Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 09:08 AM EDT

PDB ID	:	3HJ3
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

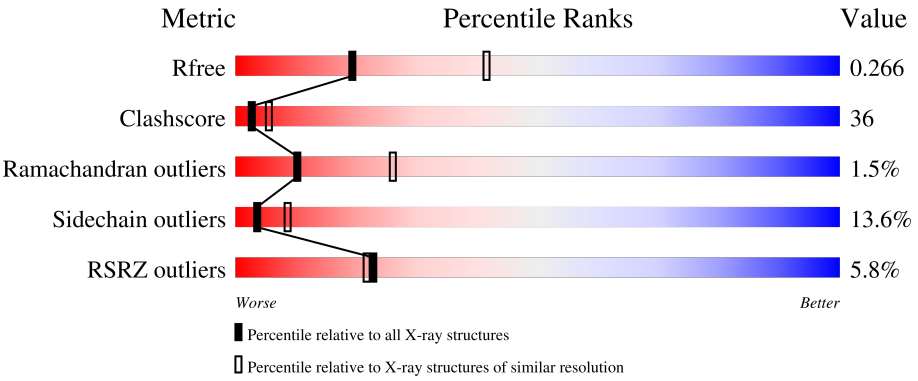
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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% 56% 32% 9%
1	B	521	3% 55% 34% 8%
1	C	521	7% 47% 40% 10%
1	D	521	10% 42% 45% 9%

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	X
2	UMP	B	607	-	-	X	X
2	UMP	C	611	-	-	X	-
3	CB3	A	604	X	-	X	-
3	CB3	B	608	X	-	-	X
3	CB3	C	612	X	-	X	X
4	MTX	D	615	-	-	X	-

2 Entry composition (i)

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.

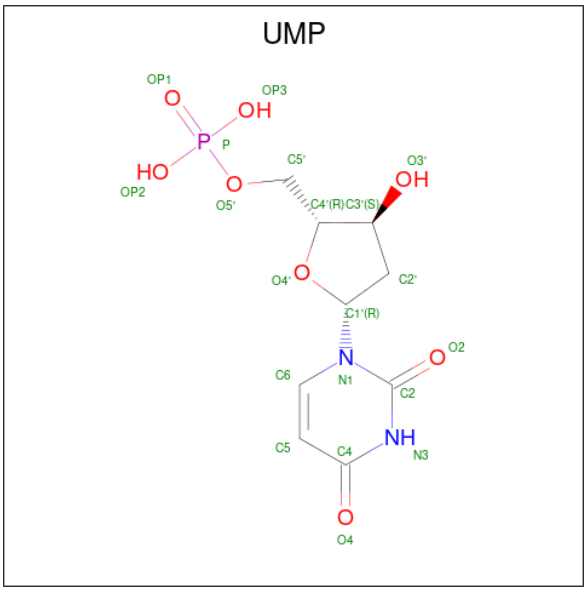
- Molecule 1 is a protein called Chain A, crystal structure of Dhfr.

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:

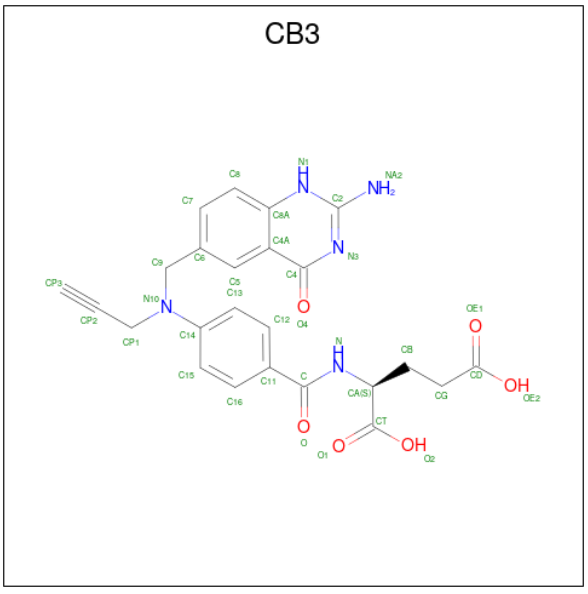
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ALA	PHE	engineered mutation	UNP Q5CGA3
B	207	ALA	PHE	engineered mutation	UNP Q5CGA3
C	207	ALA	PHE	engineered mutation	UNP Q5CGA3
D	207	ALA	PHE	engineered mutation	UNP Q5CGA3

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



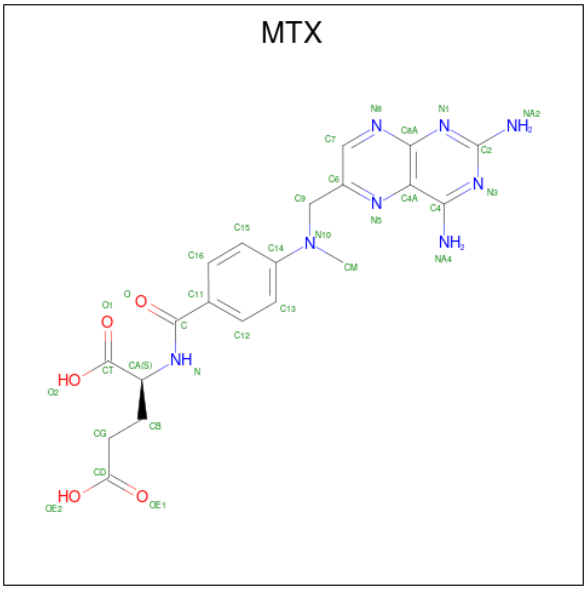
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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



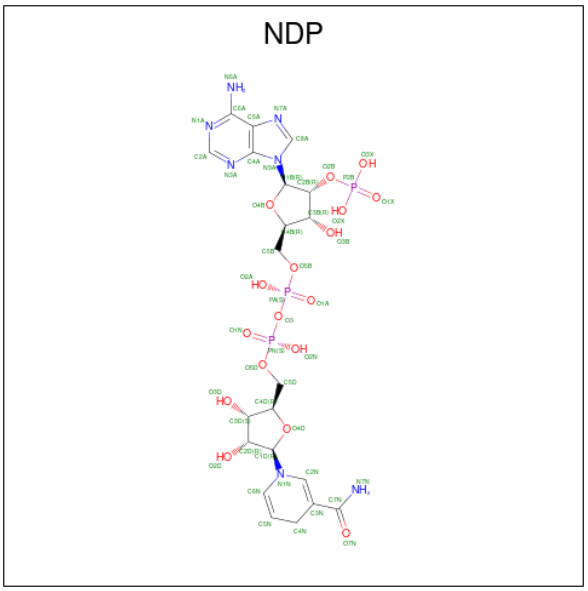
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 35 24 5 6	0	0
3	B	1	Total C N O 35 24 5 6	0	0
3	C	1	Total C N O 35 24 5 6	0	0

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).



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

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



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

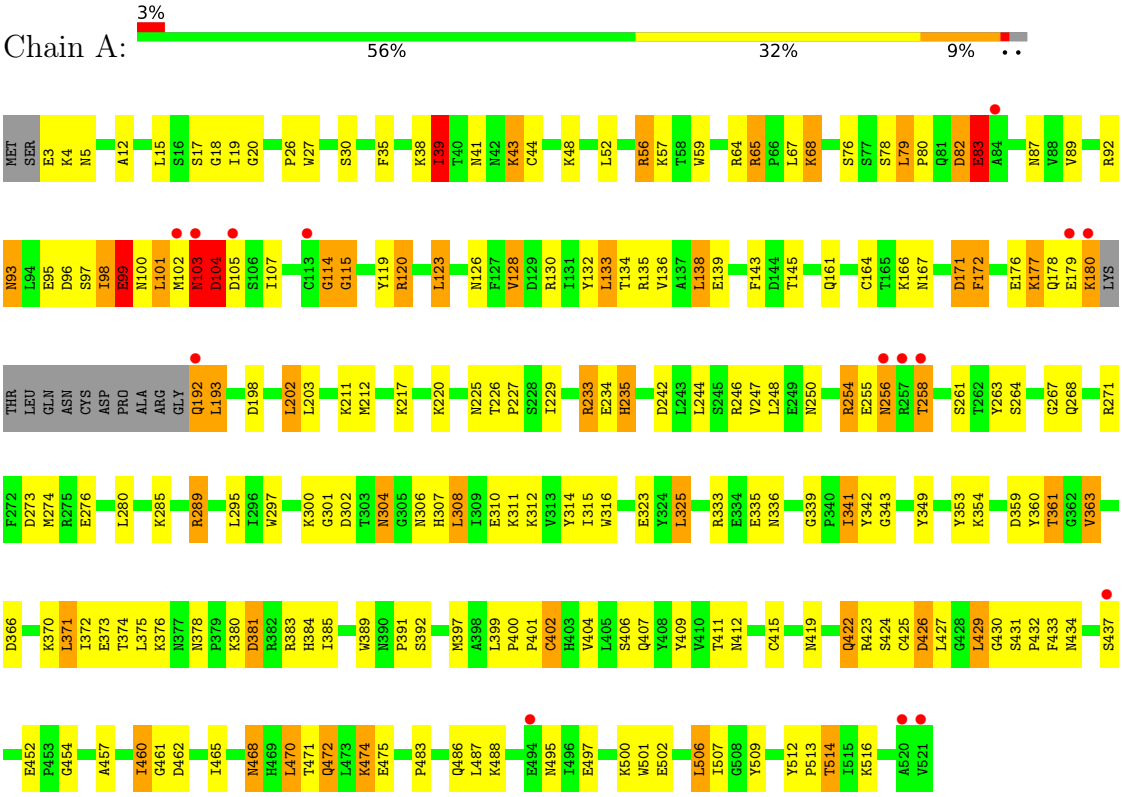
- Molecule 6 is water.

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

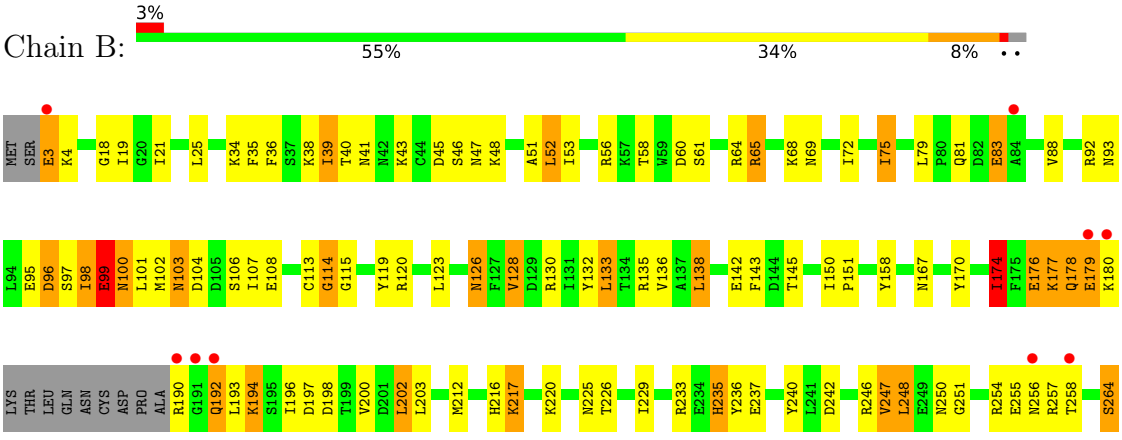
3 Residue-property plots (i)

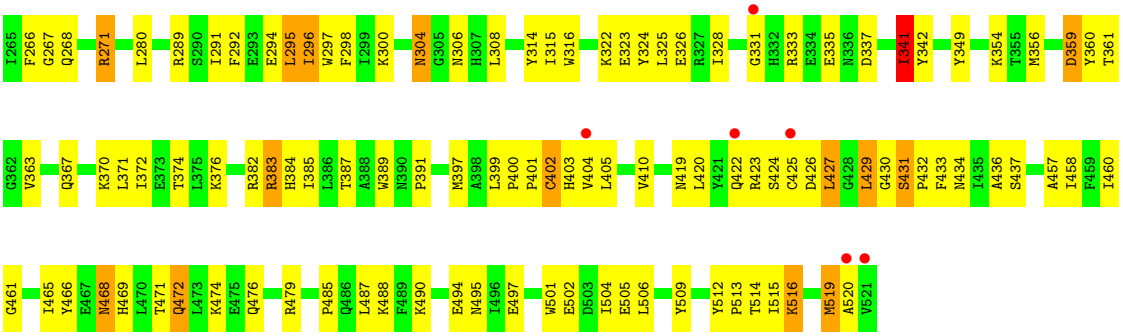
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



