



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:33 PM UTC

PDB ID : 3HJ3 / pdb_00003hj3
Title : Crystal Structure of the ChTS-DHFR F207A Non-Active Site Mutant
Authors : Anderson, K.S.; Martucci, W.E.
Deposited on : 2009-05-20
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

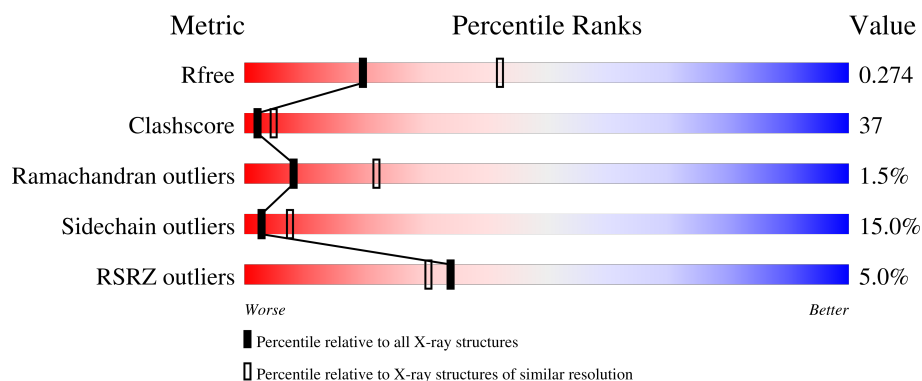
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	521	3% 52% 33% 11% ..
1	B	521	3% 53% 36% 7% ..
1	C	521	6% 45% 40% 11% ..
1	D	521	7% 41% 44% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	603	-	-	X	-
2	UMP	B	607	-	-	X	-
2	UMP	C	611	-	-	X	-
3	CB3	A	604	X	-	X	-
3	CB3	B	608	X	-	-	-
3	CB3	C	612	X	-	X	-
4	MTX	D	615	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17282 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.

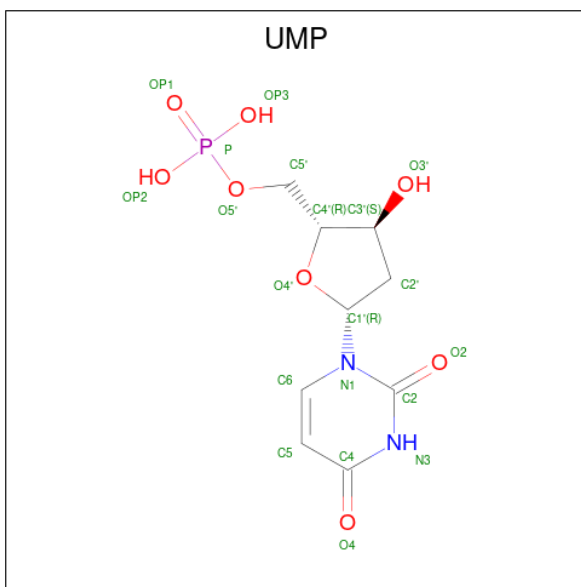
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			4131	2638	695	776	22			
1	B	510	Total	C	N	O	S	0	0	0
			4144	2645	698	779	22			
1	C	510	Total	C	N	O	S	0	0	0
			4147	2648	698	779	22			
1	D	505	Total	C	N	O	S	0	0	0
			4104	2622	690	770	22			

There are 4 discrepancies between the modelled and reference sequences:

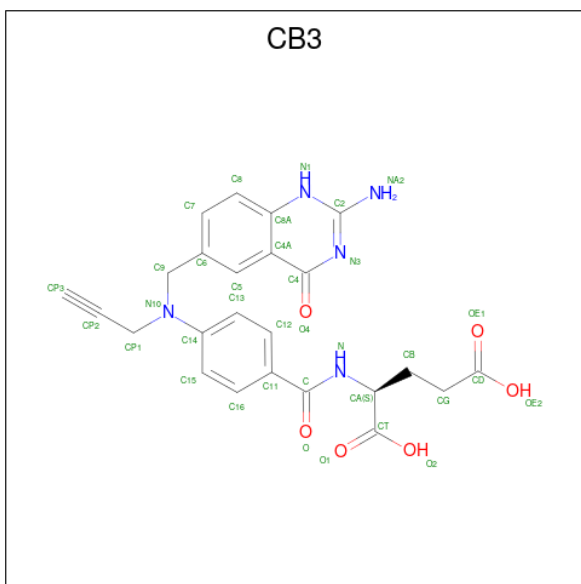
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ALA	PHE	engineered mutation	UNP Q5CGA3
B	207	ALA	PHE	engineered mutation	UNP Q5CGA3
C	207	ALA	PHE	engineered mutation	UNP Q5CGA3
D	207	ALA	PHE	engineered mutation	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



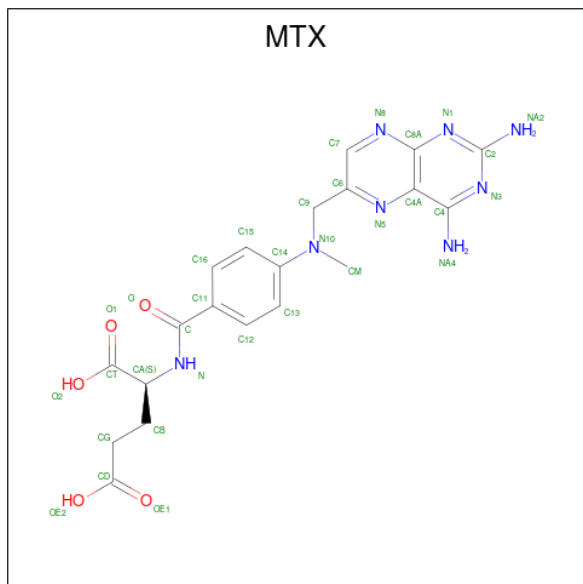
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula: $C_{24}H_{23}N_5O_6$).



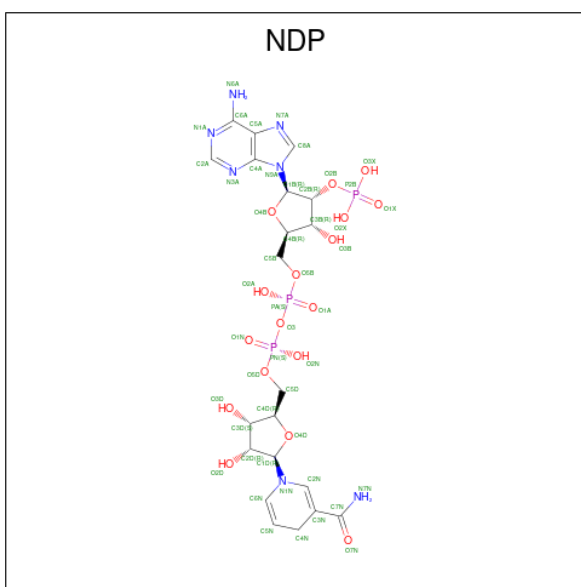
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is METHOTREXATE (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			33	20	8	5		
4	B	1	Total	C	N	O	0	0
			33	20	8	5		
4	C	1	Total	C	N	O	0	0
			33	20	8	5		
4	D	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

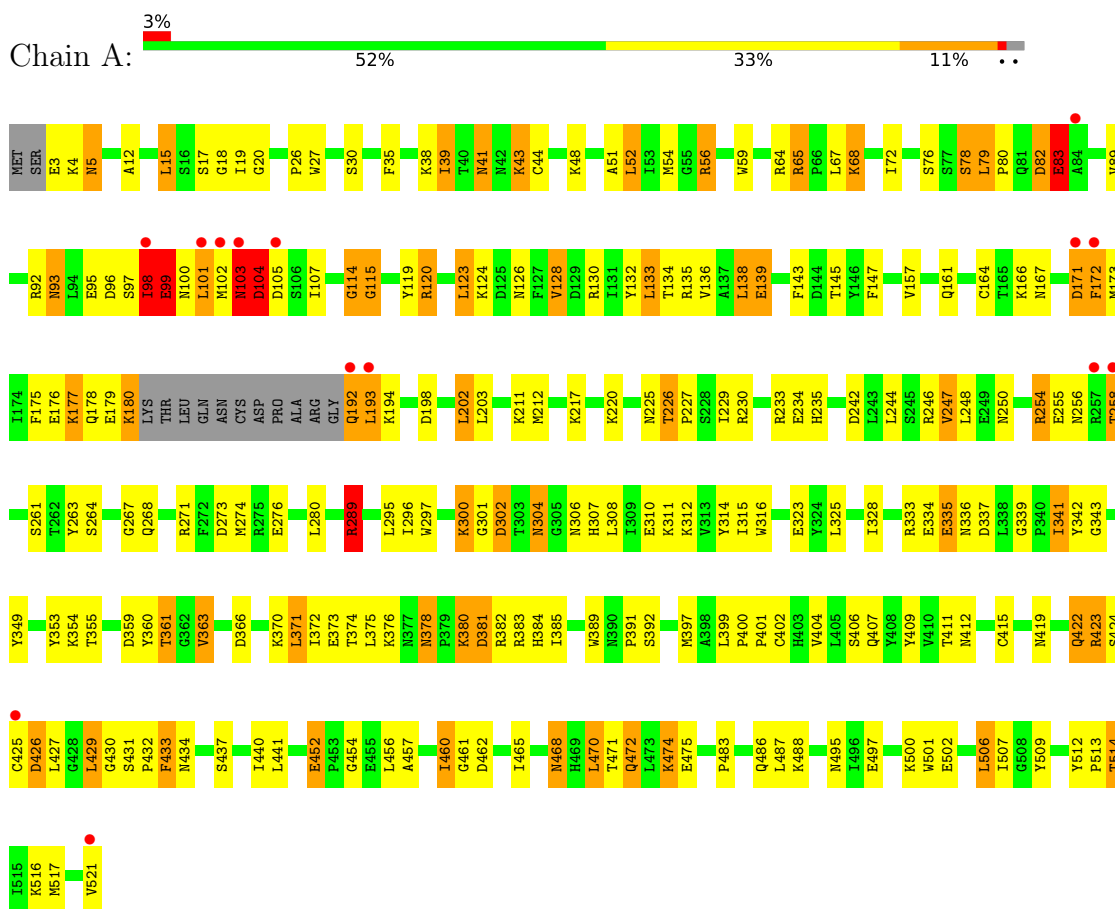
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	98	Total O 98 98	0	0
6	B	86	Total O 86 86	0	0
6	C	47	Total O 47 47	0	0
6	D	36	Total O 36 36	0	0

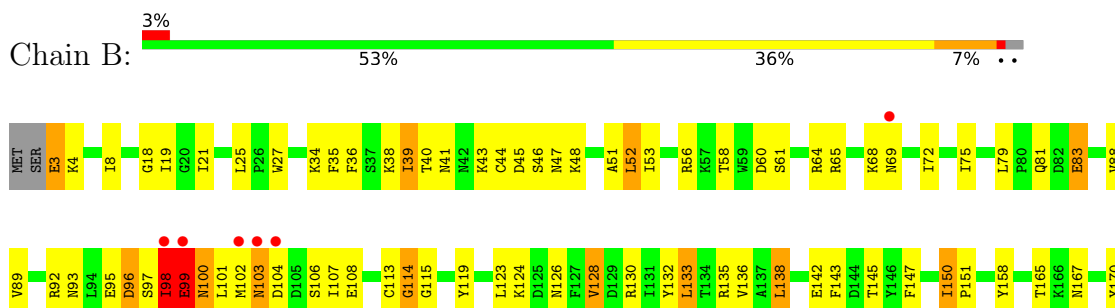
3 Residue-property plots

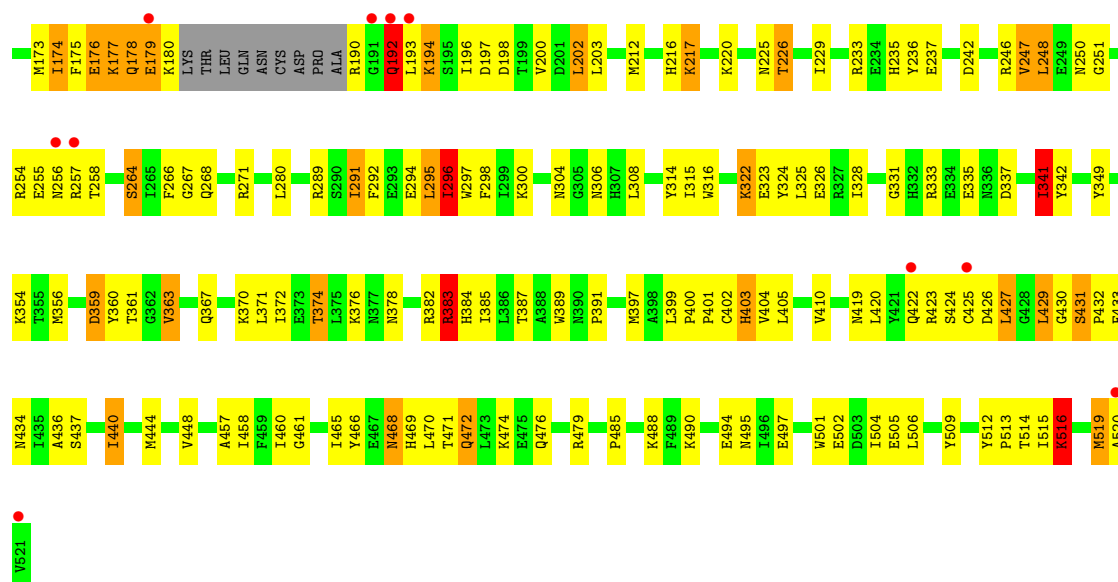
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Chain A, crystal structure of Dhfr

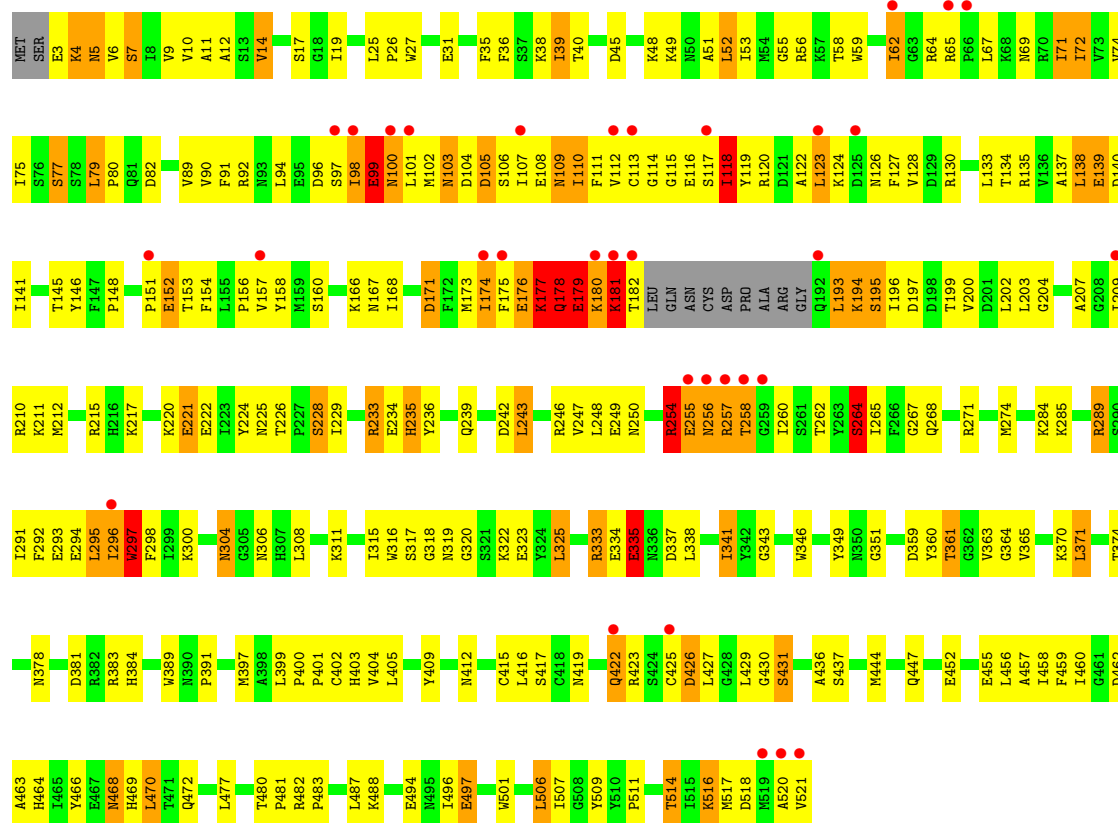
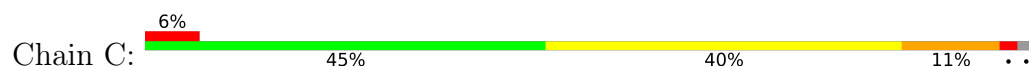


- Molecule 1: Chain A, crystal structure of Dhfr



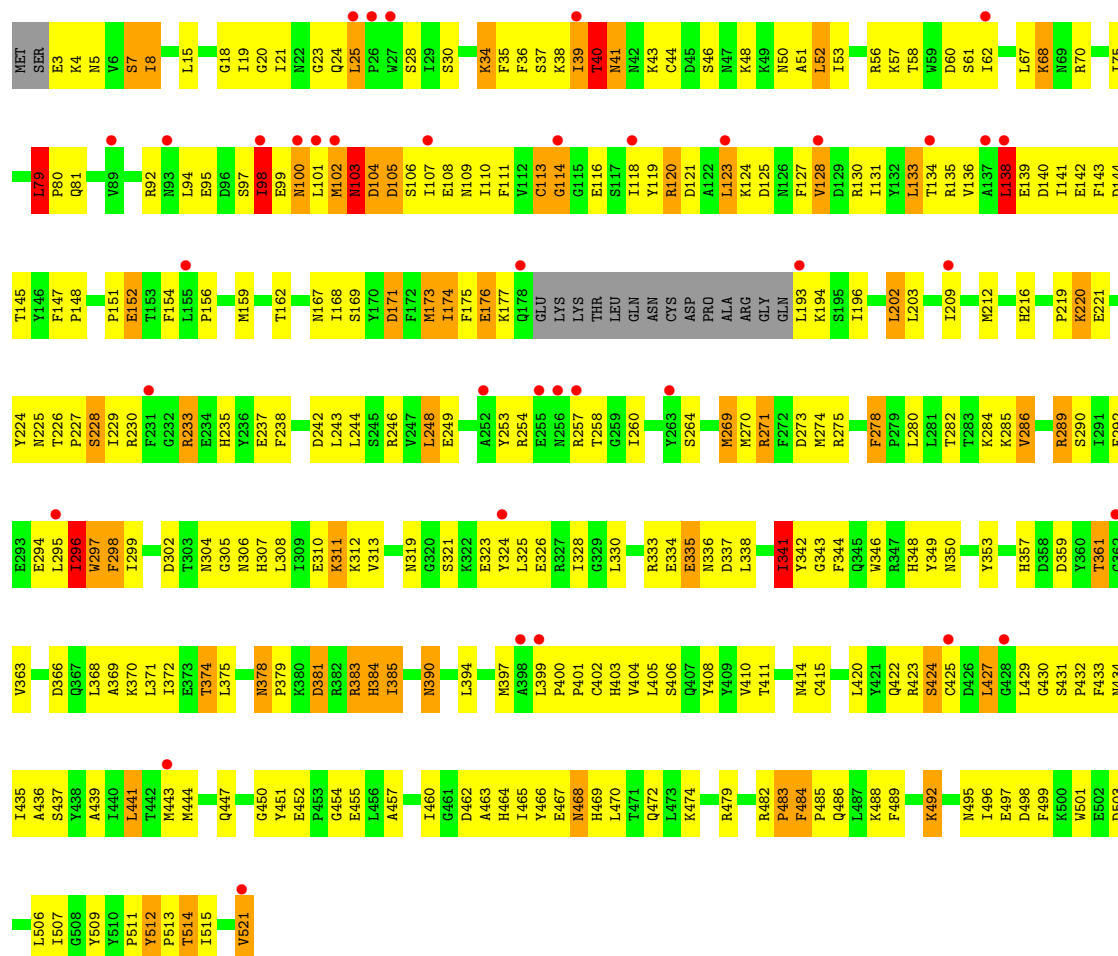


• Molecule 1: Chain A, crystal structure of Dhfr



• Molecule 1: Chain A, crystal structure of Dhfr





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.86Å 121.86Å 342.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.4 (50.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.68Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.228 , 0.274 0.229 , 0.274	Depositor DCC
R_{free} test set	4070 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17282	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CB3, UMP, MTX, NDP

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	1.01	0/4225	1.15	21/5709 (0.4%)
1	B	1.01	1/4238 (0.0%)	1.09	7/5726 (0.1%)
1	C	0.95	1/4241 (0.0%)	1.13	14/5730 (0.2%)
1	D	0.86	1/4198 (0.0%)	1.08	17/5674 (0.3%)
All	All	0.96	3/16902 (0.0%)	1.11	59/22839 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	8
1	C	0	12
1	D	0	6
All	All	0	32

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	THR	CA-CB	7.74	1.59	1.52
1	D	521	VAL	C-OXT	5.95	1.35	1.23
1	C	521	VAL	C-OXT	5.61	1.34	1.23

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	THR	CA-C-N	7.50	127.53	119.28
1	A	226	THR	C-N-CA	7.50	127.53	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	LEU	CA-C-N	7.43	127.70	119.90
1	C	79	LEU	C-N-CA	7.43	127.70	119.90
1	D	128	VAL	N-CA-C	6.99	117.71	107.37
1	C	14	VAL	N-CA-C	6.93	117.07	110.42
1	C	335	GLU	CA-C-N	-6.92	112.27	122.86
1	C	335	GLU	C-N-CA	-6.92	112.27	122.86
1	C	351	GLY	N-CA-C	-6.67	103.62	112.82
1	C	152	GLU	N-CA-C	6.58	120.57	112.54
1	D	483	PRO	CB-CA-C	-6.55	103.25	111.56
1	D	296	ILE	CB-CA-C	-6.33	104.45	110.65
1	D	100	ASN	N-CA-C	6.29	118.94	111.71
1	D	269	MET	N-CA-C	6.18	119.63	108.69
1	D	278	PHE	CB-CA-C	6.16	117.20	108.76
1	A	382	ARG	N-CA-C	6.15	120.38	112.26
1	A	378	ASN	CA-C-N	6.10	125.58	119.24
1	A	378	ASN	C-N-CA	6.10	125.58	119.24
1	D	102	MET	N-CA-C	-6.08	104.98	113.37
1	A	452	GLU	CA-C-N	-6.06	113.70	119.76
1	A	452	GLU	C-N-CA	-6.06	113.70	119.76
1	D	79	LEU	CA-C-N	6.06	126.02	119.78
1	D	79	LEU	C-N-CA	6.06	126.02	119.78
1	D	100	ASN	CB-CA-C	-6.03	99.47	110.63
1	A	147	PHE	CA-C-N	-5.92	114.17	120.03
1	A	147	PHE	C-N-CA	-5.92	114.17	120.03
1	A	423	ARG	N-CA-C	-5.91	104.92	111.36
1	D	385	ILE	N-CA-C	5.86	117.12	108.45
1	A	5	ASN	N-CA-C	5.80	118.66	109.96
1	A	328	ILE	N-CA-C	5.79	117.67	112.17
1	D	390	ASN	CB-CA-C	5.75	118.18	110.13
1	D	298	PHE	N-CA-C	-5.75	104.62	111.69
1	B	147	PHE	N-CA-C	-5.66	102.52	109.65
1	A	15	LEU	CA-C-N	-5.65	113.67	122.37
1	A	15	LEU	C-N-CA	-5.65	113.67	122.37
1	D	341	ILE	CB-CA-C	-5.64	102.03	111.29
1	D	484	PHE	N-CA-C	5.63	117.67	109.84
1	C	430	GLY	N-CA-C	5.53	119.37	112.73
1	C	298	PHE	N-CA-C	-5.52	105.26	111.28
1	C	171	ASP	CB-CA-C	-5.49	100.58	110.36
1	B	296	ILE	CB-CA-C	-5.47	103.24	112.16
1	B	516	LYS	N-CA-C	5.42	117.56	109.59
1	A	230	ARG	N-CA-C	-5.37	105.79	112.93
1	C	124	LYS	N-CA-C	-5.36	104.86	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	LEU	N-CA-C	-5.33	105.13	111.69
1	C	110	ILE	N-CA-C	5.31	115.51	107.75
1	B	440	ILE	CB-CA-C	-5.31	104.89	112.22
1	A	355	THR	N-CA-CB	5.29	119.75	111.56
1	A	41	ASN	N-CA-C	5.25	118.14	111.69
1	A	433	PHE	N-CA-C	5.19	116.63	111.07
1	A	139	GLU	N-CA-CB	-5.18	103.49	110.95
1	B	226	THR	CA-C-N	5.16	124.96	119.28
1	B	226	THR	C-N-CA	5.16	124.96	119.28
1	C	264	SER	N-CA-C	5.16	116.92	108.76
1	C	297	TRP	N-CA-C	5.15	119.82	111.37
1	B	291	ILE	N-CA-C	-5.10	105.74	110.53
1	A	335	GLU	CB-CA-C	5.06	117.42	109.84
1	D	297	TRP	N-CA-C	5.05	119.71	111.37
1	A	302	ASP	N-CA-C	5.04	117.77	109.76

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	GLY	Peptide
1	A	171	ASP	Peptide
1	A	192	GLN	Peptide
1	A	289	ARG	Sidechain
1	A	98	ILE	Peptide
1	A	99	GLU	Peptide
1	B	114	GLY	Peptide
1	B	170	TYR	Peptide
1	B	192	GLN	Peptide
1	B	3	GLU	Peptide
1	B	341	ILE	Peptide
1	B	383	ARG	Sidechain
1	B	98	ILE	Peptide
1	B	99	GLU	Peptide
1	C	112	VAL	Peptide
1	C	113	CYS	Peptide
1	C	118	ILE	Peptide
1	C	177	LYS	Peptide
1	C	178	GLN	Peptide
1	C	179	GLU	Peptide
1	C	254	ARG	Peptide
1	C	255	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	296	ILE	Peptide
1	C	341	ILE	Peptide
1	C	98	ILE	Peptide
1	C	99	GLU	Peptide
1	D	114	GLY	Peptide
1	D	138	LEU	Peptide
1	D	233	ARG	Sidechain
1	D	296	ILE	Peptide
1	D	341	ILE	Peptide
1	D	98	ILE	Peptide

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	4131	0	4066	280	0
1	B	4144	0	4077	289	3
1	C	4147	0	4086	342	3
1	D	4104	0	4039	361	0
2	A	20	0	11	7	0
2	B	20	0	11	9	0
2	C	20	0	11	9	0
3	A	35	0	21	11	0
3	B	35	0	21	8	0
3	C	35	0	21	10	0
4	A	33	0	19	1	0
4	B	33	0	19	4	0
4	C	33	0	19	6	0
4	D	33	0	20	13	0
5	A	48	0	26	4	0
5	B	48	0	26	6	0
5	C	48	0	26	7	0
5	D	48	0	26	8	0
6	A	98	0	0	31	0
6	B	86	0	0	29	0
6	C	47	0	0	29	0
6	D	36	0	0	47	0
All	All	17282	0	16545	1244	3

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 37.

