OD1	1:D:3209:ASN:C	2.63	0.40
1:D:3294:ALA:O	1:D:3297:VAL:HG22	2.21	0.40
1:D:3492:LEU:O	1:D:3496:LYS:HG3	2.21	0.40
1:A:33:ARG:NH2	5:A:4407:HOH:O	2.54	0.40
1:A:324:VAL:O	1:A:328:VAL:HG23	2.21	0.40
1:A:369:ALA:HA	1:A:370:PRO:HD3	1.92	0.40
1:B:1551:LYS:O	1:B:1555:GLU:HB2	2.21	0.40
1:D:3051:GLN:HA	1:D:3051:GLN:NE2	2.35	0.40
1:B:1468:VAL:HA	1:B:1471:PHE:CE2	2.56	0.40
1:C:2023:GLU:HA	1:C:2023:GLU:OE1	2.22	0.40
1:D:3165:ARG:NH2	2:D:3603:OXL:O1	2.45	0.40
1:A:66:LEU:CD2	1:A:70:ARG:HD3	2.51	0.40
1:A:316:ALA:N	1:A:392:VAL:HG11	2.36	0.40
1:A:343:MSE:SE	5:A:4862:HOH:O	2.89	0.40
1:B:1344:PHE:CD2	1:B:1344:PHE:C	2.99	0.40
1:B:1447:SER:HB3	1:B:1448:PRO:HD2	2.03	0.40
1:C:2057:LYS:HE2	1:C:2059:GLU:HG2	2.03	0.40
1:C:2143:VAL:HB	1:C:2237:GLU:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2454:LEU:C	1:C:2456:ASP:N	2.78	0.40
1:D:3165:ARG:O	1:D:3165:ARG:NE	2.54	0.40
1:D:3350:LEU:HD23	1:D:3350:LEU:N	2.36	0.40
1:D:3471:PHE:N	1:D:3472:PRO:CD	2.84	0.40
1:A:219:MSE:O	1:B:1056:PRO:HD2	2.22	0.40
1:A:295:GLN:HA	1:A:295:GLN:OE1	2.22	0.40
1:B:1140:ARG:NH2	1:B:1233:ASP:OD2	2.55	0.40
1:B:1150:TRP:HA	1:B:1151:PRO:HD3	1.89	0.40
1:C:2108:MSE:N	1:C:2109:PRO:CD	2.85	0.40
1:C:2217:PHE:O	1:C:2218:TYR:C	2.64	0.40
1:D:3296:LYS:HE2	1:D:3296:LYS:HB2	1.89	0.40
1:D:3461:THR:HG21	1:D:3511:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/564 (98%)	530 (96%)	19 (3%)	2 (0%)	30	34
1	B	551/564 (98%)	522 (95%)	26 (5%)	3 (0%)	24	27
1	C	551/564 (98%)	530 (96%)	17 (3%)	4 (1%)	18	19
1	D	551/564 (98%)	528 (96%)	20 (4%)	3 (0%)	24	27
All	All	2204/2256 (98%)	2110 (96%)	82 (4%)	12 (0%)	24	27

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1332	LEU
1	C	2332	LEU
1	A	397	ARG

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Mol	Chain	Res	Type
1	C	2392	VAL
1	D	3302	ILE
1	C	2397	ARG
1	B	1392	VAL
1	D	3103	ASP
1	A	270	ARG
1	D	3392	VAL
1	C	2056	PRO
1	B	1369	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	469/465 (101%)	400 (85%)	69 (15%)	3	2
1	B	469/465 (101%)	395 (84%)	74 (16%)	2	2
1	C	469/465 (101%)	400 (85%)	69 (15%)	3	2
1	D	469/465 (101%)	404 (86%)	65 (14%)	3	3
All	All	1876/1860 (101%)	1599 (85%)	277 (15%)	3	2

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	23	GLU
1	A	24	LYS
1	A	43	GLN
1	A	70	ARG
1	A	75	MSE
1	A	76	THR
1	A	85	ILE
1	A	99	ILE
1	A	100	LEU
1	A	101	GLN
1	A	104	ILE

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Mol	Chain	Res	Type
1	A	111	VAL
1	A	121	SER
1	A	123	TYR
1	A	133	LEU
1	A	140	ARG
1	A	145	SER
1	A	153	ASN
1	A	165	ARG
1	A	169	LEU
1	A	196	ASP
1	A	197	ARG
1	A	219	MSE
1	A	221	LEU
1	A	227	ARG
1	A	245	ARG
1	A	248	ARG
1	A	251	LEU
1	A	272	LYS
1	A	286	VAL
1	A	291	LEU
1	A	292	LEU
1	A	296	LYS
1	A	299	SER
1	A	300	LYS
1	A	302	ILE
1	A	306	LYS
1	A	322	LEU
1	A	327	MSE
1	A	329	GLU
1	A	335	GLN
1	A	336	GLU
1	A	339	LYS
1	A	340	LYS
1	A	346	LYS
1	A	350	LEU
1	A	355	LYS
1	A	358	ILE
1	A	371	GLU
1	A	384	LEU
1	A	385	LYS
1	A	389	ILE
1	A	392	VAL

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Mol	Chain	Res	Type
1	A	398	LEU
1	A	407	MSE
1	A	489	SER
1	A	492	LEU
1	A	499	THR
1	A	502	LEU
1	A	505	GLU
1	A	520	GLN
1	A	529	LYS
1	A	539	MSE
1	A	554	LYS
1	A	556	ARG
1	A	559	ARG
1	A	561	GLU
1	A	571	GLU
1	B	1021	ILE
1	B	1022	LYS
1	B	1024	LYS
1	B	1043	GLN
1	B	1057	LYS
1	B	1058	ILE
1	B	1070	ARG
1	B	1073	LYS
1	B	1074	LYS
1	B	1075	MSE
1	B	1085	ILE
1	B	1094	LYS
1	B	1099	ILE
1	B	1100	LEU
1	B	1111	VAL
1	B	1123	TYR
1	B	1131	LYS
1	B	1133	LEU
1	B	1140	ARG
1	B	1153	ASN
1	B	1165	ARG
1	B	1214	LYS
1	B	1224	LYS
1	B	1233	ASP
1	B	1236	ASP
1	B	1243	THR
1	B	1248	ARG

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Mol	Chain	Res	Type
1	B	1251	LEU
1	B	1267	ARG
1	B	1286	VAL
1	B	1291	LEU
1	B	1292	LEU
1	B	1296	LYS
1	B	1297	VAL
1	B	1300	LYS
1	B	1304	GLU
1	B	1306	LYS
1	B	1321	ASN
1	B	1323	ILE
1	B	1332	LEU
1	B	1346	LYS
1	B	1350	LEU
1	B	1357	LYS
1	B	1362	GLN
1	B	1363	GLU
1	B	1368	SER
1	B	1371	GLU
1	B	1372	SER
1	B	1373	ILE
1	B	1383	ILE
1	B	1384	LEU
1	B	1389	ILE
1	B	1397	ARG
1	B	1398	LEU
1	B	1402	ASP
1	B	1423	THR
1	B	1436	LEU
1	B	1438	GLU
1	B	1455	THR
1	B	1492	LEU
1	B	1499	THR
1	B	1502	LEU
1	B	1504	ASP
1	B	1505	GLU
1	B	1507	LEU
1	B	1511	ARG
1	B	1519	ILE
1	B	1520	GLN
1	B	1524	ILE