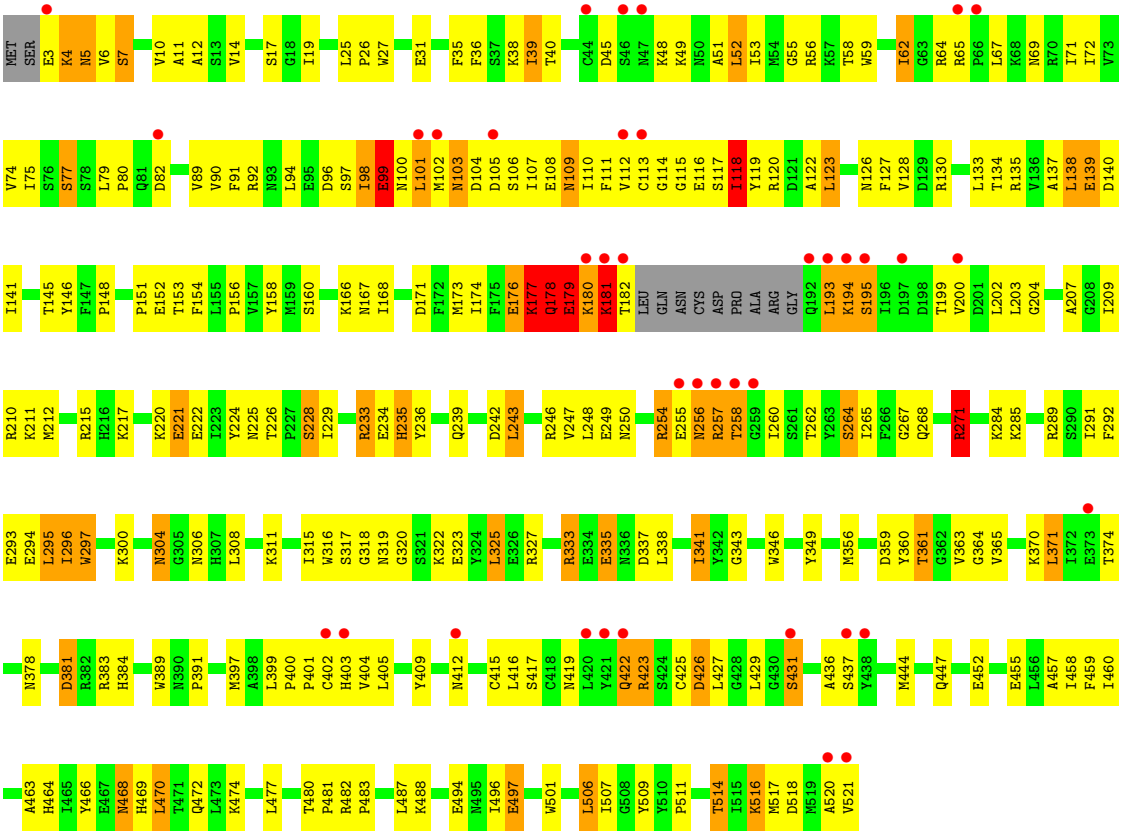
• Molecule 1: Chain A, crystal structure of Dhfr





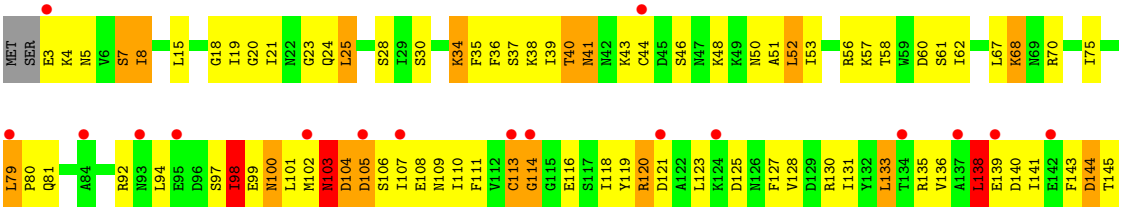
• Molecule 1: Chain A, crystal structure of Dhfr

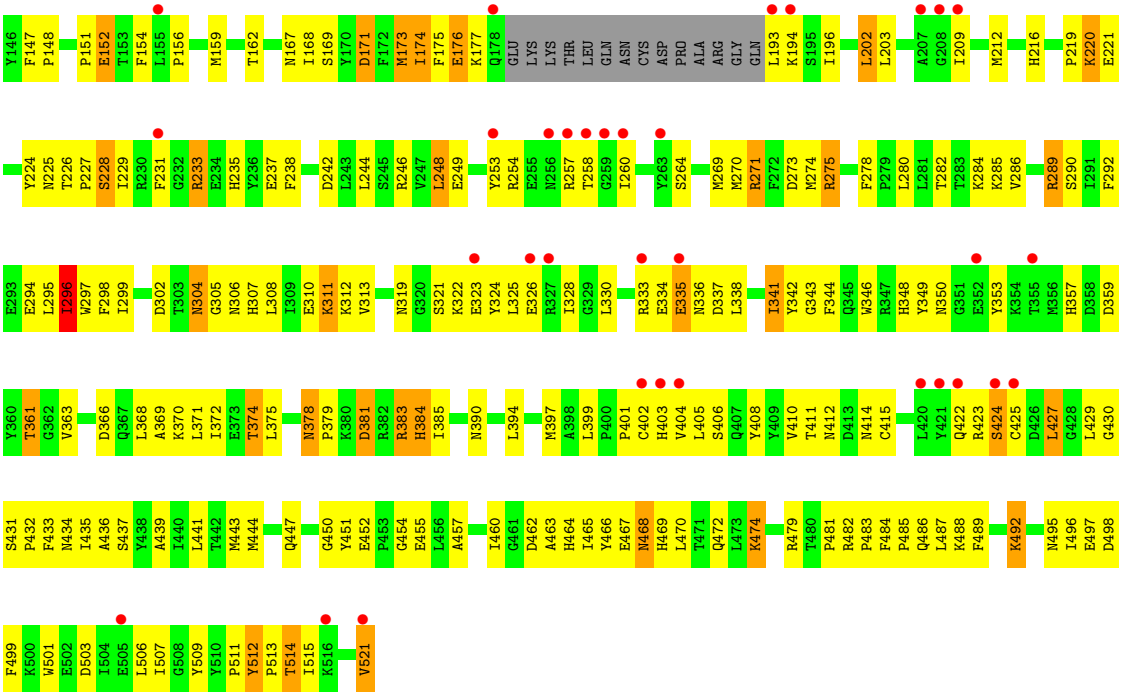
Chain C:



• Molecule 1: Chain A, crystal structure of Dhfr

Chain D:




Y146 F147 P148 P151 E152 T153 F154 L155 P156 M159 T162 N167 I168 S169 Y170 D171 F172 M173 I174 F175 E176 K177 Q178 GLU LYS LYS THR LEU GLN ASN CYS ASP PRO ALA ARG GLY GLN L193 K194 S195 I196 L202 L203 A207 G208 I209 M212 H216 P219 K220 E221
Y224 N225 T226 P227 S228 I229 R230 F231 G232 R233 E234 H235 Y236 E237 F238 D242 L243 L244 S245 R246 V247 L248 E249 Y253 R254 E255 N256 R257 T258 G259 I260 Y263 S264 M269 M270 R271 F272 D273 M274 R275 F278 P279 L280 L281 T282 T283 K284 K285 V286 R289 S290 I291 F292
E293 E294 L295 T296 W297 F298 I299 D302 T303 N304 G305 N306 H307 L308 I309 E310 K311 K312 V313 N319 G320 S321 K322 E323 Y324 L325 E326 R327 I328 G329 L330 R333 E334 E335 N336 D337 L338 I341 Y342 G343 F344 Q345 W346 R347 H348 Y349 N350 G351 E352 Y353 K354 T355 M356 H357 D358 D359
Y360 T361 G362 V363 D366 Q367 L368 A369 K370 L371 I372 E373 T374 L375 N378 P379 K380 D381 R382 R383 H384 I385 N390 L394 M397 A398 L399 P400 P401 C402 H403 V404 L405 S406 Q407 Y408 Y409 V410 T411 N412 D413 N414 C415 L420 Y421 Q422 R423 S424 C425 D426 L427 G428 L429 G430
S431 P432 F433 N434 I435 A436 S437 Y438 A439 I440 L441 T442 M443 M444 Q447 G450 Y451 E452 P453 G454 E455 L456 A457 I460 G461 D462 A463 H464 I465 Y466 E467 N468 H469 L470 T471 Q472 L473 K474 R479 T480 P481 R482 P483 F484 P485 Q486 L487 K488 F489 K492 N495 I496 E497 D498
F499 K500 W501 E502 D503 T504 E505 L506 T507 G508 Y509 Y510 P511 Y512 P513 T514 I515 K516 V521

4 Data and refinement statistics (i)

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 34.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 99.5 (34.47-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.68Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.228 , 0.274 0.219 , 0.266	Depositor DCC
R_{free} test set	4070 reflections (5.02%)	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 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MTX, UMP, CB3, 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	0.84	1/4225 (0.0%)	0.86	4/5709 (0.1%)
1	B	0.87	2/4238 (0.0%)	0.83	4/5726 (0.1%)
1	C	0.82	1/4241 (0.0%)	0.86	5/5730 (0.1%)
1	D	0.74	1/4198 (0.0%)	0.79	2/5674 (0.0%)
All	All	0.82	5/16902 (0.0%)	0.83	15/22839 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	CYS	CB-SG	-9.21	1.66	1.82
1	B	402	CYS	CB-SG	-9.01	1.67	1.82
1	D	521	VAL	C-OXT	6.37	1.35	1.23
1	C	521	VAL	C-OXT	6.01	1.34	1.23
1	B	240	TYR	CE1-CZ	5.49	1.45	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	423	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	423	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	B	75	ILE	CG1-CB-CG2	-7.13	95.72	111.40
1	B	402	CYS	CA-CB-SG	-6.15	102.93	114.00
1	A	402	CYS	CA-CB-SG	-5.80	103.55	114.00
1	A	308	LEU	CB-CG-CD2	-5.64	101.40	111.00
1	B	65	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	174	ILE	CG1-CB-CG2	-5.54	99.22	111.40
1	C	101	LEU	CA-CB-CG	5.52	127.99	115.30
1	C	356	MET	CG-SD-CE	5.51	109.02	100.20
1	D	100	ASN	CB-CA-C	-5.46	99.47	110.40
1	D	144	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	271	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	39	ILE	CG1-CB-CG2	-5.16	100.06	111.40
1	A	325	LEU	CA-CB-CG	5.12	127.08	115.30

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
1	C	296	ILE	Peptide

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Mol	Chain	Res	Type	Group
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4131	0	4066	271	0
1	B	4144	0	4077	280	3
1	C	4147	0	4086	333	3
1	D	4104	0	4039	351	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	32	0
6	B	86	0	0	30	0
6	C	47	0	0	29	0
6	D	36	0	0	47	0
All	All	17282	0	16545	1208	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 36.