All (1244) 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:402:CYS:SG	2:C:611:UMP:C6	2.20	1.33
1:B:65:ARG:HD2	6:B:593:HOH:O	1.41	1.19
1:C:211:LYS:HB3	6:C:561:HOH:O	1.39	1.18
1:C:374:THR:HG22	1:C:384:HIS:CE1	1.81	1.14
1:A:381:ASP:HB2	6:A:591:HOH:O	1.47	1.12
1:B:374:THR:HG22	1:B:384:HIS:ND1	1.63	1.12
1:D:28:SER:HB2	6:D:524:HOH:O	1.51	1.10
1:C:371:LEU:HA	6:C:560:HOH:O	1.52	1.10
1:C:4:LYS:HB3	1:C:101:LEU:HD22	1.20	1.09
1:C:5:ASN:H	1:C:5:ASN:ND2	1.36	1.08
1:A:126:ASN:HD21	1:A:177:LYS:HE2	0.91	1.08
1:D:295:LEU:HD23	1:D:295:LEU:O	1.54	1.07
1:B:126:ASN:HD21	1:B:177:LYS:HE3	0.95	1.07
1:D:37:SER:HB2	4:D:615:MTX:HG2	1.34	1.07
1:C:5:ASN:HD22	1:C:5:ASN:N	1.45	1.06
1:B:103:ASN:C	1:B:103:ASN:HD22	1.60	1.06
1:C:180:LYS:HG2	1:C:181:LYS:N	1.44	1.06
1:C:403:HIS:HD2	2:C:611:UMP:O4	1.37	1.05
1:C:158:TYR:HB3	1:C:174:ILE:HG12	1.37	1.04
1:C:4:LYS:HE3	1:C:101:LEU:HA	1.37	1.04
1:A:402:CYS:SG	2:A:603:UMP:C6	2.52	1.03
1:A:3:GLU:HA	1:A:3:GLU:OE2	1.58	1.03
1:C:494:GLU:HG2	6:C:543:HOH:O	1.55	1.03
1:A:374:THR:HB	6:A:568:HOH:O	1.57	1.03
1:A:397:MET:HE1	1:A:401:PRO:HD3	1.41	1.02
1:C:397:MET:HE1	1:C:401:PRO:CD	1.88	1.02
1:C:397:MET:CE	1:C:401:PRO:HD3	1.89	1.02
1:D:38:LYS:HA	6:D:546:HOH:O	1.57	1.02
1:D:306:ASN:ND2	1:D:336:ASN:HB2	1.73	1.01
1:A:126:ASN:ND2	1:A:177:LYS:HE2	1.74	1.01
1:C:180:LYS:HZ3	1:C:181:LYS:CB	1.72	1.01
1:C:98:ILE:HD12	1:C:127:PHE:HD1	1.22	1.01
1:C:180:LYS:NZ	1:C:181:LYS:HB3	1.76	1.01
1:D:123:LEU:HD12	1:D:128:VAL:HG11	1.40	1.01
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.43	1.00
1:D:295:LEU:HA	6:D:544:HOH:O	1.59	1.00
1:B:460:ILE:HD12	6:B:597:HOH:O	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASN:HA	1:B:103:ASN:HD21	1.22	0.99
1:A:126:ASN:HD21	1:A:177:LYS:CE	1.76	0.99
1:C:4:LYS:HB3	1:C:101:LEU:CD2	1.92	0.98
1:C:98:ILE:HD12	1:C:127:PHE:CD1	1.98	0.98
1:C:100:ASN:HA	1:C:103:ASN:ND2	1.78	0.98
1:C:518:ASP:HB3	6:C:562:HOH:O	1.62	0.98
1:D:52:LEU:HB3	1:D:113:CYS:SG	2.03	0.97
1:B:359:ASP:OD2	1:B:361:THR:HG22	1.64	0.96
4:C:613:MTX:HG2	4:C:613:MTX:O1	1.64	0.96
1:B:126:ASN:ND2	1:B:177:LYS:HE3	1.81	0.95
1:B:96:ASP:O	1:B:99:GLU:HG2	1.66	0.95
1:D:5:ASN:HD21	1:D:130:ARG:HH21	1.14	0.95
1:B:96:ASP:O	1:B:99:GLU:HB3	1.66	0.95
1:D:290:SER:HB3	1:D:313:VAL:HG11	1.49	0.95
1:A:359:ASP:OD1	1:A:361:THR:HG22	1.67	0.94
1:B:179:GLU:HG2	1:B:180:LYS:H	1.29	0.94
1:A:48:LYS:HD3	1:A:105:ASP:O	1.67	0.93
1:D:151:PRO:HG2	1:D:154:PHE:CD2	2.04	0.93
1:B:194:LYS:HB3	6:B:573:HOH:O	1.66	0.93
1:B:374:THR:CG2	1:B:384:HIS:ND1	2.32	0.93
1:D:274:MET:HB2	1:D:454:GLY:O	1.69	0.93
1:C:180:LYS:HG2	1:C:181:LYS:H	1.33	0.92
1:C:64:ARG:HD2	6:C:551:HOH:O	1.68	0.92
1:D:447:GLN:HG2	1:D:492:LYS:HE2	1.52	0.92
1:A:468:ASN:HD22	1:A:468:ASN:H	1.17	0.92
1:C:158:TYR:CB	1:C:174:ILE:HG12	2.01	0.91
1:D:366:ASP:OD1	1:D:369:ALA:HB2	1.70	0.91
1:D:50:ASN:HD22	1:D:111:PHE:HE2	1.07	0.91
1:A:424:SER:O	2:A:603:UMP:H2'	1.70	0.91
1:B:520:ALA:HB2	6:B:598:HOH:O	1.69	0.91
1:C:180:LYS:CG	1:C:181:LYS:N	2.32	0.91
1:D:271:ARG:HD3	6:D:536:HOH:O	1.71	0.91
1:A:425:CYS:SG	1:A:431:SER:HB2	2.10	0.90
1:C:256:ASN:C	1:C:256:ASN:HD22	1.80	0.90
1:C:403:HIS:CD2	2:C:611:UMP:O4	2.24	0.90
1:B:374:THR:HG22	1:B:384:HIS:CE1	2.07	0.90
1:D:136:VAL:HG12	1:D:138:LEU:CD2	2.02	0.89
1:D:275:ARG:HB3	6:D:549:HOH:O	1.72	0.89
1:B:516:LYS:HD2	6:B:569:HOH:O	1.72	0.89
1:B:304:ASN:ND2	1:B:306:ASN:H	1.71	0.89
1:C:180:LYS:NZ	1:C:180:LYS:C	2.30	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASP:HB3	1:D:107:ILE:HD13	1.53	0.89
1:C:360:TYR:O	1:C:363:VAL:HG12	1.72	0.88
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.08	0.88
1:D:94:LEU:HD23	1:D:121:ASP:HB3	1.56	0.88
1:C:180:LYS:HZ3	1:C:181:LYS:N	1.72	0.88
1:D:136:VAL:HG12	1:D:138:LEU:HD23	1.56	0.88
1:B:100:ASN:HA	1:B:103:ASN:ND2	1.88	0.87
1:A:225:ASN:O	1:A:233:ARG:NH2	2.08	0.87
1:B:52:LEU:HB3	1:B:113:CYS:SG	2.15	0.87
1:D:290:SER:HB3	1:D:313:VAL:CG1	2.05	0.87
1:D:68:LYS:CG	6:D:545:HOH:O	2.21	0.86
1:C:117:SER:O	1:C:118:ILE:HG22	1.76	0.86
1:B:96:ASP:O	1:B:99:GLU:CB	2.24	0.85
1:C:397:MET:HE1	1:C:401:PRO:HD3	0.94	0.85
1:C:225:ASN:O	1:C:233:ARG:NH2	2.08	0.85
1:B:383:ARG:C	6:B:606:HOH:O	2.20	0.85
1:C:180:LYS:HZ3	1:C:181:LYS:CA	1.90	0.85
1:C:180:LYS:NZ	1:C:181:LYS:CB	2.33	0.85
1:C:62:ILE:CG2	6:C:567:HOH:O	2.24	0.84
1:D:5:ASN:HD21	1:D:130:ARG:NH2	1.74	0.84
1:C:468:ASN:HD22	1:C:468:ASN:H	1.23	0.84
1:B:304:ASN:HD22	1:B:306:ASN:H	1.25	0.84
1:C:374:THR:HG22	1:C:384:HIS:HE1	1.40	0.84
1:C:98:ILE:O	1:C:99:GLU:HB3	1.77	0.84
1:D:50:ASN:ND2	1:D:111:PHE:HE2	1.75	0.84
1:D:427:LEU:HD21	1:D:463:ALA:HB1	1.60	0.84
1:A:361:THR:HB	6:A:620:HOH:O	1.75	0.84
1:B:397:MET:HE1	1:B:401:PRO:HD3	1.58	0.83
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.43	0.83
1:C:100:ASN:HA	1:C:103:ASN:HD21	1.40	0.83
3:C:612:CB3:HP11	6:C:538:HOH:O	1.79	0.83
1:D:171:ASP:CG	1:D:483:PRO:HB3	2.04	0.82
1:B:225:ASN:O	1:B:233:ARG:NH2	2.12	0.82
1:D:62:ILE:HD11	4:D:615:MTX:C13	2.08	0.82
1:A:4:LYS:HB3	1:A:101:LEU:CD2	2.09	0.82
1:C:180:LYS:HZ1	1:C:181:LYS:HB3	1.45	0.82
1:C:193:LEU:CD2	1:C:193:LEU:H	1.91	0.82
1:B:96:ASP:O	1:B:99:GLU:CG	2.27	0.82
1:C:48:LYS:HB3	1:C:106:SER:O	1.79	0.82
1:C:233:ARG:NH1	1:C:242:ASP:OD1	2.13	0.82
1:B:103:ASN:C	1:B:103:ASN:ND2	2.34	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLY:O	1:C:118:ILE:HG22	1.79	0.82
1:C:297:TRP:HH2	1:C:338:LEU:HD12	1.43	0.82
1:D:284:LYS:CG	6:D:553:HOH:O	2.28	0.82
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.62	0.82
1:A:380:LYS:HE3	1:A:412:ASN:HD21	1.44	0.82
1:D:468:ASN:H	1:D:468:ASN:HD22	1.24	0.82
1:D:102:MET:O	1:D:103:ASN:HB3	1.77	0.81
1:D:368:LEU:O	1:D:372:ILE:HG13	1.81	0.81
1:D:167:ASN:O	1:D:507:ILE:HG21	1.78	0.81
1:A:104:ASP:HB3	1:A:107:ILE:HG12	1.63	0.81
1:A:430:GLY:O	3:A:604:CB3:HP3	1.81	0.81
1:D:120:ARG:HG3	1:D:120:ARG:HH11	1.43	0.81
1:D:297:TRP:HH2	1:D:338:LEU:HD12	1.43	0.81
1:B:104:ASP:CB	1:B:107:ILE:HD13	2.11	0.81
1:B:422:GLN:OE1	6:B:597:HOH:O	1.99	0.81
1:D:297:TRP:HH2	1:D:338:LEU:CD1	1.94	0.81
1:C:514:THR:HG21	6:C:522:HOH:O	1.80	0.80
1:C:180:LYS:C	1:C:180:LYS:HZ2	1.88	0.80
1:C:256:ASN:C	1:C:256:ASN:ND2	2.39	0.80
1:B:374:THR:CG2	1:B:384:HIS:CE1	2.65	0.80
1:C:297:TRP:HH2	1:C:338:LEU:CD1	1.94	0.80
1:B:397:MET:HE2	1:B:399:LEU:O	1.81	0.80
1:D:334:GLU:HB3	6:D:555:HOH:O	1.81	0.80
1:B:194:LYS:CB	6:B:573:HOH:O	2.24	0.80
1:C:402:CYS:SG	2:C:611:UMP:N1	2.55	0.80
4:C:613:MTX:O1	4:C:613:MTX:CG	2.30	0.80
1:D:171:ASP:OD2	1:D:483:PRO:HB3	1.82	0.79
1:D:488:LYS:HE3	6:D:534:HOH:O	1.82	0.79
1:D:306:ASN:HD21	1:D:336:ASN:HB2	1.43	0.79
1:A:254:ARG:HD2	1:A:264:SER:HB3	1.63	0.79
1:B:472:GLN:HE21	1:B:472:GLN:N	1.81	0.79
1:C:374:THR:CG2	1:C:384:HIS:CE1	2.65	0.79
1:D:366:ASP:OD1	1:D:369:ALA:CB	2.31	0.79
1:B:4:LYS:HB3	1:B:101:LEU:HD23	1.65	0.79
1:C:167:ASN:HB3	1:C:507:ILE:HD13	1.65	0.78
1:A:495:ASN:HB3	6:A:621:HOH:O	1.84	0.78
1:C:96:ASP:O	1:C:99:GLU:HG2	1.82	0.78
1:C:293:GLU:O	1:C:296:ILE:HG22	1.83	0.78
1:D:19:ILE:O	5:D:616:NDP:H2N	1.84	0.78
1:D:282:THR:HG21	1:D:482:ARG:O	1.82	0.78
1:D:270:MET:HE2	1:D:460:ILE:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:TRP:CH2	1:D:338:LEU:HD12	2.19	0.77
1:C:6:VAL:HG22	1:C:110:ILE:HB	1.67	0.77
1:C:397:MET:HE2	1:C:400:PRO:HA	1.66	0.77
1:D:307:HIS:O	1:D:311:LYS:HE2	1.84	0.77
1:C:217:LYS:H	1:C:250:ASN:HD21	1.33	0.77
1:D:151:PRO:HG2	1:D:154:PHE:HD2	1.48	0.77
1:A:383:ARG:HH21	1:B:400:PRO:HG2	1.49	0.77
1:B:295:LEU:HD22	1:B:295:LEU:O	1.85	0.77
1:D:48:LYS:HE2	1:D:105:ASP:O	1.85	0.77
1:B:468:ASN:H	1:B:468:ASN:HD22	1.31	0.76
1:A:380:LYS:HE3	1:A:412:ASN:ND2	2.00	0.76
1:C:193:LEU:H	1:C:193:LEU:HD22	1.51	0.76
1:C:117:SER:O	1:C:118:ILE:CG2	2.33	0.76
1:A:430:GLY:HA2	3:A:604:CB3:CP3	2.15	0.76
1:C:168:ILE:HA	6:C:527:HOH:O	1.86	0.76
1:B:192:GLN:HA	1:B:192:GLN:NE2	2.01	0.76
1:D:7:SER:HB3	1:D:130:ARG:HB3	1.66	0.76
1:B:99:GLU:O	1:B:103:ASN:CG	2.28	0.75
2:C:611:UMP:H1'	3:C:612:CB3:C4	2.16	0.75
1:A:425:CYS:SG	1:A:431:SER:CB	2.75	0.75
1:A:374:THR:HG22	1:A:384:HIS:CE1	2.21	0.75
1:B:472:GLN:NE2	1:B:472:GLN:H	1.83	0.75
1:C:178:GLN:N	1:C:179:GLU:HG2	2.02	0.75
1:D:425:CYS:SG	1:D:431:SER:HB2	2.27	0.75
1:B:257:ARG:HD3	2:B:607:UMP:OP1	1.87	0.75
1:C:256:ASN:ND2	1:C:258:THR:H	1.85	0.75
1:B:403:HIS:CD2	2:B:607:UMP:O4	2.39	0.75
2:B:607:UMP:H1'	3:B:608:CB3:C4	2.17	0.75
1:A:4:LYS:HB3	1:A:101:LEU:HD22	1.68	0.75
1:B:422:GLN:HE22	1:B:434:ASN:HB3	1.50	0.75
1:D:138:LEU:HD22	1:D:168:ILE:HG23	1.69	0.75
1:D:68:LYS:HG2	6:D:545:HOH:O	1.82	0.74
1:C:193:LEU:CD2	1:C:193:LEU:N	2.48	0.74
1:D:120:ARG:HG3	1:D:120:ARG:NH1	1.97	0.74
1:A:297:TRP:CD2	1:A:308:LEU:HD21	2.23	0.74
1:C:56:ARG:HD3	5:C:614:NDP:O2X	1.88	0.74
1:C:400:PRO:HG2	1:D:383:ARG:HE	1.53	0.74
1:C:7:SER:HB3	1:C:130:ARG:HB2	1.69	0.74
1:B:341:ILE:HA	1:B:397:MET:HE3	1.69	0.74
1:C:98:ILE:O	1:C:99:GLU:CB	2.36	0.74
1:C:117:SER:O	1:C:118:ILE:CB	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ARG:HE	1:C:268:GLN:NE2	1.85	0.74
1:D:171:ASP:OD1	1:D:483:PRO:CA	2.36	0.74
1:D:284:LYS:HG3	6:D:553:HOH:O	1.86	0.74
1:C:67:LEU:HD12	1:C:72:ILE:CD1	2.18	0.73
1:D:40:THR:CG2	1:D:70:ARG:HD2	2.18	0.73
1:A:506:LEU:HD13	1:A:509:TYR:HB2	1.70	0.73
1:C:4:LYS:CB	1:C:101:LEU:HD22	2.11	0.73
1:D:75:ILE:O	5:D:616:NDP:H1B	1.88	0.73
1:C:304:ASN:ND2	1:C:306:ASN:H	1.87	0.73
1:A:99:GLU:O	1:A:103:ASN:ND2	2.21	0.73
1:A:103:ASN:CG	1:A:104:ASP:N	2.47	0.73
1:C:399:LEU:HD21	3:C:612:CB3:C8	2.18	0.73
1:D:36:PHE:O	1:D:40:THR:HB	1.88	0.73
1:C:402:CYS:SG	2:C:611:UMP:H6	2.08	0.73
1:C:254:ARG:NH2	1:D:410:VAL:O	2.21	0.72
1:D:467:GLU:HA	1:D:470:LEU:HD13	1.69	0.72
1:A:103:ASN:O	1:A:104:ASP:C	2.31	0.72
1:B:384:HIS:N	6:B:606:HOH:O	2.22	0.72
1:A:103:ASN:ND2	1:A:103:ASN:C	2.47	0.72
1:D:216:HIS:ND1	6:D:551:HOH:O	2.23	0.72
1:A:133:LEU:C	1:A:133:LEU:HD22	2.14	0.72
1:C:99:GLU:O	1:C:102:MET:HG2	1.90	0.72
1:D:40:THR:HG21	1:D:70:ARG:HH11	1.54	0.72
1:C:256:ASN:HD22	1:C:258:THR:H	1.36	0.72
1:D:225:ASN:O	1:D:233:ARG:NH2	2.23	0.72
1:A:422:GLN:CD	1:A:425:CYS:HB2	2.15	0.72
1:D:136:VAL:CG1	1:D:138:LEU:HD21	2.20	0.72
1:A:19:ILE:O	5:A:606:NDP:H2N	1.89	0.72
1:A:374:THR:CB	6:A:568:HOH:O	2.23	0.72
1:D:305:GLY:HA3	1:D:336:ASN:HD22	1.52	0.72
1:C:378:ASN:O	1:C:381:ASP:HB2	1.89	0.71
1:D:68:LYS:HG3	6:D:545:HOH:O	1.86	0.71
1:B:402:CYS:SG	2:B:607:UMP:C6	2.83	0.71
1:B:422:GLN:HE22	1:B:434:ASN:CB	2.03	0.71
1:D:423:ARG:HG3	1:D:424:SER:N	2.04	0.71
1:B:34:LYS:HE3	6:B:594:HOH:O	1.90	0.71
1:B:104:ASP:HB3	1:B:107:ILE:HD13	1.70	0.71
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.71	0.71
1:C:31:GLU:HG3	6:C:563:HOH:O	1.89	0.71
1:C:62:ILE:HG22	6:C:567:HOH:O	1.86	0.71
1:C:193:LEU:HD22	1:C:193:LEU:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ARG:CB	6:D:549:HOH:O	2.35	0.71
1:A:310:GLU:HB3	6:A:559:HOH:O	1.90	0.71
1:C:304:ASN:HD22	1:C:306:ASN:H	1.36	0.71
1:A:161:GLN:NE2	6:A:611:HOH:O	2.23	0.71
1:C:212:MET:SD	1:D:273:ASP:HB2	2.31	0.71
1:D:135:ARG:HD3	1:D:173:MET:SD	2.30	0.71
1:A:133:LEU:C	1:A:133:LEU:CD2	2.63	0.70
4:D:615:MTX:HB2	4:D:615:MTX:O	1.90	0.70
2:A:603:UMP:H1'	3:A:604:CB3:C4	2.21	0.70
1:A:397:MET:CE	1:A:401:PRO:HD3	2.21	0.70
1:C:51:ALA:C	1:C:52:LEU:HD23	2.17	0.70
1:D:306:ASN:ND2	1:D:336:ASN:CB	2.54	0.70
1:A:389:TRP:CE2	1:B:385:ILE:HG21	2.27	0.70
1:B:3:GLU:HG3	1:B:4:LYS:H	1.56	0.70
1:A:341:ILE:HA	1:A:397:MET:HE3	1.74	0.70
1:C:193:LEU:HD23	1:C:193:LEU:O	1.92	0.70
1:D:271:ARG:HG2	1:D:271:ARG:HH11	1.57	0.70
1:A:65:ARG:HG3	1:A:65:ARG:NH1	2.03	0.70
1:A:422:GLN:NE2	1:A:425:CYS:HB2	2.06	0.70
1:D:156:PRO:O	1:D:228:SER:HB2	1.91	0.70
1:B:179:GLU:HG2	1:B:180:LYS:N	2.06	0.69
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.72	0.69
1:C:487:LEU:O	1:C:488:LYS:HD3	1.91	0.69
1:D:4:LYS:HE3	1:D:107:ILE:O	1.92	0.69
1:D:295:LEU:O	1:D:295:LEU:CD2	2.37	0.69
1:C:371:LEU:CA	6:C:560:HOH:O	2.20	0.69
1:B:468:ASN:HD22	1:B:468:ASN:N	1.86	0.69
1:A:304:ASN:HD22	1:A:304:ASN:C	2.01	0.69
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.28	0.69
1:C:514:THR:HG22	6:C:524:HOH:O	1.91	0.69
1:B:98:ILE:O	1:B:99:GLU:HB3	1.91	0.69
1:C:4:LYS:HG2	1:C:101:LEU:HD23	1.74	0.69
1:B:179:GLU:CG	1:B:180:LYS:H	2.04	0.69
1:C:297:TRP:CH2	1:C:338:LEU:HD12	2.25	0.69
1:D:40:THR:HG22	1:D:70:ARG:CD	2.22	0.69
1:C:117:SER:O	1:C:118:ILE:HB	1.92	0.69
1:B:420:LEU:HD21	1:B:422:GLN:HE21	1.56	0.68
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.73	0.68
1:A:430:GLY:CA	3:A:604:CB3:HP3	2.22	0.68
1:B:75:ILE:O	5:B:610:NDP:H1B	1.93	0.68
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:N	1:B:52:LEU:HD23	2.08	0.68
1:D:337:ASP:HB2	6:D:555:HOH:O	1.94	0.68
1:C:100:ASN:H	1:C:100:ASN:HD22	1.39	0.68
1:C:158:TYR:O	1:C:173:MET:HB2	1.94	0.68
1:C:363:VAL:HG22	1:C:364:GLY:N	2.07	0.68
1:B:315:ILE:HD12	3:B:608:CB3:HP12	1.76	0.68
1:C:180:LYS:HZ1	1:C:182:THR:H	1.41	0.68
1:C:389:TRP:HB2	1:C:404:VAL:CG1	2.22	0.68
1:A:103:ASN:CG	1:A:104:ASP:H	2.01	0.68
1:C:374:THR:HG22	1:C:384:HIS:ND1	2.08	0.68
1:D:62:ILE:CG2	1:D:62:ILE:O	2.41	0.68
1:C:399:LEU:CD2	3:C:612:CB3:C8	2.71	0.68
1:B:314:TYR:C	6:B:596:HOH:O	2.36	0.68
1:D:58:THR:HG23	4:D:615:MTX:HM2	1.76	0.68
1:D:334:GLU:O	1:D:335:GLU:C	2.37	0.68
1:A:383:ARG:HH21	1:B:400:PRO:CG	2.06	0.67
1:D:452:GLU:HG2	6:D:532:HOH:O	1.94	0.67
1:A:130:ARG:HD2	1:A:132:TYR:CE1	2.30	0.67
1:A:246:ARG:HH11	1:A:268:GLN:HE21	1.39	0.67
1:D:62:ILE:O	1:D:62:ILE:HG22	1.93	0.67
1:A:267:GLY:O	1:B:271:ARG:NH2	2.28	0.67
1:A:297:TRP:CE2	1:A:308:LEU:HD21	2.29	0.67
1:D:136:VAL:CG1	1:D:138:LEU:CD2	2.72	0.67
1:D:271:ARG:HH11	1:D:271:ARG:CG	2.08	0.67
1:D:466:TYR:HB3	1:D:468:ASN:HD21	1.60	0.67
1:A:430:GLY:C	3:A:604:CB3:HP3	2.20	0.67
1:B:271:ARG:HG3	1:B:271:ARG:HH11	1.60	0.67
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.77	0.67
1:D:325:LEU:HD23	1:D:333:ARG:HB3	1.77	0.67
1:D:341:ILE:HA	1:D:397:MET:HE3	1.77	0.67
1:B:136:VAL:HG12	1:B:138:LEU:HD22	1.77	0.66
1:D:427:LEU:HD23	1:D:464:HIS:N	2.09	0.66
1:D:138:LEU:HD22	1:D:168:ILE:CG2	2.25	0.66
1:C:26:PRO:HG2	1:C:27:TRP:CZ3	2.30	0.66
1:D:116:GLU:HB2	1:D:145:THR:HG23	1.77	0.66
1:D:411:THR:OG1	1:D:415:CYS:HB2	1.95	0.66
1:C:349:TYR:OH	1:D:349:TYR:OH	2.01	0.66
1:D:492:LYS:HE3	6:D:539:HOH:O	1.96	0.66
1:C:256:ASN:O	1:C:258:THR:N	2.29	0.66
1:C:323:GLU:H	1:C:323:GLU:CD	2.03	0.66
1:D:479:ARG:HB3	1:D:512:TYR:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:SER:O	2:A:603:UMP:C2'	2.44	0.65
1:C:4:LYS:NZ	1:C:107:ILE:O	2.29	0.65
4:D:615:MTX:O	4:D:615:MTX:CB	2.42	0.65
1:A:98:ILE:O	1:A:99:GLU:HB3	1.95	0.65
1:A:217:LYS:HB2	1:A:250:ASN:HD21	1.61	0.65
1:A:130:ARG:NH1	1:A:176:GLU:OE2	2.29	0.65
1:D:125:ASP:HB3	1:D:127:PHE:CE1	2.32	0.65
1:D:342:TYR:OH	1:D:402:CYS:N	2.20	0.65
1:B:128:VAL:HG13	6:B:536:HOH:O	1.96	0.65
1:D:120:ARG:HH11	1:D:120:ARG:CG	2.10	0.65
1:B:81:GLN:OE1	1:B:92:ARG:NH2	2.30	0.65
1:D:38:LYS:HD3	6:D:546:HOH:O	1.96	0.65
1:A:310:GLU:CB	6:A:559:HOH:O	2.44	0.65
1:C:422:GLN:CD	1:C:425:CYS:HB2	2.21	0.65
1:D:40:THR:CG2	1:D:70:ARG:HH11	2.08	0.65
1:D:235:HIS:CE1	1:D:237:GLU:HB2	2.32	0.65
1:C:193:LEU:O	1:C:195:SER:N	2.30	0.65
1:C:48:LYS:HG2	1:C:106:SER:HA	1.78	0.64
1:D:40:THR:HG22	1:D:70:ARG:HD3	1.78	0.64
1:C:468:ASN:H	1:C:468:ASN:ND2	1.94	0.64
1:D:20:GLY:HA3	1:D:145:THR:HB	1.79	0.64
1:A:383:ARG:NH2	1:B:400:PRO:HG2	2.12	0.64
1:D:469:HIS:HA	1:D:472:GLN:OE1	1.98	0.64
1:B:196:ILE:O	1:B:200:VAL:HG23	1.97	0.64
1:D:260:ILE:HG21	1:D:468:ASN:ND2	2.11	0.64
1:D:439:ALA:O	1:D:443:MET:HG3	1.98	0.64
1:C:12:ALA:HB1	1:C:17:SER:HA	1.77	0.64
1:D:171:ASP:OD1	1:D:483:PRO:HA	1.97	0.64
1:B:36:PHE:O	1:B:40:THR:HG23	1.97	0.64
1:C:180:LYS:CG	1:C:181:LYS:H	2.05	0.64
1:D:116:GLU:HB2	1:D:145:THR:CG2	2.27	0.64
1:A:179:GLU:O	1:A:180:LYS:HE2	1.98	0.64
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.80	0.64
1:C:180:LYS:HZ3	1:C:180:LYS:C	1.97	0.64
1:D:298:PHE:CD2	6:D:544:HOH:O	2.50	0.64
1:A:254:ARG:O	1:A:261:SER:HB3	1.97	0.64
1:C:152:GLU:C	1:C:154:PHE:H	2.04	0.64
1:C:239:GLN:HG3	1:C:271:ARG:O	1.98	0.64
1:D:50:ASN:ND2	1:D:111:PHE:CE2	2.57	0.64
1:B:167:ASN:ND2	1:B:488:LYS:HE3	2.12	0.64
1:B:294:GLU:O	1:B:297:TRP:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ILE:HA	6:D:522:HOH:O	1.97	0.64
1:D:229:ILE:HG22	1:D:233:ARG:HG2	1.80	0.64
1:D:305:GLY:CA	1:D:336:ASN:HD22	2.11	0.64
1:B:359:ASP:CG	1:B:361:THR:HG22	2.23	0.63
1:A:297:TRP:CG	1:A:308:LEU:HD21	2.34	0.63
1:C:67:LEU:HD12	1:C:72:ILE:HD11	1.80	0.63
1:A:135:ARG:NH1	1:A:171:ASP:OD2	2.21	0.63
1:A:35:PHE:CZ	1:A:39:ILE:HD13	2.33	0.63
1:D:466:TYR:HB3	1:D:468:ASN:ND2	2.12	0.63
1:A:179:GLU:O	1:A:180:LYS:CG	2.47	0.63
1:B:331:GLY:N	6:B:577:HOH:O	2.30	0.63
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.14	0.63
1:C:178:GLN:H	1:C:179:GLU:HG2	1.64	0.62
1:C:284:LYS:HE2	6:C:529:HOH:O	1.99	0.62
1:D:305:GLY:C	1:D:336:ASN:HD22	2.06	0.62
1:A:246:ARG:HH11	1:A:268:GLN:NE2	1.97	0.62
1:C:98:ILE:CD1	1:C:127:PHE:CD1	2.80	0.62
1:C:397:MET:CE	1:C:400:PRO:HA	2.29	0.62
1:D:344:PHE:CE2	1:D:353:TYR:HD1	2.17	0.62
1:B:246:ARG:HE	1:B:268:GLN:NE2	1.98	0.62
1:D:359:ASP:OD1	1:D:361:THR:HB	1.98	0.62
1:A:289:ARG:NH2	1:A:311:LYS:O	2.32	0.62
1:A:308:LEU:N	1:A:308:LEU:HD22	2.15	0.62
4:C:613:MTX:N5	5:C:614:NDP:H42N	2.14	0.62
1:D:40:THR:CG2	1:D:70:ARG:CD	2.77	0.62
1:D:58:THR:CG2	4:D:615:MTX:HM2	2.29	0.62
1:D:298:PHE:HD2	6:D:544:HOH:O	1.81	0.62
1:B:304:ASN:HD22	1:B:304:ASN:C	2.08	0.62
1:C:371:LEU:N	6:C:560:HOH:O	2.30	0.62
1:C:423:ARG:HD3	1:D:385:ILE:HD11	1.82	0.62
1:D:275:ARG:HD3	6:D:552:HOH:O	1.98	0.62
1:A:472:GLN:HE21	1:A:472:GLN:H	1.47	0.62
1:B:19:ILE:O	5:B:610:NDP:H2N	2.00	0.62
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.82	0.62
1:A:359:ASP:OD1	1:A:361:THR:CG2	2.46	0.62
1:D:101:LEU:C	1:D:103:ASN:H	2.07	0.62
1:A:402:CYS:SG	2:A:603:UMP:H6	2.21	0.61
1:D:48:LYS:HG2	1:D:106:SER:HA	1.82	0.61
1:D:295:LEU:CA	6:D:544:HOH:O	2.33	0.61
1:D:136:VAL:HG12	1:D:138:LEU:HD21	1.78	0.61
1:A:297:TRP:CD1	1:A:308:LEU:HD21	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ILE:HG22	1:C:118:ILE:HD11	1.82	0.61
1:A:335:GLU:O	1:A:336:ASN:HB2	2.00	0.61
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.81	0.61
1:A:130:ARG:HD2	1:A:132:TYR:CZ	2.35	0.61
1:A:136:VAL:HG12	1:A:138:LEU:HD22	1.82	0.61
1:C:468:ASN:HD22	1:C:468:ASN:N	1.91	0.61
1:D:104:ASP:C	1:D:106:SER:H	2.07	0.61
1:A:103:ASN:ND2	1:A:104:ASP:N	2.48	0.61
1:C:102:MET:HG3	1:C:103:ASN:HB3	1.82	0.61
1:D:171:ASP:OD1	1:D:483:PRO:HB3	2.01	0.61
1:B:138:LEU:HD23	1:B:138:LEU:H	1.66	0.61
1:C:55:GLY:HA3	5:C:614:NDP:O2A	2.00	0.61
1:C:243:LEU:HD12	1:C:243:LEU:O	2.00	0.61
1:A:35:PHE:CE1	1:A:39:ILE:HD13	2.35	0.61
1:A:300:LYS:HD3	1:A:497:GLU:HB2	1.83	0.61
1:C:215:ARG:HD3	1:D:275:ARG:NH2	2.16	0.61
1:C:422:GLN:CG	1:C:425:CYS:HB2	2.30	0.61
1:D:147:PHE:CD2	1:D:148:PRO:HD2	2.35	0.61
1:D:455:GLU:HG3	6:D:525:HOH:O	2.01	0.61
1:A:233:ARG:NH1	1:A:242:ASP:OD1	2.33	0.60
1:B:233:ARG:NH1	1:B:242:ASP:OD1	2.33	0.60
1:B:472:GLN:HE21	1:B:472:GLN:H	1.42	0.60
1:A:468:ASN:HD22	1:A:468:ASN:N	1.85	0.60
1:B:360:TYR:O	1:B:363:VAL:HG12	2.01	0.60
1:C:180:LYS:O	1:C:181:LYS:C	2.43	0.60
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.35	0.60
1:A:82:ASP:OD1	1:A:83:GLU:N	2.34	0.60
1:C:422:GLN:HG2	1:C:425:CYS:HB2	1.83	0.60
1:D:465:ILE:HG23	6:D:538:HOH:O	2.00	0.60
1:C:4:LYS:HD2	1:C:108:GLU:O	2.02	0.60
1:C:49:LYS:N	1:C:106:SER:O	2.30	0.60
1:C:419:ASN:HD22	1:C:457:ALA:HB3	1.65	0.60
1:D:509:TYR:HA	6:D:550:HOH:O	2.00	0.60
1:C:116:GLU:HG3	1:C:146:TYR:O	2.01	0.60
1:C:374:THR:CG2	1:C:384:HIS:ND1	2.64	0.60
1:D:295:LEU:HD23	1:D:295:LEU:C	2.25	0.60
1:A:354:LYS:HD2	6:A:550:HOH:O	2.01	0.60
4:D:615:MTX:HG1	4:D:615:MTX:O1	2.02	0.60
1:C:178:GLN:HA	1:C:179:GLU:HG3	1.83	0.60
1:D:432:PRO:HA	1:D:435:ILE:HD12	1.84	0.60
1:A:4:LYS:HD2	1:A:107:ILE:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:H	1:A:468:ASN:ND2	1.93	0.59
1:C:359:ASP:OD1	1:C:361:THR:HG22	2.01	0.59
1:D:39:ILE:HG23	1:D:40:THR:H	1.67	0.59
1:C:135:ARG:NH1	1:C:171:ASP:OD2	2.36	0.59
1:C:167:ASN:O	1:C:507:ILE:HG21	2.01	0.59
1:D:405:LEU:C	1:D:405:LEU:HD23	2.28	0.59
1:A:430:GLY:HA2	3:A:604:CB3:HP3	1.82	0.59
1:B:138:LEU:N	1:B:138:LEU:CD2	2.65	0.59
1:C:10:VAL:HG22	1:C:11:ALA:H	1.68	0.59
1:C:11:ALA:O	1:C:19:ILE:HG22	2.03	0.59
1:A:407:GLN:OE1	1:B:423:ARG:HA	2.02	0.59
1:D:171:ASP:OD1	1:D:483:PRO:CB	2.50	0.59
1:A:271:ARG:NH2	1:B:267:GLY:O	2.36	0.59
1:C:415:CYS:HA	1:C:452:GLU:O	2.03	0.59
1:A:99:GLU:OE2	1:A:99:GLU:C	2.46	0.59
1:A:426:ASP:OD2	1:A:426:ASP:C	2.46	0.59
1:D:104:ASP:C	1:D:106:SER:N	2.60	0.59
1:B:255:GLU:H	1:B:255:GLU:CD	2.11	0.59
1:C:156:PRO:O	1:C:228:SER:HB2	2.03	0.59
1:D:479:ARG:HD3	1:D:512:TYR:CD2	2.38	0.59
1:C:117:SER:C	1:C:118:ILE:HG22	2.27	0.58
1:C:315:ILE:HG22	3:C:612:CB3:HG1	1.85	0.58
1:D:108:GLU:HG2	1:D:109:ASN:ND2	2.18	0.58
1:C:320:GLY:O	1:C:335:GLU:O	2.22	0.58
1:D:67:LEU:HD22	4:D:615:MTX:HA	1.85	0.58
4:D:615:MTX:N5	5:D:616:NDP:H42N	2.18	0.58
1:D:21:ILE:HA	1:D:144:ASP:OD2	2.03	0.58
1:D:56:ARG:HD3	5:D:616:NDP:O2X	2.03	0.58
1:B:425:CYS:CB	6:B:597:HOH:O	2.51	0.58
1:D:342:TYR:CZ	1:D:401:PRO:HA	2.38	0.58
1:A:12:ALA:HB1	1:A:17:SER:HA	1.85	0.58
1:D:294:GLU:O	1:D:297:TRP:HB3	2.02	0.58
1:D:450:GLY:HA2	6:D:523:HOH:O	2.02	0.58
1:A:48:LYS:CD	1:A:105:ASP:O	2.44	0.58
1:C:19:ILE:O	5:C:614:NDP:H2N	2.03	0.58
1:D:374:THR:O	1:D:378:ASN:O	2.22	0.58
1:D:512:TYR:HB3	1:D:513:PRO:CD	2.34	0.58
1:A:193:LEU:HD13	6:A:536:HOH:O	2.02	0.58
1:D:162:THR:OG1	1:D:484:PHE:HB2	2.04	0.58
1:B:58:THR:O	1:B:61:SER:HB2	2.04	0.58
1:D:512:TYR:HB3	1:D:513:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:TYR:O	1:D:346:TRP:CD1	2.57	0.58
1:B:193:LEU:CB	6:B:524:HOH:O	2.51	0.57
1:B:256:ASN:O	1:B:258:THR:O	2.22	0.57
1:B:295:LEU:HD22	1:B:295:LEU:C	2.29	0.57
1:A:411:THR:HB	6:A:562:HOH:O	2.02	0.57
1:D:128:VAL:O	1:D:154:PHE:HZ	1.87	0.57
1:D:171:ASP:OD2	1:D:483:PRO:CB	2.51	0.57
1:B:422:GLN:NE2	1:B:434:ASN:HB3	2.19	0.57
1:C:209:ILE:H	1:C:209:ILE:HD12	1.70	0.57
1:B:420:LEU:HD21	1:B:422:GLN:NE2	2.19	0.57
1:B:512:TYR:HB3	1:B:513:PRO:HD2	1.85	0.57
1:C:423:ARG:NH1	2:C:611:UMP:OP3	2.28	0.57
1:C:247:VAL:HG12	1:C:265:ILE:CD1	2.35	0.57
1:B:246:ARG:HE	1:B:268:GLN:HE22	1.53	0.57
1:C:180:LYS:NZ	1:C:180:LYS:O	2.35	0.57
1:B:41:ASN:HD21	1:B:69:ASN:HB2	1.70	0.57
1:B:217:LYS:HB2	1:B:250:ASN:HD21	1.70	0.57
1:C:256:ASN:O	1:C:258:THR:O	2.23	0.57
1:D:507:ILE:HG22	6:D:522:HOH:O	2.03	0.57
1:D:92:ARG:O	5:D:616:NDP:H2A	2.05	0.57
1:D:285:LYS:HB3	1:D:514:THR:HG22	1.85	0.57
1:D:408:TYR:N	1:D:408:TYR:CD2	2.72	0.57
1:A:179:GLU:O	1:A:180:LYS:HG3	2.04	0.56
1:B:114:GLY:HA3	1:B:119:TYR:CZ	2.40	0.56
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.70	0.56
1:A:4:LYS:CB	1:A:101:LEU:HD22	2.33	0.56
1:A:54:MET:HE3	1:A:72:ILE:HG23	1.86	0.56
1:A:246:ARG:HE	1:A:268:GLN:NE2	2.02	0.56
1:A:471:THR:HG23	6:A:610:HOH:O	2.06	0.56
1:C:4:LYS:CB	1:C:101:LEU:CD2	2.76	0.56
1:C:304:ASN:HD22	1:C:304:ASN:C	2.12	0.56
1:C:363:VAL:CG2	1:C:364:GLY:N	2.68	0.56
1:D:75:ILE:O	1:D:75:ILE:HG22	2.04	0.56
1:B:419:ASN:ND2	1:B:457:ALA:HB3	2.20	0.56
1:C:3:GLU:HG3	1:C:4:LYS:H	1.70	0.56
1:C:137:ALA:O	1:C:138:LEU:HD13	2.05	0.56
1:D:104:ASP:O	1:D:107:ILE:N	2.21	0.56
1:D:447:GLN:HG3	6:D:539:HOH:O	2.04	0.56
1:A:389:TRP:CH2	1:B:385:ILE:HD12	2.41	0.56
1:B:216:HIS:HD2	6:B:551:HOH:O	1.89	0.56
1:B:425:CYS:HB2	6:B:597:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:H	1:C:193:LEU:HD23	1.67	0.56
1:C:460:ILE:HG21	1:C:463:ALA:HB2	1.88	0.56
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.88	0.56
1:A:103:ASN:C	1:A:103:ASN:HD22	2.13	0.56
1:C:217:LYS:N	1:C:250:ASN:HD21	2.04	0.56
1:D:37:SER:O	1:D:41:ASN:HB2	2.06	0.56
1:D:104:ASP:CB	1:D:107:ILE:HD13	2.32	0.56
1:D:344:PHE:CE2	1:D:353:TYR:CD1	2.94	0.56
1:A:247:VAL:HG22	1:A:465:ILE:HD12	1.88	0.56
2:A:603:UMP:OP1	1:B:383:ARG:NH1	2.39	0.56
1:B:138:LEU:HD23	1:B:138:LEU:O	2.06	0.56
1:B:468:ASN:H	1:B:468:ASN:ND2	2.02	0.56
1:C:151:PRO:O	1:C:154:PHE:HB2	2.04	0.56
1:A:374:THR:HG22	1:A:384:HIS:HE1	1.67	0.55
1:B:520:ALA:HB3	3:B:608:CB3:NA2	2.21	0.55
1:A:133:LEU:CD2	1:A:134:THR:N	2.69	0.55
1:A:383:ARG:HE	1:B:400:PRO:HG2	1.71	0.55
1:B:100:ASN:CA	1:B:103:ASN:HD21	2.07	0.55
1:A:52:LEU:HD23	1:A:52:LEU:N	2.20	0.55
1:B:192:GLN:HA	1:B:192:GLN:HE21	1.72	0.55
1:A:385:ILE:CD1	1:B:423:ARG:HD3	2.36	0.55
1:B:138:LEU:H	1:B:138:LEU:CD2	2.20	0.55
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.88	0.55
1:A:304:ASN:ND2	1:A:306:ASN:H	2.04	0.55
1:B:43:LYS:NZ	1:B:48:LYS:O	2.33	0.55
1:D:4:LYS:HB2	1:D:101:LEU:CD2	2.36	0.55
1:C:135:ARG:HB2	1:C:171:ASP:HB2	1.88	0.55
1:B:247:VAL:CG2	1:B:465:ILE:HD12	2.36	0.55
1:C:178:GLN:CA	1:C:179:GLU:HG2	2.37	0.55
1:C:234:GLU:HG2	1:C:234:GLU:O	2.07	0.55
1:D:297:TRP:CH2	1:D:338:LEU:CD1	2.82	0.55
1:B:502:GLU:H	1:B:502:GLU:CD	2.14	0.55
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.89	0.55
1:D:28:SER:HA	6:D:535:HOH:O	2.07	0.55
1:D:138:LEU:HD23	1:D:138:LEU:N	2.22	0.55
1:D:468:ASN:HD22	1:D:468:ASN:N	2.01	0.55
1:A:472:GLN:HE21	1:A:472:GLN:N	2.05	0.55
1:A:472:GLN:H	1:A:472:GLN:NE2	2.05	0.55
1:C:7:SER:HB3	1:C:130:ARG:CB	2.36	0.55
1:C:412:ASN:OD1	1:D:253:TYR:O	2.24	0.55
1:D:422:GLN:CD	1:D:425:CYS:HB2	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.42	0.54
1:D:56:ARG:HG3	1:D:79:LEU:HD12	1.90	0.54
1:D:307:HIS:O	1:D:311:LYS:CE	2.54	0.54
1:A:102:MET:O	1:A:103:ASN:CB	2.55	0.54
1:C:10:VAL:HG22	1:C:11:ALA:N	2.21	0.54
1:D:242:ASP:O	1:D:246:ARG:HB2	2.06	0.54
1:A:39:ILE:HD12	1:B:202:LEU:HD23	1.88	0.54
1:A:217:LYS:H	1:A:250:ASN:ND2	2.04	0.54
1:A:304:ASN:HD22	1:A:306:ASN:H	1.55	0.54
1:D:15:LEU:HB2	1:D:139:GLU:HG2	1.88	0.54
1:B:323:GLU:O	1:B:326:GLU:HB3	2.07	0.54
1:C:294:GLU:O	1:C:297:TRP:HB3	2.08	0.54
1:D:278:PHE:CE1	1:D:439:ALA:HB1	2.43	0.54
1:B:51:ALA:C	1:B:52:LEU:HD23	2.31	0.54
1:C:402:CYS:O	1:C:404:VAL:HG23	2.08	0.54
1:D:343:GLY:HA2	1:D:346:TRP:HB2	1.89	0.54
1:D:430:GLY:O	1:D:433:PHE:HB2	2.08	0.54
1:A:173:MET:HE2	1:A:175:PHE:CZ	2.43	0.54
1:A:120:ARG:NH1	6:A:538:HOH:O	2.24	0.54
1:A:304:ASN:HD21	1:A:306:ASN:HB2	1.73	0.54
1:A:422:GLN:HE22	1:A:434:ASN:ND2	2.06	0.54
1:C:319:ASN:ND2	1:C:399:LEU:HD22	2.23	0.54
1:D:284:LYS:HD2	6:D:553:HOH:O	2.07	0.54
1:A:5:ASN:ND2	1:A:130:ARG:HH21	2.05	0.54
1:A:104:ASP:CB	1:A:107:ILE:HG12	2.38	0.54
1:A:374:THR:CG2	6:A:568:HOH:O	2.53	0.54
1:B:3:GLU:HB3	6:B:567:HOH:O	2.08	0.54
1:B:466:TYR:O	1:B:469:HIS:HB2	2.07	0.54
1:C:114:GLY:HA3	1:C:119:TYR:CZ	2.43	0.54
1:C:274:MET:HE2	1:C:456:LEU:HB2	1.89	0.54
1:D:79:LEU:HD23	1:D:80:PRO:HD2	1.90	0.54
1:D:457:ALA:HB2	6:D:536:HOH:O	2.08	0.54
1:A:385:ILE:HD11	1:B:423:ARG:HD3	1.89	0.53
1:B:304:ASN:ND2	1:B:306:ASN:HB2	2.23	0.53
1:B:397:MET:CE	1:B:401:PRO:HD3	2.34	0.53
1:B:403:HIS:HD2	2:B:607:UMP:O4	1.90	0.53
4:C:613:MTX:O	4:C:613:MTX:HB2	2.08	0.53
1:D:15:LEU:N	1:D:139:GLU:OE1	2.37	0.53
1:D:324:TYR:O	1:D:328:ILE:HG12	2.08	0.53
1:A:401:PRO:O	1:A:423:ARG:NE	2.39	0.53
1:B:100:ASN:CA	1:B:103:ASN:ND2	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:HD11	1:C:145:THR:HG22	1.90	0.53
1:C:399:LEU:CD2	3:C:612:CB3:H8	2.37	0.53
1:D:378:ASN:O	1:D:384:HIS:HE1	1.92	0.53
1:B:472:GLN:N	1:B:472:GLN:NE2	2.46	0.53
1:C:289:ARG:NH2	1:C:311:LYS:O	2.41	0.53
1:C:178:GLN:CA	1:C:179:GLU:CG	2.85	0.53
1:D:290:SER:CB	1:D:313:VAL:CG1	2.84	0.53
1:B:104:ASP:HB3	1:B:107:ILE:CD1	2.38	0.53
1:C:509:TYR:O	1:C:511:PRO:HD3	2.08	0.53
1:D:344:PHE:CZ	1:D:353:TYR:HD1	2.27	0.53
1:D:349:TYR:CD2	1:D:350:ASN:HB2	2.43	0.53