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Mol	Chain	Res	Type
1	B	1531	THR
1	B	1547	GLU
1	B	1549	LYS
1	B	1557	THR
1	B	1561	GLU
1	C	2021	ILE
1	C	2022	LYS
1	C	2023	GLU
1	C	2026	LYS
1	C	2043	GLN
1	C	2066	LEU
1	C	2070	ARG
1	C	2085	ILE
1	C	2086	MSE
1	C	2094	LYS
1	C	2099	ILE
1	C	2100	LEU
1	C	2104	ILE
1	C	2111	VAL
1	C	2122	GLN
1	C	2123	TYR
1	C	2133	LEU
1	C	2140	ARG
1	C	2146	ILE
1	C	2165	ARG
1	C	2169	LEU
1	C	2221	LEU
1	C	2223	GLN
1	C	2224	LYS
1	C	2225	ARG
1	C	2251	LEU
1	C	2286	VAL
1	C	2291	LEU
1	C	2292	LEU
1	C	2296	LYS
1	C	2297	VAL
1	C	2300	LYS
1	C	2306	LYS
1	C	2328	VAL
1	C	2330	ASN
1	C	2333	SER
1	C	2339	LYS

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Mol	Chain	Res	Type
1	C	2346	LYS
1	C	2350	LEU
1	C	2355	LYS
1	C	2357	LYS
1	C	2363	GLU
1	C	2375	ASP
1	C	2378	GLU
1	C	2384	LEU
1	C	2385	LYS
1	C	2389	ILE
1	C	2392	VAL
1	C	2398	LEU
1	C	2436	LEU
1	C	2438	GLU
1	C	2453	LYS
1	C	2454	LEU
1	C	2455	THR
1	C	2458	ARG
1	C	2492	LEU
1	C	2500	SER
1	C	2502	LEU
1	C	2507	LEU
1	C	2520	GLN
1	C	2531	THR
1	C	2539	MSE
1	C	2547	GLU
1	C	2551	LYS
1	C	2556	ARG
1	C	2559	ARG
1	C	2561	GLU
1	C	2563	ASP
1	C	2571	GLU
1	D	3022	LYS
1	D	3043	GLN
1	D	3057	LYS
1	D	3066	LEU
1	D	3070	ARG
1	D	3074	LYS
1	D	3076	THR
1	D	3085	ILE
1	D	3099	ILE
1	D	3100	LEU

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Mol	Chain	Res	Type
1	D	3111	VAL
1	D	3123	TYR
1	D	3133	LEU
1	D	3140	ARG
1	D	3146	ILE
1	D	3153	ASN
1	D	3156	LYS
1	D	3165	ARG
1	D	3169	LEU
1	D	3193	ILE
1	D	3205	VAL
1	D	3221	LEU
1	D	3229	GLN
1	D	3245	ARG
1	D	3248	ARG
1	D	3251	LEU
1	D	3266	LEU
1	D	3272	LYS
1	D	3286	VAL
1	D	3291	LEU
1	D	3292	LEU
1	D	3296	LYS
1	D	3297	VAL
1	D	3300	LYS
1	D	3306	LYS
1	D	3322	LEU
1	D	3327	MSE
1	D	3329	GLU
1	D	3333	SER
1	D	3336	GLU
1	D	3339	LYS
1	D	3346	LYS
1	D	3350	LEU
1	D	3352	LYS
1	D	3355	LYS
1	D	3358	ILE
1	D	3363	GLU
1	D	3371	GLU
1	D	3384	LEU
1	D	3389	ILE
1	D	3412	GLU
1	D	3438	GLU

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Mol	Chain	Res	Type
1	D	3489	SER
1	D	3492	LEU
1	D	3502	LEU
1	D	3507	LEU
1	D	3518	ASN
1	D	3520	GLN
1	D	3529	LYS
1	D	3531	THR
1	D	3538	LYS
1	D	3547	GLU
1	D	3551	LYS
1	D	3559	ARG
1	D	3571	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	64	GLN
1	A	69	HIS
1	A	125	HIS
1	A	153	ASN
1	A	261	ASN
1	A	305	HIS
1	A	330	ASN
1	A	411	ASN
1	A	482	ASN
1	A	485	HIS
1	A	520	GLN
1	B	1043	GLN
1	B	1051	GLN
1	B	1064	GLN
1	B	1069	HIS
1	B	1154	HIS
1	B	1229	GLN
1	B	1261	ASN
1	B	1411	ASN
1	B	1425	GLN
1	B	1485	HIS
1	B	1518	ASN
1	B	1520	GLN
1	C	2064	GLN

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Mol	Chain	Res	Type
1	C	2069	HIS
1	C	2122	GLN
1	C	2154	HIS
1	C	2261	ASN
1	C	2425	GLN
1	C	2520	GLN
1	D	3051	GLN
1	D	3064	GLN
1	D	3069	HIS
1	D	3122	GLN
1	D	3125	HIS
1	D	3153	ASN
1	D	3229	GLN
1	D	3230	GLN
1	D	3261	ASN
1	D	3482	ASN
1	D	3485	HIS
1	D	3518	ASN
1	D	3520	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAD	C	2601	-	46,48,48	1.83	9 (19%)	64,73,73	1.85	12 (18%)
4	NAD	C	2602	-	46,48,48	2.67	13 (28%)	64,73,73	1.86	11 (17%)
4	NAD	A	601	-	46,48,48	2.01	12 (26%)	64,73,73	1.84	10 (15%)
4	NAD	D	3601	-	46,48,48	2.01	13 (28%)	64,73,73	1.85	11 (17%)
2	OXL	B	1603	3	5,5,5	1.68	2 (40%)	6,6,6	2.46	2 (33%)
4	NAD	B	1602	-	46,48,48	2.31	13 (28%)	64,73,73	1.84	11 (17%)
2	OXL	A	603	3	5,5,5	1.93	2 (40%)	6,6,6	2.27	2 (33%)
4	NAD	D	3602	-	46,48,48	2.23	9 (19%)	64,73,73	1.86	11 (17%)
2	OXL	C	2603	3	5,5,5	1.68	2 (40%)	6,6,6	2.41	2 (33%)
4	NAD	B	1601	-	46,48,48	1.93	12 (26%)	64,73,73	1.86	11 (17%)
2	OXL	D	3603	3	5,5,5	1.74	2 (40%)	6,6,6	2.34	2 (33%)
4	NAD	A	602	-	46,48,48	2.26	13 (28%)	64,73,73	1.86	11 (17%)