All (1208) 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:C:180:LYS:HG2	1:C:181:LYS:N	1.44	1.06
1:C:180:LYS:HZ3	1:C:181:LYS:CB	1.69	1.05
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: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:C:397:MET:HE1	1:C:401:PRO:CD	1.89	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:B:103:ASN:C	1:B:103:ASN:HD22	1.60	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
1:B:100:ASN:HA	1:B:103:ASN:HD21	1.22	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:397:MET:HE1	1:C:401:PRO:HD3	0.95	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:256:ASN:C	1:C:256:ASN:HD22	1.80	0.86
1:C:180:LYS:HZ3	1:C:181:LYS:CA	1.89	0.85
1:B:96:ASP:O	1:B:99:GLU:CB	2.24	0.85
1:C:225:ASN:O	1:C:233:ARG:NH2	2.08	0.85
1:C:180:LYS:HZ3	1:C:181:LYS:N	1.74	0.85
1:C:62:ILE:CG2	6:C:567:HOH:O	2.24	0.84
1:C:180:LYS:NZ	1:C:180:LYS:C	2.30	0.84
1:D:5:ASN:HD21	1:D:130:ARG:NH2	1.74	0.84
1:C:180:LYS:NZ	1:C:181:LYS:CB	2.33	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: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
1:A:397:MET:HE1	1:A:401:PRO:HD3	1.61	0.83
3:C:612:CB3:HP11	6:C:538:HOH:O	1.79	0.83
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ASN:H	1:D:468:ASN:HD22	1.24	0.82
1:C:397:MET:HE2	1:C:400:PRO:HA	1.62	0.81
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:C:180:LYS:C	1:C:180:LYS:HZ2	1.84	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: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: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:B:383:ARG:C	6:B:606:HOH:O	2.20	0.79
1:D:306:ASN:HD21	1:D:336:ASN:HB2	1.43	0.79
1:B:103:ASN:C	1:B:103:ASN:ND2	2.34	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:171:ASP:CG	1:D:483:PRO:HB3	2.04	0.78
1:C:180:LYS:HZ1	1:C:181:LYS:HB3	1.49	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: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:D:307:HIS:O	1:D:311:LYS:HE2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:256:ASN:C	1:C:256:ASN:ND2	2.39	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:B:341:ILE:HG22	1:B:397:MET:HE2	1.67	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:57:LYS:NZ	6:A:589:HOH:O	2.21	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: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:B:384:HIS:N	6:B:606:HOH:O	2.22	0.72
1:D:216:HIS:ND1	6:D:551:HOH:O	2.23	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: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:B:397:MET:HE3	6:B:570:HOH:O	1.91	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
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:B:99:GLU:O	1:B:103:ASN:CG	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:A:103:ASN:CG	1:A:104:ASP:N	2.47	0.68
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:389:TRP:HB2	1:C:404:VAL:CG1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:LEU:CD2	3:C:612:CB3:C8	2.71	0.68
1:A:103:ASN:O	1:A:104:ASP:C	2.31	0.68
1:C:180:LYS:HZ1	1:C:182:THR:H	1.41	0.68
1:D:58:THR:HG23	4:D:615:MTX:HM2	1.76	0.68
1:A:103:ASN:ND2	1:A:103:ASN:C	2.47	0.67
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:133:LEU:C	1:A:133:LEU:HD22	2.14	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:A:422:GLN:CD	1:A:425:CYS:HB2	2.15	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: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: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:D:479:ARG:HB3	1:D:512:TYR:CE2	2.31	0.66
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
1:C:51:ALA:C	1:C:52:LEU:HD23	2.17	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:133:LEU:C	1:A:133:LEU:CD2	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:304:ASN:HD22	1:A:304:ASN:C	2.01	0.64
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: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: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
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: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:103:ASN:CG	1:A:104:ASP:H	2.01	0.63
1:B:314:TYR:C	6:B:596:HOH:O	2.36	0.63
1:A:35:PHE:CZ	1:A:39:ILE:HD13	2.33	0.63
1:D:334:GLU:O	1:D:335:GLU:C	2.37	0.63
1:D:466:TYR:HB3	1:D:468:ASN:ND2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:430:GLY:C	3:A:604:CB3:HP3	2.20	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: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: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
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: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:C:323:GLU:H	1:C:323:GLU:CD	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:422:GLN:CD	1:C:425:CYS:HB2	2.21	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
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:B:397:MET:HE1	1:B:399:LEU:O	2.01	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: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:D:341:ILE:HA	1:D:397:MET:HE3	1.83	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:C:152:GLU:C	1:C:154:PHE:H	2.04	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:359:ASP:CG	1:B:361:THR:HG22	2.23	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: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:B:397:MET:CE	1:B:401:PRO:HD3	2.34	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:305:GLY:C	1:D:336:ASN:HD22	2.06	0.58
1:D:512:TYR:HB3	1:D:513:PRO:HD2	1.85	0.58
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: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:304:ASN:HD22	1:B:304:ASN:C	2.08	0.57
1:B:420:LEU:HD21	1:B:422:GLN:NE2	2.19	0.57
1:C:180:LYS:NZ	1:C:180:LYS:O	2.35	0.57
1:B:512:TYR:HB3	1:B:513:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:101:LEU:C	1:D:103:ASN:H	2.07	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: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: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
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: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
1:C:180:LYS:O	1:C:181:LYS:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASP:C	1:D:106:SER:H	2.07	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:D:295:LEU:HD23	1:D:295:LEU:C	2.25	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: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: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:A:426:ASP:OD2	1:A:426:ASP:C	2.46	0.54
1:D:15:LEU:HB2	1:D:139:GLU:HG2	1.88	0.54
1:B:255:GLU:H	1:B:255:GLU:CD	2.11	0.54
1:B:323:GLU:O	1:B:326:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:405:LEU:C	1:D:405:LEU:HD23	2.28	0.54
1:C:117:SER:C	1:C:118:ILE:HG22	2.27	0.54
1:C:402:CYS:O	1:C:404:VAL:HG23	2.08	0.54
1:D:104:ASP:C	1:D:106:SER:N	2.60	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: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:99:GLU:OE2	1:A:99:GLU:C	2.46	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:324:TYR:CE2	1:D:328:ILE:HD13	2.44	0.53
1:B:295:LEU:HD22	1:B:295:LEU:C	2.29	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: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:211:LYS:CB	6:C:561:HOH:O	2.19	0.52
1:A:172:PHE:N	1:A:172:PHE:CD2	2.77	0.52
1:B:257:ARG:HD3	2:B:607:UMP:P	2.49	0.52
1:A:103:ASN:C	1:A:103:ASN:HD22	2.13	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
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:297:TRP:CH2	1:C:338:LEU:CD1	2.85	0.52
1:C:304:ASN:HD22	1:C:304:ASN:C	2.12	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:HA	1:A:397:MET:HE2	1.92	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: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:A:380:LYS:HD2	1:B:254:ARG:CZ	2.41	0.50
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:409:TYR:HH	1:B:264:SER:HG	1.56	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: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:A:468:ASN:N	1:A:468:ASN:ND2	2.57	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:B:468:ASN:N	1:B:468:ASN:ND2	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LYS:O	1:D:177:LYS:HG2	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: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:B:502:GLU:H	1:B:502:GLU:CD	2.14	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:N	1:C:460:ILE:HD13	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:C:98:ILE:CD1	1:C:127:PHE:HD1	2.09	0.50
1:D:422:GLN:CD	1:D:425:CYS:HB2	2.31	0.50
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: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:A:65:ARG:HH11	1:A:65:ARG:CG	2.19	0.49
1:B:51:ALA:C	1:B:52:LEU:HD23	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:179:GLU:CG	1:B:180:LYS:N	2.72	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:C:459:PHE:C	1:C:460:ILE:HD13	2.33	0.49
1:D:120:ARG:NH1	1:D:148:PRO:HB3	2.26	0.49
1:A:3:GLU:OE2	1:A:3:GLU:CA	2.33	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: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
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: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:B:104:ASP:C	1:B:106:SER:N	2.66	0.48
1:D:436:ALA:O	1:D:439:ALA:HB3	2.13	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: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:C:153:THR:O	1:C:177:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:171:ASP:CG	1:D:483:PRO:CB	2.81	0.48
1:C:19:ILE:CG1	1:C:145:THR:HG22	2.44	0.48
1:C:152:GLU:C	1:C:154:PHE:N	2.66	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
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:C:323:GLU:CD	1:C:323:GLU:N	2.66	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:A:128:VAL:N	6:A:527:HOH:O	2.40	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:468:ASN:ND2	1:C:468:ASN:N	2.60	0.47
1:D:348:HIS:O	1:D:349:TYR:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:THR:O	1:C:177:LYS:HA	2.13	0.47
1:D:295:LEU:CD2	1:D:295:LEU:C	2.82	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: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:397:MET:HE2	6:D:531:HOH:O	2.15	0.47
1:A:383:ARG:NE	1:B:400:PRO:HG2	2.29	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:D:159:MET:HE1	1:D:481:PRO:O	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
1:C:193:LEU:O	1:C:194:LYS:C	2.52	0.47
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:53:ILE:HG23	1:D:75:ILE:HD13	1.96	0.47
1:A:323:GLU:H	1:A:323:GLU:CD	2.18	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:422:GLN:NE2	1:B:434:ASN:CG	2.68	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:D:390:ASN:O	1:D:394:LEU:HG	2.15	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:275:ARG:C	6:D:549:HOH:O	2.54	0.46
1:B:192:GLN:NE2	1:B:192:GLN:CA	2.70	0.46
1:C:177:LYS:HE3	1:C:177:LYS:HB3	1.28	0.46
1:D:270:MET:CE	1:D:460:ILE:HD11	2.45	0.46
1:C:11:ALA:HA	1:C:134:THR:O	2.15	0.46
1:D:512:TYR:HD1	1:D:512:TYR:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:370:LYS:C	6:C:560:HOH:O	2.54	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
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:469:HIS:HA	1:C:472:GLN:OE1	2.16	0.46
1:D:103:ASN:CG	1:D:104:ASP:N	2.67	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:A:500:LYS:O	1:A:501:TRP:C	2.54	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
4:A:605:MTX:N5	5:A:606:NDP:H42N	2.31	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: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: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:96:ASP:C	1:A:98:ILE:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:THR:HG21	6:A:548:HOH:O	2.16	0.45
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.75	0.45
1:D:455:GLU:N	6:D:525:HOH:O	2.50	0.45
1:A:96:ASP:C	1:A:98:ILE:N	2.70	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
1:D:173:MET:HE3	1:D:173:MET:HB3	1.77	0.45
1:D:290:SER:HA	1:D:313:VAL:HG21	1.98	0.45
1:D:310:GLU:C	1:D:312:LYS:H	2.19	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:A:487:LEU:C	1:A:487:LEU:HD23	2.36	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: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:D:467:GLU:C	1:D:469:HIS:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:341:ILE:HA	1:D:397:MET:CE	2.46	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: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: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:D:40:THR:HG23	1:D:52:LEU:HD21	1.99	0.44
1:D:97:SER:C	1:D:99:GLU:H	2.20	0.44
1:A:297:TRP:CE2	1:A:308:LEU:CD2	2.98	0.44
1:B:258:THR:HG21	1:B:520:ALA:HB1	1.98	0.44
1:B:397:MET:HE1	1:B:401:PRO:HD3	1.99	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: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: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:429:LEU:O	1:A:432:PRO:HD2	2.17	0.44
1:D:434:ASN:O	1:D:435:ILE:C	2.55	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: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:D:482:ARG:NH1	1:D:511:PRO:C	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:225:ASN:O	1:D:226:THR:C	2.56	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:B:52:LEU:N	1:B:52:LEU:CD2	2.80	0.43
1:A:164:CYS:HB2	1:A:276:GLU:O	2.18	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:C:292:PHE:HE1	1:C:444:MET:HE3	1.83	0.43
1:D:103:ASN:ND2	1:D:103:ASN:C	2.71	0.43
1:D:366:ASP:OD1	1:D:369:ALA:HB3	2.16	0.43
1:A:103:ASN:O	1:A:104:ASP:O	2.36	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: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: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:225:ASN:O	1:B:226:THR:C	2.56	0.43
1:B:433:PHE:O	1:B:437:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASN:O	1:C:257:ARG:C	2.57	0.43
1:C:257:ARG:HG2	2:C:611:UMP:OP2	2.18	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
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:C:243:LEU:HD12	1:C:243:LEU:C	2.38	0.43
1:D:244:LEU:HD12	1:D:465:ILE:HD11	2.00	0.43
1:A:234:GLU:O	1:A:235:HIS:C	2.57	0.43
1:A:460:ILE:HG22	1:A:461:GLY:N	2.34	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:198:ASP:O	1:A:202:LEU:HD22	2.19	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: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: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:A:502:GLU:CD	1:A:502:GLU:H	2.23	0.42
1:B:126:ASN:C	1:B:126:ASN:HD22	2.23	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:D:101:LEU:C	1:D:103:ASN:N	2.71	0.42
1:D:292:PHE:CD2	1:D:292:PHE:C	2.92	0.42
1:A:59:TRP:CH2	1:A:64:ARG:C	2.93	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:180:LYS:HZ3	1:C:181:LYS:HB2	1.73	0.42
1:C:361:THR:O	1:C:361:THR:HG23	2.19	0.42
1:C:105:ASP:N	1:C:105:ASP:OD1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:104:ASP:CG	1:B:107:ILE:HD13	2.40	0.42
1:C:207:ALA:O	1:C:210:ARG:HB2	2.20	0.42
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:D:46:SER:C	1:D:48:LYS:H	2.22	0.42
1:A:171:ASP:CG	1:A:483:PRO:HG3	2.39	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: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:273:ASP:CG	6:A:611:HOH:O	2.58	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:N	2.72	0.42
1:D:103:ASN:CG	1:D:104:ASP:H	2.23	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:35:PHE:O	1:C:36:PHE:C	2.58	0.42
1:C:296:ILE:O	1:C:300:LYS:HG2	2.20	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:426:ASP:OD2	1:C:426:ASP:C	2.58	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:D:220:LYS:HB2	1:D:220:LYS:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:TRP:NE1	1:B:385:ILE:CG2	2.83	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
1:A:104:ASP:HB3	1:A:107:ILE:CG1	2.41	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:285:LYS:NZ	6:A:548:HOH:O	2.51	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
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:A:349:TYR:CD2	1:B:391:PRO:HG2	2.56	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:359:ASP:CG	1:C:361:THR:HG22	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:405:LEU:C	1:B:405:LEU:HD23	2.41	0.41
1:C:317:SER:O	1:C:318:GLY:C	2.58	0.41
1:D:51:ALA:C	1:D:52:LEU:HD23	2.42	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: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:C:293:GLU:C	1:C:296:ILE:HG22	2.38	0.41
1:D:219:PRO:HA	1:D:249:GLU:HG2	2.03	0.41
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: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:A:304:ASN:C	1:A:304:ASN:ND2	2.72	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:133:LEU:C	1:D:133:LEU:CD2	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:341:ILE:O	1:A:342:TYR:C	2.60	0.40
1:A:397:MET:HE1	1:A:401:PRO:CD	2.42	0.40
1:B:3:GLU:HG3	1:B:4:LYS:N	2.31	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:C:455:GLU:OE1	1:D:212:MET:HE3	2.21	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: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:341:ILE:HG13	1:D:342:TYR:N	2.36	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	504/521 (97%)	468 (93%)	28 (6%)	8 (2%)	9 24
1	B	506/521 (97%)	473 (94%)	28 (6%)	5 (1%)	15 37
1	C	506/521 (97%)	462 (91%)	37 (7%)	7 (1%)	11 28
1	D	501/521 (96%)	439 (88%)	51 (10%)	11 (2%)	6 17
All	All	2017/2084 (97%)	1842 (91%)	144 (7%)	31 (2%)	10 26