1:A:15:LEU:HB2	1:A:139:GLU:HG2	1.90	0.53
1:C:79:LEU:HD22	1:C:90:VAL:HG21	1.89	0.53
1:C:459:PHE:C	1:C:460:ILE:HD13	2.33	0.53
1:D:324:TYR:CE2	1:D:328:ILE:HD13	2.44	0.53
1:B:35:PHE:CE1	1:B:39:ILE:HD13	2.44	0.53
1:A:126:ASN:ND2	1:A:177:LYS:CE	2.51	0.53
1:C:516:LYS:CE	6:C:533:HOH:O	2.56	0.53
1:D:171:ASP:CG	1:D:483:PRO:CB	2.81	0.53
1:C:152:GLU:C	1:C:154:PHE:N	2.66	0.53
1:C:256:ASN:ND2	1:C:258:THR:HG23	2.24	0.53
1:D:62:ILE:HD11	4:D:615:MTX:C12	2.39	0.53
1:B:242:ASP:O	1:B:246:ARG:HG3	2.09	0.52
1:C:75:ILE:O	5:C:614:NDP:H1B	2.08	0.52
1:C:100:ASN:CA	1:C:103:ASN:ND2	2.63	0.52
1:D:275:ARG:HD3	1:D:415:CYS:SG	2.49	0.52
1:D:495:ASN:O	1:D:498:ASP:HB2	2.09	0.52
1:A:83:GLU:OE2	1:A:83:GLU:HA	2.07	0.52
1:A:99:GLU:O	1:A:102:MET:O	2.27	0.52
1:C:323:GLU:CD	1:C:323:GLU:N	2.66	0.52
1:D:348:HIS:O	1:D:349:TYR:C	2.52	0.52
1:C:211:LYS:CB	6:C:561:HOH:O	2.19	0.52
1:D:295:LEU:CD2	1:D:295:LEU:C	2.82	0.52
1:A:172:PHE:N	1:A:172:PHE:CD2	2.77	0.52
1:C:173:MET:HE2	1:C:175:PHE:CZ	2.44	0.52
1:B:257:ARG:HD3	2:B:607:UMP:P	2.49	0.52
1:C:180:LYS:O	1:C:182:THR:N	2.43	0.52
1:C:423:ARG:HD3	1:D:385:ILE:CD1	2.40	0.52
1:D:30:SER:O	1:D:34:LYS:HB2	2.10	0.52
1:D:220:LYS:HB2	1:D:220:LYS:NZ	2.25	0.52
1:A:430:GLY:CA	3:A:604:CB3:CP3	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:CE1	1:B:237:GLU:HB2	2.44	0.52
1:C:98:ILE:O	1:C:99:GLU:CG	2.57	0.52
1:C:115:GLY:O	1:C:118:ILE:CG2	2.53	0.52
1:C:193:LEU:O	1:C:194:LYS:C	2.52	0.52
1:C:297:TRP:CH2	1:C:338:LEU:CD1	2.85	0.52
1:D:295:LEU:O	1:D:299:ILE:HG13	2.10	0.52
1:D:447:GLN:HG2	1:D:492:LYS:CE	2.34	0.52
1:A:102:MET:O	1:A:103:ASN:HB3	2.09	0.51
1:A:323:GLU:H	1:A:323:GLU:CD	2.18	0.51
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.45	0.51
1:B:192:GLN:HE21	1:B:192:GLN:CA	2.22	0.51
1:B:422:GLN:NE2	1:B:434:ASN:CG	2.68	0.51
3:C:612:CB3:H13	3:C:612:CB3:CP2	2.40	0.51
1:A:431:SER:HB3	1:A:432:PRO:HD3	1.92	0.51
1:B:246:ARG:HH11	1:B:268:GLN:NE2	2.08	0.51
1:C:119:TYR:O	1:C:123:LEU:HD23	2.10	0.51
1:C:256:ASN:ND2	1:C:256:ASN:O	2.43	0.51
1:D:44:CYS:HB2	1:D:108:GLU:OE1	2.10	0.51
1:B:304:ASN:HD21	1:B:306:ASN:HB2	1.74	0.51
1:A:217:LYS:H	1:A:250:ASN:HD21	1.57	0.51
1:B:225:ASN:N	6:B:574:HOH:O	2.40	0.51
1:B:458:ILE:HG22	1:B:460:ILE:HD11	1.91	0.51
1:D:5:ASN:O	1:D:110:ILE:HB	2.10	0.51
1:D:289:ARG:HG3	1:D:501:TRP:CZ2	2.45	0.51
1:A:44:CYS:HB2	6:A:545:HOH:O	2.11	0.51
1:B:126:ASN:HD21	1:B:177:LYS:CE	1.90	0.51
1:C:180:LYS:NZ	1:C:182:THR:H	2.08	0.51
1:C:363:VAL:CG2	1:C:364:GLY:H	2.24	0.51
1:D:8:ILE:HD12	1:D:119:TYR:CE1	2.46	0.51
1:C:48:LYS:CB	1:C:106:SER:O	2.56	0.51
1:D:3:GLU:OE2	1:D:3:GLU:HA	2.09	0.51
1:D:275:ARG:C	6:D:549:HOH:O	2.54	0.51
1:D:334:GLU:N	6:D:555:HOH:O	2.24	0.51
1:A:217:LYS:N	1:A:250:ASN:HD21	2.09	0.51
1:A:254:ARG:HD2	1:A:264:SER:CB	2.37	0.51
1:B:25:LEU:HD11	4:B:609:MTX:H7	1.93	0.51
1:B:426:ASP:HB3	1:B:430:GLY:H	1.76	0.51
3:B:608:CB3:CP2	3:B:608:CB3:H13	2.41	0.51
1:C:293:GLU:HA	1:C:296:ILE:HG22	1.92	0.51
1:D:52:LEU:HB3	1:D:113:CYS:HG	1.71	0.51
1:A:380:LYS:HD2	1:B:254:ARG:CZ	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:NE	1:B:268:GLN:HE22	2.09	0.50
1:C:174:ILE:HD11	1:D:196:ILE:HG12	1.92	0.50
1:D:171:ASP:OD2	1:D:171:ASP:N	2.43	0.50
1:D:235:HIS:CD2	6:D:526:HOH:O	2.65	0.50
1:D:444:MET:HG2	1:D:499:PHE:CE1	2.46	0.50
1:A:312:LYS:HG2	1:A:314:TYR:OH	2.11	0.50
1:A:500:LYS:O	1:A:501:TRP:C	2.54	0.50
1:B:246:ARG:HH11	1:B:268:GLN:HE21	1.58	0.50
1:B:466:TYR:HB3	1:B:468:ASN:HD21	1.76	0.50
1:C:236:TYR:OH	1:D:212:MET:HB3	2.12	0.50
1:D:103:ASN:CG	1:D:104:ASP:N	2.67	0.50
1:D:328:ILE:CD1	1:D:330:LEU:HD12	2.41	0.50
1:A:263:TYR:CE2	1:A:470:LEU:HD21	2.46	0.50
1:B:136:VAL:HG12	1:B:138:LEU:CD2	2.41	0.50
1:B:193:LEU:N	1:B:193:LEU:HD23	2.26	0.50
1:C:289:ARG:HG3	1:C:501:TRP:CE2	2.46	0.50
1:C:423:ARG:CD	1:D:385:ILE:HD11	2.41	0.50
1:D:171:ASP:OD2	1:D:483:PRO:CG	2.59	0.50
1:D:177:LYS:O	1:D:177:LYS:HG2	2.11	0.50
1:D:397:MET:HE2	6:D:531:HOH:O	2.11	0.50
1:D:468:ASN:H	1:D:468:ASN:ND2	2.01	0.50
1:A:371:LEU:HD22	1:A:375:LEU:HG	1.94	0.50
1:B:190:ARG:HA	1:B:197:ASP:OD1	2.12	0.50
1:B:192:GLN:HG2	6:B:592:HOH:O	2.11	0.50
1:C:100:ASN:HA	1:C:103:ASN:HD22	1.70	0.50
1:C:304:ASN:HD21	1:C:306:ASN:HB2	1.77	0.50
1:D:4:LYS:HD2	1:D:101:LEU:HA	1.94	0.50
1:D:104:ASP:HB2	1:D:107:ILE:HB	1.92	0.50
1:A:96:ASP:C	1:A:98:ILE:H	2.20	0.50
1:A:254:ARG:NH2	1:B:410:VAL:O	2.44	0.50
1:A:366:ASP:O	1:A:370:LYS:HG3	2.12	0.50
1:C:180:LYS:NZ	1:C:181:LYS:CA	2.67	0.50
1:D:284:LYS:CD	6:D:553:HOH:O	2.56	0.50
1:B:466:TYR:HB3	1:B:468:ASN:ND2	2.25	0.50
1:C:264:SER:HB2	1:C:464:HIS:HB3	1.94	0.50
1:C:381:ASP:O	1:C:384:HIS:CD2	2.65	0.50
1:C:460:ILE:HD13	1:C:460:ILE:N	2.26	0.50
1:D:67:LEU:CD2	4:D:615:MTX:HA	2.42	0.50
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.46	0.50
1:A:487:LEU:C	1:A:487:LEU:HD23	2.36	0.50
1:C:98:ILE:CD1	1:C:127:PHE:HD1	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:HB2	1:A:454:GLY:O	2.11	0.50
1:A:400:PRO:HD2	1:B:383:ARG:NH1	2.27	0.50
1:C:246:ARG:HE	1:C:268:GLN:HE22	1.60	0.50
1:D:128:VAL:O	1:D:154:PHE:CZ	2.65	0.50
1:D:130:ARG:NH1	1:D:176:GLU:OE2	2.45	0.50
1:D:310:GLU:C	1:D:312:LYS:H	2.19	0.50
1:D:447:GLN:CG	6:D:539:HOH:O	2.59	0.50
1:D:486:GLN:HB2	1:D:507:ILE:HB	1.94	0.50
1:A:64:ARG:NH2	1:A:79:LEU:HD21	2.26	0.49
1:A:133:LEU:HD22	1:A:134:THR:N	2.26	0.49
1:B:132:TYR:HA	1:B:174:ILE:HG22	1.94	0.49
1:C:53:ILE:HG23	1:C:75:ILE:HD13	1.94	0.49
1:C:62:ILE:HG21	6:C:567:HOH:O	2.03	0.49
1:C:158:TYR:HB2	1:C:174:ILE:HG12	1.90	0.49
1:D:467:GLU:C	1:D:469:HIS:H	2.20	0.49
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.19	0.49
1:B:255:GLU:HB2	6:B:540:HOH:O	2.11	0.49
1:B:316:TRP:N	6:B:596:HOH:O	2.45	0.49
1:A:26:PRO:HB2	1:A:27:TRP:CE3	2.46	0.49
1:A:360:TYR:O	1:A:363:VAL:HG13	2.12	0.49
1:A:409:TYR:HH	1:B:264:SER:HG	1.59	0.49
1:D:224:TYR:O	1:D:227:PRO:HG3	2.12	0.49
1:D:342:TYR:OH	1:D:401:PRO:HA	2.12	0.49
1:D:427:LEU:HD23	1:D:464:HIS:H	1.77	0.49
1:C:370:LYS:C	6:C:560:HOH:O	2.54	0.49
1:A:470:LEU:O	1:A:474:LYS:HD3	2.12	0.49
1:B:372:ILE:O	1:B:376:LYS:HG3	2.13	0.49
1:A:246:ARG:HE	1:A:268:GLN:HE22	1.60	0.49
1:A:342:TYR:CE1	1:A:401:PRO:HB3	2.48	0.49
1:A:378:ASN:O	1:A:381:ASP:HB3	2.11	0.49
1:B:53:ILE:HG23	1:B:75:ILE:HD13	1.94	0.49
1:B:130:ARG:HG3	1:B:130:ARG:HH11	1.78	0.49
1:D:97:SER:C	1:D:99:GLU:H	2.20	0.49
1:D:120:ARG:NH1	1:D:148:PRO:HB3	2.26	0.49
1:A:399:LEU:CD2	3:A:604:CB3:H8	2.43	0.49
1:B:194:LYS:HG2	1:B:198:ASP:OD1	2.12	0.49
1:B:367:GLN:OE1	1:B:387:THR:HG22	2.13	0.49
1:D:135:ARG:HH22	1:D:159:MET:HE2	1.78	0.49
1:B:280:LEU:HD23	1:B:509:TYR:CE2	2.47	0.49
1:C:138:LEU:HD22	1:C:168:ILE:CG2	2.42	0.49
1:D:67:LEU:HD22	4:D:615:MTX:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:LEU:O	1:D:97:SER:OG	2.24	0.49
1:D:271:ARG:CG	1:D:271:ARG:NH1	2.69	0.49
1:C:3:GLU:CG	1:C:4:LYS:H	2.26	0.49
1:D:19:ILE:HB	5:D:616:NDP:N7N	2.28	0.49
1:D:485:PRO:HB3	1:D:509:TYR:HB2	1.95	0.49
1:A:507:ILE:N	1:A:507:ILE:HD12	2.27	0.49
1:B:95:GLU:O	1:B:98:ILE:O	2.31	0.49
1:D:434:ASN:O	1:D:435:ILE:C	2.55	0.49
1:A:82:ASP:O	1:A:83:GLU:HG2	2.13	0.48
1:C:343:GLY:HA2	1:C:346:TRP:HB2	1.95	0.48
3:A:604:CB3:CP2	3:A:604:CB3:H13	2.41	0.48
1:D:436:ALA:O	1:D:439:ALA:HB3	2.13	0.48
1:D:482:ARG:NH1	1:D:511:PRO:C	2.71	0.48
1:A:333:ARG:NE	6:A:615:HOH:O	2.25	0.48
1:C:262:THR:HG22	1:C:466:TYR:CD1	2.49	0.48
1:D:57:LYS:O	1:D:60:ASP:HB2	2.13	0.48
1:D:225:ASN:O	1:D:226:THR:C	2.56	0.48
1:D:280:LEU:HD11	1:D:286:VAL:HB	1.95	0.48
1:D:296:ILE:HG13	1:D:296:ILE:O	2.12	0.48
1:D:429:LEU:O	1:D:432:PRO:HD2	2.13	0.48
1:A:115:GLY:HA3	5:A:606:NDP:PA	2.53	0.48
1:A:271:ARG:HD3	1:B:212:MET:CE	2.43	0.48
1:B:104:ASP:C	1:B:106:SER:N	2.66	0.48
1:C:153:THR:O	1:C:177:LYS:HG2	2.14	0.48
1:C:292:PHE:HE1	1:C:444:MET:CE	2.27	0.48
1:D:23:GLY:HA3	6:D:527:HOH:O	2.13	0.48
1:B:295:LEU:O	1:B:298:PHE:HB2	2.14	0.48
1:C:139:GLU:O	1:C:140:ASP:HB2	2.13	0.48
1:D:116:GLU:CB	1:D:145:THR:HG23	2.44	0.48
1:D:341:ILE:HG22	1:D:397:MET:HB3	1.94	0.48
1:A:226:THR:HG22	1:A:229:ILE:HG13	1.95	0.48
1:B:304:ASN:ND2	1:B:306:ASN:N	2.53	0.48
1:A:96:ASP:C	1:A:98:ILE:N	2.70	0.48
1:C:19:ILE:CG1	1:C:145:THR:HG22	2.44	0.48
1:D:103:ASN:C	1:D:103:ASN:ND2	2.71	0.48
1:D:295:LEU:HD23	6:D:544:HOH:O	2.13	0.48
1:A:212:MET:HB3	1:B:236:TYR:OH	2.14	0.48
1:B:132:TYR:CD2	1:B:174:ILE:CG2	2.97	0.48
1:D:441:LEU:HD12	1:D:441:LEU:O	2.14	0.48
1:A:4:LYS:HE2	1:A:101:LEU:HA	1.95	0.48
1:B:266:PHE:HA	1:B:461:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:LYS:NZ	1:B:505:GLU:HG3	2.29	0.48
1:C:97:SER:O	1:C:100:ASN:ND2	2.46	0.48
1:D:226:THR:N	1:D:227:PRO:HD3	2.29	0.48
1:D:19:ILE:HD11	1:D:145:THR:HG22	1.95	0.48
1:D:151:PRO:CG	1:D:154:PHE:CD2	2.90	0.48
1:D:334:GLU:OE2	1:D:357:HIS:HE1	1.96	0.48
1:A:211:LYS:HE3	6:A:595:HOH:O	2.14	0.47
1:C:180:LYS:HG2	1:C:181:LYS:CA	2.38	0.47
1:C:260:ILE:HD12	1:C:520:ALA:CB	2.44	0.47
1:D:101:LEU:C	1:D:103:ASN:N	2.71	0.47
1:A:128:VAL:N	6:A:527:HOH:O	2.40	0.47
1:A:234:GLU:O	1:A:235:HIS:C	2.57	0.47
1:B:97:SER:O	1:B:99:GLU:HG3	2.14	0.47
1:B:266:PHE:CD1	1:B:461:GLY:O	2.67	0.47
1:B:466:TYR:OH	3:B:608:CB3:NA2	2.46	0.47
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.14	0.47
1:B:132:TYR:CD2	1:B:174:ILE:HG21	2.49	0.47
1:C:243:LEU:HD12	1:C:243:LEU:C	2.38	0.47
1:A:4:LYS:CE	1:A:101:LEU:HA	2.44	0.47
1:A:56:ARG:HD3	5:A:606:NDP:O1X	2.14	0.47
1:A:315:ILE:HG13	1:A:316:TRP:CD1	2.49	0.47
1:B:194:LYS:HB2	6:B:573:HOH:O	2.03	0.47
1:B:217:LYS:H	1:B:250:ASN:HD21	1.62	0.47
1:B:298:PHE:CE1	1:B:342:TYR:HB2	2.48	0.47
1:C:153:THR:O	1:C:177:LYS:HA	2.13	0.47
1:D:472:GLN:HB3	1:D:515:ILE:HG21	1.96	0.47
1:A:193:LEU:HD12	6:A:526:HOH:O	2.14	0.47
1:B:126:ASN:C	1:B:126:ASN:HD22	2.23	0.47
1:C:516:LYS:HE2	6:C:533:HOH:O	2.12	0.47
1:D:4:LYS:CD	1:D:101:LEU:HA	2.45	0.47
1:D:233:ARG:HB3	1:D:238:PHE:CD2	2.50	0.47
1:D:292:PHE:CD2	1:D:292:PHE:C	2.92	0.47
1:A:59:TRP:CH2	1:A:64:ARG:C	2.93	0.47
1:A:383:ARG:NE	1:B:400:PRO:HG2	2.29	0.47
1:A:502:GLU:CD	1:A:502:GLU:H	2.23	0.47
1:B:45:ASP:OD1	1:B:47:ASN:HB2	2.14	0.47
1:B:69:ASN:O	6:B:571:HOH:O	2.20	0.47
1:B:324:TYR:O	1:B:328:ILE:HG12	2.15	0.47
1:A:119:TYR:O	1:A:123:LEU:HD22	2.13	0.47
1:A:372:ILE:O	1:A:376:LYS:HG2	2.15	0.47
4:B:609:MTX:N5	5:B:610:NDP:H42N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASN:HD22	1:C:257:ARG:N	2.11	0.47
1:C:256:ASN:HD21	1:C:258:THR:HG23	1.80	0.47
1:D:4:LYS:HB2	1:D:101:LEU:HD23	1.96	0.47
1:D:46:SER:C	1:D:48:LYS:H	2.22	0.47
1:D:53:ILE:HG23	1:D:75:ILE:HD13	1.96	0.47
1:B:257:ARG:CD	2:B:607:UMP:OP1	2.61	0.47
1:D:130:ARG:HG2	1:D:175:PHE:O	2.14	0.47
1:D:254:ARG:HD2	1:D:264:SER:HB3	1.96	0.47
1:A:18:GLY:HA3	1:A:143:PHE:CD1	2.50	0.47
1:A:133:LEU:HD23	1:A:134:THR:N	2.29	0.47
1:B:104:ASP:CG	1:B:107:ILE:HD13	2.40	0.47
1:C:116:GLU:O	1:C:120:ARG:HB2	2.15	0.47
1:C:138:LEU:HD22	1:C:168:ILE:HG21	1.96	0.47
1:C:204:GLY:HA2	6:C:561:HOH:O	2.14	0.47
1:C:256:ASN:O	1:C:257:ARG:C	2.57	0.47
1:D:390:ASN:O	1:D:394:LEU:HG	2.15	0.47
1:A:171:ASP:CG	1:A:483:PRO:HG3	2.39	0.47
1:B:403:HIS:HB2	1:B:420:LEU:HD11	1.97	0.47
1:C:153:THR:O	1:C:177:LYS:CG	2.63	0.47
1:B:519:MET:HG3	3:B:608:CB3:H16	1.98	0.46
1:D:103:ASN:CG	1:D:104:ASP:H	2.23	0.46
1:C:35:PHE:O	1:C:36:PHE:C	2.58	0.46
1:C:177:LYS:HE3	1:C:177:LYS:HB3	1.28	0.46
1:C:247:VAL:C	1:C:249:GLU:N	2.72	0.46
1:B:440:ILE:CG2	1:B:444:MET:HE3	2.44	0.46
1:C:11:ALA:HA	1:C:134:THR:O	2.15	0.46
1:C:426:ASP:OD2	1:C:426:ASP:C	2.58	0.46
1:D:512:TYR:HD1	1:D:512:TYR:H	1.64	0.46
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.50	0.46
1:D:337:ASP:CB	6:D:555:HOH:O	2.59	0.46
1:A:64:ARG:HH22	1:A:79:LEU:HD21	1.80	0.46
1:A:337:ASP:OD2	1:A:353:TYR:OH	2.32	0.46
1:A:361:THR:HG23	1:A:361:THR:O	2.15	0.46
1:B:420:LEU:HG	1:B:422:GLN:HG3	1.97	0.46
1:C:363:VAL:HG22	1:C:364:GLY:H	1.77	0.46
1:C:402:CYS:HB2	2:C:611:UMP:C4	2.50	0.46
1:D:290:SER:HB3	1:D:313:VAL:HG13	1.90	0.46
1:A:114:GLY:HA3	1:A:119:TYR:CZ	2.51	0.46
1:C:284:LYS:NZ	6:C:547:HOH:O	2.48	0.46
1:D:48:LYS:HA	1:D:106:SER:O	2.15	0.46
1:A:82:ASP:O	1:A:83:GLU:CG	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:HB3	1:B:101:LEU:CD2	2.43	0.46
1:C:19:ILE:HB	5:C:614:NDP:N7N	2.31	0.46
1:C:359:ASP:CG	1:C:361:THR:HG22	2.40	0.46
1:C:469:HIS:HA	1:C:472:GLN:OE1	2.16	0.46
1:D:135:ARG:NH2	1:D:159:MET:HE2	2.31	0.46
1:D:328:ILE:HD11	1:D:330:LEU:HD12	1.98	0.46
1:A:76:SER:O	1:A:92:ARG:HD3	2.15	0.46
1:A:342:TYR:CE1	1:A:401:PRO:CB	2.98	0.46
1:C:25:LEU:HD12	6:C:549:HOH:O	2.15	0.46
1:C:77:SER:O	1:C:92:ARG:NH1	2.49	0.46
1:C:247:VAL:HG12	1:C:265:ILE:HD13	1.98	0.46
1:A:68:LYS:HB2	6:A:602:HOH:O	2.15	0.46
1:A:273:ASP:CG	6:A:611:HOH:O	2.58	0.46
4:A:605:MTX:N5	5:A:606:NDP:H42N	2.31	0.46
1:B:225:ASN:O	1:B:226:THR:C	2.56	0.46
1:B:296:ILE:HG23	1:B:297:TRP:N	2.29	0.46
1:B:315:ILE:HG13	1:B:316:TRP:CD1	2.51	0.46
1:C:496:ILE:O	1:C:496:ILE:HG13	2.16	0.46
1:D:116:GLU:OE2	1:D:145:THR:HA	2.16	0.46
1:A:274:MET:HE2	1:A:456:LEU:HB2	1.98	0.45
1:B:360:TYR:O	1:B:363:VAL:CG1	2.64	0.45
1:C:96:ASP:O	1:C:99:GLU:CG	2.59	0.45
1:C:317:SER:O	1:C:318:GLY:C	2.58	0.45
1:D:492:LYS:CE	6:D:539:HOH:O	2.60	0.45
1:A:419:ASN:ND2	1:A:457:ALA:HB3	2.30	0.45
1:B:133:LEU:HD13	1:B:135:ARG:HG2	1.98	0.45
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.98	0.45
1:C:399:LEU:HD21	3:C:612:CB3:H8	1.96	0.45
1:D:39:ILE:HG23	1:D:40:THR:N	2.31	0.45
1:A:180:LYS:HE3	1:A:180:LYS:HB2	1.56	0.45
1:A:423:ARG:HD3	1:B:385:ILE:HD11	1.98	0.45
1:A:514:THR:HG21	6:A:548:HOH:O	2.16	0.45
1:B:179:GLU:CG	1:B:180:LYS:N	2.72	0.45
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.75	0.45
1:C:293:GLU:C	1:C:296:ILE:HG22	2.38	0.45
1:D:51:ALA:C	1:D:52:LEU:HD23	2.42	0.45
1:D:455:GLU:N	6:D:525:HOH:O	2.50	0.45
1:B:72:ILE:HB	1:B:88:VAL:HG22	1.99	0.45
1:B:176:GLU:HB3	1:B:178:GLN:HE21	1.82	0.45
1:B:247:VAL:O	1:B:251:GLY:N	2.47	0.45
1:B:314:TYR:HA	6:B:596:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:SER:HA	1:D:313:VAL:HG21	1.98	0.45
1:D:507:ILE:N	1:D:507:ILE:HD12	2.31	0.45
1:A:383:ARG:HH21	1:B:400:PRO:CD	2.30	0.45
1:A:400:PRO:CD	1:B:383:ARG:NH1	2.80	0.45
1:B:21:ILE:O	1:B:21:ILE:HG23	2.17	0.45
1:B:495:ASN:OD1	1:B:497:GLU:OE2	2.33	0.45
1:C:35:PHE:O	1:C:39:ILE:HG23	2.17	0.45
1:C:226:THR:OG1	1:C:480:THR:HG23	2.16	0.45
1:D:151:PRO:CG	1:D:154:PHE:HD2	2.26	0.45
1:A:423:ARG:NH1	2:A:603:UMP:OP3	2.37	0.45
1:A:495:ASN:HB2	6:A:576:HOH:O	2.16	0.45
1:B:403:HIS:CD2	1:B:403:HIS:H	2.33	0.45
1:C:148:PRO:CB	6:C:542:HOH:O	2.65	0.45
1:C:320:GLY:O	1:C:325:LEU:HD22	2.17	0.45
1:D:103:ASN:ND2	1:D:104:ASP:OD1	2.49	0.45
1:D:133:LEU:CD2	1:D:133:LEU:C	2.90	0.45
1:D:349:TYR:O	1:D:350:ASN:CB	2.63	0.45
1:D:427:LEU:CD2	1:D:463:ALA:HB1	2.38	0.45
1:A:93:ASN:HD21	1:A:95:GLU:HB3	1.81	0.45
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.52	0.45
1:B:60:ASP:OD1	1:B:64:ARG:NH1	2.43	0.45
1:C:90:VAL:HG12	1:C:91:PHE:N	2.32	0.45
1:C:130:ARG:NH1	1:C:130:ARG:HG3	2.32	0.45
1:C:516:LYS:HE2	1:C:517:MET:N	2.32	0.45
1:A:192:GLN:O	1:A:193:LEU:HD22	2.17	0.45
1:B:420:LEU:CD2	1:B:422:GLN:NE2	2.80	0.45
1:B:427:LEU:HA	1:B:431:SER:HB2	1.99	0.45
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.82	0.45
1:D:114:GLY:HA3	1:D:119:TYR:CZ	2.52	0.45
1:D:319:ASN:HD22	1:D:399:LEU:HB2	1.81	0.45
1:B:291:ILE:HG12	1:B:433:PHE:CD2	2.52	0.45
1:C:226:THR:HG22	1:C:229:ILE:HG13	1.98	0.45
1:D:299:ILE:HD13	1:D:496:ILE:HD11	1.97	0.45
1:D:423:ARG:CG	1:D:424:SER:N	2.78	0.45
1:B:257:ARG:HD3	2:B:607:UMP:OP2	2.16	0.45
1:C:138:LEU:HD21	1:C:168:ILE:HG12	1.99	0.45
1:C:246:ARG:HE	1:C:268:GLN:HE21	1.62	0.45
1:D:36:PHE:CD1	1:D:36:PHE:C	2.95	0.45
1:A:135:ARG:HB2	1:A:171:ASP:HB2	1.98	0.44
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.51	0.44
1:B:27:TRP:CD1	1:B:27:TRP:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:THR:HA	1:C:111:PHE:CE2	2.51	0.44
1:D:97:SER:O	1:D:99:GLU:N	2.50	0.44
1:A:301:GLY:HA2	1:A:343:GLY:O	2.17	0.44
1:B:271:ARG:HG3	1:B:271:ARG:NH1	2.27	0.44
1:B:502:GLU:CD	1:B:502:GLU:N	2.75	0.44
1:D:40:THR:HG23	1:D:52:LEU:HD21	1.99	0.44
1:A:297:TRP:CE2	1:A:308:LEU:CD2	2.98	0.44
1:A:334:GLU:O	1:A:335:GLU:C	2.60	0.44
1:B:173:MET:HE2	1:B:175:PHE:CZ	2.52	0.44
1:B:258:THR:HG21	1:B:520:ALA:HB1	1.98	0.44
1:B:423:ARG:HG3	1:B:424:SER:N	2.32	0.44
1:D:136:VAL:HG11	1:D:138:LEU:HD21	1.99	0.44
1:A:79:LEU:HD22	1:A:80:PRO:HD2	1.98	0.44
1:A:304:ASN:ND2	1:A:306:ASN:HB2	2.33	0.44
1:A:341:ILE:O	1:A:342:TYR:C	2.60	0.44
1:A:389:TRP:CH2	1:B:385:ILE:CD1	3.01	0.44
1:B:79:LEU:O	1:B:92:ARG:NH2	2.45	0.44
1:B:405:LEU:C	1:B:405:LEU:HD23	2.41	0.44
1:D:489:PHE:HA	1:D:503:ASP:O	2.18	0.44
1:B:247:VAL:HG21	1:B:465:ILE:HG13	2.00	0.44
1:B:429:LEU:HD12	1:B:429:LEU:HA	1.74	0.44
1:C:195:SER:OG	1:D:174:ILE:HD11	2.18	0.44
1:D:278:PHE:CE1	1:D:439:ALA:CB	3.00	0.44
1:A:99:GLU:C	1:A:99:GLU:CD	2.85	0.44
1:A:429:LEU:O	1:A:432:PRO:HD2	2.17	0.44
1:D:341:ILE:HA	1:D:397:MET:CE	2.46	0.44
1:A:97:SER:O	1:A:100:ASN:ND2	2.50	0.44
1:A:99:GLU:OE2	1:A:100:ASN:N	2.51	0.44
1:A:233:ARG:NH1	1:A:242:ASP:CG	2.76	0.44
1:B:103:ASN:O	1:B:104:ASP:C	2.60	0.44
1:B:280:LEU:HD23	1:B:509:TYR:CD2	2.53	0.44
1:B:403:HIS:NE2	2:B:607:UMP:O4	2.50	0.44
1:C:94:LEU:HD21	1:C:122:ALA:HB2	2.00	0.44
1:D:40:THR:HG23	1:D:70:ARG:HD2	1.96	0.44
1:A:179:GLU:O	1:A:180:LYS:CD	2.66	0.44
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.80	0.44
1:B:138:LEU:HD23	1:B:138:LEU:N	2.27	0.44
1:C:506:LEU:HA	1:C:506:LEU:HD23	1.75	0.44
1:D:25:LEU:HG	6:D:528:HOH:O	2.16	0.44
1:A:102:MET:O	1:A:103:ASN:ND2	2.51	0.44
1:C:52:LEU:HD23	1:C:52:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ILE:O	1:C:71:ILE:HG22	2.18	0.44
1:C:295:LEU:O	1:C:295:LEU:HD22	2.18	0.44
1:D:67:LEU:HD22	4:D:615:MTX:CT	2.48	0.44
1:D:92:ARG:O	5:D:616:NDP:C2A	2.66	0.44
1:D:194:LYS:HE2	1:D:194:LYS:HB3	1.81	0.44
1:A:67:LEU:N	6:A:609:HOH:O	2.23	0.43
1:B:167:ASN:HD22	1:B:488:LYS:HE3	1.79	0.43
1:A:389:TRP:NE1	1:B:385:ILE:HG21	2.32	0.43
1:B:333:ARG:CG	1:B:337:ASP:HB3	2.45	0.43
1:B:476:GLN:HA	1:B:479:ARG:HD2	2.00	0.43
1:C:5:ASN:OD1	1:C:109:ASN:OD1	2.36	0.43
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.76	0.43
1:A:426:ASP:O	1:A:426:ASP:CG	2.60	0.43
1:B:52:LEU:N	1:B:52:LEU:CD2	2.80	0.43
1:C:98:ILE:C	1:C:99:GLU:CG	2.89	0.43
1:A:164:CYS:HB2	1:A:276:GLU:O	2.18	0.43
1:B:99:GLU:C	1:B:101:LEU:H	2.26	0.43
1:B:193:LEU:HD23	1:B:193:LEU:H	1.83	0.43
1:C:59:TRP:CD1	1:C:74:VAL:HG21	2.52	0.43
1:D:310:GLU:C	1:D:312:LYS:N	2.75	0.43
1:D:366:ASP:OD1	1:D:369:ALA:HB3	2.16	0.43
1:B:56:ARG:HD3	5:B:610:NDP:O1X	2.18	0.43
1:C:409:TYR:O	1:C:416:LEU:HA	2.18	0.43
1:D:39:ILE:C	1:D:41:ASN:H	2.27	0.43
1:D:58:THR:O	1:D:61:SER:N	2.51	0.43
1:C:108:GLU:HB3	1:C:109:ASN:ND2	2.34	0.43
1:C:399:LEU:HD22	3:C:612:CB3:H8	2.01	0.43
1:C:466:TYR:HB3	1:C:468:ASN:ND2	2.34	0.43
1:B:295:LEU:C	1:B:295:LEU:CD2	2.92	0.43
1:C:19:ILE:HB	5:C:614:NDP:H71N	1.84	0.43
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.82	0.43
1:C:158:TYR:HB3	1:C:174:ILE:H	1.83	0.43
1:C:300:LYS:HE2	6:C:536:HOH:O	2.19	0.43
1:C:458:ILE:HG22	1:C:460:ILE:HD11	2.01	0.43
1:A:389:TRP:HB2	1:A:404:VAL:HG13	2.01	0.43
1:A:424:SER:OG	1:B:382:ARG:HD2	2.18	0.43
1:B:433:PHE:O	1:B:437:SER:HB2	2.19	0.43
1:C:257:ARG:HG2	2:C:611:UMP:OP2	2.18	0.43
1:D:133:LEU:HD22	1:D:134:THR:C	2.44	0.43
1:A:415:CYS:HA	1:A:452:GLU:O	2.19	0.43
1:B:43:LYS:HB2	1:B:108:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ASP:HA	1:B:356:MET:SD	2.59	0.43
1:C:100:ASN:HD22	1:C:100:ASN:N	2.11	0.43
1:C:100:ASN:CA	1:C:103:ASN:HD22	2.30	0.43
1:D:244:LEU:HD12	1:D:465:ILE:HD11	2.00	0.43
1:A:103:ASN:O	1:A:104:ASP:O	2.36	0.43
1:A:514:THR:HG23	6:A:522:HOH:O	2.19	0.43
1:B:18:GLY:HA3	1:B:143:PHE:CD1	2.54	0.43
1:B:458:ILE:HG22	1:B:460:ILE:CD1	2.49	0.43
1:C:480:THR:HA	1:C:481:PRO:HD3	1.86	0.43
1:A:51:ALA:C	1:A:52:LEU:HD23	2.44	0.42
1:A:198:ASP:O	1:A:202:LEU:HD22	2.19	0.42
1:A:460:ILE:HG22	1:A:461:GLY:N	2.34	0.42
1:B:422:GLN:NE2	1:B:434:ASN:OD1	2.52	0.42
1:C:79:LEU:HA	1:C:80:PRO:HD3	1.78	0.42
1:C:455:GLU:OE1	1:D:212:MET:HE3	2.19	0.42
1:D:173:MET:HB3	1:D:173:MET:HE3	1.67	0.42
1:D:334:GLU:CB	6:D:555:HOH:O	2.53	0.42
1:B:19:ILE:HB	5:B:610:NDP:N7N	2.34	0.42
1:C:55:GLY:N	1:C:118:ILE:HD13	2.34	0.42
1:D:39:ILE:C	1:D:41:ASN:N	2.77	0.42
1:D:342:TYR:CE1	1:D:401:PRO:HB3	2.54	0.42
1:D:512:TYR:N	1:D:512:TYR:CD1	2.87	0.42
1:A:179:GLU:O	1:A:180:LYS:CE	2.66	0.42
1:A:229:ILE:HG22	1:A:233:ARG:HG2	2.00	0.42
1:C:193:LEU:C	1:C:195:SER:N	2.75	0.42
1:C:462:ASP:C	1:C:462:ASP:OD2	2.62	0.42
1:D:21:ILE:HA	1:D:144:ASP:CG	2.44	0.42
1:D:57:LYS:HB2	5:D:616:NDP:O3	2.20	0.42
1:D:100:ASN:O	1:D:103:ASN:O	2.37	0.42
1:A:193:LEU:HD13	1:A:193:LEU:HA	1.75	0.42
1:A:226:THR:N	1:A:227:PRO:HD3	2.35	0.42
1:B:322:LYS:HB2	6:B:572:HOH:O	2.19	0.42
1:C:361:THR:O	1:C:361:THR:HG23	2.19	0.42
1:A:166:LYS:O	1:A:167:ASN:HB2	2.19	0.42
1:A:304:ASN:HD22	1:A:306:ASN:N	2.16	0.42
1:B:53:ILE:HG23	1:B:75:ILE:CD1	2.50	0.42
1:D:118:ILE:O	1:D:118:ILE:HG22	2.18	0.42
1:A:15:LEU:HB2	1:A:139:GLU:CG	2.49	0.42
1:A:171:ASP:OD1	6:A:533:HOH:O	2.21	0.42
1:C:74:VAL:C	1:C:75:ILE:HD12	2.45	0.42
1:C:207:ALA:O	1:C:210:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:GLY:HA2	1:C:460:ILE:O	2.19	0.42
1:C:425:CYS:SG	1:C:431:SER:CB	3.07	0.42
1:A:462:ASP:OD1	1:B:382:ARG:HG2	2.19	0.42
1:A:486:GLN:HA	6:A:524:HOH:O	2.18	0.42
1:B:4:LYS:HE2	1:B:101:LEU:O	2.20	0.42
1:B:100:ASN:HA	1:B:103:ASN:CG	2.45	0.42
1:C:154:PHE:HA	1:C:176:GLU:O	2.20	0.42
1:D:269:MET:HG3	1:D:269:MET:O	2.18	0.42
1:D:290:SER:CB	1:D:313:VAL:HG11	2.33	0.42
1:A:423:ARG:CD	1:B:385:ILE:HD11	2.49	0.42
1:C:247:VAL:C	1:C:249:GLU:H	2.27	0.42
1:D:403:HIS:CD2	1:D:403:HIS:H	2.38	0.42
1:D:465:ILE:HG22	1:D:466:TYR:O	2.20	0.42
1:A:429:LEU:HA	6:A:551:HOH:O	2.19	0.42
1:B:115:GLY:HA2	5:B:610:NDP:O5D	2.20	0.42
1:B:229:ILE:HG22	1:B:233:ARG:HG2	2.00	0.42
1:B:422:GLN:NE2	1:B:434:ASN:CB	2.75	0.42
1:B:479:ARG:CZ	1:B:515:ILE:HD11	2.50	0.42
3:B:608:CB3:CP2	6:B:604:HOH:O	2.67	0.42
1:C:4:LYS:NZ	1:C:107:ILE:HG22	2.34	0.42
1:C:105:ASP:OD1	1:C:105:ASP:N	2.52	0.42
1:C:296:ILE:O	1:C:300:LYS:HG2	2.20	0.42
1:D:3:GLU:CD	1:D:4:LYS:H	2.28	0.42
1:D:8:ILE:O	1:D:8:ILE:HG13	2.06	0.42
1:A:217:LYS:HB2	1:A:250:ASN:ND2	2.31	0.41
1:C:5:ASN:ND2	1:C:5:ASN:N	2.18	0.41
1:C:14:VAL:HG21	1:C:483:PRO:HD2	2.01	0.41
1:C:160:SER:O	1:C:235:HIS:HB2	2.19	0.41
1:C:497:GLU:H	1:C:497:GLU:HG2	1.64	0.41
1:D:18:GLY:HA3	1:D:143:PHE:CD1	2.54	0.41
1:D:98:ILE:O	1:D:98:ILE:HG22	2.20	0.41
1:D:121:ASP:O	1:D:125:ASP:HB2	2.20	0.41
1:A:389:TRP:NE1	1:B:385:ILE:CG2	2.83	0.41
1:B:341:ILE:HG22	1:B:397:MET:HE3	2.02	0.41
1:C:45:ASP:OD2	1:C:48:LYS:HE3	2.20	0.41
1:C:333:ARG:HD3	6:C:537:HOH:O	2.19	0.41
1:C:470:LEU:HD12	1:C:470:LEU:HA	1.94	0.41
1:D:43:LYS:NZ	1:D:46:SER:HA	2.34	0.41
1:B:19:ILE:HD11	1:B:145:THR:HG22	2.02	0.41
1:C:221:GLU:O	1:C:221:GLU:HG3	2.20	0.41
1:D:290:SER:CB	1:D:313:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASP:HB3	1:A:107:ILE:CG1	2.41	0.41
1:A:126:ASN:CG	1:A:126:ASN:O	2.63	0.41
1:B:130:ARG:HD2	1:B:132:TYR:CE1	2.56	0.41
1:B:158:TYR:HB3	1:B:174:ILE:HG12	2.02	0.41
1:B:248:LEU:HD13	1:B:465:ILE:HD12	2.01	0.41
1:C:203:LEU:HD13	1:D:35:PHE:CD1	2.56	0.41
1:D:260:ILE:HD12	1:D:260:ILE:N	2.35	0.41
1:D:341:ILE:HB	6:D:531:HOH:O	2.21	0.41
1:A:193:LEU:HA	6:A:536:HOH:O	2.21	0.41
1:A:406:SER:HA	1:A:419:ASN:O	2.20	0.41
1:B:58:THR:CG2	4:B:609:MTX:HM2	2.51	0.41
1:B:324:TYR:CE2	1:B:328:ILE:HD13	2.55	0.41
1:C:27:TRP:CD1	1:C:27:TRP:C	2.99	0.41
3:C:612:CB3:C6	3:C:612:CB3:H15	2.50	0.41
4:C:613:MTX:O	4:C:613:MTX:CB	2.58	0.41
1:D:220:LYS:HB2	1:D:220:LYS:HZ3	1.86	0.41
1:A:78:SER:O	1:A:79:LEU:C	2.63	0.41
1:A:349:TYR:CD2	1:B:391:PRO:HG2	2.56	0.41
1:A:409:TYR:OH	1:B:264:SER:OG	2.31	0.41
1:A:487:LEU:HD23	1:A:488:LYS:N	2.35	0.41
1:B:114:GLY:CA	1:B:119:TYR:CZ	3.03	0.41
1:B:341:ILE:HG13	1:B:342:TYR:N	2.35	0.41
3:B:608:CB3:C6	3:B:608:CB3:H15	2.50	0.41
1:C:9:VAL:O	1:C:119:TYR:OH	2.30	0.41
1:D:270:MET:CE	1:D:460:ILE:HD11	2.45	0.41
1:A:276:GLU:O	1:A:486:GLN:NE2	2.49	0.41
1:A:297:TRP:NE1	1:A:308:LEU:HD21	2.35	0.41
1:A:383:ARG:CZ	1:B:400:PRO:HG2	2.51	0.41
1:B:98:ILE:H	1:B:98:ILE:HG12	1.60	0.41
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.90	0.41
1:B:271:ARG:NH1	1:B:271:ARG:CG	2.84	0.41
1:C:19:ILE:HG13	1:C:145:THR:HG22	2.02	0.41
1:C:225:ASN:HB3	6:C:557:HOH:O	2.19	0.41
1:C:315:ILE:HG13	1:C:316:TRP:CD1	2.55	0.41
1:C:482:ARG:HB3	1:C:483:PRO:HD2	2.02	0.41
1:D:381:ASP:HB3	6:D:537:HOH:O	2.20	0.41
1:A:280:LEU:HA	6:A:543:HOH:O	2.20	0.41
1:A:433:PHE:CD2	3:A:604:CB3:H13	2.56	0.41
3:A:604:CB3:C6	3:A:604:CB3:H15	2.51	0.41
1:B:193:LEU:O	1:B:197:ASP:OD2	2.39	0.41
1:B:331:GLY:CA	6:B:577:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ASN:O	1:D:307:HIS:HB2	2.20	0.41
1:A:19:ILE:HD11	1:A:145:THR:HG22	2.02	0.41
1:A:41:ASN:O	1:A:43:LYS:HG2	2.21	0.41
1:A:96:ASP:O	1:A:99:GLU:HG2	2.21	0.41
1:A:138:LEU:N	1:A:138:LEU:CD2	2.84	0.41
1:A:138:LEU:HD23	1:A:138:LEU:O	2.21	0.41
1:A:302:ASP:OD2	1:A:307:HIS:ND1	2.31	0.41
1:A:440:ILE:O	1:A:441:LEU:C	2.64	0.41
1:A:472:GLN:O	1:A:475:GLU:HB3	2.19	0.41
1:B:296:ILE:CG2	1:B:297:TRP:N	2.84	0.41
1:B:337:ASP:CG	1:B:356:MET:HB3	2.46	0.41
1:D:248:LEU:HD12	1:D:248:LEU:HA	1.96	0.41
1:D:466:TYR:O	1:D:469:HIS:HB2	2.20	0.41
1:A:517:MET:HE3	6:A:574:HOH:O	2.21	0.41
1:B:93:ASN:OD1	1:B:96:ASP:HB2	2.21	0.41
1:B:99:GLU:HG3	1:B:100:ASN:N	2.35	0.41
1:B:292:PHE:CE1	1:B:504:ILE:HD11	2.56	0.41
1:B:432:PRO:HG2	6:B:582:HOH:O	2.21	0.41
1:D:219:PRO:HA	1:D:249:GLU:HG2	2.03	0.41
1:A:133:LEU:HD22	1:A:134:THR:C	2.46	0.40
1:A:512:TYR:HB3	1:A:513:PRO:HD2	2.02	0.40
1:B:300:LYS:HG2	1:B:497:GLU:HB2	2.03	0.40
1:C:153:THR:HB	1:C:177:LYS:HG2	2.04	0.40
1:C:180:LYS:HG2	1:C:181:LYS:CB	2.51	0.40
1:C:180:LYS:HG2	1:C:181:LYS:HB2	2.03	0.40
1:C:285:LYS:NZ	6:C:522:HOH:O	2.52	0.40
1:C:334:GLU:O	1:C:335:GLU:C	2.63	0.40
1:D:53:ILE:HD12	1:D:53:ILE:N	2.36	0.40
1:D:140:ASP:O	1:D:141:ILE:HG23	2.21	0.40
1:D:244:LEU:CD1	1:D:465:ILE:HD11	2.51	0.40
1:C:19:ILE:CD1	1:C:145:THR:HG22	2.50	0.40
1:C:31:GLU:CG	6:C:563:HOH:O	2.60	0.40
1:C:58:THR:HG22	4:C:613:MTX:HM2	2.04	0.40
1:D:162:THR:CG2	1:D:169:SER:HB3	2.51	0.40
1:D:482:ARG:HB3	1:D:483:PRO:HD2	2.02	0.40
1:A:256:ASN:O	1:A:258:THR:O	2.38	0.40
1:A:341:ILE:HG13	1:A:342:TYR:N	2.36	0.40
1:A:383:ARG:NH2	1:B:400:PRO:CD	2.84	0.40
1:B:460:ILE:N	1:B:460:ILE:HD13	2.35	0.40
1:D:133:LEU:HD13	1:D:135:ARG:HG2	2.02	0.40
1:B:3:GLU:HG3	1:B:4:LYS:N	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:PHE:CD1	1:B:36:PHE:C	2.99	0.40
1:B:247:VAL:CG2	1:B:465:ILE:CD1	2.98	0.40
1:B:485:PRO:HB3	1:B:509:TYR:HA	2.03	0.40
1:C:225:ASN:HB2	1:C:477:LEU:HD23	2.03	0.40
1:D:125:ASP:CB	1:D:127:PHE:CE1	3.01	0.40
1:D:321:SER:HA	1:D:335:GLU:OE1	2.21	0.40
1:D:324:TYR:CZ	1:D:328:ILE:HG21	2.56	0.40
1:D:474:LYS:HB2	1:D:474:LYS:HE3	1.90	0.40
1:A:246:ARG:NE	1:A:268:GLN:HE22	2.19	0.40
1:B:304:ASN:HD21	1:B:306:ASN:CB	2.33	0.40
4:B:609:MTX:H13	4:B:609:MTX:HM1	1.77	0.40
1:C:4:LYS:CG	1:C:101:LEU:HD23	2.47	0.40
1:C:196:ILE:O	1:C:197:ASP:C	2.64	0.40
1:C:199:THR:O	1:C:203:LEU:HB2	2.21	0.40
1:C:249:GLU:HG3	1:C:250:ASN:OD1	2.22	0.40
1:D:97:SER:C	1:D:99:GLU:N	2.79	0.40
1:D:375:LEU:HD23	1:D:375:LEU:HA	1.87	0.40
1:D:414:ASN:OD1	1:D:451:TYR:HE2	2.05	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:OE1	1:C:166:LYS:NZ[5_555]	1.67	0.53
1:B:3:GLU:OE1	1:C:166:LYS:CE[5_555]	1.99	0.21
1:B:3:GLU:CD	1:C:166:LYS:NZ[5_555]	2.07	0.13