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

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

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2602	NAD	C2N-N1N	10.90	1.47	1.35
4	A	602	NAD	C2N-N1N	8.72	1.44	1.35
4	B	1602	NAD	C2N-N1N	7.91	1.43	1.35
4	B	1602	NAD	O4D-C1D	7.74	1.51	1.40
4	A	601	NAD	C2N-N1N	7.25	1.42	1.35
4	D	3602	NAD	C2N-N1N	7.12	1.42	1.35
4	C	2602	NAD	O4D-C1D	7.08	1.50	1.40
4	D	3601	NAD	C2N-N1N	7.04	1.42	1.35
4	D	3602	NAD	O4D-C1D	6.82	1.49	1.40
4	C	2602	NAD	C6N-N1N	6.59	1.50	1.35
4	C	2601	NAD	C2N-N1N	6.51	1.42	1.35
4	B	1601	NAD	C2N-N1N	6.13	1.41	1.35
4	A	602	NAD	O4D-C1D	5.84	1.48	1.40
4	C	2602	NAD	C4N-C3N	4.53	1.46	1.39
4	B	1601	NAD	C5A-N7A	-4.52	1.30	1.39
4	B	1601	NAD	C6N-N1N	4.38	1.45	1.35
4	A	602	NAD	C5A-N7A	-4.34	1.31	1.39
4	D	3602	NAD	C5A-N7A	-4.25	1.31	1.39
4	A	602	NAD	C6N-N1N	4.21	1.44	1.35
4	B	1602	NAD	PN-O3	4.18	1.64	1.59
4	A	601	NAD	C5A-N7A	-4.18	1.31	1.39
4	C	2601	NAD	C6N-N1N	4.13	1.44	1.35
4	D	3602	NAD	C6N-N1N	4.13	1.44	1.35
4	D	3601	NAD	C6N-N1N	4.11	1.44	1.35
4	D	3601	NAD	C5A-N7A	-4.11	1.31	1.39
4	A	601	NAD	C6N-N1N	4.11	1.44	1.35
4	C	2602	NAD	C5A-N7A	-4.04	1.31	1.39
4	D	3601	NAD	O4D-C1D	3.99	1.46	1.40
4	C	2601	NAD	C5A-N7A	-3.93	1.31	1.39
4	B	1602	NAD	C5A-N7A	-3.76	1.32	1.39
4	D	3601	NAD	C3N-C7N	3.66	1.56	1.50
4	B	1602	NAD	C6N-N1N	3.60	1.43	1.35
4	D	3602	NAD	PN-O3	3.57	1.63	1.59
4	A	602	NAD	C3N-C7N	3.44	1.55	1.50
4	A	601	NAD	O4D-C1D	3.40	1.45	1.40
4	C	2601	NAD	C5A-C4A	-3.38	1.33	1.39
4	B	1601	NAD	O4D-C1D	3.23	1.45	1.40
4	D	3601	NAD	C5A-C4A	-3.21	1.33	1.39
4	A	601	NAD	C5A-C4A	-3.20	1.33	1.39
4	D	3602	NAD	C4N-C3N	3.15	1.44	1.39
4	A	601	NAD	C3N-C7N	3.08	1.55	1.50
4	A	601	NAD	C4N-C3N	3.01	1.44	1.39
4	D	3602	NAD	C5A-C4A	-2.97	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1602	NAD	C4N-C3N	2.97	1.43	1.39
4	D	3602	NAD	O4D-C4D	2.95	1.51	1.45
4	B	1601	NAD	C5A-C4A	-2.88	1.33	1.39
4	A	602	NAD	C5A-C4A	-2.86	1.34	1.39
4	C	2602	NAD	C5A-C4A	-2.84	1.34	1.39
2	A	603	OXL	O4-C2	-2.83	1.22	1.30
4	B	1601	NAD	C8A-N7A	2.78	1.37	1.31
4	C	2602	NAD	O4B-C1B	2.74	1.48	1.42
4	D	3602	NAD	C8A-N7A	2.72	1.36	1.31
4	B	1602	NAD	C5A-C4A	-2.70	1.34	1.39
4	C	2602	NAD	C5N-C4N	2.66	1.43	1.38
2	D	3603	OXL	O4-C2	-2.61	1.23	1.30
2	C	2603	OXL	O4-C2	-2.60	1.23	1.30
4	C	2602	NAD	C8A-N7A	2.59	1.36	1.31
2	B	1603	OXL	O4-C2	-2.59	1.23	1.30
4	D	3601	NAD	C4N-C3N	2.57	1.43	1.39
2	A	603	OXL	O3-C1	-2.55	1.23	1.30
2	B	1603	OXL	O3-C1	-2.53	1.23	1.30
2	D	3603	OXL	O3-C1	-2.52	1.23	1.30
4	B	1602	NAD	C3N-C7N	2.52	1.54	1.50
4	B	1601	NAD	C3N-C7N	2.49	1.54	1.50
4	A	602	NAD	C8A-N7A	2.48	1.36	1.31
4	C	2601	NAD	C8A-N7A	2.46	1.36	1.31
4	C	2602	NAD	C2A-N3A	2.45	1.38	1.33
4	A	602	NAD	O4D-C4D	2.43	1.50	1.45
4	D	3601	NAD	O4B-C1B	2.40	1.47	1.42
2	C	2603	OXL	O3-C1	-2.40	1.24	1.30
4	A	601	NAD	C2A-N3A	2.40	1.38	1.33
4	B	1602	NAD	C8A-N7A	2.38	1.36	1.31
4	D	3601	NAD	C2A-N3A	2.37	1.38	1.33
4	B	1601	NAD	C4A-N9A	-2.35	1.32	1.37
4	A	601	NAD	C4A-N9A	-2.35	1.32	1.37
4	D	3601	NAD	C4A-N9A	-2.32	1.32	1.37
4	D	3601	NAD	C5N-C4N	2.31	1.42	1.38
4	C	2601	NAD	C3N-C7N	2.31	1.54	1.50
4	A	602	NAD	C4N-C3N	2.31	1.42	1.39
4	A	601	NAD	C2A-N1A	2.29	1.38	1.33
4	B	1602	NAD	C2A-N1A	2.28	1.38	1.33
4	D	3601	NAD	C8A-N7A	2.27	1.36	1.31
4	B	1601	NAD	C5N-C4N	2.26	1.42	1.38
4	A	601	NAD	O4B-C1B	2.26	1.47	1.42
4	B	1601	NAD	C4N-C3N	2.25	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	NAD	C2A-N3A	2.23	1.37	1.33
4	C	2601	NAD	C4A-N9A	-2.22	1.33	1.37
4	B	1602	NAD	O4D-C4D	2.20	1.49	1.45
4	B	1601	NAD	O4D-C4D	2.19	1.49	1.45
4	B	1602	NAD	C2A-N3A	2.16	1.37	1.33
4	D	3601	NAD	C2A-N1A	2.15	1.37	1.33
4	A	602	NAD	C2A-N1A	2.14	1.37	1.33
4	B	1601	NAD	C2A-N1A	2.13	1.37	1.33
4	A	602	NAD	C2A-N3A	2.12	1.37	1.33
4	A	602	NAD	PN-O3	2.11	1.61	1.59
4	C	2602	NAD	C2N-C3N	2.09	1.42	1.39
4	A	601	NAD	C5N-C4N	2.09	1.42	1.38
4	C	2601	NAD	C2A-N1A	2.04	1.37	1.33
4	A	602	NAD	C2N-C3N	2.03	1.42	1.39
4	C	2602	NAD	O3B-C3B	2.03	1.48	1.43
4	C	2602	NAD	C2A-N1A	2.02	1.37	1.33
4	B	1602	NAD	O4B-C1B	2.01	1.46	1.42