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

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Mol	Chain	Res	Type
1	A	115	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	457/469 (97%)	399 (87%)	58 (13%)	4 10
1	B	458/469 (98%)	405 (88%)	53 (12%)	5 12
1	C	459/469 (98%)	385 (84%)	74 (16%)	2 6
1	D	454/469 (97%)	391 (86%)	63 (14%)	3 8
All	All	1828/1876 (97%)	1580 (86%)	248 (14%)	3 8

All (248) 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	56	ARG
1	A	65	ARG
1	A	68	LYS
1	A	78	SER
1	A	79	LEU
1	A	83	GLU
1	A	87	ASN
1	A	89	VAL
1	A	93	ASN
1	A	99	GLU
1	A	103	ASN
1	A	104	ASP
1	A	120	ARG
1	A	123	LEU
1	A	128	VAL
1	A	133	LEU
1	A	138	LEU

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Mol	Chain	Res	Type
1	A	172	PHE
1	A	177	LYS
1	A	178	GLN
1	A	180	LYS
1	A	193	LEU
1	A	202	LEU
1	A	203	LEU
1	A	220	LYS
1	A	233	ARG
1	A	235	HIS
1	A	244	LEU
1	A	248	LEU
1	A	254	ARG
1	A	255	GLU
1	A	256	ASN
1	A	258	THR
1	A	295	LEU
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	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	B	39	ILE
1	B	46	SER
1	B	52	LEU
1	B	68	LYS

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Mol	Chain	Res	Type
1	B	83	GLU
1	B	96	ASP
1	B	99	GLU
1	B	102	MET
1	B	103	ASN
1	B	120	ARG
1	B	123	LEU
1	B	126	ASN
1	B	128	VAL
1	B	133	LEU
1	B	138	LEU
1	B	142	GLU
1	B	174	ILE
1	B	176	GLU
1	B	177	LYS
1	B	178	GLN
1	B	179	GLU
1	B	194	LYS
1	B	202	LEU
1	B	203	LEU
1	B	217	LYS
1	B	220	LYS
1	B	235	HIS
1	B	247	VAL
1	B	248	LEU
1	B	264	SER
1	B	271	ARG
1	B	295	LEU
1	B	296	ILE
1	B	304	ASN
1	B	308	LEU
1	B	325	LEU
1	B	335	GLU
1	B	359	ASP
1	B	370	LYS
1	B	371	LEU
1	B	427	LEU
1	B	429	LEU
1	B	431	SER
1	B	468	ASN
1	B	471	THR
1	B	472	GLN

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Mol	Chain	Res	Type
1	B	474	LYS
1	B	487	LEU
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	77	SER
1	C	82	ASP
1	C	89	VAL
1	C	99	GLU
1	C	103	ASN
1	C	104	ASP
1	C	109	ASN
1	C	123	LEU
1	C	126	ASN
1	C	128	VAL
1	C	133	LEU
1	C	138	LEU
1	C	139	GLU
1	C	141	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

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Mol	Chain	Res	Type
1	C	228	SER
1	C	233	ARG
1	C	235	HIS
1	C	243	LEU
1	C	256	ASN
1	C	257	ARG
1	C	258	THR
1	C	264	SER
1	C	271	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	327	ARG
1	C	333	ARG
1	C	335	GLU
1	C	361	THR
1	C	365	VAL
1	C	371	LEU
1	C	381	ASP
1	C	383	ARG
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	474	LYS
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

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Mol	Chain	Res	Type
1	D	25	LEU
1	D	34	LYS
1	D	41	ASN
1	D	52	LEU
1	D	68	LYS
1	D	79	LEU
1	D	81	GLN
1	D	103	ASN
1	D	104	ASP
1	D	113	CYS
1	D	120	ARG
1	D	133	LEU
1	D	138	LEU
1	D	152	GLU
1	D	171	ASP
1	D	173	MET
1	D	174	ILE
1	D	176	GLU
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	231	PHE
1	D	248	LEU
1	D	257	ARG
1	D	258	THR
1	D	271	ARG
1	D	275	ARG
1	D	289	ARG
1	D	296	ILE
1	D	304	ASN
1	D	308	LEU
1	D	311	LYS
1	D	322	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

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Mol	Chain	Res	Type
1	D	374	THR
1	D	378	ASN
1	D	381	ASP
1	D	383	ARG
1	D	404	VAL
1	D	406	SER
1	D	412	ASN
1	D	424	SER
1	D	427	LEU
1	D	437	SER
1	D	468	ASN
1	D	474	LYS
1	D	487	LEU
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 (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	93	ASN
1	A	103	ASN
1	A	126	ASN
1	A	167	ASN
1	A	250	ASN
1	A	256	ASN
1	A	268	GLN
1	A	304	ASN
1	A	306	ASN
1	A	336	ASN
1	A	357	HIS
1	A	412	ASN
1	A	419	ASN
1	A	434	ASN
1	A	468	ASN
1	A	472	GLN
1	A	476	GLN
1	B	5	ASN
1	B	24	GLN

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Mol	Chain	Res	Type
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	412	ASN
1	B	419	ASN
1	B	422	GLN
1	B	434	ASN
1	B	468	ASN
1	B	472	GLN
1	B	476	GLN
1	C	5	ASN
1	C	24	GLN
1	C	47	ASN
1	C	100	ASN
1	C	103	ASN
1	C	167	ASN
1	C	256	ASN
1	C	268	GLN
1	C	304	ASN
1	C	306	ASN
1	C	319	ASN
1	C	357	HIS
1	C	412	ASN
1	C	414	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

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Mol	Chain	Res	Type
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	304	ASN
1	D	306	ASN
1	D	336	ASN
1	D	357	HIS
1	D	412	ASN
1	D	414	ASN
1	D	419	ASN
1	D	422	GLN
1	D	434	ASN
1	D	464	HIS
1	D	468	ASN
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 monosaccharides 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	$\#\|Z\| > 2$
2	UMP	C	611	-	21,21,21	2.96	5 (23%)	31,31,31	2.18	9 (29%)
4	MTX	D	615	-	35,35,35	1.61	6 (17%)	46,49,49	2.21	18 (39%)
3	CB3	B	608	-	36,37,37	2.01	8 (22%)	46,51,51	1.97	6 (13%)
5	NDP	A	606	-	45,52,52	1.44	3 (6%)	53,80,80	1.15	3 (5%)
5	NDP	B	610	-	45,52,52	1.31	4 (8%)	53,80,80	1.19	6 (11%)
4	MTX	A	605	-	35,35,35	1.91	12 (34%)	46,49,49	1.82	11 (23%)
3	CB3	C	612	-	36,37,37	1.96	9 (25%)	46,51,51	1.96	5 (10%)
5	NDP	C	614	-	45,52,52	1.26	4 (8%)	53,80,80	1.14	4 (7%)
5	NDP	D	616	-	45,52,52	1.31	4 (8%)	53,80,80	1.37	8 (15%)
4	MTX	C	613	-	35,35,35	1.78	9 (25%)	46,49,49	1.97	12 (26%)
3	CB3	A	604	-	36,37,37	2.11	12 (33%)	46,51,51	2.01	6 (13%)
2	UMP	A	603	-	21,21,21	3.01	7 (33%)	31,31,31	2.18	9 (29%)
4	MTX	B	609	-	35,35,35	1.90	10 (28%)	46,49,49	2.06	10 (21%)
2	UMP	B	607	-	21,21,21	2.95	5 (23%)	31,31,31	2.22	9 (29%)

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
2	UMP	C	611	-	-	3/10/22/22	0/2/2/2
4	MTX	D	615	-	-	4/25/25/25	0/3/3/3
3	CB3	B	608	-	1/1/5/6	7/27/28/28	0/3/3/3
5	NDP	A	606	-	-	2/30/77/77	0/5/5/5
5	NDP	B	610	-	-	6/30/77/77	0/5/5/5
4	MTX	A	605	-	-	5/25/25/25	0/3/3/3
3	CB3	C	612	-	1/1/5/6	7/27/28/28	0/3/3/3
5	NDP	C	614	-	-	7/30/77/77	0/5/5/5
5	NDP	D	616	-	-	4/30/77/77	0/5/5/5
4	MTX	C	613	-	-	5/25/25/25	0/3/3/3
2	UMP	A	603	-	-	3/10/22/22	0/2/2/2
3	CB3	A	604	-	1/1/5/6	7/27/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MTX	B	609	-	-	2/25/25/25	0/3/3/3
2	UMP	B	607	-	-	3/10/22/22	0/2/2/2