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	504/521 (97%)	468 (93%)	28 (6%)	8 (2%)	7 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	506/521 (97%)	473 (94%)	28 (6%)	5 (1%)	12	32
1	C	506/521 (97%)	462 (91%)	37 (7%)	7 (1%)	9	23
1	D	501/521 (96%)	439 (88%)	51 (10%)	11 (2%)	5	14
All	All	2017/2084 (97%)	1842 (91%)	144 (7%)	31 (2%)	8	22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	C	118	ILE
1	C	178	GLN
1	C	181	LYS
1	D	103	ASN
1	D	335	GLU
1	A	99	GLU
1	A	101	LEU
1	A	103	ASN
1	A	104	ASP
1	B	99	GLU
1	D	40	THR
1	D	98	ILE
1	D	105	ASP
1	D	462	ASP
1	A	82	ASP
1	B	83	GLU
1	B	100	ASN
1	B	341	ILE
1	C	99	GLU
1	C	194	LYS
1	D	384	HIS
1	B	354	LYS
1	D	379	PRO
1	D	512	TYR
1	C	179	GLU
1	C	341	ILE
1	D	152	GLU
1	D	221	GLU
1	A	341	ILE
1	A	115	GLY

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	457/469 (97%)	392 (86%)	65 (14%)	3	8
1	B	458/469 (98%)	395 (86%)	63 (14%)	3	9
1	C	459/469 (98%)	380 (83%)	79 (17%)	2	6
1	D	454/469 (97%)	387 (85%)	67 (15%)	3	8
All	All	1828/1876 (97%)	1554 (85%)	274 (15%)	3	7