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2602	NAD	C5A-C4A-N3A	-6.20	118.18	126.72
4	A	602	NAD	C5A-C4A-N3A	-6.08	118.35	126.72
4	D	3602	NAD	C5A-C4A-N3A	-6.07	118.36	126.72
4	B	1601	NAD	C5A-C4A-N3A	-5.97	118.50	126.72
4	B	1602	NAD	C5A-C4A-N3A	-5.96	118.52	126.72
4	A	601	NAD	C5A-C4A-N3A	-5.89	118.60	126.72
4	C	2601	NAD	C5A-C4A-N3A	-5.82	118.71	126.72
4	D	3601	NAD	C5A-C4A-N3A	-5.79	118.75	126.72
4	D	3602	NAD	N3A-C2A-N1A	-5.20	120.70	128.58
4	A	601	NAD	N3A-C2A-N1A	-5.16	120.76	128.58
4	B	1601	NAD	N3A-C2A-N1A	-5.16	120.77	128.58
4	A	602	NAD	C6A-C5A-N7A	-5.16	122.14	132.09
4	C	2601	NAD	N3A-C2A-N1A	-5.15	120.79	128.58
4	B	1601	NAD	C6A-C5A-N7A	-5.13	122.20	132.09
4	B	1602	NAD	N3A-C2A-N1A	-5.12	120.83	128.58
4	C	2601	NAD	C6A-C5A-C4A	5.11	124.16	117.18
4	A	602	NAD	C6A-C5A-C4A	5.10	124.14	117.18
4	D	3601	NAD	N3A-C2A-N1A	-5.09	120.88	128.58
4	C	2601	NAD	C6A-C5A-N7A	-5.08	122.30	132.09
4	C	2602	NAD	C6A-C5A-C4A	5.06	124.09	117.18
4	A	601	NAD	C6A-C5A-C4A	5.05	124.07	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3601	NAD	C6A-C5A-C4A	5.03	124.05	117.18
4	A	601	NAD	C6A-C5A-N7A	-5.03	122.40	132.09
4	D	3602	NAD	C6A-C5A-N7A	-5.01	122.44	132.09
4	A	602	NAD	N3A-C4A-N9A	4.99	135.65	127.17
4	A	602	NAD	N3A-C2A-N1A	-4.98	121.04	128.58
4	B	1602	NAD	C6A-C5A-N7A	-4.96	122.52	132.09
4	C	2602	NAD	C6A-C5A-N7A	-4.96	122.54	132.09
4	D	3601	NAD	C6A-C5A-N7A	-4.94	122.56	132.09
4	C	2602	NAD	N3A-C2A-N1A	-4.94	121.10	128.58
4	B	1601	NAD	C6A-C5A-C4A	4.94	123.92	117.18
4	C	2602	NAD	N3A-C4A-N9A	4.92	135.53	127.17
4	B	1602	NAD	C6A-C5A-C4A	4.92	123.89	117.18
4	D	3602	NAD	C6A-C5A-C4A	4.92	123.89	117.18
4	B	1602	NAD	N3A-C4A-N9A	4.90	135.50	127.17
4	A	601	NAD	N3A-C4A-N9A	4.89	135.49	127.17
4	C	2601	NAD	N3A-C4A-N9A	4.88	135.47	127.17
4	D	3601	NAD	N3A-C4A-N9A	4.81	135.35	127.17
4	D	3602	NAD	N3A-C4A-N9A	4.80	135.32	127.17
4	B	1601	NAD	N3A-C4A-N9A	4.79	135.31	127.17
2	C	2603	OXL	O3-C1-C2	4.04	120.66	112.83
2	B	1603	OXL	O3-C1-C2	3.92	120.42	112.83
4	D	3601	NAD	N9A-C8A-N7A	-3.87	108.44	113.94
2	B	1603	OXL	O4-C2-C1	3.83	120.27	112.83
4	C	2601	NAD	N9A-C8A-N7A	-3.83	108.50	113.94
4	A	601	NAD	N9A-C8A-N7A	-3.81	108.52	113.94
4	B	1602	NAD	N9A-C8A-N7A	-3.73	108.64	113.94
2	D	3603	OXL	O4-C2-C1	3.72	120.05	112.83
2	D	3603	OXL	O3-C1-C2	3.70	120.00	112.83
4	C	2602	NAD	N9A-C8A-N7A	-3.68	108.71	113.94
2	A	603	OXL	O4-C2-C1	3.64	119.89	112.83
4	D	3602	NAD	N9A-C8A-N7A	-3.61	108.81	113.94
4	A	602	NAD	N9A-C8A-N7A	-3.58	108.86	113.94
4	B	1601	NAD	N9A-C8A-N7A	-3.57	108.86	113.94
2	A	603	OXL	O3-C1-C2	3.57	119.76	112.83
2	C	2603	OXL	O4-C2-C1	3.54	119.70	112.83
4	D	3602	NAD	C2A-N3A-C4A	3.30	119.89	111.83
4	C	2602	NAD	C2A-N3A-C4A	3.29	119.86	111.83
4	B	1602	NAD	C2A-N3A-C4A	3.28	119.84	111.83
4	B	1601	NAD	C2A-N3A-C4A	3.27	119.82	111.83
4	A	602	NAD	C2A-N3A-C4A	3.24	119.75	111.83
4	A	601	NAD	C2A-N3A-C4A	3.23	119.71	111.83
4	D	3602	NAD	C6N-N1N-C2N	-3.17	119.18	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3601	NAD	C2A-N3A-C4A	3.16	119.56	111.83
4	C	2601	NAD	C2A-N3A-C4A	3.15	119.53	111.83
4	D	3601	NAD	C4D-O4D-C1D	-3.09	107.10	109.92
4	B	1601	NAD	C4D-O4D-C1D	-2.94	107.23	109.92
4	A	601	NAD	C4D-O4D-C1D	-2.89	107.28	109.92
4	B	1601	NAD	C4A-C5A-N7A	2.88	113.88	110.58
4	A	602	NAD	C6N-N1N-C2N	-2.88	119.43	121.88
4	A	602	NAD	C4A-C5A-N7A	2.74	113.72	110.58
4	D	3602	NAD	C4A-C5A-N7A	2.70	113.67	110.58
4	B	1602	NAD	C4A-C5A-N7A	2.63	113.59	110.58
4	C	2601	NAD	C4A-C5A-N7A	2.58	113.53	110.58
4	A	601	NAD	C4A-C5A-N7A	2.57	113.53	110.58
4	B	1601	NAD	O4B-C1B-N9A	2.56	113.00	108.09
4	C	2602	NAD	C2D-C3D-C4D	2.55	107.54	102.61
4	D	3601	NAD	O4B-C1B-N9A	2.53	112.94	108.09
4	B	1602	NAD	C6N-N1N-C2N	-2.51	119.74	121.88
4	C	2601	NAD	O4B-C1B-N9A	2.49	112.88	108.09
4	B	1602	NAD	C2D-C3D-C4D	2.49	107.41	102.61
4	C	2601	NAD	C4D-O4D-C1D	-2.48	107.65	109.92
4	D	3601	NAD	C4A-C5A-N7A	2.45	113.38	110.58
4	C	2602	NAD	C4A-C5A-N7A	2.44	113.38	110.58
4	C	2602	NAD	C3N-C7N-N7N	-2.43	114.74	117.74
4	A	602	NAD	C2D-C3D-C4D	2.30	107.05	102.61
4	C	2602	NAD	C5N-C4N-C3N	2.28	122.61	120.36
4	A	602	NAD	C3B-C2B-C1B	2.28	105.77	101.46
4	D	3602	NAD	C2D-C3D-C4D	2.27	107.00	102.61
4	A	601	NAD	O4B-C1B-N9A	2.24	112.39	108.09
4	D	3601	NAD	C6N-N1N-C2N	-2.17	120.03	121.88
4	C	2601	NAD	C4A-N9A-C8A	2.13	107.97	105.74
4	B	1602	NAD	C3B-C2B-C1B	2.10	105.44	101.46
4	D	3602	NAD	C3B-C2B-C1B	2.09	105.42	101.46
4	C	2601	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
4	B	1601	NAD	C3N-C7N-N7N	-2.05	115.21	117.74

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAD	O4D-C1D-N1N-C6N
4	A	602	NAD	C5B-O5B-PA-O1A
4	A	602	NAD	C5B-O5B-PA-O2A
4	A	602	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
4	B	1601	NAD	O4D-C1D-N1N-C6N
4	B	1602	NAD	C5B-O5B-PA-O2A
4	B	1602	NAD	C5B-O5B-PA-O3
4	C	2601	NAD	O4D-C1D-N1N-C6N
4	C	2602	NAD	C5B-O5B-PA-O2A
4	C	2602	NAD	C5B-O5B-PA-O3
4	C	2602	NAD	PA-O3-PN-O5D
4	D	3601	NAD	O4D-C1D-N1N-C6N
4	D	3602	NAD	C5B-O5B-PA-O1A
4	D	3602	NAD	C5B-O5B-PA-O2A
4	D	3602	NAD	C5B-O5B-PA-O3
4	A	602	NAD	PA-O3-PN-O5D
4	B	1602	NAD	PA-O3-PN-O5D
4	D	3602	NAD	PA-O3-PN-O5D
4	C	2602	NAD	C3D-C4D-C5D-O5D
4	B	1602	NAD	C4D-C5D-O5D-PN
4	A	602	NAD	PA-O3-PN-O1N
4	B	1602	NAD	PN-O3-PA-O1A
4	D	3602	NAD	PA-O3-PN-O1N
4	D	3602	NAD	C4D-C5D-O5D-PN
4	A	602	NAD	C4D-C5D-O5D-PN
4	C	2602	NAD	C4D-C5D-O5D-PN
4	A	601	NAD	O4D-C1D-N1N-C2N
4	B	1601	NAD	O4D-C1D-N1N-C2N
4	C	2601	NAD	O4D-C1D-N1N-C2N
4	D	3601	NAD	O4D-C1D-N1N-C2N
4	B	1602	NAD	PA-O3-PN-O1N
4	C	2602	NAD	PN-O3-PA-O1A
4	C	2602	NAD	PN-O3-PA-O2A
4	A	602	NAD	C3D-C4D-C5D-O5D
4	A	602	NAD	PN-O3-PA-O2A
4	C	2601	NAD	PN-O3-PA-O2A
4	D	3602	NAD	PN-O3-PA-O2A
4	B	1602	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