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	UMP	C6-C5	8.45	1.54	1.35
2	A	603	UMP	C6-C5	8.44	1.54	1.35
2	C	611	UMP	C6-C5	8.42	1.54	1.35
3	A	604	CB3	CP1-CP2	5.76	1.54	1.47
2	A	603	UMP	C6-N1	5.74	1.51	1.38
2	B	607	UMP	C6-N1	5.70	1.51	1.38
2	C	611	UMP	C6-N1	5.69	1.51	1.38
2	C	611	UMP	C5-C4	5.61	1.56	1.43
5	A	606	NDP	C4N-C3N	-5.58	1.38	1.49
2	B	607	UMP	C5-C4	5.49	1.55	1.43
3	B	608	CB3	CP1-CP2	5.46	1.54	1.47
2	A	603	UMP	C5-C4	5.44	1.55	1.43
4	C	613	MTX	C-N	-5.41	1.22	1.34
4	B	609	MTX	C-N	-5.35	1.22	1.34
3	A	604	CB3	O4-C4	5.08	1.37	1.24
3	B	608	CB3	O4-C4	4.98	1.37	1.24
5	D	616	NDP	C4N-C3N	-4.94	1.40	1.49
3	C	612	CB3	O4-C4	4.92	1.36	1.24
5	C	614	NDP	C4N-C3N	-4.90	1.40	1.49
3	C	612	CB3	CP1-CP2	4.90	1.53	1.47
3	A	604	CB3	CP1-N10	4.84	1.50	1.46
5	B	610	NDP	C4N-C3N	-4.63	1.40	1.49
3	C	612	CB3	CP1-N10	4.49	1.50	1.46
4	A	605	MTX	C-N	-4.41	1.24	1.34
4	D	615	MTX	C-N	-4.32	1.24	1.34
3	B	608	CB3	CP1-N10	4.26	1.50	1.46
5	D	616	NDP	C6N-C5N	4.22	1.40	1.33
2	A	603	UMP	C2-N1	4.03	1.44	1.38
5	A	606	NDP	C4N-C5N	-4.02	1.38	1.48
5	B	610	NDP	C6N-C5N	3.99	1.40	1.33
2	C	611	UMP	C2-N1	3.95	1.44	1.38
4	A	605	MTX	C8A-N8	-3.81	1.31	1.37
2	B	607	UMP	C2-N1	3.79	1.44	1.38
4	C	613	MTX	C8A-N8	-3.78	1.31	1.37
5	C	614	NDP	C6N-C5N	3.59	1.39	1.33
5	C	614	NDP	C4N-C5N	-3.47	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	615	MTX	O-C	3.38	1.30	1.23
4	B	609	MTX	C8A-N8	-3.32	1.32	1.37
2	A	603	UMP	P-OP1	3.31	1.61	1.50
3	A	604	CB3	C9-N10	3.31	1.51	1.46
4	A	605	MTX	O-C	3.28	1.30	1.23
2	C	611	UMP	P-OP1	3.25	1.61	1.50
4	D	615	MTX	C8A-N8	-3.20	1.32	1.37
5	B	610	NDP	C4N-C5N	-3.19	1.40	1.48
3	C	612	CB3	C9-N10	3.18	1.50	1.46
5	A	606	NDP	C6N-C5N	3.16	1.39	1.33
5	D	616	NDP	C4N-C5N	-3.15	1.40	1.48
2	B	607	UMP	P-OP1	3.13	1.60	1.50
4	C	613	MTX	O-C	3.09	1.29	1.23
3	B	608	CB3	C9-N10	3.05	1.50	1.46
4	A	605	MTX	C4A-N5	-2.95	1.31	1.37
4	A	605	MTX	C4A-C8A	-2.92	1.35	1.40
4	B	609	MTX	O2-CT	-2.77	1.21	1.30
4	C	613	MTX	C4A-C8A	-2.68	1.35	1.40
3	C	612	CB3	C11-C	2.68	1.55	1.50
3	B	608	CB3	C11-C	2.64	1.55	1.50
4	B	609	MTX	O-C	2.63	1.28	1.23
4	A	605	MTX	C2-N3	-2.61	1.30	1.35
3	A	604	CB3	C11-C	2.60	1.55	1.50
4	A	605	MTX	C8A-N1	-2.58	1.31	1.36
4	C	613	MTX	O2-CT	-2.56	1.22	1.30
4	B	609	MTX	C2-N3	-2.53	1.30	1.35
3	A	604	CB3	C8-C7	2.50	1.41	1.36
4	C	613	MTX	C8A-N1	-2.50	1.31	1.36
3	B	608	CB3	C15-C14	2.47	1.44	1.39
4	A	605	MTX	C4-N3	-2.46	1.29	1.33
4	A	605	MTX	C4-C4A	-2.45	1.34	1.43
4	B	609	MTX	OE2-CD	-2.41	1.22	1.30
2	A	603	UMP	O4'-C1'	2.41	1.47	1.42
4	A	605	MTX	O2-CT	-2.40	1.22	1.30
3	B	608	CB3	C8-C7	2.39	1.41	1.36
3	C	612	CB3	C15-C14	2.39	1.44	1.39
3	C	612	CB3	C8-C7	2.32	1.41	1.36
5	D	616	NDP	O4B-C1B	2.29	1.44	1.41
2	A	603	UMP	O4'-C4'	2.28	1.50	1.45
4	D	615	MTX	C4A-C8A	-2.26	1.36	1.40
3	C	612	CB3	C16-C15	2.23	1.42	1.38
3	A	604	CB3	C16-C15	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	MTX	OE2-CD	-2.22	1.23	1.30
3	A	604	CB3	C15-C14	2.22	1.43	1.39
4	D	615	MTX	C8A-N1	-2.17	1.32	1.36
4	B	609	MTX	CA-CT	-2.17	1.47	1.52
4	C	613	MTX	C12-C11	-2.15	1.35	1.39
4	B	609	MTX	C4A-N5	-2.15	1.33	1.37
3	A	604	CB3	C4-N3	2.13	1.36	1.33
5	B	610	NDP	O4B-C1B	2.10	1.44	1.41
4	B	609	MTX	C16-C11	-2.10	1.35	1.39
3	B	608	CB3	C16-C15	2.09	1.42	1.38
5	C	614	NDP	O4B-C1B	2.09	1.44	1.41
4	D	615	MTX	O2-CT	-2.08	1.23	1.30
4	C	613	MTX	C4-C4A	-2.08	1.35	1.43
3	A	604	CB3	CA-N	2.07	1.50	1.45
4	C	613	MTX	C4A-N5	-2.06	1.33	1.37
4	A	605	MTX	CA-CT	-2.05	1.47	1.52
3	C	612	CB3	C4-N3	2.04	1.36	1.33
3	A	604	CB3	C5-C6	2.02	1.42	1.37
4	B	609	MTX	C11-C	-2.01	1.46	1.50
3	A	604	CB3	CG-CD	2.01	1.55	1.50

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	604	CB3	C4A-C8A-N1	-7.57	119.49	123.60
3	B	608	CB3	C4A-C8A-N1	-7.15	119.72	123.60
3	C	612	CB3	C4A-C8A-N1	-6.86	119.88	123.60
3	A	604	CB3	C4A-C4-N3	-6.74	119.70	124.40
3	C	612	CB3	C4A-C4-N3	-6.73	119.71	124.40
3	B	608	CB3	C4A-C4-N3	-6.69	119.74	124.40
4	B	609	MTX	C6-C9-N10	-6.08	103.18	113.60
4	D	615	MTX	C6-C9-N10	-5.89	103.50	113.60
4	D	615	MTX	CB-CA-N	-5.76	99.23	110.88
2	B	607	UMP	C5-C6-N1	-5.64	112.37	121.81
2	C	611	UMP	C5-C6-N1	-5.56	112.49	121.81
2	A	603	UMP	C5-C6-N1	-5.51	112.58	121.81
4	A	605	MTX	C6-C9-N10	-5.50	104.18	113.60
2	A	603	UMP	C6-C5-C4	-5.40	112.13	119.52
5	D	616	NDP	N3A-C2A-N1A	-5.35	120.32	128.68
2	B	607	UMP	C6-C5-C4	-5.32	112.25	119.52
3	C	612	CB3	N1-C2-N3	-5.29	120.17	127.22
4	C	613	MTX	C6-C9-N10	-5.25	104.60	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	611	UMP	C6-C5-C4	-5.22	112.39	119.52
3	B	608	CB3	N1-C2-N3	-5.18	120.31	127.22
3	A	604	CB3	N1-C2-N3	-5.17	120.33	127.22
4	B	609	MTX	C4A-C4-N3	-5.11	117.66	121.01
4	C	613	MTX	CG-CB-CA	-4.92	103.95	113.16
5	B	610	NDP	N3A-C2A-N1A	-4.91	121.01	128.68
5	C	614	NDP	N3A-C2A-N1A	-4.72	121.30	128.68
2	B	607	UMP	N3-C2-N1	4.62	121.03	114.89
4	B	609	MTX	CB-CA-N	-4.62	101.54	110.88
2	C	611	UMP	N3-C2-N1	4.50	120.86	114.89
4	C	613	MTX	N1-C2-N3	-4.48	121.24	127.22
2	A	603	UMP	N3-C2-N1	4.42	120.75	114.89
5	A	606	NDP	N3A-C2A-N1A	-4.41	121.78	128.68
4	D	615	MTX	CB-CG-CD	-4.03	101.82	112.51
2	B	607	UMP	C5-C4-N3	3.98	120.79	114.84
4	B	609	MTX	N8-C8A-N1	3.97	120.35	115.82
4	B	609	MTX	C13-C14-N10	-3.96	115.93	121.62
2	C	611	UMP	C5-C4-N3	3.92	120.71	114.84
4	D	615	MTX	C2-N1-C8A	3.91	119.83	115.36
2	A	603	UMP	C5-C4-N3	3.91	120.69	114.84
4	D	615	MTX	N1-C2-N3	-3.84	122.10	127.22
4	A	605	MTX	N8-C8A-N1	3.77	120.13	115.82
4	A	605	MTX	C4A-C4-N3	-3.71	118.57	121.01
4	C	613	MTX	C2-N1-C8A	3.61	119.47	115.36
4	B	609	MTX	N1-C2-N3	-3.60	122.43	127.22
4	A	605	MTX	N1-C2-N3	-3.43	122.65	127.22
4	D	615	MTX	C13-C14-N10	-3.43	116.69	121.62
2	C	611	UMP	O4'-C1'-N1	3.40	113.93	107.86
3	C	612	CB3	C2-N3-C4	3.38	121.29	115.93
2	A	603	UMP	O4'-C1'-N1	3.37	113.89	107.86
4	A	605	MTX	C6-C7-N8	-3.35	119.84	123.13
2	B	607	UMP	O4'-C1'-N1	3.35	113.85	107.86
3	B	608	CB3	C2-N3-C4	3.33	121.22	115.93
3	A	604	CB3	C2-N3-C4	3.27	121.12	115.93
5	D	616	NDP	O4D-C1D-N1N	3.25	114.40	108.06
4	C	613	MTX	O-C-N	-3.25	116.48	122.45
4	C	613	MTX	C4A-C4-N3	-3.16	118.94	121.01
4	D	615	MTX	OE1-CD-CG	-3.11	113.10	123.08
2	B	607	UMP	O4-C4-C5	-3.03	119.83	125.16
4	C	613	MTX	C6-C7-N8	-3.02	120.17	123.13
4	C	613	MTX	N8-C8A-N1	3.01	119.25	115.82
4	B	609	MTX	C7-N8-C8A	3.01	119.71	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	613	MTX	C7-N8-C8A	2.98	119.69	116.69
4	A	605	MTX	C7-N8-C8A	2.98	119.69	116.69
2	C	611	UMP	O4-C4-C5	-2.94	119.99	125.16
4	A	605	MTX	CB-CA-CT	-2.93	103.30	110.35
2	A	603	UMP	O4-C4-C5	-2.89	120.08	125.16
2	B	607	UMP	OP3-P-OP2	2.84	118.49	107.64
2	A	603	UMP	OP3-P-OP2	2.84	118.47	107.64
4	D	615	MTX	C9-C6-N5	2.83	121.49	116.96
2	C	611	UMP	OP3-P-OP2	2.80	118.33	107.64
4	B	609	MTX	C2-N1-C8A	2.80	118.55	115.36
4	A	605	MTX	C13-C14-N10	-2.79	117.61	121.62
4	D	615	MTX	OE2-CD-CG	2.67	122.61	114.03
5	C	614	NDP	O3X-P2B-O2X	2.64	117.71	107.64
4	C	613	MTX	C13-C14-N10	-2.60	117.89	121.62
4	B	609	MTX	C6-C7-N8	-2.59	120.59	123.13
5	C	614	NDP	O4D-C1D-N1N	2.54	113.02	108.06
4	D	615	MTX	O2-CT-CA	2.53	121.81	113.40
4	D	615	MTX	C6-C7-N8	-2.49	120.69	123.13
5	D	616	NDP	C1B-N9A-C4A	-2.46	122.31	126.64
4	D	615	MTX	CG-CB-CA	-2.46	108.55	113.16
4	A	605	MTX	C2-N1-C8A	2.46	118.16	115.36
5	B	610	NDP	O3X-P2B-O1X	2.44	120.23	110.68
4	B	609	MTX	CG-CB-CA	-2.44	108.60	113.16
5	B	610	NDP	C1D-N1N-C2N	-2.43	117.07	121.11
5	A	606	NDP	PN-O3-PA	-2.41	124.57	132.83
5	C	614	NDP	C4A-C5A-N7A	-2.40	106.89	109.40
2	B	607	UMP	O2-C2-N1	-2.36	119.65	122.79
4	D	615	MTX	N8-C8A-N1	2.35	118.50	115.82
4	D	615	MTX	C7-N8-C8A	2.34	119.05	116.69
5	D	616	NDP	O3X-P2B-O2X	2.34	116.58	107.64
3	C	612	CB3	CA-N-C	2.31	127.26	121.60
5	B	610	NDP	O4D-C1D-N1N	2.30	112.56	108.06
5	D	616	NDP	C3N-C2N-N1N	-2.30	119.81	123.10
2	C	611	UMP	O2-C2-N1	-2.26	119.78	122.79
5	A	606	NDP	C4A-C5A-N7A	-2.26	107.05	109.40
2	B	607	UMP	C4-N3-C2	-2.25	123.61	126.58
5	D	616	NDP	C3N-C7N-N7N	-2.22	113.72	117.67
5	B	610	NDP	O4B-C1B-C2B	-2.19	102.78	106.59
4	A	605	MTX	O2-CT-CA	2.19	120.67	113.40
3	B	608	CB3	CA-N-C	2.18	126.93	121.60
5	D	616	NDP	C1D-N1N-C2N	-2.14	117.55	121.11
4	D	615	MTX	C4-C4A-N5	2.13	121.97	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	611	UMP	C4-N3-C2	-2.12	123.79	126.58
4	C	613	MTX	NA2-C2-N3	2.11	120.54	117.25
5	D	616	NDP	O2B-P2B-O1X	-2.11	101.26	109.39
5	B	610	NDP	C2B-C3B-C4B	-2.09	97.45	101.99
4	A	605	MTX	CA-N-C	2.08	126.69	121.60
4	C	613	MTX	C11-C-N	2.08	121.05	117.06
2	A	603	UMP	O2-C2-N1	-2.08	120.02	122.79
2	A	603	UMP	C4-N3-C2	-2.07	123.86	126.58
4	D	615	MTX	C9-C6-C7	-2.06	118.00	121.60
3	A	604	CB3	CA-N-C	2.05	126.62	121.60
4	D	615	MTX	NA2-C2-N3	2.05	120.44	117.25
3	B	608	CB3	C6-C5-C4A	-2.02	119.62	122.65
3	A	604	CB3	C6-C5-C4A	-2.02	119.63	122.65
4	D	615	MTX	CT-CA-N	2.01	115.31	110.55