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	39	ILE
1	A	43	LYS
1	A	52	LEU
1	A	56	ARG
1	A	65	ARG
1	A	68	LYS
1	A	78	SER
1	A	79	LEU
1	A	83	GLU
1	A	89	VAL
1	A	93	ASN
1	A	98	ILE
1	A	99	GLU
1	A	103	ASN
1	A	104	ASP
1	A	120	ARG
1	A	123	LEU
1	A	124	LYS
1	A	128	VAL
1	A	133	LEU
1	A	138	LEU
1	A	157	VAL
1	A	172	PHE

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Mol	Chain	Res	Type
1	A	177	LYS
1	A	178	GLN
1	A	180	LYS
1	A	193	LEU
1	A	194	LYS
1	A	202	LEU
1	A	203	LEU
1	A	220	LYS
1	A	244	LEU
1	A	247	VAL
1	A	248	LEU
1	A	254	ARG
1	A	255	GLU
1	A	258	THR
1	A	289	ARG
1	A	295	LEU
1	A	296	ILE
1	A	300	LYS
1	A	304	ASN
1	A	325	LEU
1	A	361	THR
1	A	363	VAL
1	A	371	LEU
1	A	373	GLU
1	A	380	LYS
1	A	381	ASP
1	A	392	SER
1	A	422	GLN
1	A	426	ASP
1	A	427	LEU
1	A	429	LEU
1	A	437	SER
1	A	460	ILE
1	A	468	ASN
1	A	470	LEU
1	A	472	GLN
1	A	474	LYS
1	A	506	LEU
1	A	514	THR
1	A	516	LYS
1	A	521	VAL
1	B	8	ILE

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Mol	Chain	Res	Type
1	B	39	ILE
1	B	44	CYS
1	B	46	SER
1	B	52	LEU
1	B	68	LYS
1	B	83	GLU
1	B	89	VAL
1	B	96	ASP
1	B	98	ILE
1	B	99	GLU
1	B	102	MET
1	B	103	ASN
1	B	123	LEU
1	B	124	LYS
1	B	128	VAL
1	B	133	LEU
1	B	138	LEU
1	B	142	GLU
1	B	150	ILE
1	B	165	THR
1	B	174	ILE
1	B	176	GLU
1	B	177	LYS
1	B	178	GLN
1	B	179	GLU
1	B	192	GLN
1	B	194	LYS
1	B	202	LEU
1	B	203	LEU
1	B	217	LYS
1	B	220	LYS
1	B	247	VAL
1	B	248	LEU
1	B	264	SER
1	B	295	LEU
1	B	296	ILE
1	B	308	LEU
1	B	322	LYS
1	B	325	LEU
1	B	335	GLU
1	B	359	ASP
1	B	363	VAL

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Mol	Chain	Res	Type
1	B	370	LYS
1	B	371	LEU
1	B	374	THR
1	B	378	ASN
1	B	383	ARG
1	B	403	HIS
1	B	427	LEU
1	B	429	LEU
1	B	431	SER
1	B	448	VAL
1	B	468	ASN
1	B	470	LEU
1	B	471	THR
1	B	472	GLN
1	B	474	LYS
1	B	494	GLU
1	B	506	LEU
1	B	514	THR
1	B	516	LYS
1	B	519	MET
1	C	4	LYS
1	C	5	ASN
1	C	7	SER
1	C	39	ILE
1	C	52	LEU
1	C	62	ILE
1	C	65	ARG
1	C	69	ASN
1	C	71	ILE
1	C	72	ILE
1	C	77	SER
1	C	82	ASP
1	C	89	VAL
1	C	99	GLU
1	C	100	ASN
1	C	103	ASN
1	C	104	ASP
1	C	105	ASP
1	C	109	ASN
1	C	123	LEU
1	C	126	ASN
1	C	128	VAL

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Mol	Chain	Res	Type
1	C	133	LEU
1	C	138	LEU
1	C	139	GLU
1	C	141	ILE
1	C	157	VAL
1	C	174	ILE
1	C	176	GLU
1	C	177	LYS
1	C	179	GLU
1	C	180	LYS
1	C	181	LYS
1	C	193	LEU
1	C	195	SER
1	C	200	VAL
1	C	202	LEU
1	C	220	LYS
1	C	221	GLU
1	C	222	GLU
1	C	224	TYR
1	C	228	SER
1	C	233	ARG
1	C	235	HIS
1	C	243	LEU
1	C	254	ARG
1	C	255	GLU
1	C	256	ASN
1	C	257	ARG
1	C	258	THR
1	C	264	SER
1	C	289	ARG
1	C	295	LEU
1	C	297	TRP
1	C	304	ASN
1	C	308	LEU
1	C	322	LYS
1	C	325	LEU
1	C	333	ARG
1	C	335	GLU
1	C	361	THR
1	C	365	VAL
1	C	371	LEU
1	C	383	ARG

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Mol	Chain	Res	Type
1	C	405	LEU
1	C	417	SER
1	C	422	GLN
1	C	426	ASP
1	C	427	LEU
1	C	429	LEU
1	C	431	SER
1	C	437	SER
1	C	447	GLN
1	C	468	ASN
1	C	470	LEU
1	C	497	GLU
1	C	506	LEU
1	C	514	THR
1	C	516	LYS
1	D	7	SER
1	D	8	ILE
1	D	24	GLN
1	D	25	LEU
1	D	34	LYS
1	D	39	ILE
1	D	40	THR
1	D	41	ASN
1	D	52	LEU
1	D	68	LYS
1	D	79	LEU
1	D	81	GLN
1	D	95	GLU
1	D	103	ASN
1	D	104	ASP
1	D	113	CYS
1	D	120	ARG
1	D	123	LEU
1	D	124	LYS
1	D	133	LEU
1	D	138	LEU
1	D	142	GLU
1	D	152	GLU
1	D	171	ASP
1	D	173	MET
1	D	174	ILE
1	D	176	GLU

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Mol	Chain	Res	Type
1	D	193	LEU
1	D	202	LEU
1	D	203	LEU
1	D	209	ILE
1	D	220	LYS
1	D	228	SER
1	D	230	ARG
1	D	248	LEU
1	D	257	ARG
1	D	258	THR
1	D	271	ARG
1	D	286	VAL
1	D	289	ARG
1	D	296	ILE
1	D	308	LEU
1	D	311	LYS
1	D	323	GLU
1	D	326	GLU
1	D	361	THR
1	D	363	VAL
1	D	370	LYS
1	D	371	LEU
1	D	374	THR
1	D	378	ASN
1	D	381	ASP
1	D	383	ARG
1	D	400	PRO
1	D	404	VAL
1	D	406	SER
1	D	420	LEU
1	D	424	SER
1	D	427	LEU
1	D	437	SER
1	D	441	LEU
1	D	468	ASN
1	D	492	LYS
1	D	497	GLU
1	D	506	LEU
1	D	514	THR
1	D	521	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	41	ASN
1	A	93	ASN
1	A	103	ASN
1	A	109	ASN
1	A	126	ASN
1	A	167	ASN
1	A	214	ASN
1	A	250	ASN
1	A	268	GLN
1	A	304	ASN
1	A	306	ASN
1	A	336	ASN
1	A	412	ASN
1	A	419	ASN
1	A	422	GLN
1	A	434	ASN
1	A	468	ASN
1	A	472	GLN
1	A	476	GLN
1	B	5	ASN
1	B	24	GLN
1	B	41	ASN
1	B	103	ASN
1	B	126	ASN
1	B	167	ASN
1	B	178	GLN
1	B	192	GLN
1	B	214	ASN
1	B	250	ASN
1	B	268	GLN
1	B	304	ASN
1	B	306	ASN
1	B	319	ASN
1	B	336	ASN
1	B	357	HIS
1	B	378	ASN
1	B	412	ASN
1	B	419	ASN
1	B	422	GLN
1	B	434	ASN
1	B	468	ASN
1	B	472	GLN

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Mol	Chain	Res	Type
1	B	476	GLN
1	B	495	ASN
1	C	5	ASN
1	C	24	GLN
1	C	41	ASN
1	C	47	ASN
1	C	100	ASN
1	C	103	ASN
1	C	167	ASN
1	C	178	GLN
1	C	250	ASN
1	C	256	ASN
1	C	268	GLN
1	C	304	ASN
1	C	306	ASN
1	C	336	ASN
1	C	377	ASN
1	C	412	ASN
1	C	419	ASN
1	C	422	GLN
1	C	434	ASN
1	C	464	HIS
1	C	468	ASN
1	C	476	GLN
1	D	5	ASN
1	D	24	GLN
1	D	47	ASN
1	D	103	ASN
1	D	109	ASN
1	D	216	HIS
1	D	250	ASN
1	D	256	ASN
1	D	268	GLN
1	D	306	ASN
1	D	336	ASN
1	D	357	HIS
1	D	414	ASN
1	D	419	ASN
1	D	422	GLN
1	D	434	ASN
1	D	464	HIS
1	D	468	ASN

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Mol	Chain	Res	Type
1	D	476	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	CB3	B	608	-	37,37,37	2.36	9 (24%)	50,51,51	1.05	2 (4%)
2	UMP	B	607	-	21,21,21	2.99	5 (23%)	30,31,31	2.34	9 (30%)
5	NDP	B	610	-	51,52,52	1.33	6 (11%)	71,80,80	1.62	14 (19%)
5	NDP	C	614	-	51,52,52	1.32	6 (11%)	71,80,80	1.72	13 (18%)
5	NDP	D	616	-	51,52,52	1.44	6 (11%)	71,80,80	1.72	17 (23%)
2	UMP	C	611	-	21,21,21	3.00	5 (23%)	30,31,31	2.29	9 (30%)
4	MTX	D	615	-	35,35,35	1.60	7 (20%)	47,49,49	2.18	16 (34%)
3	CB3	C	612	-	37,37,37	2.32	8 (21%)	50,51,51	1.05	2 (4%)
5	NDP	A	606	-	51,52,52	1.40	3 (5%)	71,80,80	1.62	11 (15%)
2	UMP	A	603	-	21,21,21	3.05	7 (33%)	30,31,31	2.30	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTX	C	613	-	35,35,35	1.78	10 (28%)	47,49,49	1.93	11 (23%)
3	CB3	A	604	-	37,37,37	2.43	10 (27%)	50,51,51	0.98	1 (2%)
4	MTX	B	609	-	35,35,35	1.92	10 (28%)	47,49,49	1.94	10 (21%)
4	MTX	A	605	-	35,35,35	1.91	12 (34%)	47,49,49	1.76	10 (21%)

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	CB3	B	608	-	1/1/5/6	7/27/28/28	0/3/3/3
2	UMP	B	607	-	-	3/10/22/22	0/2/2/2
5	NDP	B	610	-	-	5/34/77/77	0/5/5/5
5	NDP	C	614	-	-	7/34/77/77	0/5/5/5
5	NDP	D	616	-	-	4/34/77/77	0/5/5/5
2	UMP	C	611	-	-	2/10/22/22	0/2/2/2
4	MTX	D	615	-	-	3/25/25/25	0/3/3/3
3	CB3	C	612	-	1/1/5/6	7/27/28/28	0/3/3/3
5	NDP	A	606	-	-	3/34/77/77	0/5/5/5
2	UMP	A	603	-	-	2/10/22/22	0/2/2/2
4	MTX	C	613	-	-	6/25/25/25	0/3/3/3
3	CB3	A	604	-	1/1/5/6	7/27/28/28	0/3/3/3
4	MTX	B	609	-	-	2/25/25/25	0/3/3/3
4	MTX	A	605	-	-	5/25/25/25	0/3/3/3

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	UMP	C6-C5	8.48	1.54	1.35
2	A	603	UMP	C6-C5	8.47	1.54	1.35
2	C	611	UMP	C6-C5	8.45	1.54	1.35
3	A	604	CB3	O4-C4	8.22	1.37	1.23
3	B	608	CB3	O4-C4	8.06	1.37	1.23
3	C	612	CB3	O4-C4	7.96	1.36	1.23
5	A	606	NDP	C4N-C3N	-5.85	1.38	1.50
2	A	603	UMP	C6-N1	5.77	1.51	1.38
2	B	607	UMP	C6-N1	5.74	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	611	UMP	C6-N1	5.72	1.51	1.38
2	C	611	UMP	C5-C4	5.68	1.56	1.43
2	B	607	UMP	C5-C4	5.56	1.55	1.43
2	A	603	UMP	C5-C4	5.51	1.55	1.43
3	A	604	CB3	CP1-CP2	5.18	1.54	1.46
5	D	616	NDP	C4N-C3N	-5.18	1.40	1.50
5	C	614	NDP	C4N-C3N	-5.14	1.40	1.50
4	C	613	MTX	C-N	-5.12	1.22	1.34
4	B	609	MTX	C-N	-5.06	1.22	1.34
3	A	604	CB3	CP1-N10	4.95	1.50	1.46
3	B	608	CB3	CP1-CP2	4.92	1.54	1.46
5	B	610	NDP	C4N-C3N	-4.86	1.40	1.50
3	C	612	CB3	C4A-C4	-4.72	1.40	1.48
3	C	612	CB3	CP1-N10	4.59	1.50	1.46
3	B	608	CB3	C4A-C4	-4.50	1.40	1.48
5	D	616	NDP	PA-O3	4.48	1.64	1.59
3	C	612	CB3	CP1-CP2	4.42	1.53	1.46
3	B	608	CB3	CP1-N10	4.36	1.50	1.46
3	A	604	CB3	C4A-C4	-4.33	1.40	1.48
4	A	605	MTX	C-N	-4.18	1.24	1.34
2	A	603	UMP	C2-N1	4.12	1.44	1.38
4	D	615	MTX	C-N	-4.10	1.24	1.34
5	A	606	NDP	C4N-C5N	-4.09	1.38	1.49
2	C	611	UMP	C2-N1	4.04	1.44	1.38
2	B	607	UMP	C2-N1	3.87	1.44	1.38
4	A	605	MTX	C8A-N8	-3.72	1.31	1.37
4	C	613	MTX	C8A-N8	-3.69	1.31	1.37
5	C	614	NDP	C4N-C5N	-3.54	1.39	1.49
2	A	603	UMP	P-OP1	3.46	1.61	1.50
5	D	616	NDP	PN-O3	3.45	1.63	1.59
2	C	611	UMP	P-OP1	3.40	1.61	1.50
5	B	610	NDP	PN-O3	3.37	1.63	1.59
2	B	607	UMP	P-OP1	3.26	1.60	1.50
5	B	610	NDP	C4N-C5N	-3.26	1.40	1.49
4	B	609	MTX	C8A-N8	-3.26	1.32	1.37
3	A	604	CB3	C9-N10	3.22	1.51	1.46
5	D	616	NDP	C4N-C5N	-3.21	1.40	1.49
4	D	615	MTX	C8A-N8	-3.14	1.32	1.37
4	A	605	MTX	C4A-C8A	-3.11	1.35	1.40
3	C	612	CB3	C9-N10	3.10	1.50	1.46
3	B	608	CB3	C9-N10	2.97	1.50	1.46
4	D	615	MTX	O-C	2.94	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	609	MTX	O2-CT	-2.88	1.21	1.30
4	A	605	MTX	C4A-N5	-2.87	1.31	1.37
4	C	613	MTX	C4A-C8A	-2.86	1.35	1.40
4	A	605	MTX	O-C	2.85	1.30	1.23
5	C	614	NDP	PA-O3	2.75	1.62	1.59
5	C	614	NDP	PN-O3	2.72	1.62	1.59
4	C	613	MTX	O-C	2.68	1.29	1.23
4	A	605	MTX	C2-N3	-2.68	1.30	1.35
4	C	613	MTX	O2-CT	-2.66	1.22	1.30
4	B	609	MTX	C2-N3	-2.59	1.30	1.35
3	B	608	CB3	C15-C14	2.58	1.44	1.39
5	D	616	NDP	C6N-C5N	2.55	1.40	1.33
3	C	612	CB3	C11-C	2.53	1.55	1.50
4	A	605	MTX	C4-N3	-2.53	1.29	1.33
4	C	613	MTX	C12-C11	-2.51	1.35	1.39
4	A	605	MTX	C8A-N1	-2.50	1.31	1.36
3	B	608	CB3	C11-C	2.50	1.55	1.50
4	A	605	MTX	O2-CT	-2.50	1.22	1.30
3	C	612	CB3	C15-C14	2.49	1.44	1.39
4	B	609	MTX	OE2-CD	-2.48	1.22	1.30
4	A	605	MTX	C4-C4A	-2.47	1.34	1.43
3	C	612	CB3	C16-C15	2.47	1.42	1.38
3	A	604	CB3	C16-C15	2.47	1.42	1.38
3	A	604	CB3	C11-C	2.46	1.55	1.50
4	B	609	MTX	C16-C11	-2.45	1.35	1.39
5	C	614	NDP	C5A-N7A	-2.43	1.34	1.39
4	C	613	MTX	C8A-N1	-2.42	1.31	1.36
5	B	610	NDP	C6N-C5N	2.42	1.40	1.33
4	D	615	MTX	C4A-C8A	-2.41	1.36	1.40
2	A	603	UMP	O4'-C1'	2.41	1.47	1.42
5	B	610	NDP	C4A-N9A	-2.32	1.32	1.37
3	B	608	CB3	C16-C15	2.32	1.42	1.38
3	A	604	CB3	C15-C14	2.31	1.43	1.39
2	A	603	UMP	O4'-C4'	2.29	1.50	1.45
4	B	609	MTX	CA-CT	-2.28	1.47	1.52
4	A	605	MTX	OE2-CD	-2.28	1.23	1.30
4	B	609	MTX	O-C	2.28	1.28	1.23
5	A	606	NDP	C8A-N7A	2.26	1.36	1.31
5	D	616	NDP	C4A-N9A	-2.25	1.33	1.37
5	B	610	NDP	C5A-N7A	-2.24	1.35	1.39
4	B	609	MTX	C12-C11	-2.20	1.36	1.39
5	C	614	NDP	C6N-C5N	2.19	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	615	MTX	O2-CT	-2.17	1.23	1.30
4	C	613	MTX	C16-C11	-2.16	1.36	1.39
4	A	605	MTX	CA-CT	-2.16	1.47	1.52
4	D	615	MTX	C8A-N1	-2.11	1.32	1.36
4	C	613	MTX	C4-C4A	-2.10	1.35	1.43
4	B	609	MTX	C4A-N5	-2.09	1.33	1.37
3	A	604	CB3	CA-N	2.09	1.50	1.45
4	D	615	MTX	OE2-CD	-2.05	1.24	1.30
3	A	604	CB3	CG-CD	2.02	1.55	1.50
3	B	608	CB3	C8A-N1	-2.02	1.36	1.39
4	C	613	MTX	C4A-N5	-2.01	1.33	1.37