6 monomers are involved in 9 short contacts:

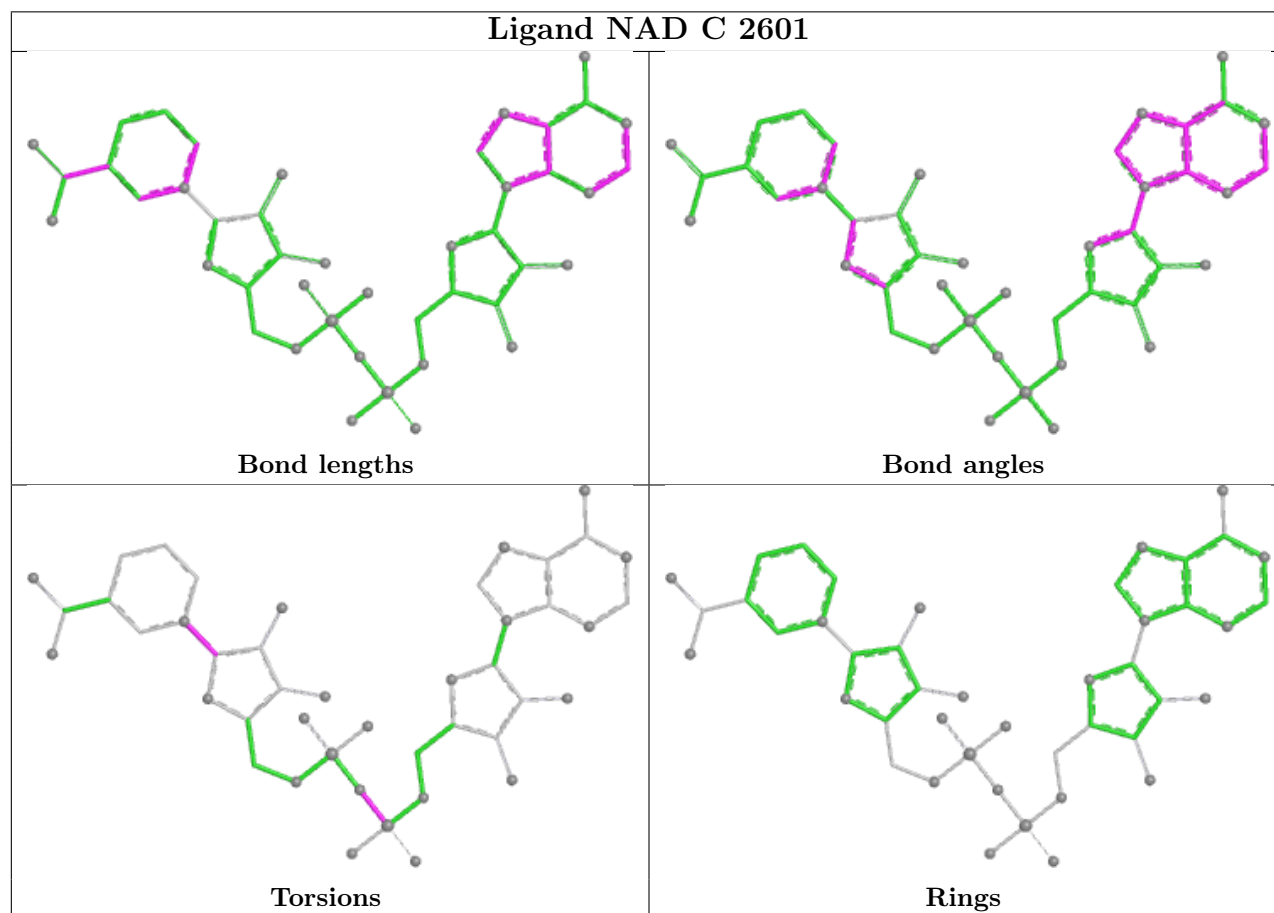
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2601	NAD	1	0
4	C	2602	NAD	1	0
4	A	601	NAD	2	0