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 (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	610	NDP	C2B-O2B-P2B-O1X
5	B	610	NDP	C2B-O2B-P2B-O3X
5	C	614	NDP	C5B-O5B-PA-O1A
5	C	614	NDP	C5B-O5B-PA-O2A
5	C	614	NDP	C3B-C4B-C5B-O5B
4	A	605	MTX	N-CA-CB-CG
3	A	604	CB3	CB-CA-N-C
3	B	608	CB3	CB-CA-N-C
3	C	612	CB3	CB-CA-N-C
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
4	C	613	MTX	C13-C14-N10-CM
4	C	613	MTX	CT-CA-N-C
5	C	614	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	A	604	CB3	N-CA-CT-O2
3	B	608	CB3	N-CA-CT-O2
3	C	612	CB3	N-CA-CT-O2
4	D	615	MTX	CB-CA-N-C
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
5	A	606	NDP	C2B-O2B-P2B-O3X
4	A	605	MTX	C6-C9-N10-CM
4	C	613	MTX	C6-C9-N10-CM
5	A	606	NDP	O4D-C1D-N1N-C2N
5	B	610	NDP	C4D-C5D-O5D-PN
3	A	604	CB3	CB-CA-CT-O2
3	B	608	CB3	CB-CA-CT-O2
3	C	612	CB3	CB-CA-CT-O1
5	C	614	NDP	O4D-C1D-N1N-C2N
4	D	615	MTX	N-CA-CB-CG
4	B	609	MTX	C13-C14-N10-CM
4	B	609	MTX	C15-C14-N10-CM
3	A	604	CB3	CB-CA-CT-O1
3	B	608	CB3	CB-CA-CT-O1
3	C	612	CB3	CB-CA-CT-O2
5	B	610	NDP	O4D-C1D-N1N-C2N
5	D	616	NDP	O4D-C1D-N1N-C2N
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	A	605	MTX	OE1-CD-CG-CB
4	A	605	MTX	OE2-CD-CG-CB
3	C	612	CB3	OE1-CD-CG-CB
3	A	604	CB3	OE1-CD-CG-CB
3	B	608	CB3	OE1-CD-CG-CB
2	B	607	UMP	O4'-C4'-C5'-O5'
4	C	613	MTX	CB-CA-N-C
3	A	604	CB3	OE2-CD-CG-CB
5	C	614	NDP	C5B-O5B-PA-O3
3	C	612	CB3	OE2-CD-CG-CB
2	A	603	UMP	O4'-C4'-C5'-O5'
2	C	611	UMP	O4'-C4'-C5'-O5'
3	B	608	CB3	OE2-CD-CG-CB
5	B	610	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
5	D	616	NDP	C2N-C3N-C7N-N7N
4	D	615	MTX	CT-CA-N-C
2	A	603	UMP	C2'-C1'-N1-C6
2	B	607	UMP	C2'-C1'-N1-C6
2	C	611	UMP	C2'-C1'-N1-C6
5	B	610	NDP	C2D-C1D-N1N-C2N

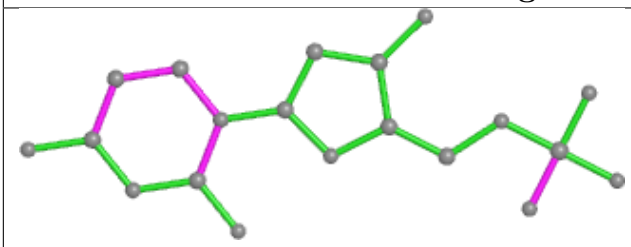
There are no ring outliers.

14 monomers are involved in 96 short contacts:

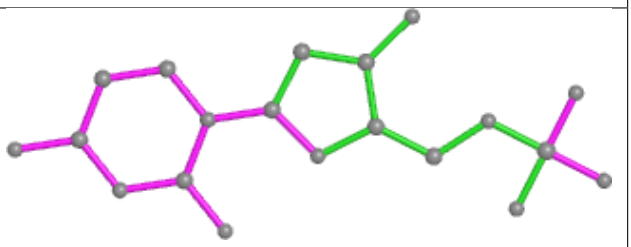
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	611	UMP	9	0
4	D	615	MTX	13	0
3	B	608	CB3	8	0
5	A	606	NDP	4	0
5	B	610	NDP	6	0
4	A	605	MTX	1	0
3	C	612	CB3	10	0
5	C	614	NDP	7	0
5	D	616	NDP	8	0
4	C	613	MTX	6	0
3	A	604	CB3	11	0
2	A	603	UMP	7	0
4	B	609	MTX	4	0
2	B	607	UMP	9	0