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	615	MTX	CB-CA-N	-5.90	99.23	110.91
2	B	607	UMP	C5-C6-N1	-5.83	112.37	121.84
2	A	603	UMP	C6-C5-C4	-5.79	112.13	119.53
2	C	611	UMP	C5-C6-N1	-5.75	112.49	121.84
4	B	609	MTX	C6-C9-N10	-5.70	103.18	112.95
2	B	607	UMP	C6-C5-C4	-5.70	112.25	119.53
2	A	603	UMP	C5-C6-N1	-5.69	112.58	121.84
2	C	611	UMP	C6-C5-C4	-5.59	112.39	119.53
5	C	614	NDP	C5A-C4A-N3A	-5.53	119.10	126.72
4	D	615	MTX	C6-C9-N10	-5.51	103.50	112.95
5	D	616	NDP	N3A-C2A-N1A	-5.46	120.32	128.58
5	A	606	NDP	C5A-C4A-N3A	-5.36	119.33	126.72
5	C	614	NDP	C2B-C1B-N9A	-5.29	105.05	113.75
4	A	605	MTX	C6-C9-N10	-5.12	104.18	112.95
5	B	610	NDP	N3A-C2A-N1A	-5.00	121.01	128.58
4	C	613	MTX	CG-CB-CA	-4.99	103.95	113.16
4	C	613	MTX	C6-C9-N10	-4.87	104.60	112.95
5	C	614	NDP	N3A-C2A-N1A	-4.81	121.30	128.58
4	B	609	MTX	CB-CA-N	-4.73	101.54	110.91
2	B	607	UMP	N3-C2-N1	4.72	121.03	114.89
5	B	610	NDP	C5A-C4A-N3A	-4.70	120.24	126.72
4	C	613	MTX	N1-C2-N3	-4.69	121.24	127.21
2	C	611	UMP	N3-C2-N1	4.58	120.86	114.89
2	A	603	UMP	N3-C2-N1	4.50	120.75	114.89
5	A	606	NDP	N3A-C2A-N1A	-4.49	121.78	128.58
5	D	616	NDP	C5A-C4A-N3A	-4.36	120.72	126.72
2	B	607	UMP	C5-C4-N3	4.28	120.79	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	C5-C4-N3	4.22	120.71	114.80
4	B	609	MTX	N8-C8A-N1	4.21	120.35	115.77
2	A	603	UMP	C5-C4-N3	4.20	120.69	114.80
5	B	610	NDP	C2B-C1B-N9A	-4.13	106.96	113.75
4	B	609	MTX	C13-C14-N10	-4.06	115.93	121.59
4	D	615	MTX	C2-N1-C8A	4.03	119.83	115.48
4	D	615	MTX	N1-C2-N3	-4.02	122.10	127.21
4	D	615	MTX	CB-CG-CD	-4.00	101.82	112.49
4	A	605	MTX	N8-C8A-N1	4.00	120.13	115.77
5	B	610	NDP	N9A-C8A-N7A	-3.84	108.50	113.94
5	D	616	NDP	N9A-C8A-N7A	-3.79	108.56	113.94
4	B	609	MTX	N1-C2-N3	-3.76	122.43	127.21
5	D	616	NDP	C2B-C1B-N9A	-3.70	107.66	113.75
4	C	613	MTX	C2-N1-C8A	3.70	119.47	115.48
5	C	614	NDP	C2A-N3A-C4A	3.65	120.75	111.83
5	A	606	NDP	C2A-N3A-C4A	3.61	120.66	111.83
4	A	605	MTX	N1-C2-N3	-3.59	122.65	127.21
5	A	606	NDP	C2B-C1B-N9A	-3.59	107.85	113.75
5	D	616	NDP	C2A-N3A-C4A	3.58	120.56	111.83
4	D	615	MTX	C13-C14-N10	-3.51	116.69	121.59
5	D	616	NDP	C4A-N9A-C8A	3.49	109.40	105.74
5	A	606	NDP	N9A-C8A-N7A	-3.47	109.01	113.94
5	C	614	NDP	N9A-C8A-N7A	-3.44	109.05	113.94
4	A	605	MTX	C6-C7-N8	-3.44	119.84	123.14
2	C	611	UMP	O4'-C1'-N1	3.42	113.93	107.86
5	B	610	NDP	N3A-C4A-N9A	3.41	132.97	127.17
2	A	603	UMP	O4'-C1'-N1	3.39	113.89	107.86
2	B	607	UMP	O4'-C1'-N1	3.37	113.85	107.86
5	A	606	NDP	N3A-C4A-N9A	3.33	132.83	127.17
5	D	616	NDP	O4D-C1D-N1N	3.31	114.40	108.08
5	C	614	NDP	N3A-C4A-N9A	3.29	132.77	127.17
5	B	610	NDP	C2A-N3A-C4A	3.27	119.82	111.83
5	B	610	NDP	C4A-N9A-C8A	3.24	109.14	105.74
5	C	614	NDP	C4A-C5A-N7A	-3.23	106.89	110.58
4	C	613	MTX	N8-C8A-N1	3.20	119.25	115.77
4	D	615	MTX	OE1-CD-CG	-3.15	113.10	123.09
5	D	616	NDP	N3A-C4A-N9A	3.15	132.52	127.17
4	C	613	MTX	O-C-N	-3.15	116.48	122.47
2	B	607	UMP	O4-C4-C5	-3.09	119.83	125.16
4	C	613	MTX	C6-C7-N8	-3.09	120.17	123.14
5	A	606	NDP	C4A-C5A-N7A	-3.09	107.05	110.58
4	A	605	MTX	C9-N10-C14	3.07	123.89	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	611	UMP	O4-C4-C5	-3.00	119.99	125.16
5	C	614	NDP	O4B-C1B-N9A	2.99	113.83	108.09
4	A	605	MTX	CB-CA-CT	-2.97	103.30	110.35
5	C	614	NDP	C5A-N7A-C8A	2.97	108.11	103.45
2	A	603	UMP	O4-C4-C5	-2.95	120.08	125.16
3	C	612	CB3	CP2-CP1-N10	-2.93	110.74	113.45
4	A	605	MTX	C13-C14-N10	-2.86	117.61	121.59
2	B	607	UMP	OP3-P-OP2	2.85	118.49	107.80
2	A	603	UMP	OP3-P-OP2	2.85	118.47	107.80
4	B	609	MTX	C2-N1-C8A	2.84	118.55	115.48
2	C	611	UMP	OP3-P-OP2	2.81	118.33	107.80
5	C	614	NDP	P2B-O2B-C2B	-2.77	116.04	123.43
5	A	606	NDP	C4A-N9A-C8A	2.75	108.62	105.74
4	D	615	MTX	OE2-CD-CG	2.72	122.61	114.00
4	D	615	MTX	C9-C6-N5	2.71	121.49	117.09
4	B	609	MTX	C4A-C4-N3	-2.69	117.66	120.84
4	B	609	MTX	C6-C7-N8	-2.66	120.59	123.14
4	C	613	MTX	C13-C14-N10	-2.66	117.89	121.59
5	C	614	NDP	O3X-P2B-O2X	2.64	117.71	107.80
3	B	608	CB3	CP2-CP1-N10	-2.61	111.04	113.45
5	C	614	NDP	O4D-C1D-N1N	2.59	113.02	108.08
5	A	606	NDP	C5A-N7A-C8A	2.57	107.48	103.45
4	D	615	MTX	C6-C7-N8	-2.56	120.69	123.14
4	C	613	MTX	C9-N10-C14	2.56	123.27	120.17
4	D	615	MTX	N8-C8A-N1	2.51	118.50	115.77
4	D	615	MTX	CG-CB-CA	-2.50	108.55	113.16
4	A	605	MTX	C2-N1-C8A	2.48	118.16	115.48
4	B	609	MTX	CG-CB-CA	-2.47	108.60	113.16
5	B	610	NDP	C1D-N1N-C2N	-2.47	117.07	121.14
4	D	615	MTX	O2-CT-CA	2.45	121.81	113.51
2	B	607	UMP	C4-N3-C2	-2.42	123.61	126.61
2	B	607	UMP	O2-C2-N1	-2.42	119.65	122.80
5	B	610	NDP	O3X-P2B-O1X	2.41	120.23	110.83
3	C	612	CB3	CA-N-C	2.37	127.26	121.56
5	B	610	NDP	O4D-C1D-N1N	2.35	112.56	108.08
5	D	616	NDP	O3X-P2B-O2X	2.34	116.58	107.80
2	C	611	UMP	O2-C2-N1	-2.32	119.78	122.80
5	D	616	NDP	C3N-C2N-N1N	-2.31	119.81	123.20
5	D	616	NDP	O4B-C1B-N9A	2.31	112.52	108.09
5	B	610	NDP	C5A-N7A-C8A	2.28	107.04	103.45
2	C	611	UMP	C4-N3-C2	-2.28	123.79	126.61
5	D	616	NDP	O2B-P2B-O1X	-2.27	101.26	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	CB3	CA-N-C	2.24	126.93	121.56
5	D	616	NDP	C3N-C7N-N7N	-2.22	113.72	117.67
2	A	603	UMP	C4-N3-C2	-2.22	123.86	126.61
5	A	606	NDP	O4B-C1B-N9A	2.22	112.34	108.09
5	B	610	NDP	O4B-C1B-C2B	-2.21	102.78	106.59
4	C	613	MTX	NA2-C2-N3	2.21	120.54	117.22
5	D	616	NDP	C1D-N1N-C2N	-2.18	117.55	121.14
4	C	613	MTX	C11-C-N	2.16	121.05	117.04
4	D	615	MTX	NA2-C2-N3	2.14	120.44	117.22
4	A	605	MTX	CA-N-C	2.14	126.69	121.56
5	D	616	NDP	C5A-N7A-C8A	2.13	106.80	103.45
2	A	603	UMP	O2-C2-N1	-2.13	120.02	122.80
4	D	615	MTX	C4-C4A-N5	2.13	121.97	120.33
5	C	614	NDP	C5A-C4A-N9A	2.13	108.13	105.81
4	A	605	MTX	O2-CT-CA	2.12	120.67	113.51
5	B	610	NDP	O3X-P2B-O2B	-2.11	97.61	105.85
5	B	610	NDP	C2B-C3B-C4B	-2.11	97.45	101.99
3	A	604	CB3	CA-N-C	2.11	126.62	121.56
5	A	606	NDP	C6A-C5A-N7A	2.09	136.12	132.09
4	D	615	MTX	CT-CA-N	2.05	115.31	110.57
5	D	616	NDP	C5A-C6A-N6A	-2.02	118.29	123.29
4	B	609	MTX	C15-C14-N10	2.01	124.40	121.59
5	D	616	NDP	C5D-C4D-C3D	-2.01	107.97	115.21

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	604	CB3	CA
3	B	608	CB3	CA
3	C	612	CB3	CA

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	614	NDP	C5B-O5B-PA-O1A
5	C	614	NDP	C5B-O5B-PA-O2A
5	C	614	NDP	C5B-O5B-PA-O3
4	A	605	MTX	N-CA-CB-CG
5	C	614	NDP	C3B-C4B-C5B-O5B
3	A	604	CB3	CB-CA-N-C
3	B	608	CB3	CB-CA-N-C
3	C	612	CB3	CB-CA-N-C

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Mol	Chain	Res	Type	Atoms
4	A	605	MTX	CT-CA-CB-CG
4	D	615	MTX	CT-CA-CB-CG
2	A	603	UMP	C2'-C1'-N1-C2
2	B	607	UMP	C2'-C1'-N1-C2
2	C	611	UMP	C2'-C1'-N1-C2
5	C	614	NDP	O4B-C4B-C5B-O5B
3	A	604	CB3	N-CA-CT-O2
3	B	608	CB3	N-CA-CT-O2
4	C	613	MTX	CT-CA-N-C
4	D	615	MTX	CB-CA-N-C
4	C	613	MTX	C13-C14-N10-CM
3	C	612	CB3	N-CA-CT-O2
4	C	613	MTX	C15-C14-N10-CM
3	A	604	CB3	N-CA-CT-O1
3	B	608	CB3	N-CA-CT-O1
3	C	612	CB3	N-CA-CT-O1
4	A	605	MTX	C6-C9-N10-CM
5	A	606	NDP	O4D-C1D-N1N-C2N
3	A	604	CB3	CB-CA-CT-O2
3	B	608	CB3	CB-CA-CT-O2
3	C	612	CB3	CB-CA-CT-O2
4	D	615	MTX	N-CA-CB-CG
5	B	610	NDP	C2B-O2B-P2B-O3X
4	B	609	MTX	C13-C14-N10-CM
4	B	609	MTX	C15-C14-N10-CM
3	C	612	CB3	CB-CA-CT-O1
5	B	610	NDP	C4D-C5D-O5D-PN
5	B	610	NDP	O4D-C1D-N1N-C2N
5	D	616	NDP	O4D-C1D-N1N-C2N
3	A	604	CB3	CB-CA-CT-O1
3	B	608	CB3	CB-CA-CT-O1
4	A	605	MTX	OE1-CD-CG-CB
5	B	610	NDP	C2N-C3N-C7N-N7N
5	C	614	NDP	O4D-C1D-N1N-C2N
5	D	616	NDP	C2N-C3N-C7N-N7N
4	A	605	MTX	OE2-CD-CG-CB
5	D	616	NDP	C4D-C5D-O5D-PN
5	C	614	NDP	C2D-C1D-N1N-C2N
5	D	616	NDP	C2D-C1D-N1N-C2N
4	C	613	MTX	C6-C9-N10-CM
3	C	612	CB3	OE1-CD-CG-CB
4	C	613	MTX	CB-CA-N-C

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Mol	Chain	Res	Type	Atoms
3	A	604	CB3	OE1-CD-CG-CB
5	A	606	NDP	C2B-O2B-P2B-O2X
5	A	606	NDP	C2B-O2B-P2B-O3X
3	A	604	CB3	OE2-CD-CG-CB
3	B	608	CB3	OE1-CD-CG-CB
2	A	603	UMP	C2'-C1'-N1-C6
3	C	612	CB3	OE2-CD-CG-CB
2	B	607	UMP	C2'-C1'-N1-C6
2	C	611	UMP	C2'-C1'-N1-C6
5	B	610	NDP	C2B-O2B-P2B-O1X
3	B	608	CB3	OE2-CD-CG-CB
4	C	613	MTX	CB-CA-CT-O1
2	B	607	UMP	O4'-C4'-C5'-O5'

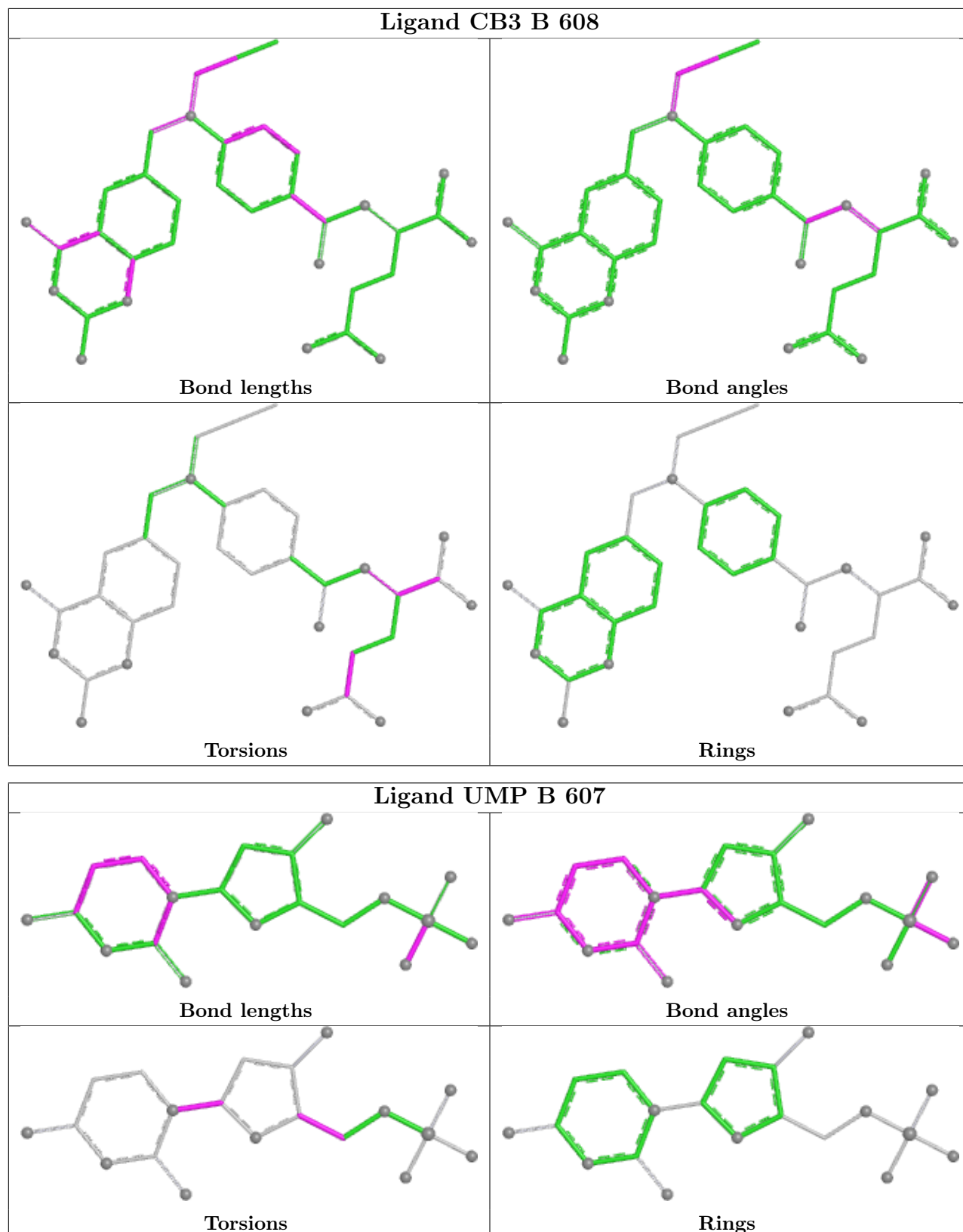
There are no ring outliers.

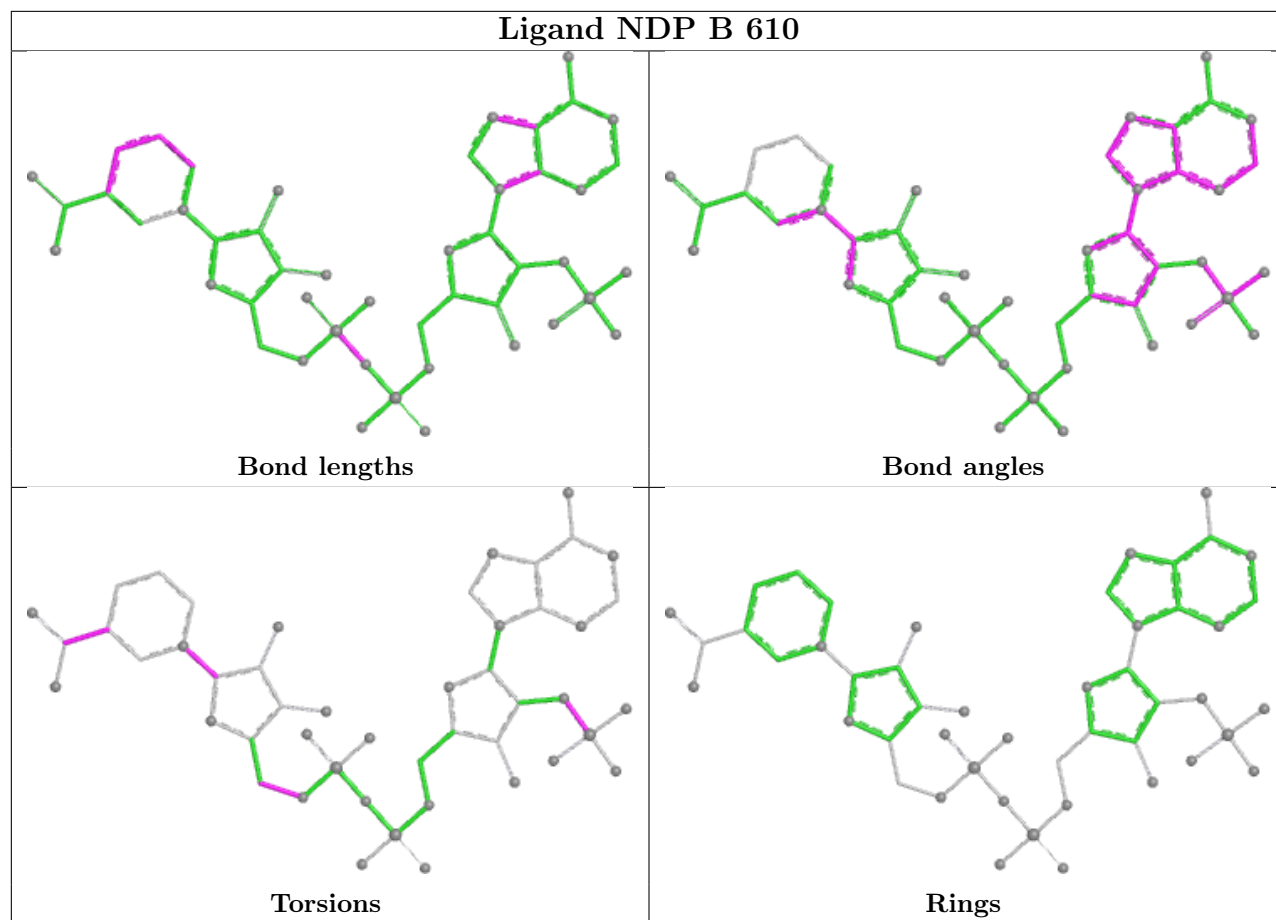
14 monomers are involved in 96 short contacts:

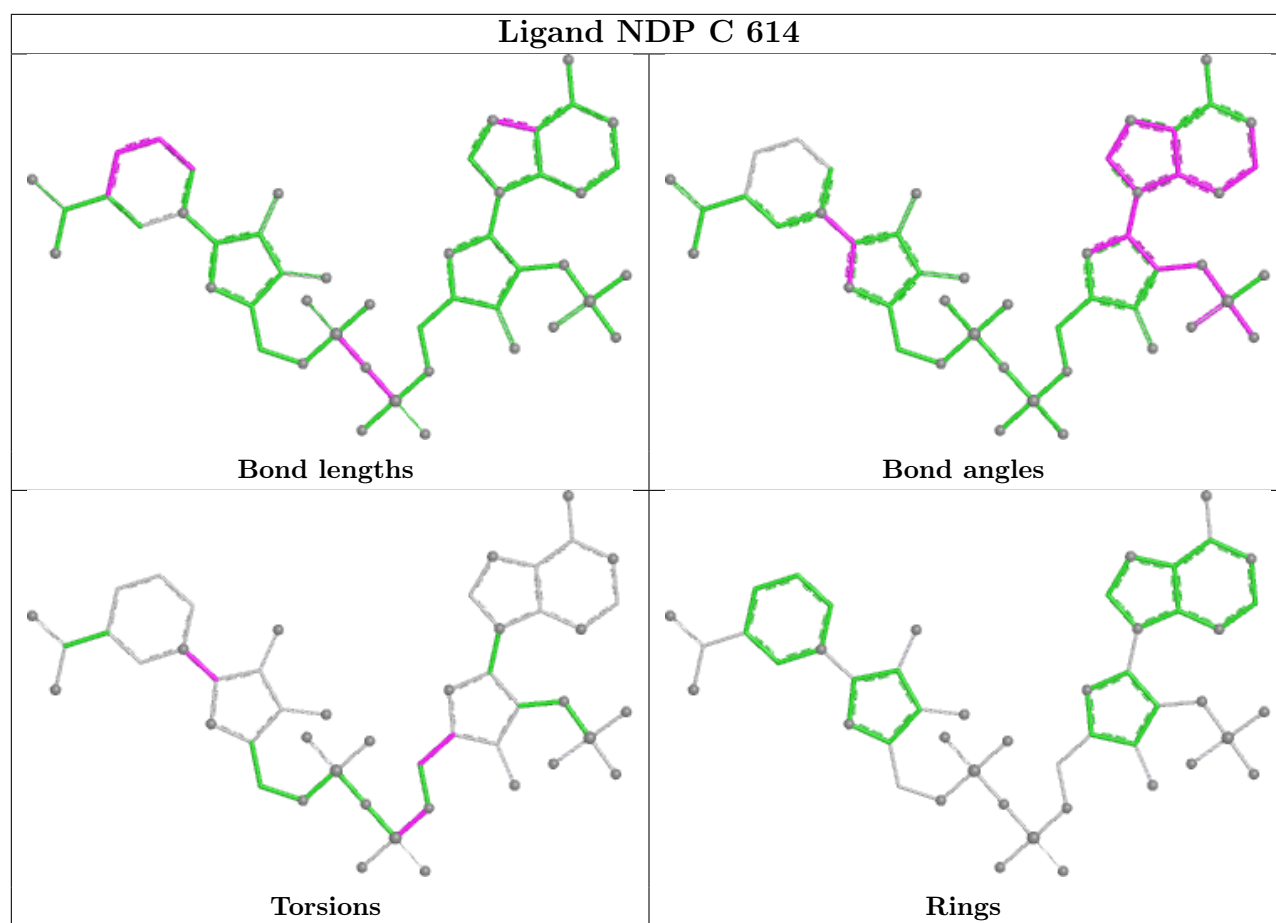
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	608	CB3	8	0
2	B	607	UMP	9	0
5	B	610	NDP	6	0
5	C	614	NDP	7	0
5	D	616	NDP	8	0
2	C	611	UMP	9	0
4	D	615	MTX	13	0
3	C	612	CB3	10	0
5	A	606	NDP	4	0
2	A	603	UMP	7	0
4	C	613	MTX	6	0
3	A	604	CB3	11	0
4	B	609	MTX	4	0
4	A	605	MTX	1	0

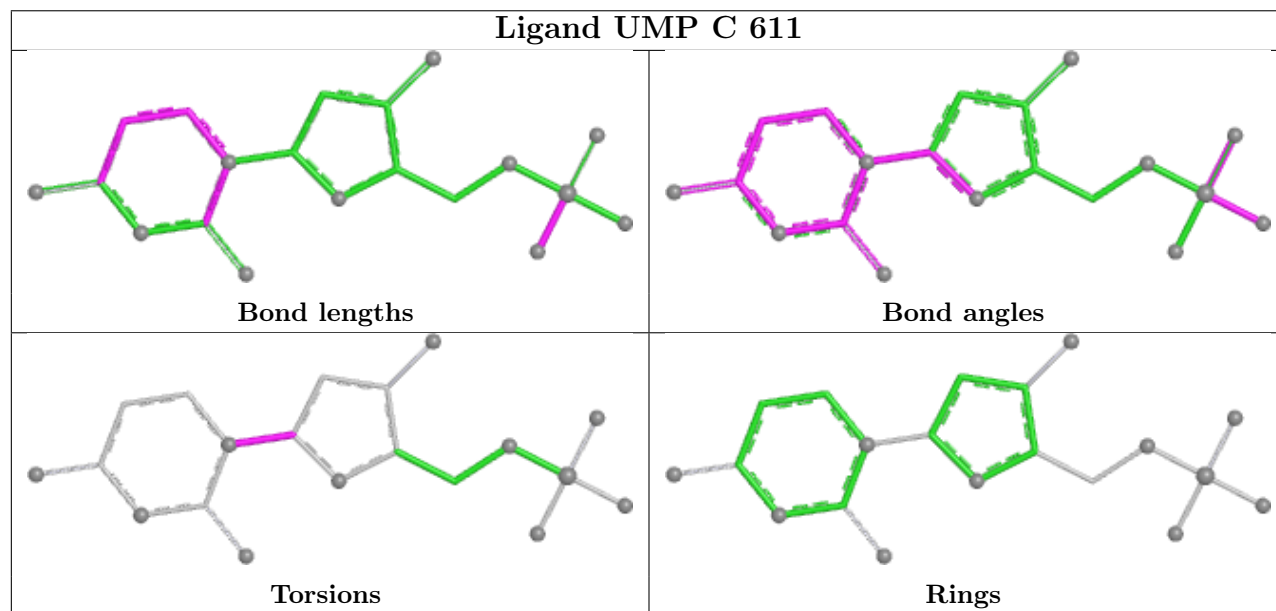
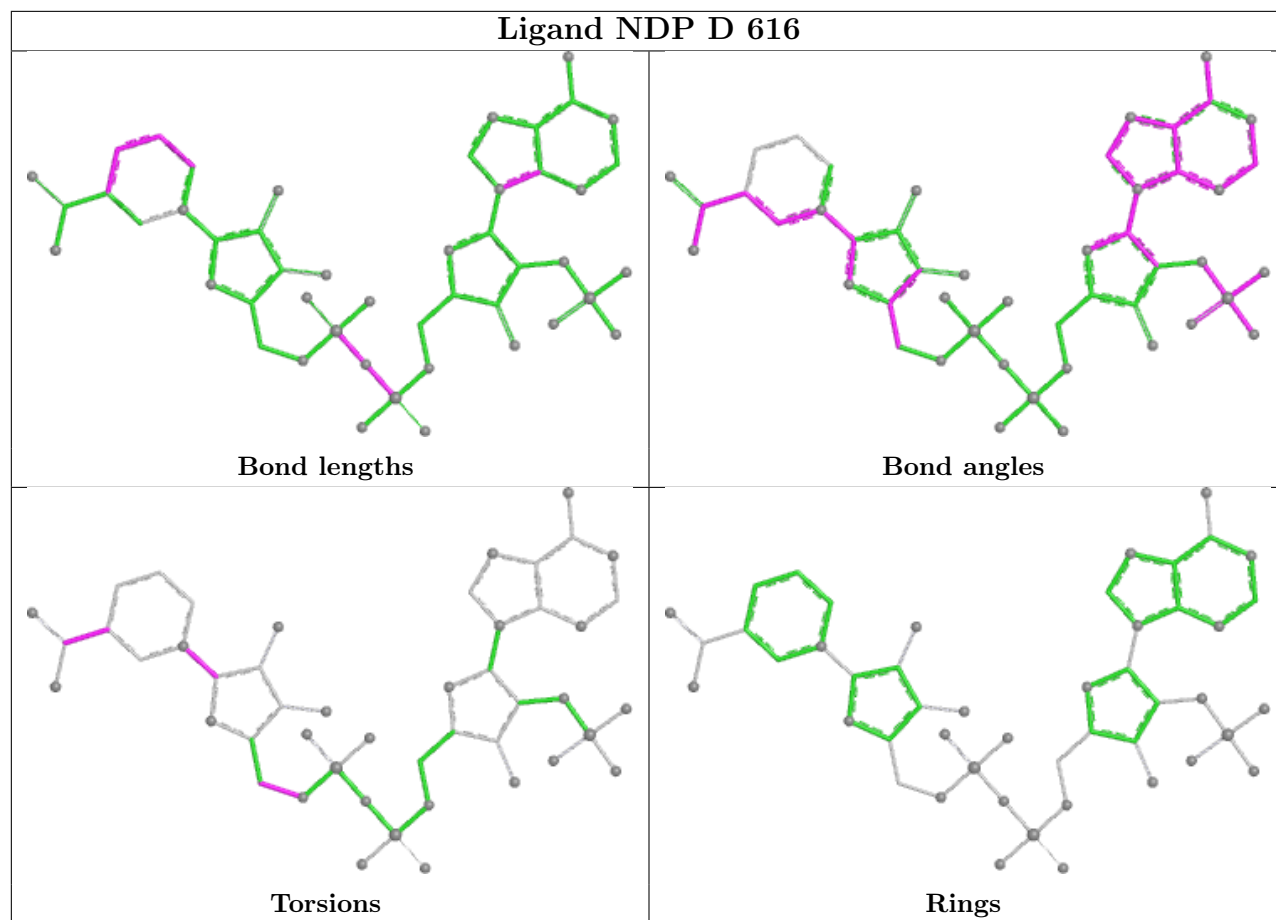
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