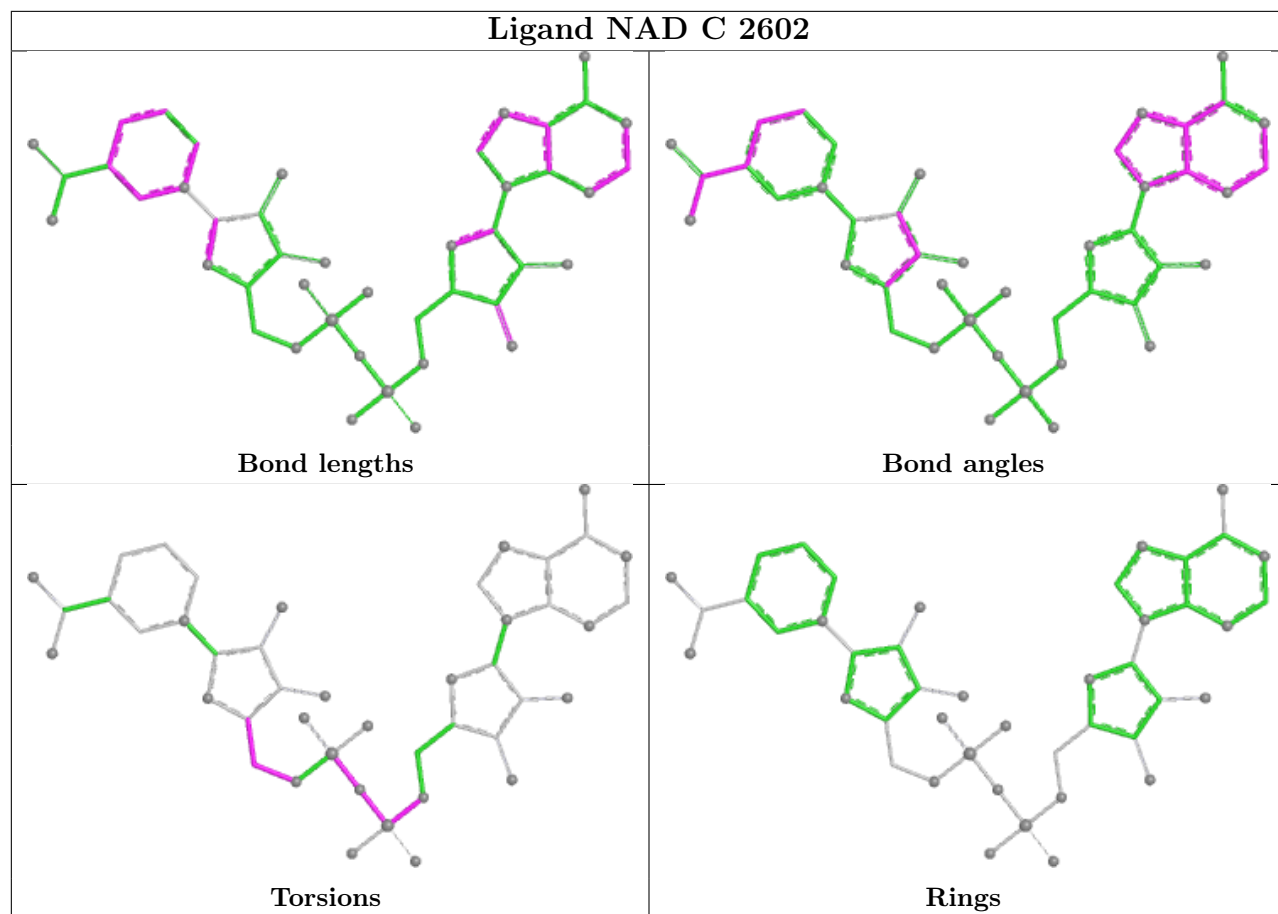
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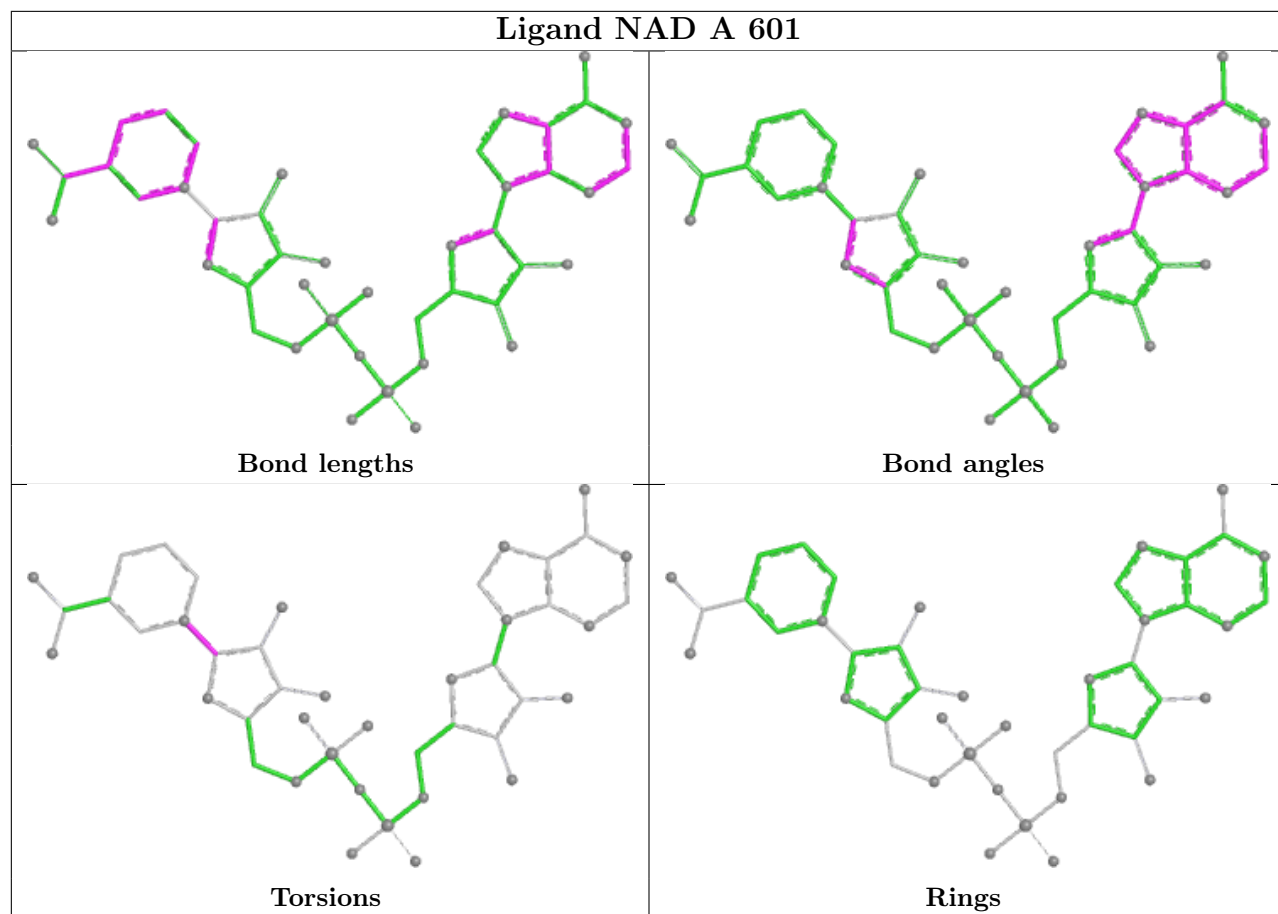
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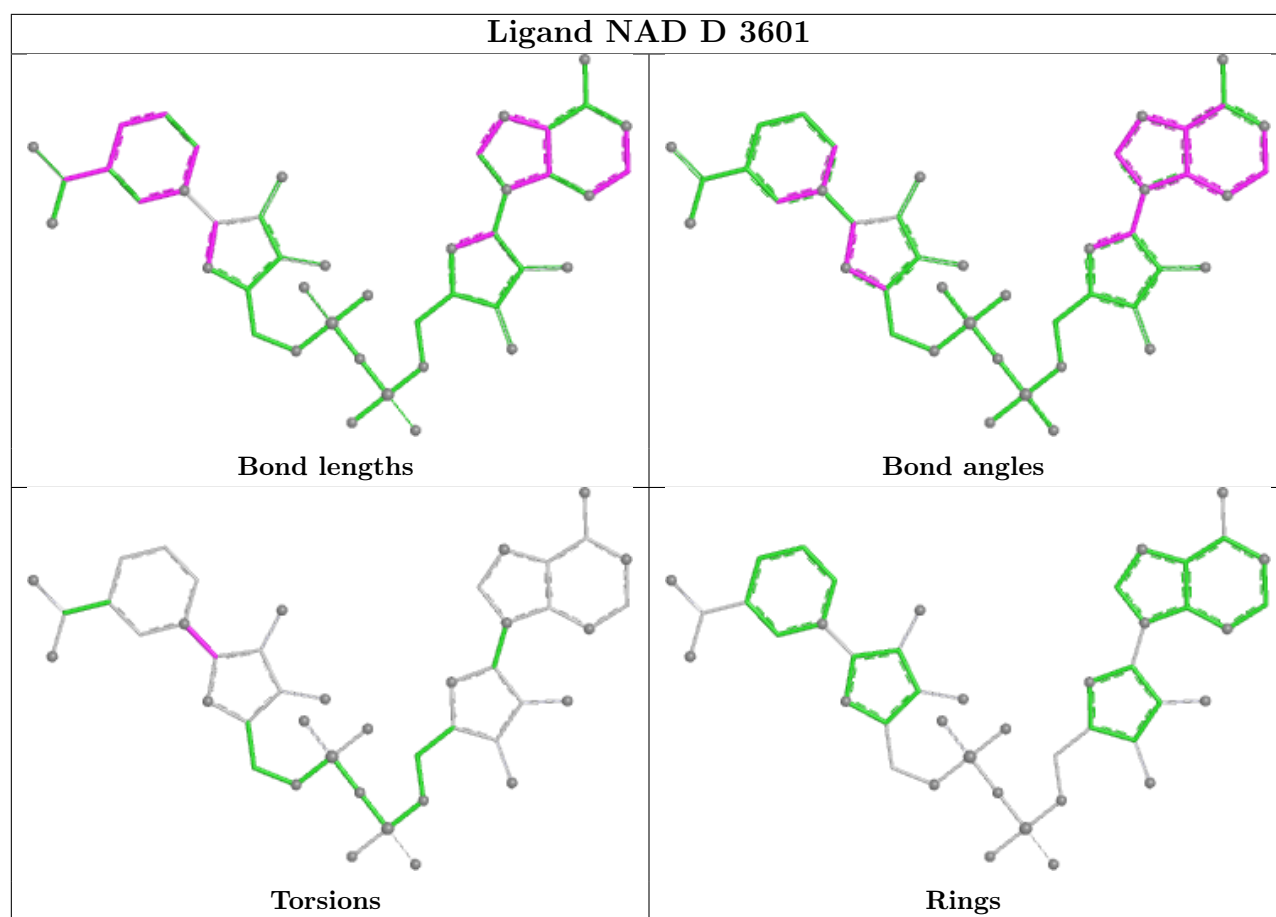
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3602	NAD	1	0
4	B	1601	NAD	3	0
2	D	3603	OXL	1	0