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

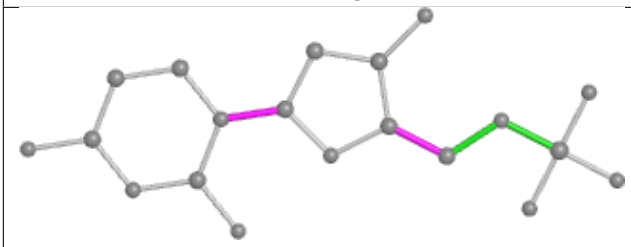
Ligand UMP C 611



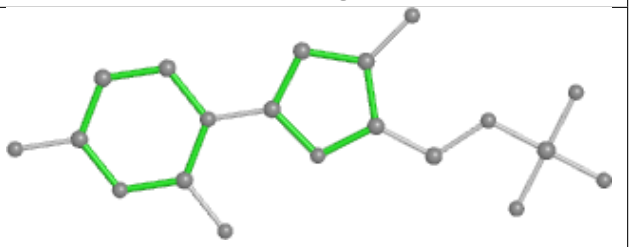
Bond lengths



Bond angles

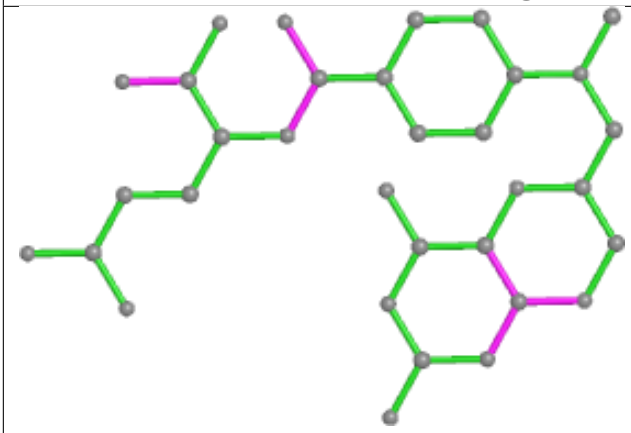


Torsions

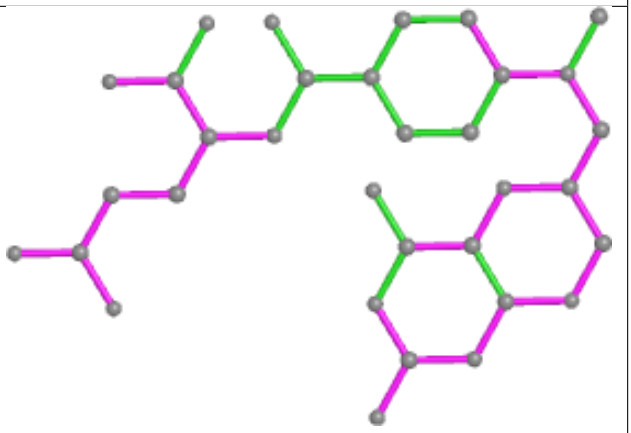


Rings

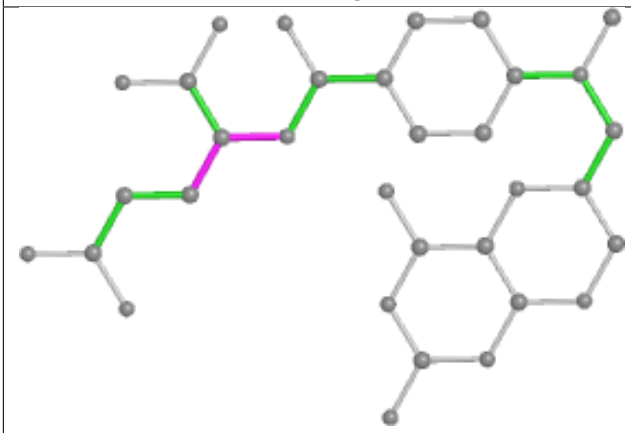
Ligand MTX D 615



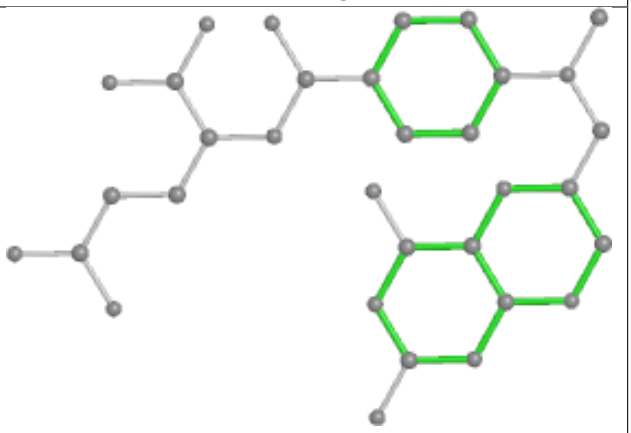
Bond lengths



Bond angles

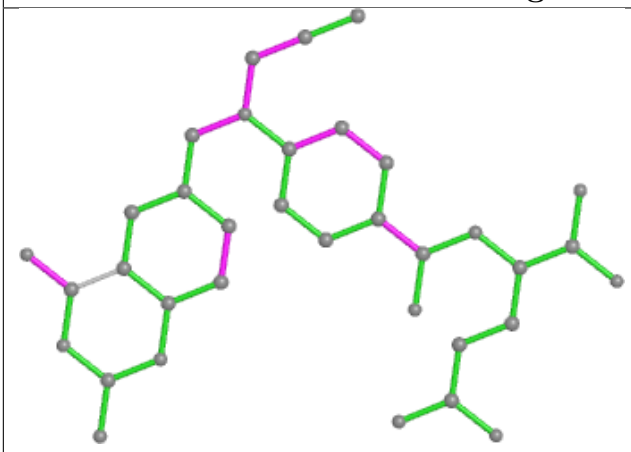


Torsions

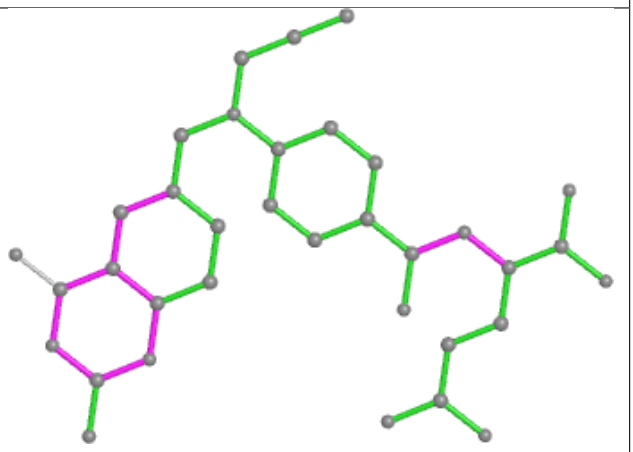


Rings

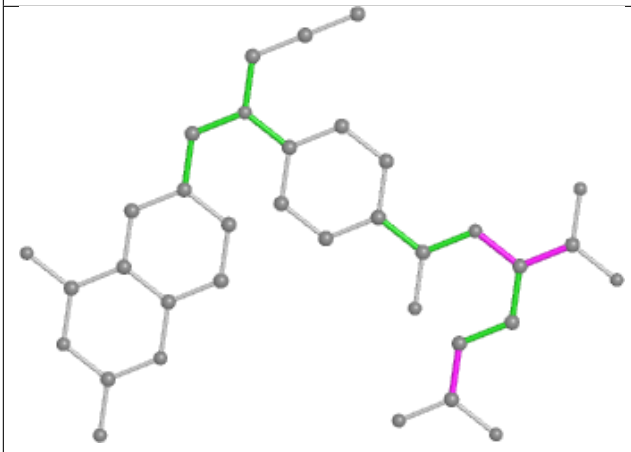
Ligand CB3 B 608



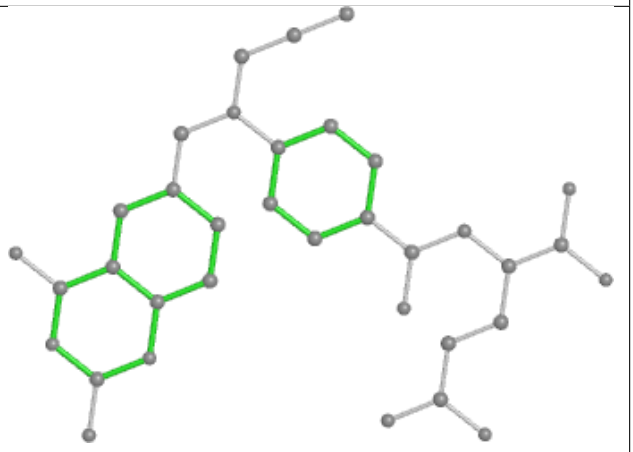
Bond lengths



Bond angles

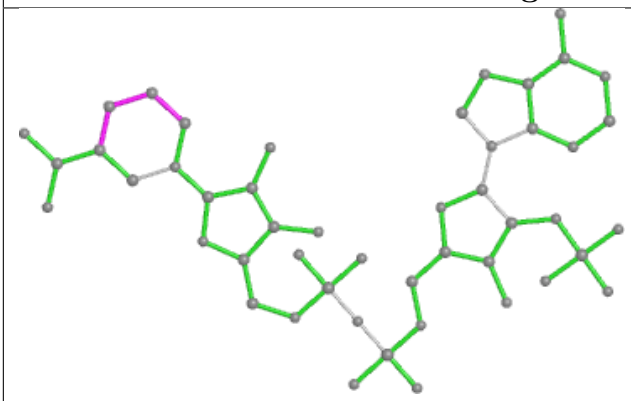


Torsions

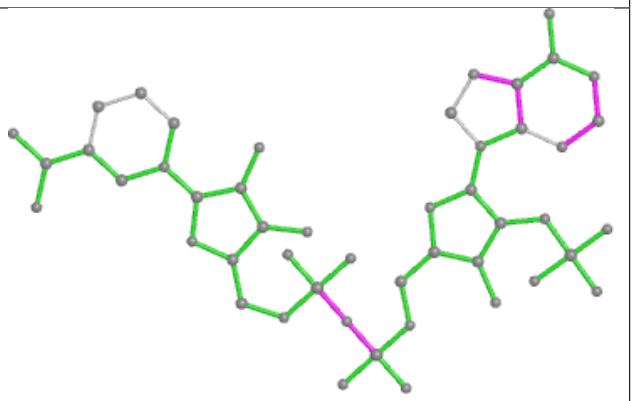


Rings

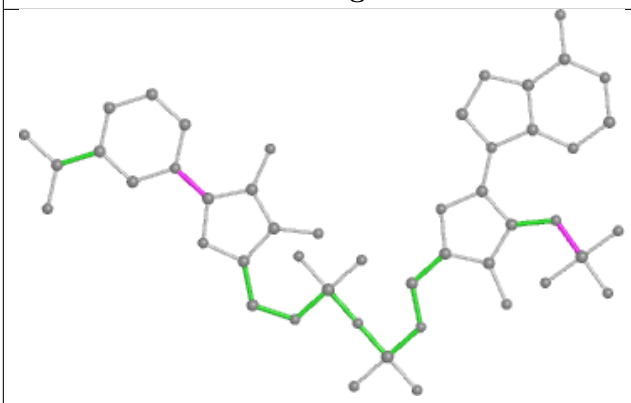
Ligand NDP A 606



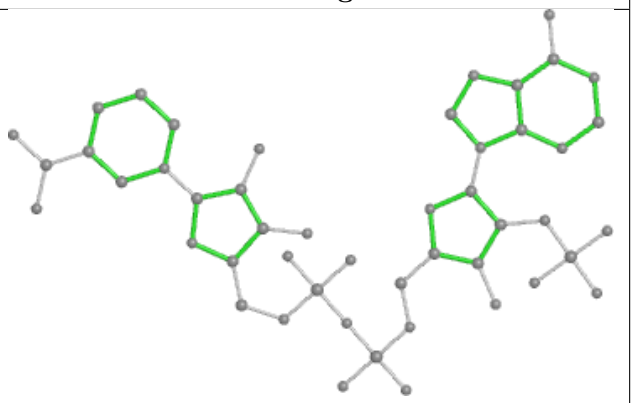
Bond lengths



Bond angles

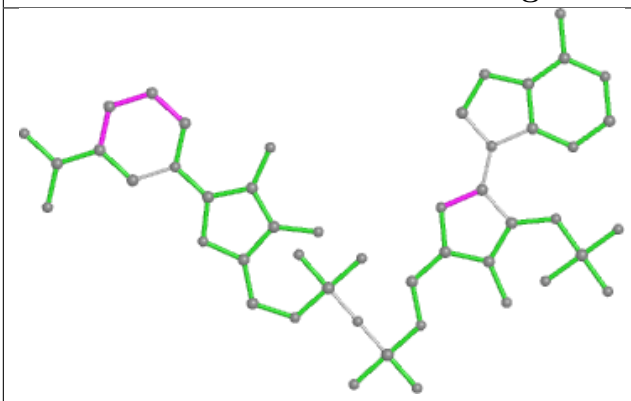


Torsions

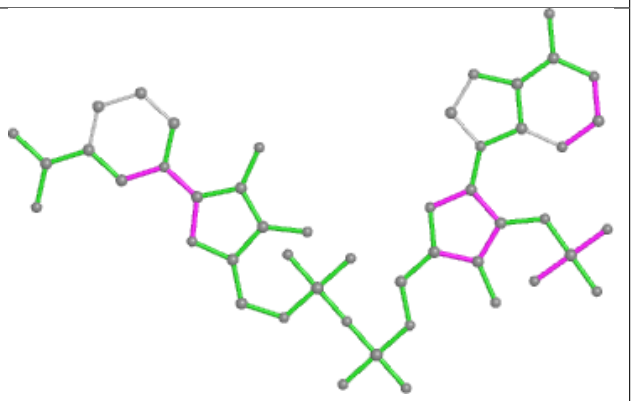


Rings

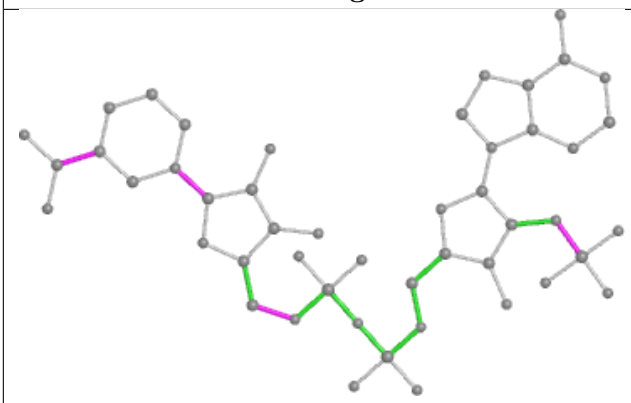
Ligand NDP B 610



Bond lengths



Bond angles



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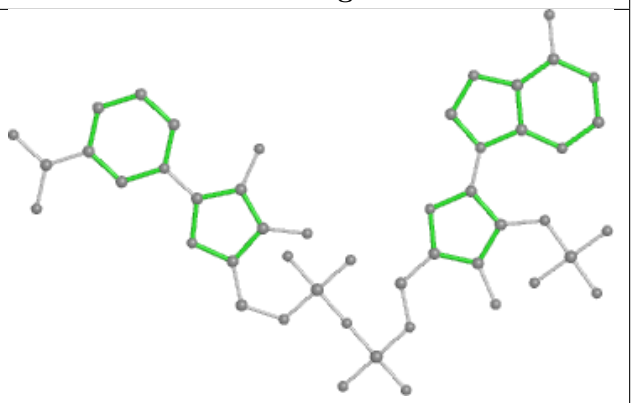
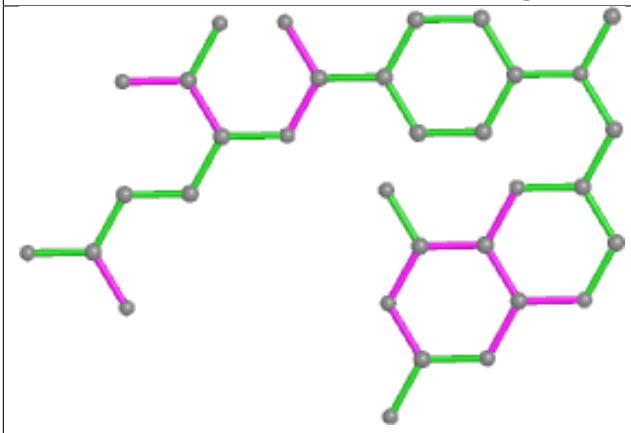


Rings

Ligand MTX A 605



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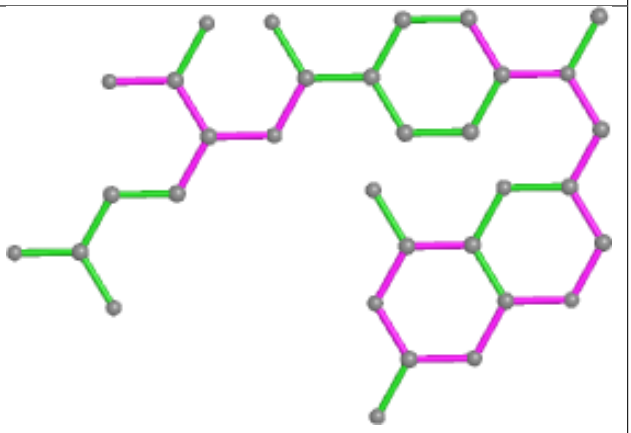
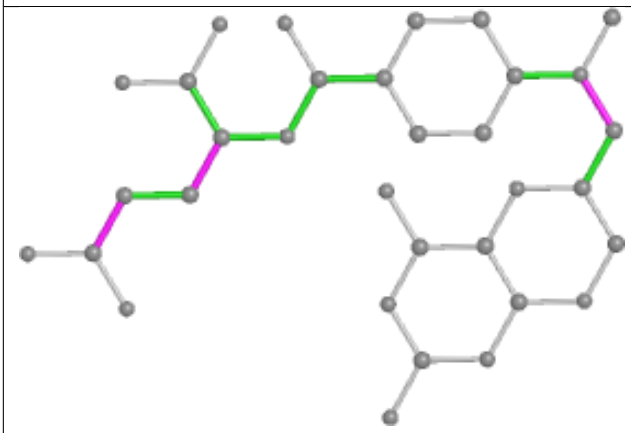