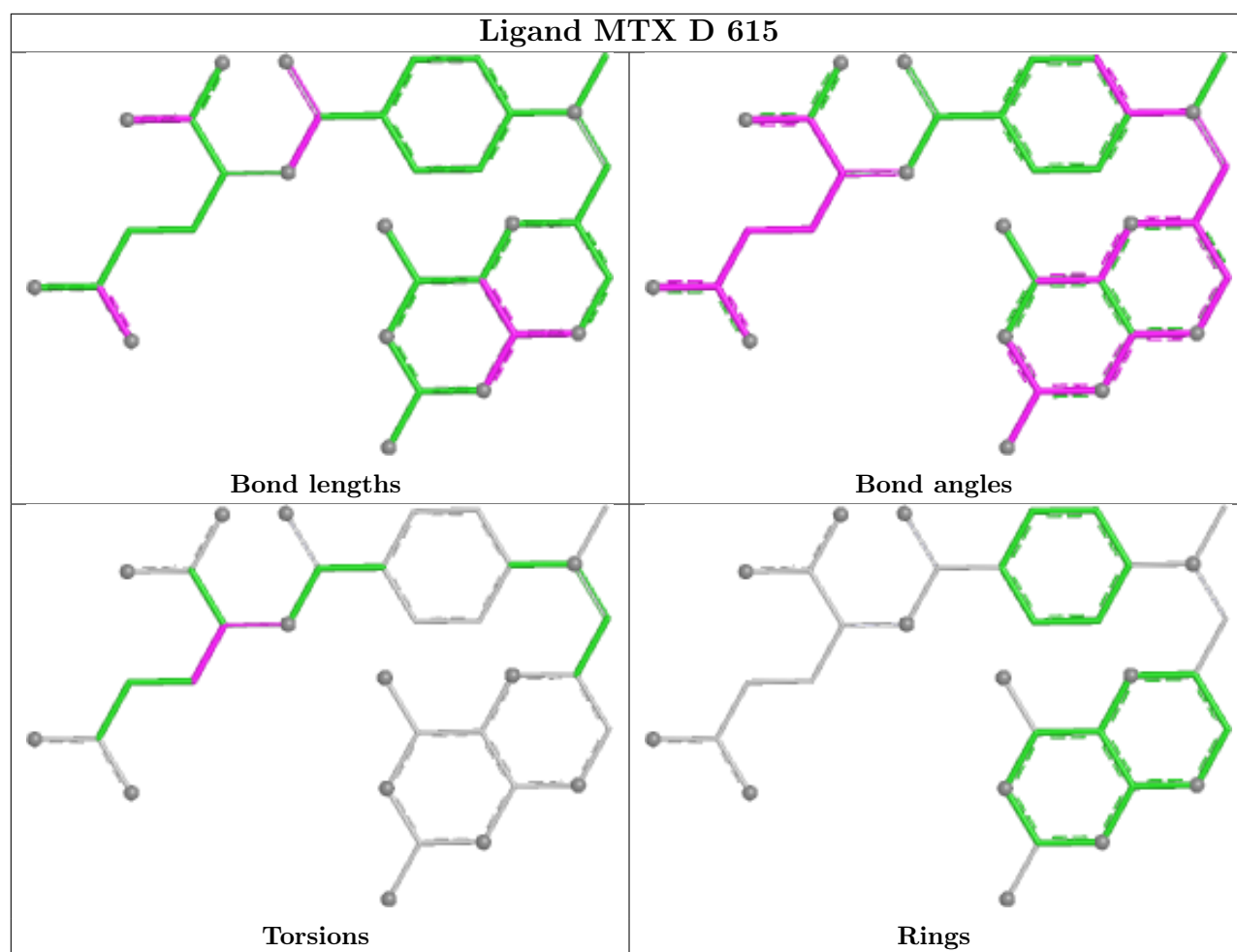
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

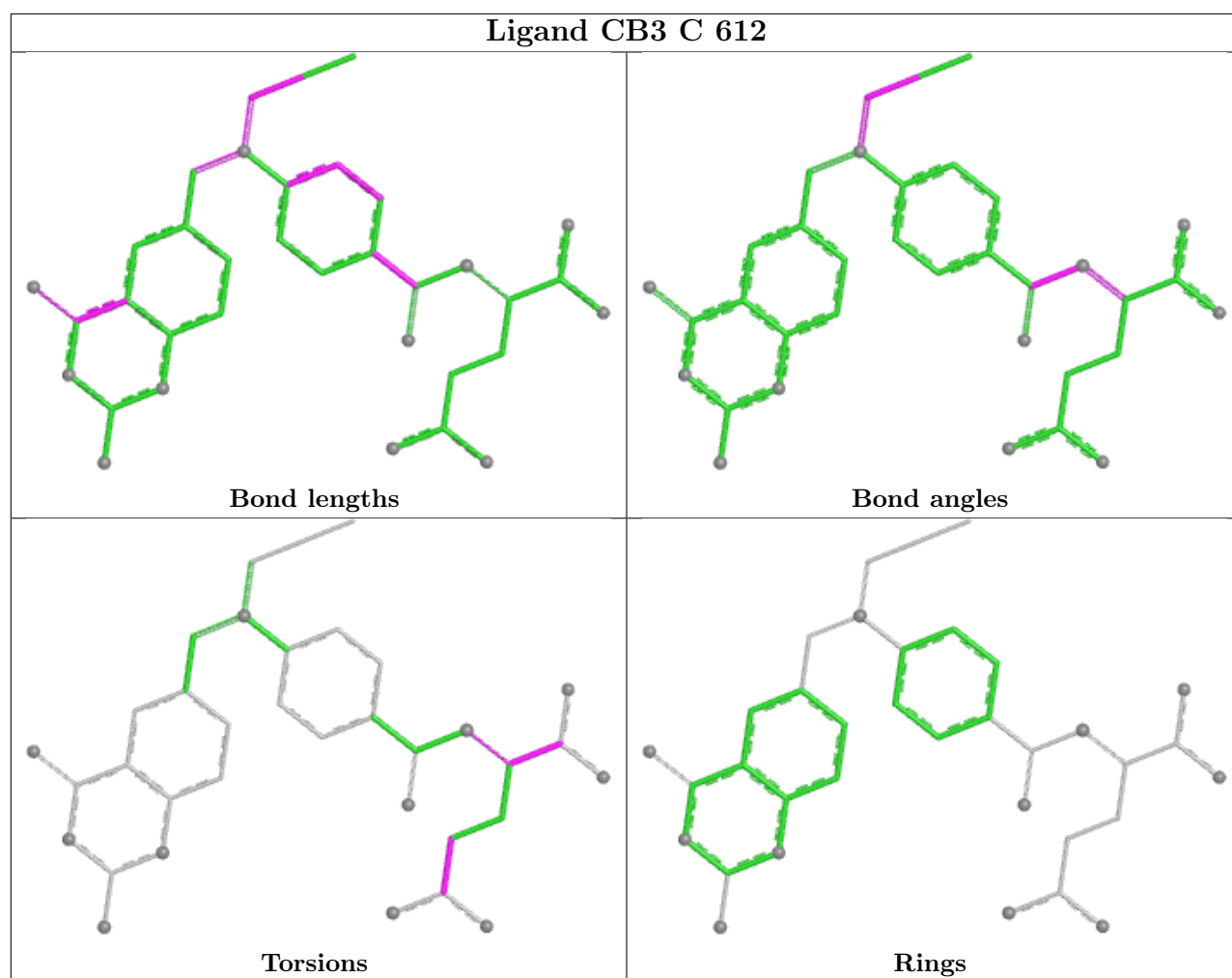


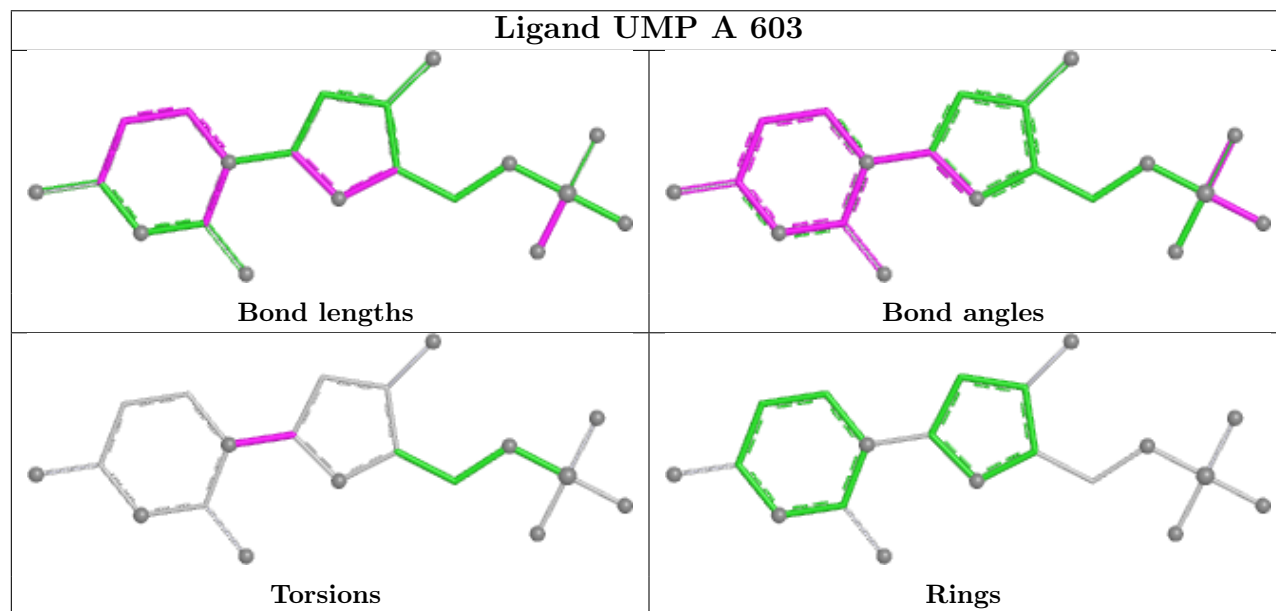
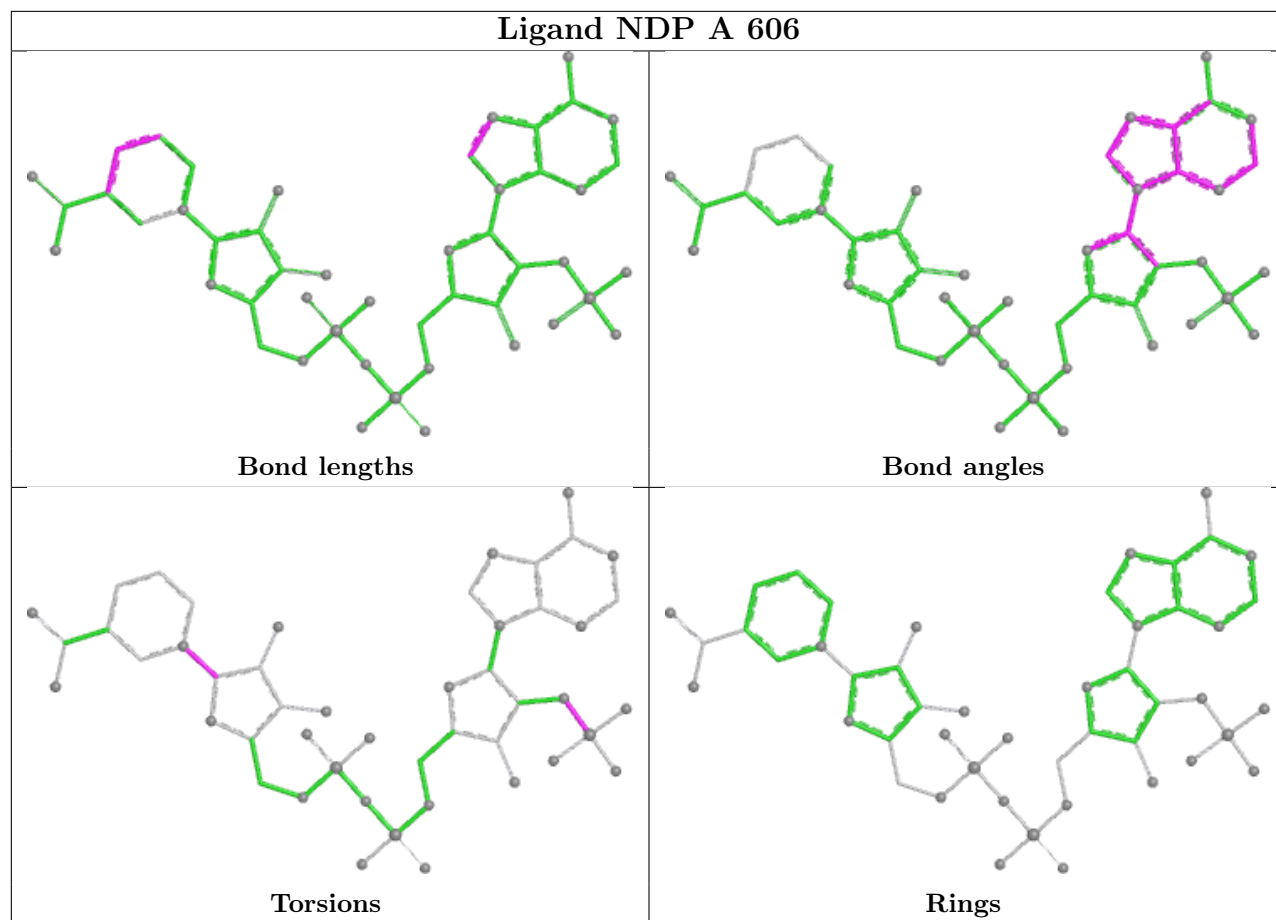


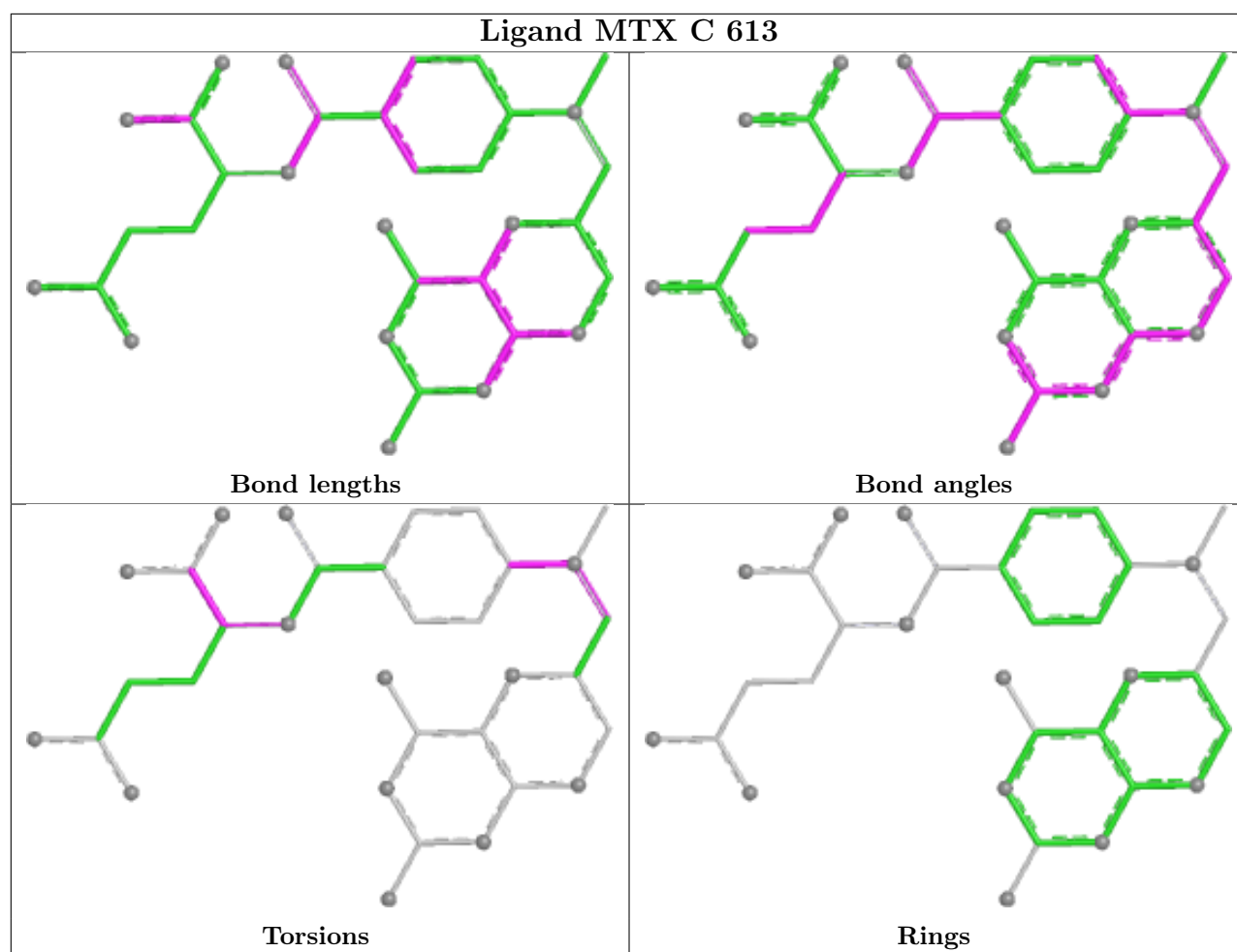


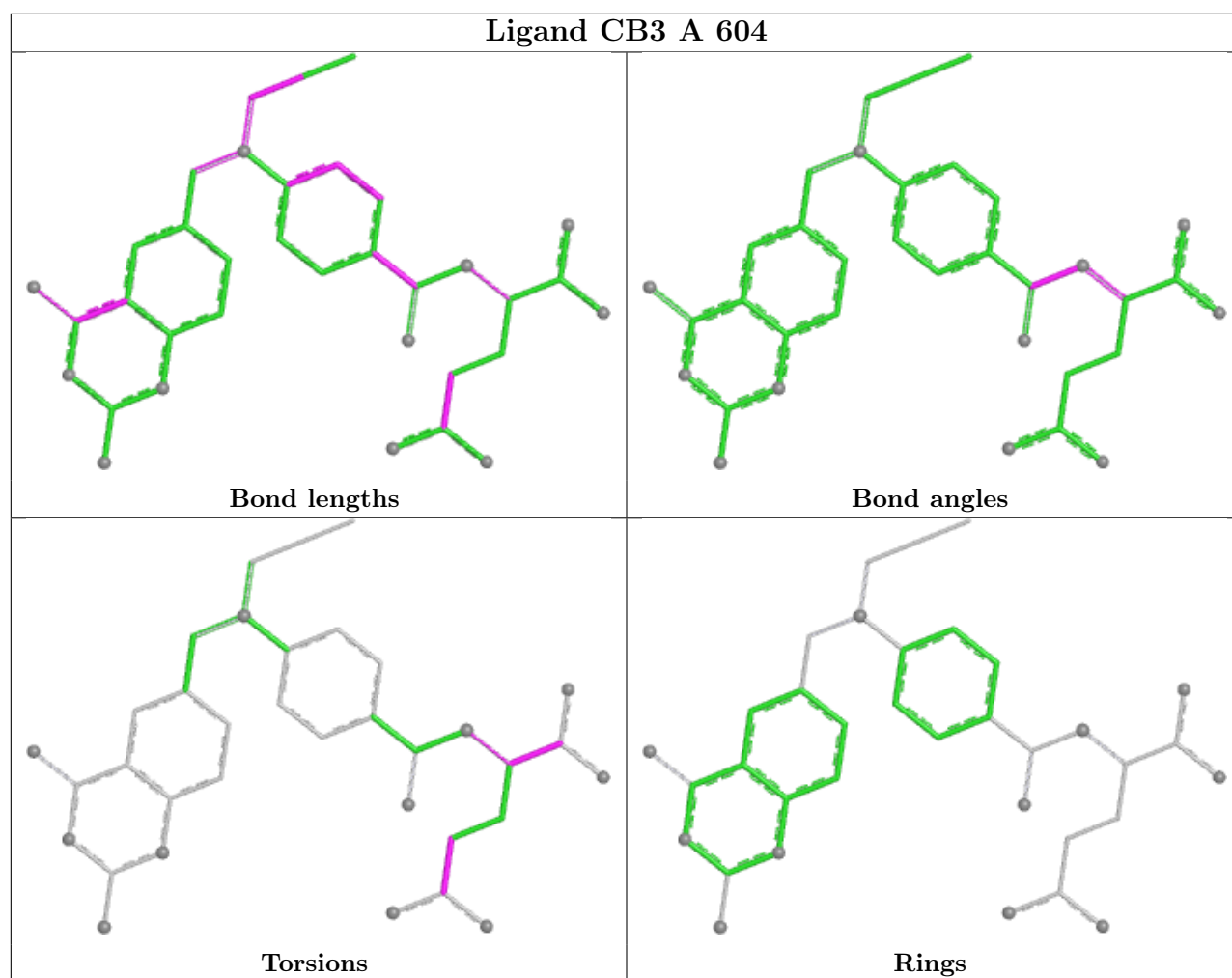


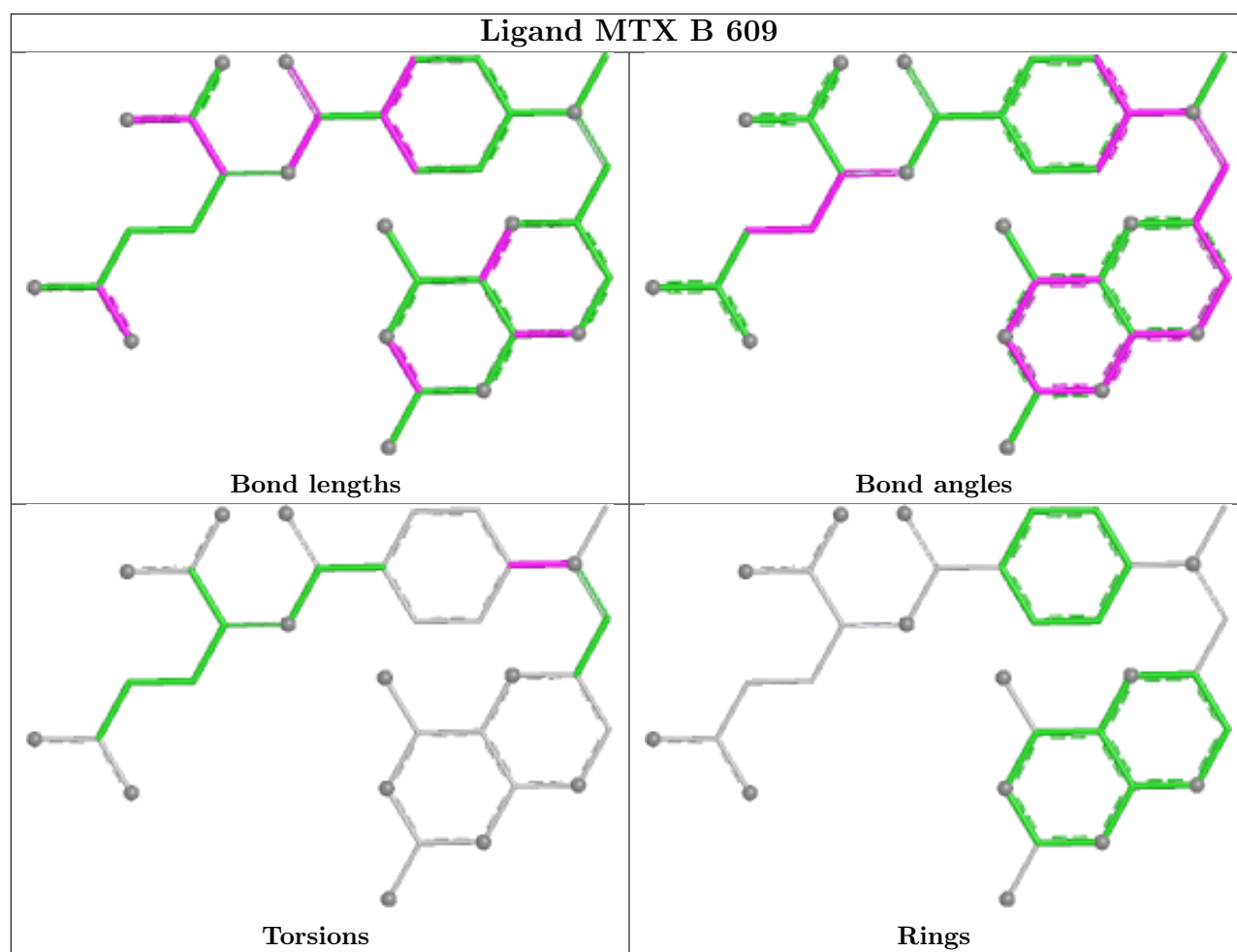


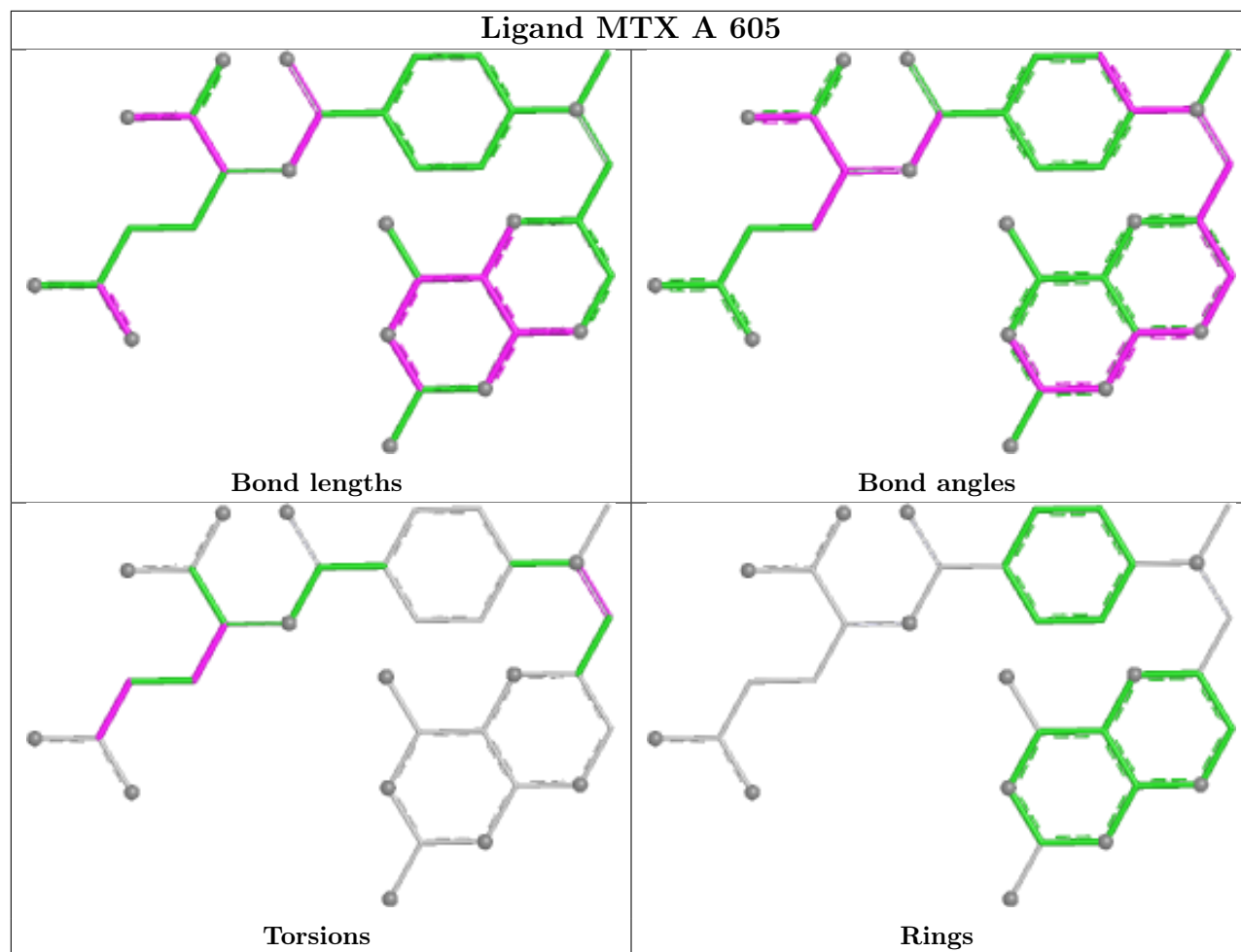












5.7 Other polymers [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	508/521 (97%)	-0.23	14 (2%) 55 51	19, 38, 67, 100	0
1	B	510/521 (97%)	-0.15	16 (3%) 51 48	22, 39, 75, 129	0
1	C	510/521 (97%)	0.41	33 (6%) 25 22	33, 54, 98, 126	0
1	D	505/521 (96%)	0.89	38 (7%) 20 17	41, 73, 101, 126	0
All	All	2033/2084 (97%)	0.23	101 (4%) 34 30	19, 50, 94, 129	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	422	GLN	5.6
1	B	425	CYS	5.0
1	C	256	ASN	4.9
1	C	258	THR	4.7
1	D	101	LEU	4.3
1	D	257	ARG	4.2
1	D	521	VAL	3.9
1	B	103	ASN	3.8
1	C	101	LEU	3.8
1	B	520	ALA	3.7
1	C	255	GLU	3.6
1	C	519	MET	3.6
1	B	521	VAL	3.5
1	D	399	LEU	3.5
1	D	62	ILE	3.4
1	C	257	ARG	3.4
1	C	521	VAL	3.3
1	D	128	VAL	3.3
1	C	259	GLY	3.2
1	C	113	CYS	3.2
1	D	193	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	100	ASN	3.2
1	A	171	ASP	3.1
1	D	178	GLN	3.1
1	D	209	ILE	3.1
1	C	425	CYS	3.1
1	C	181	LYS	3.0
1	D	114	GLY	3.0
1	C	520	ALA	2.9
1	A	103	ASN	2.9
1	C	209	ILE	2.9
1	B	104	ASP	2.9
1	D	256	ASN	2.8
1	A	521	VAL	2.8
1	C	174	ILE	2.8
1	C	182	THR	2.8
1	A	193	LEU	2.7
1	D	107	ILE	2.7
1	D	123	LEU	2.7
1	C	117	SER	2.7
1	D	39	ILE	2.7
1	B	69	ASN	2.7
1	C	97	SER	2.7
1	D	93	ASN	2.7
1	C	112	VAL	2.7
1	A	105	ASP	2.7
1	A	98	ILE	2.7
1	B	179	GLU	2.6
1	D	26	PRO	2.6
1	A	102	MET	2.6
1	A	425	CYS	2.6
1	A	84	ALA	2.6
1	D	27	TRP	2.5
1	A	172	PHE	2.5
1	B	256	ASN	2.5
1	C	192	GLN	2.5
1	D	155	LEU	2.4
1	D	255	GLU	2.4
1	A	192	GLN	2.4
1	D	252	ALA	2.4
1	B	192	GLN	2.4
1	B	191	GLY	2.4
1	D	89	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	123	LEU	2.3
1	C	98	ILE	2.3
1	D	98	ILE	2.3
1	C	157	VAL	2.3
1	C	296	ILE	2.2
1	D	137	ALA	2.2
1	B	99	GLU	2.2
1	C	180	LYS	2.2
1	B	257	ARG	2.2
1	D	428	GLY	2.2
1	B	98	ILE	2.2
1	C	107	ILE	2.2
1	A	257	ARG	2.2
1	C	422	GLN	2.2
1	D	295	LEU	2.2
1	B	102	MET	2.2
1	D	231	PHE	2.2
1	D	425	CYS	2.2
1	C	66	PRO	2.2
1	D	263	TYR	2.2
1	B	193	LEU	2.2
1	D	138	LEU	2.2
1	C	175	PHE	2.1
1	C	65	ARG	2.1
1	D	134	THR	2.1
1	D	443	MET	2.1
1	C	62	ILE	2.1
1	D	118	ILE	2.1
1	C	125	ASP	2.1
1	A	258	THR	2.1
1	C	151	PRO	2.1
1	D	102	MET	2.1
1	A	101	LEU	2.1
1	C	100	ASN	2.1
1	D	398	ALA	2.0
1	D	362	GLY	2.0
1	D	324	TYR	2.0
1	D	25	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