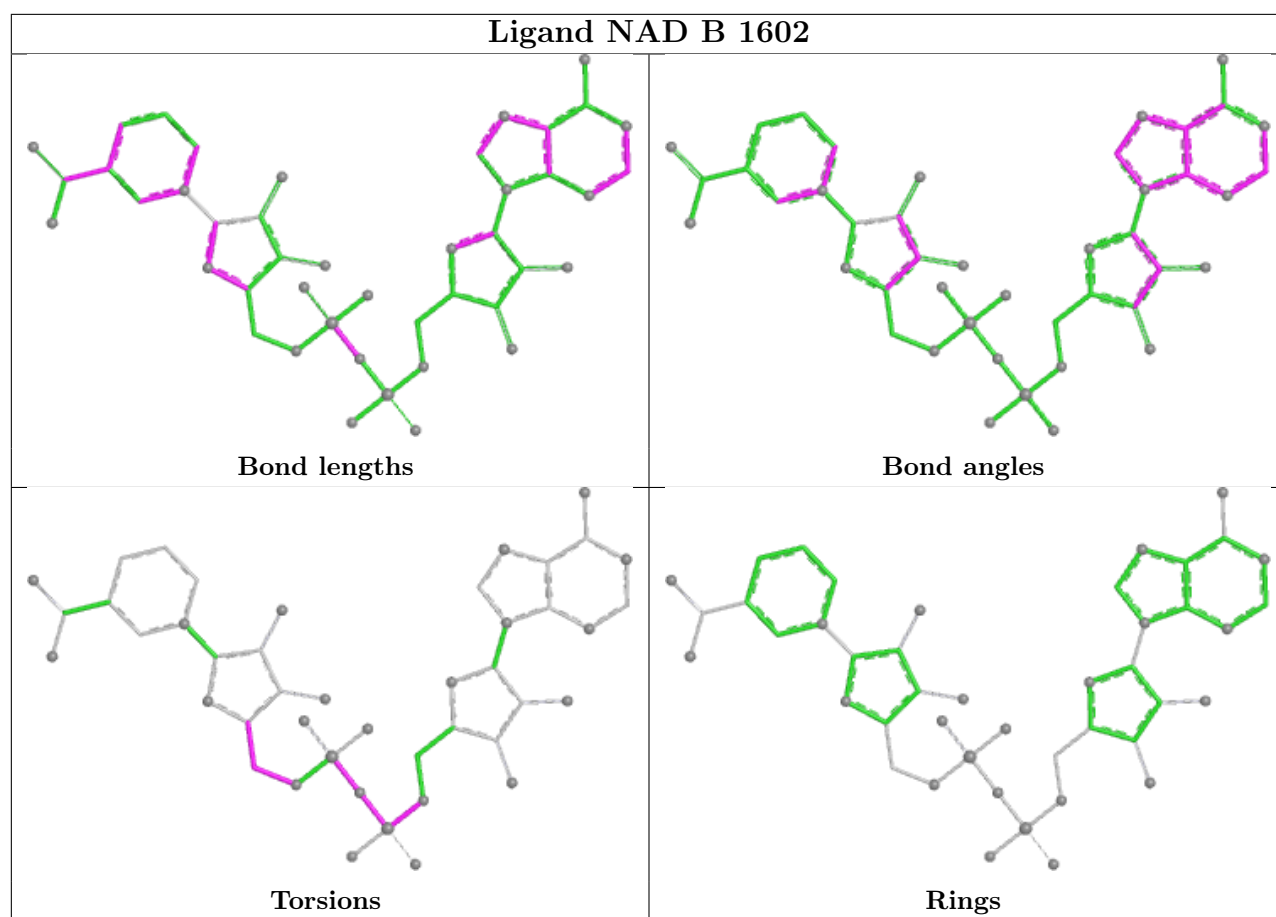
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



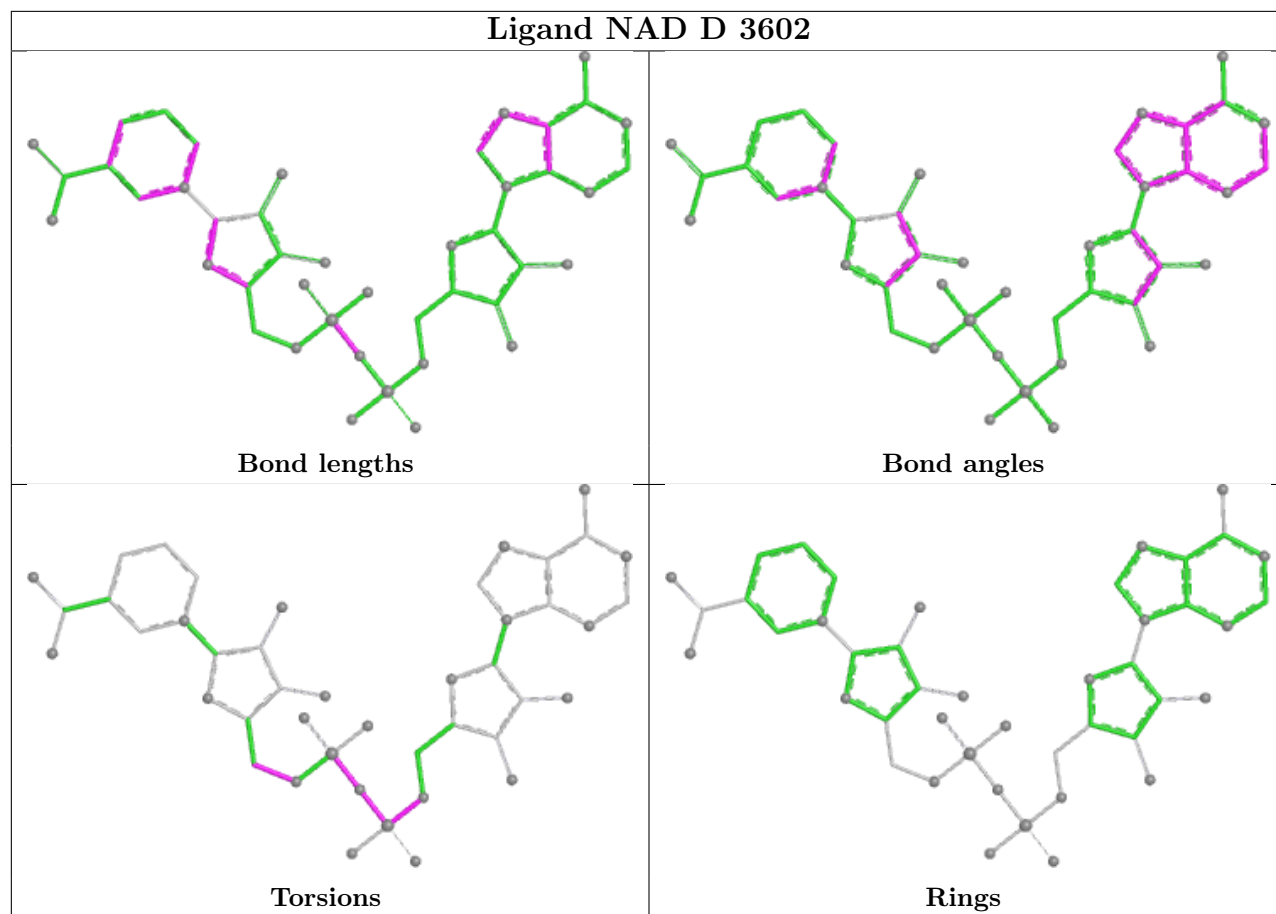


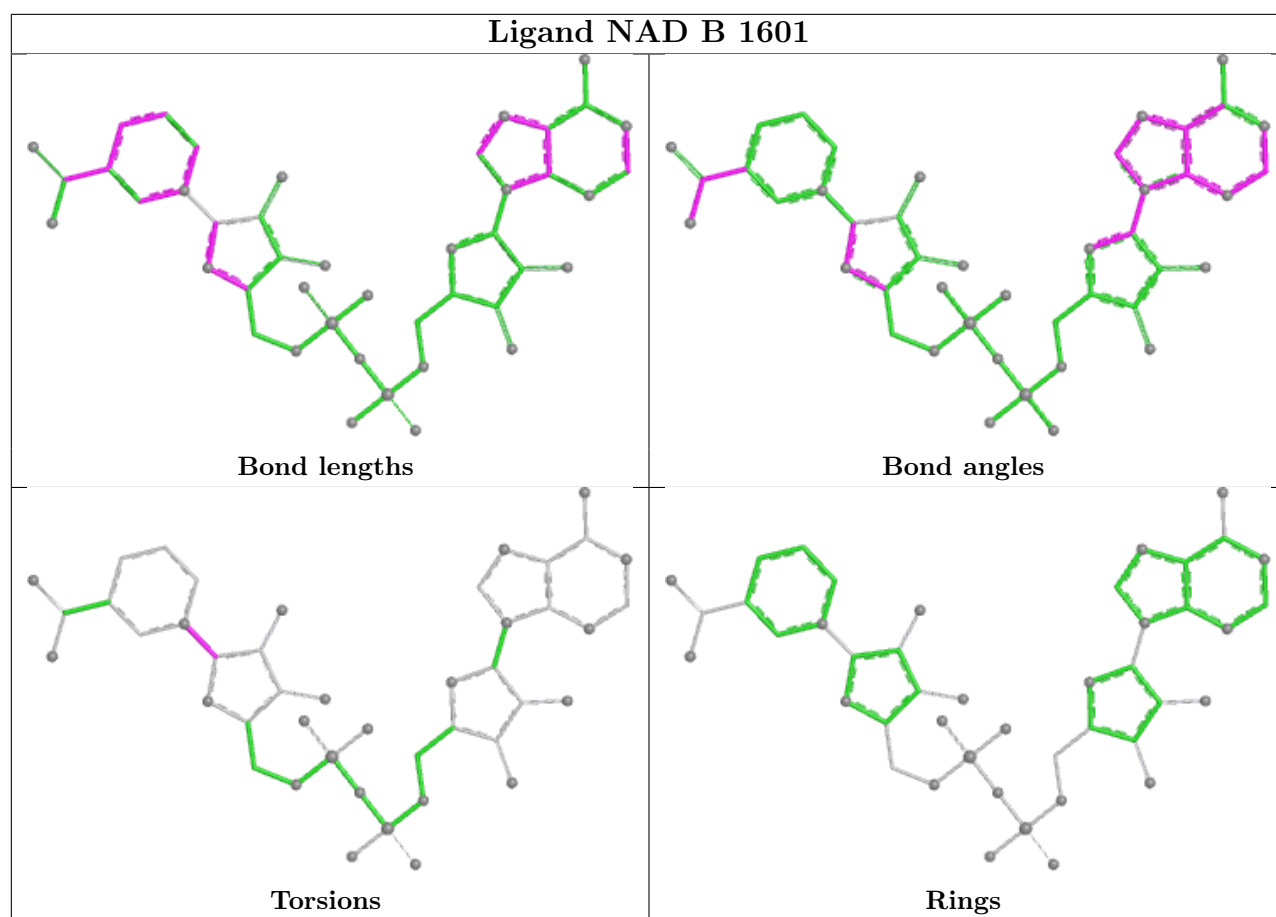


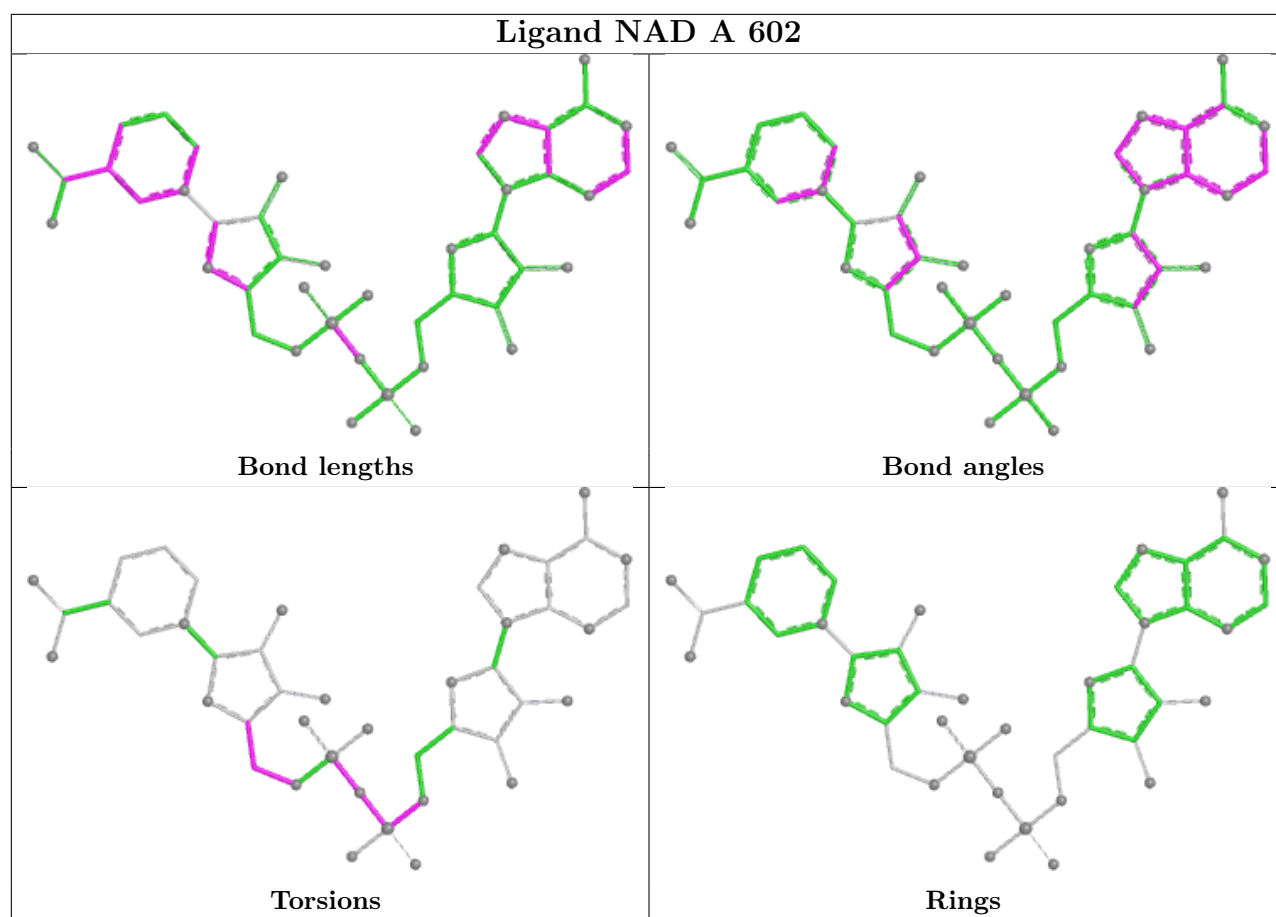




Ligand NAD D 3602







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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.