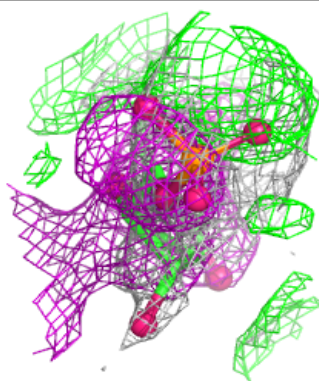
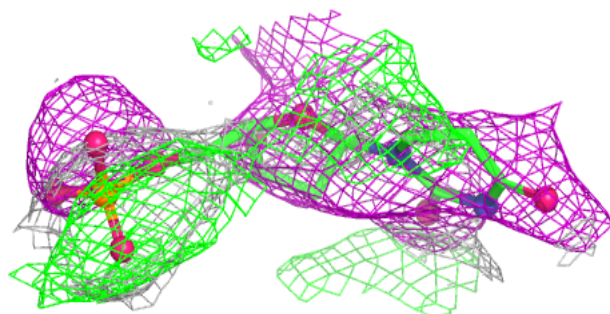
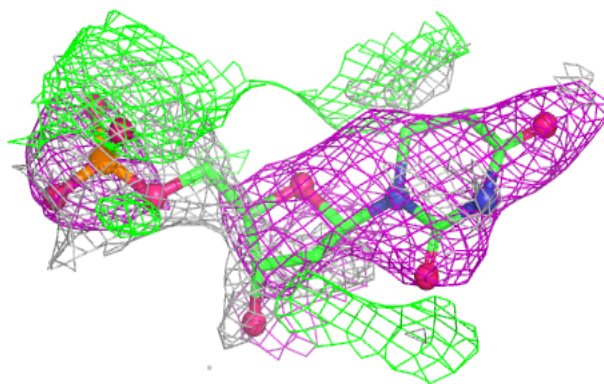
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UMP	B	607	20/20	0.44	0.27	52,66,72,72	0
3	CB3	C	612	35/35	0.52	0.25	65,69,76,76	0
3	CB3	B	608	35/35	0.63	0.22	63,69,76,76	0
2	UMP	A	603	20/20	0.64	0.26	55,68,73,73	0
2	UMP	C	611	20/20	0.65	0.21	55,66,73,73	0
3	CB3	A	604	35/35	0.71	0.21	66,71,77,78	0
4	MTX	D	615	33/33	0.87	0.13	65,70,133,151	0
5	NDP	D	616	48/48	0.91	0.10	54,74,151,159	0
4	MTX	C	613	33/33	0.93	0.11	52,63,100,144	0
5	NDP	C	614	48/48	0.94	0.10	50,74,118,195	0
4	MTX	A	605	33/33	0.95	0.08	28,40,56,79	0
4	MTX	B	609	33/33	0.95	0.07	27,38,51,73	0
5	NDP	A	606	48/48	0.97	0.07	27,38,50,69	0
5	NDP	B	610	48/48	0.98	0.05	24,33,46,49	0

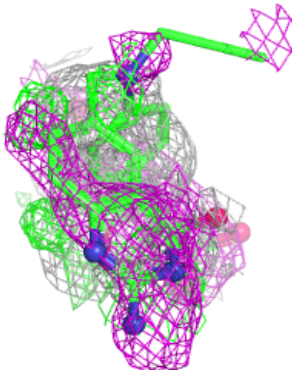
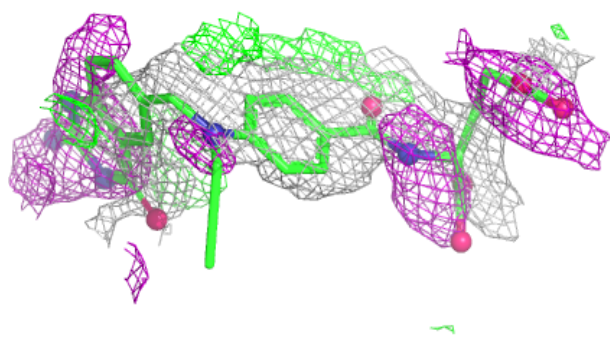
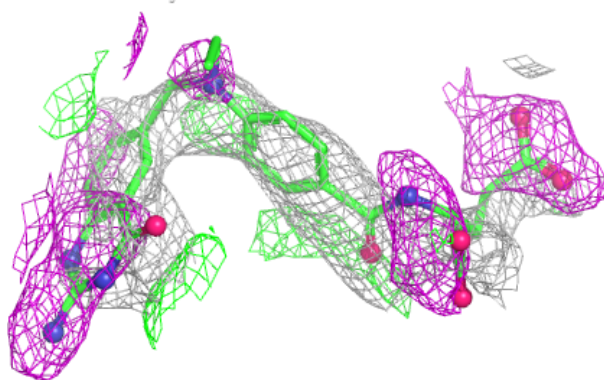
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMP B 607:

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

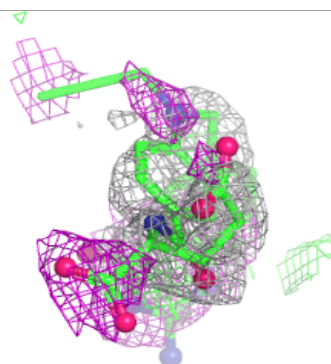
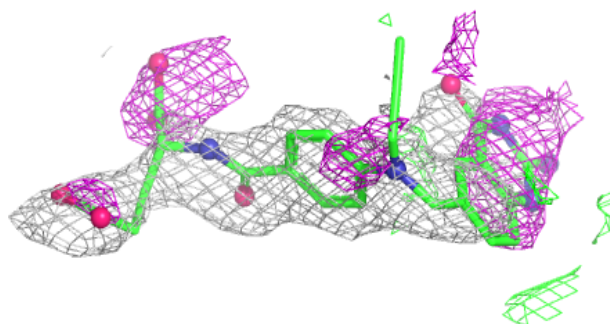
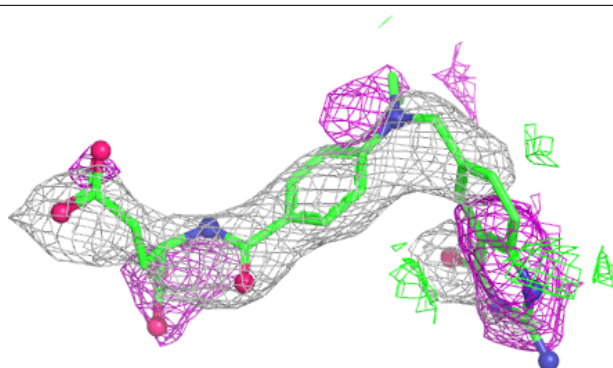
**Electron density around CB3 C 612:**

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

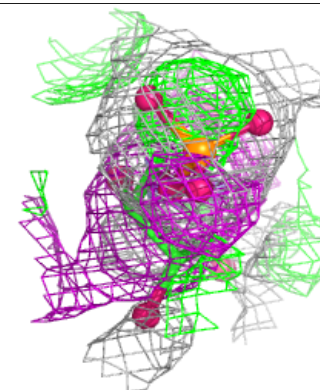
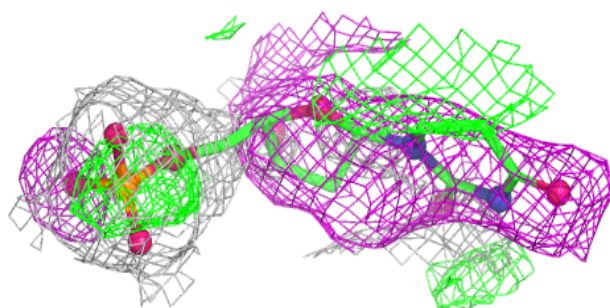
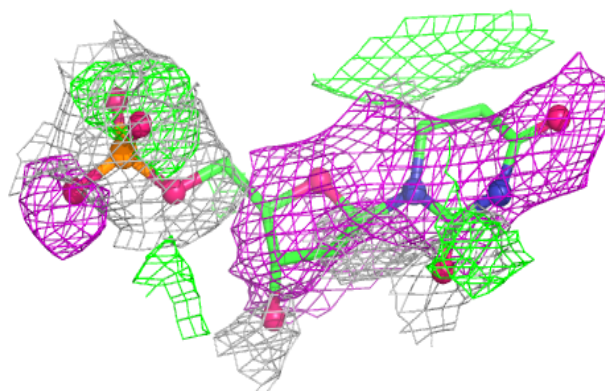


Electron density around CB3 B 608:

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

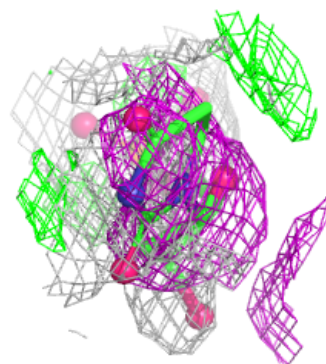
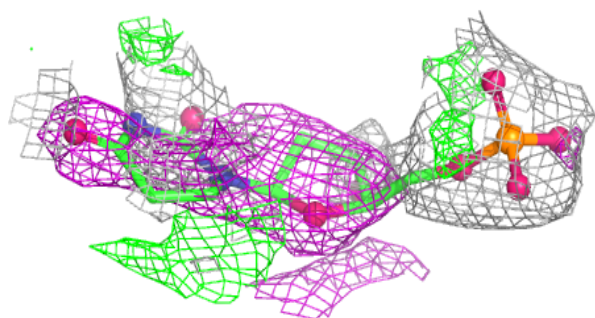
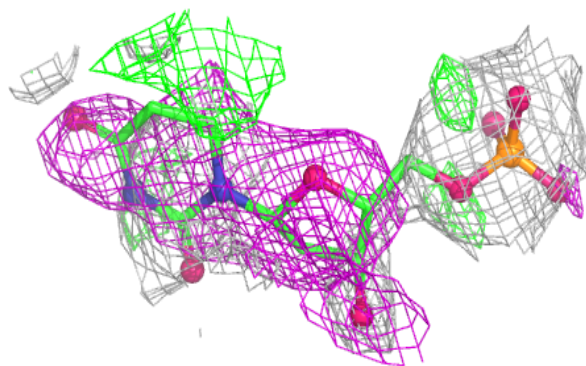
**Electron density around UMP A 603:**

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

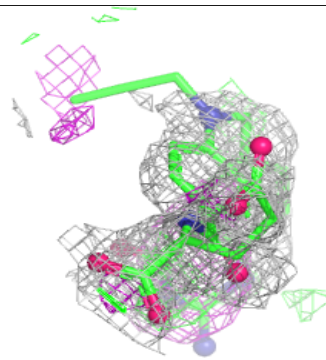
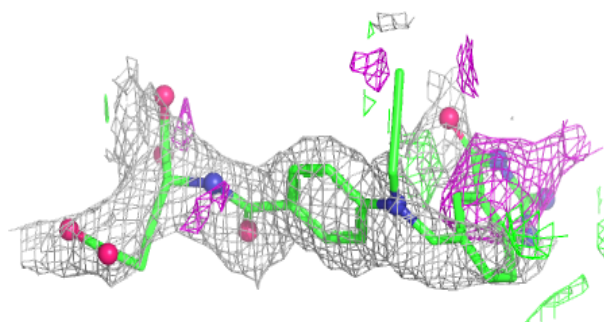
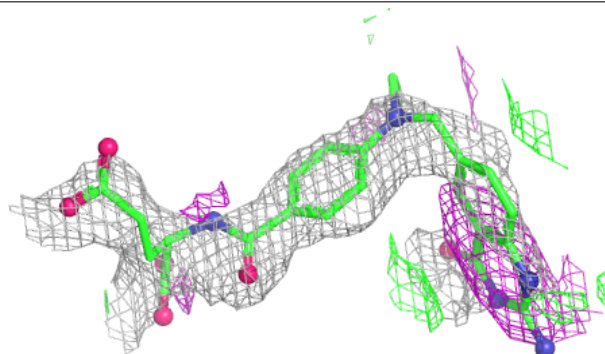


Electron density around UMP C 611:

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

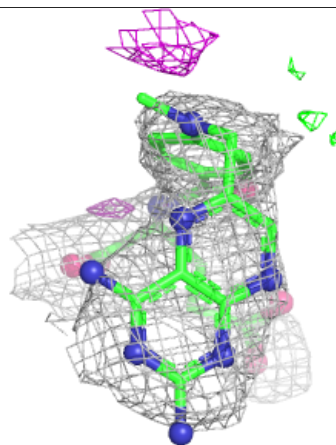
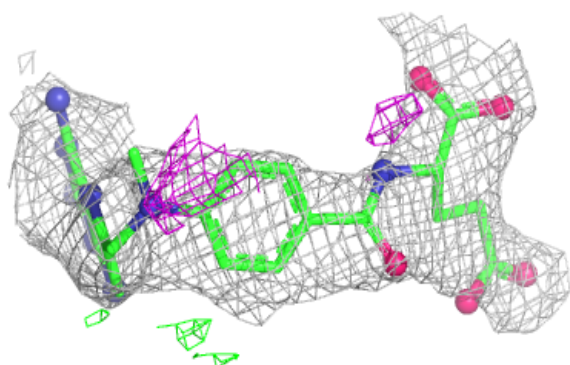
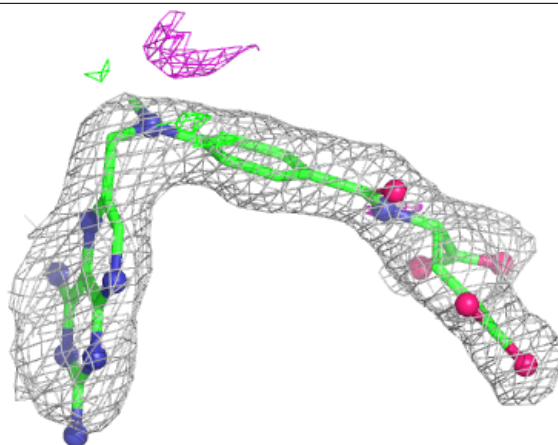
**Electron density around CB3 A 604:**

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

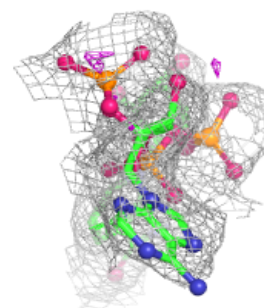
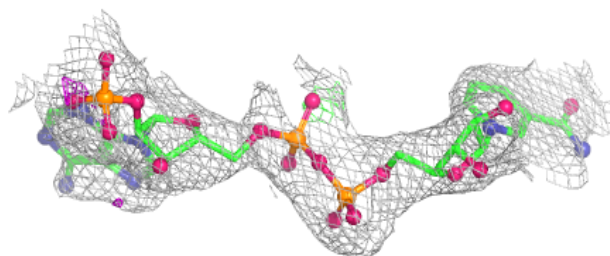
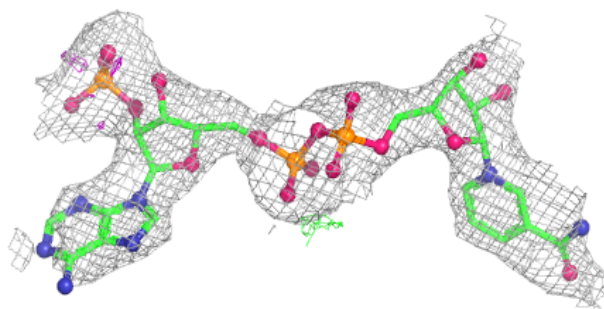


Electron density around MTX D 615:

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

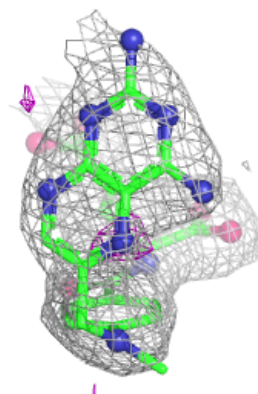
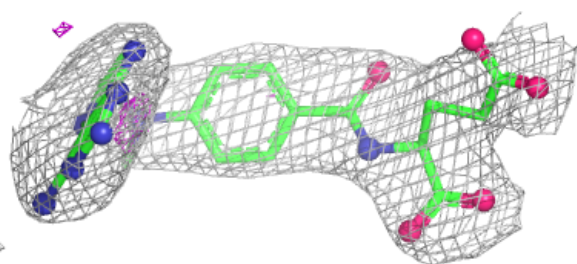
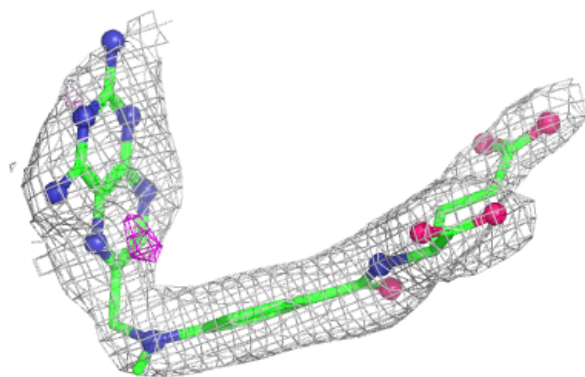
**Electron density around NDP D 616:**

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

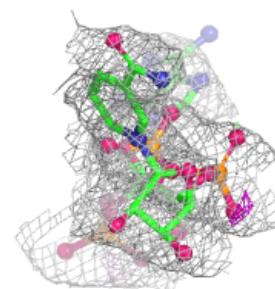
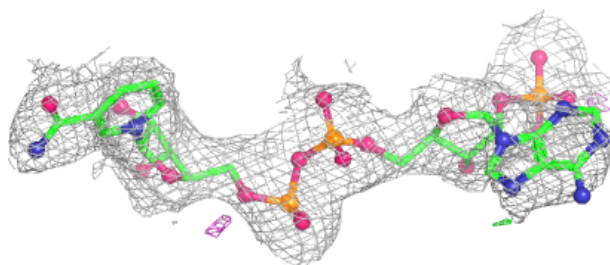
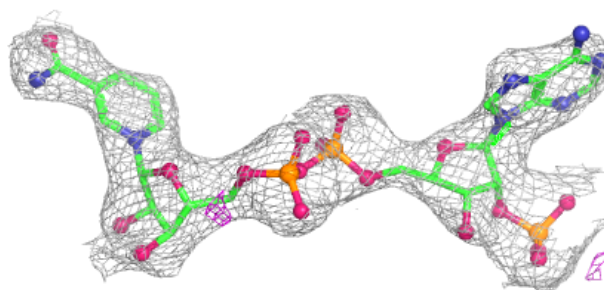


Electron density around MTX C 613:

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

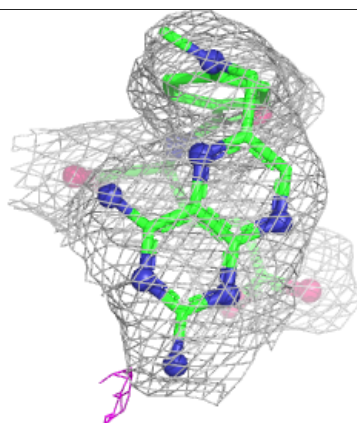
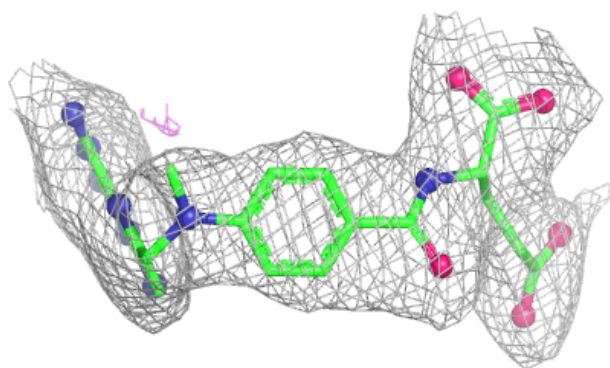
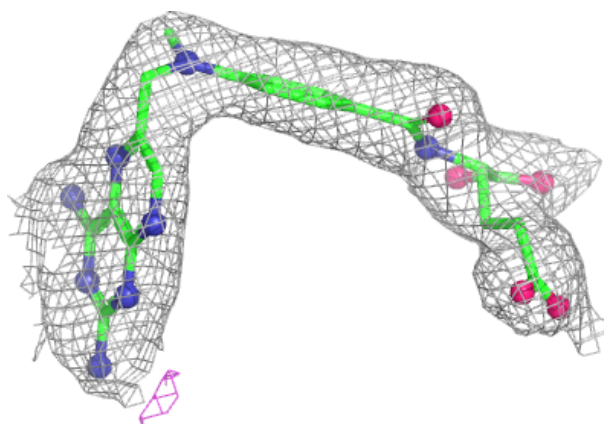
**Electron density around NDP C 614:**

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

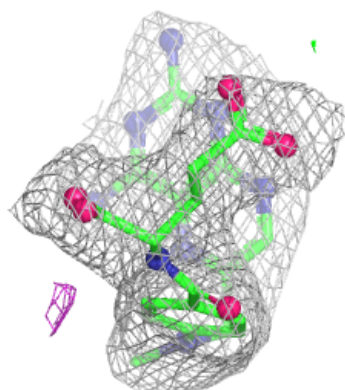
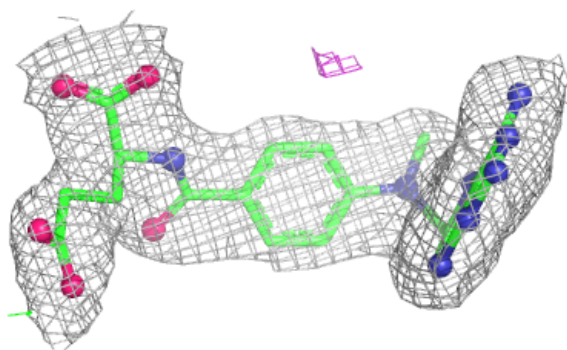
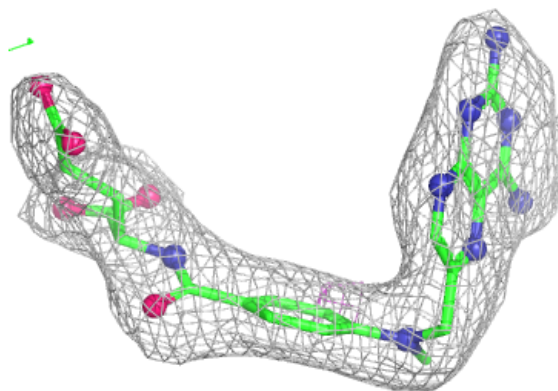


Electron density around MTX A 605:

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

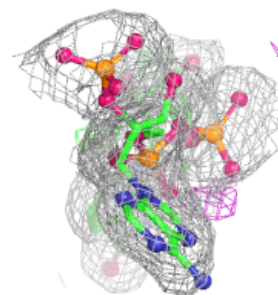
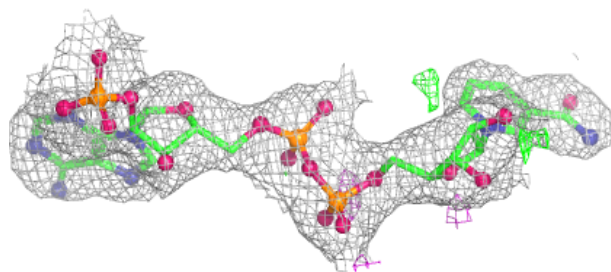
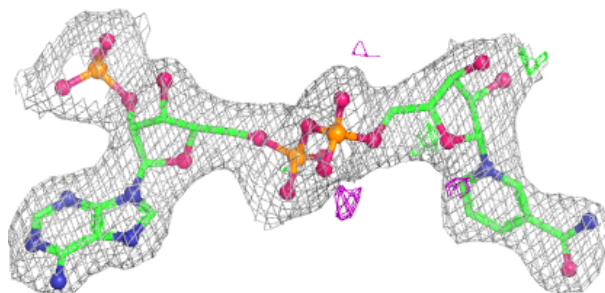
**Electron density around MTX B 609:**

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

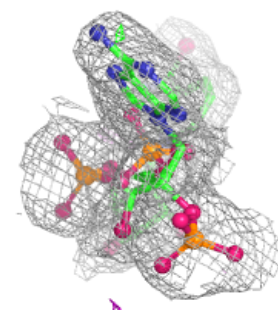
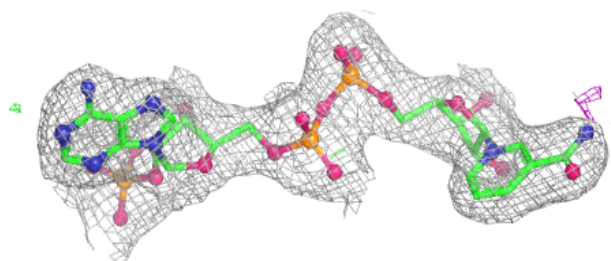
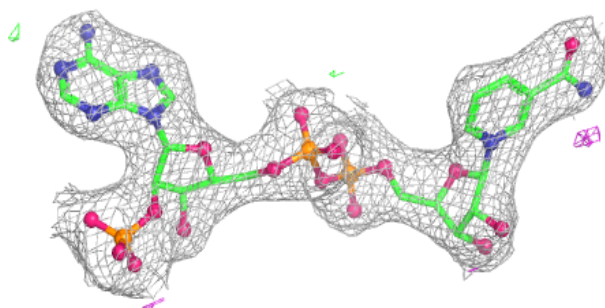


Electron density around NDP A 606:

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

**Electron density around NDP B 610:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.