Bond angles



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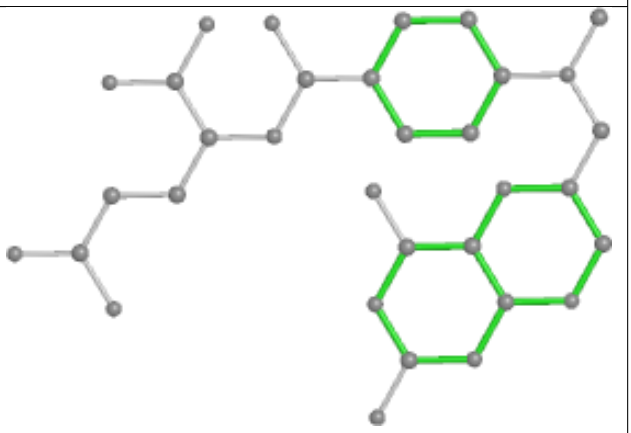
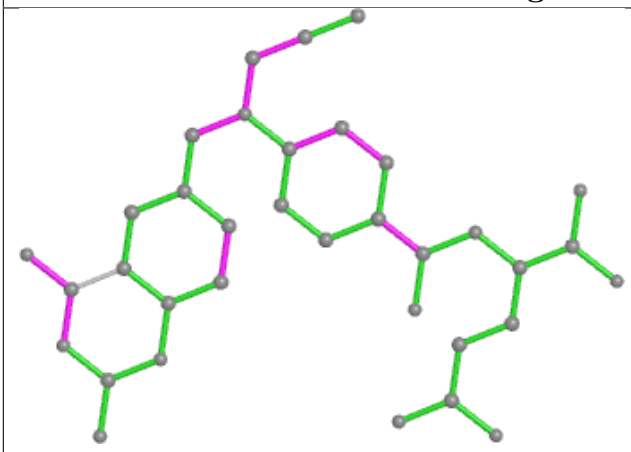
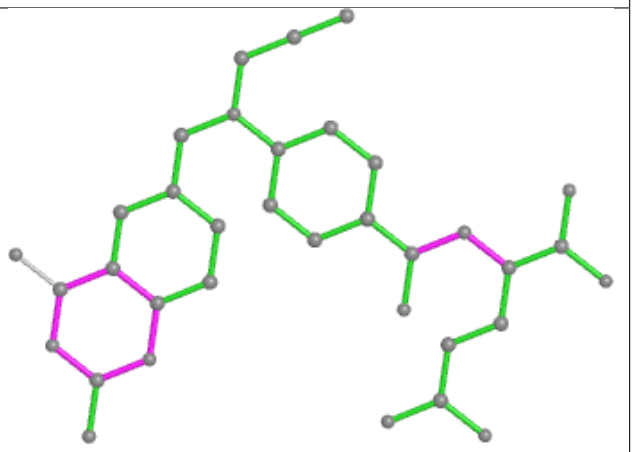


Rings

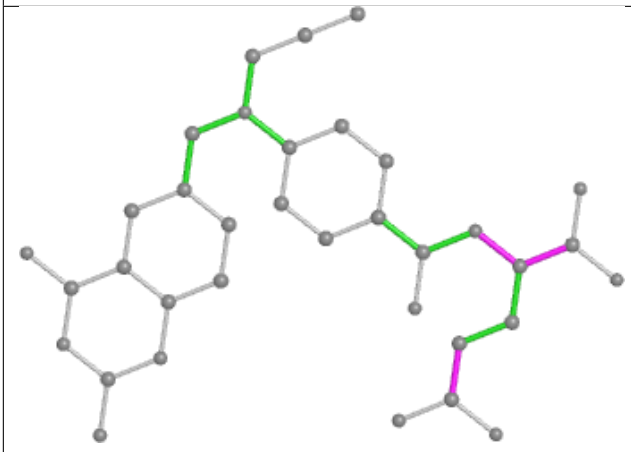
Ligand CB3 C 612



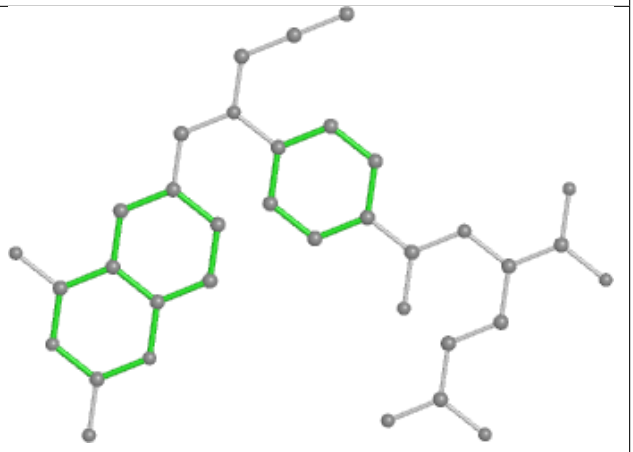
Bond lengths



Bond angles

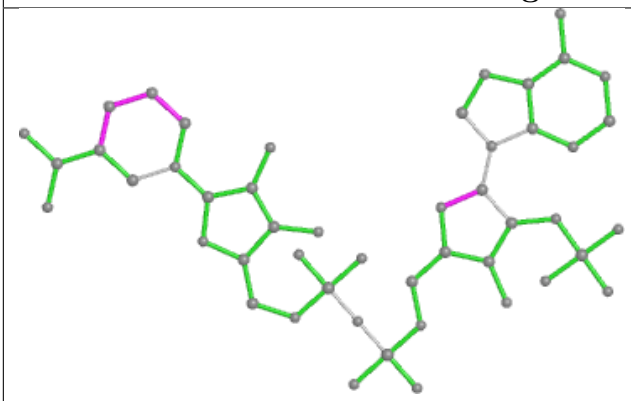


Torsions

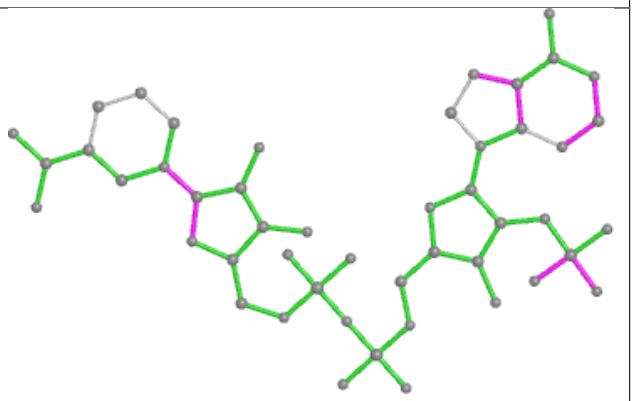


Rings

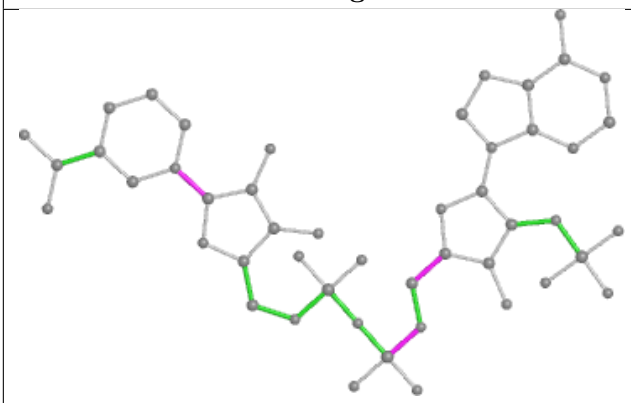
Ligand NDP C 614



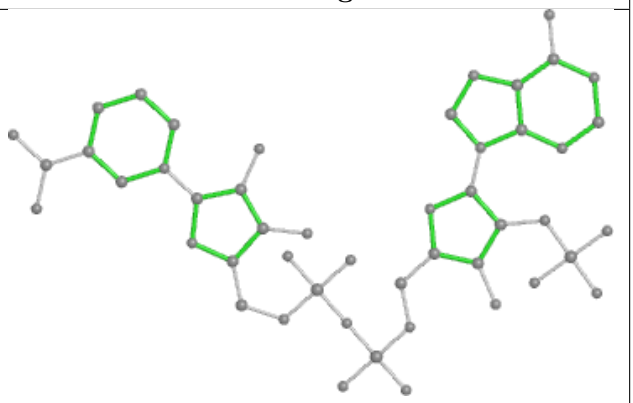
Bond lengths



Bond angles

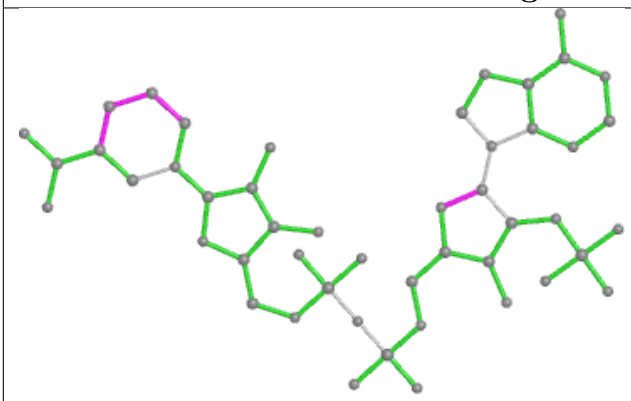


Torsions

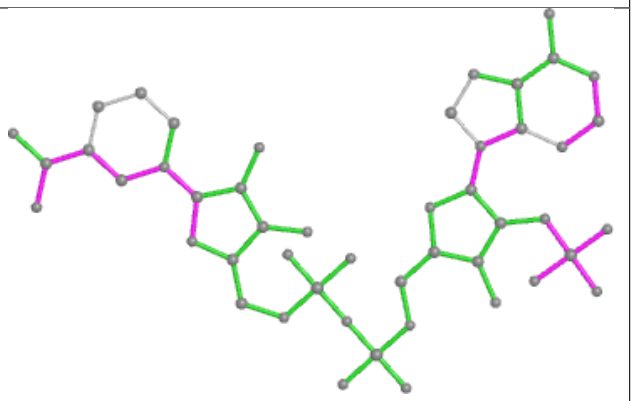


Rings

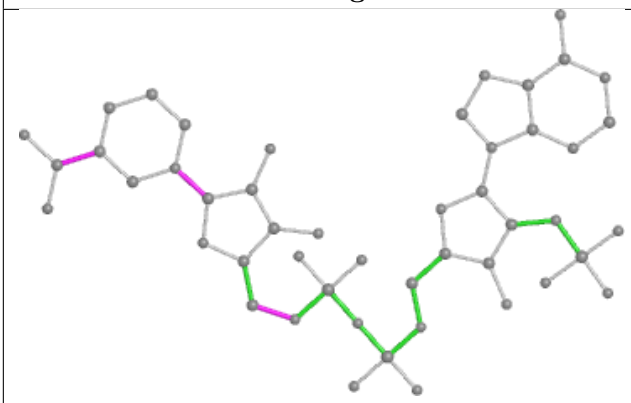
Ligand NDP D 616



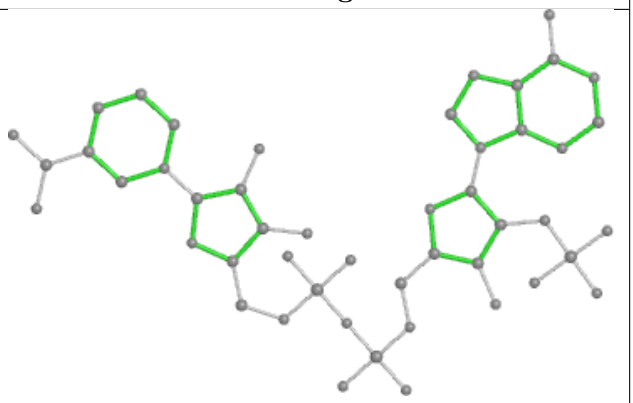
Bond lengths



Bond angles

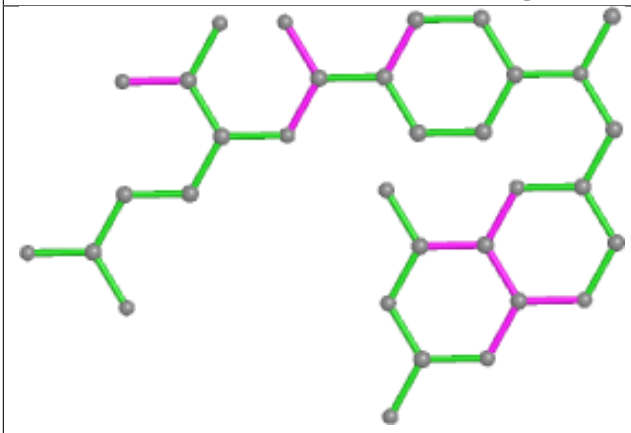


Torsions

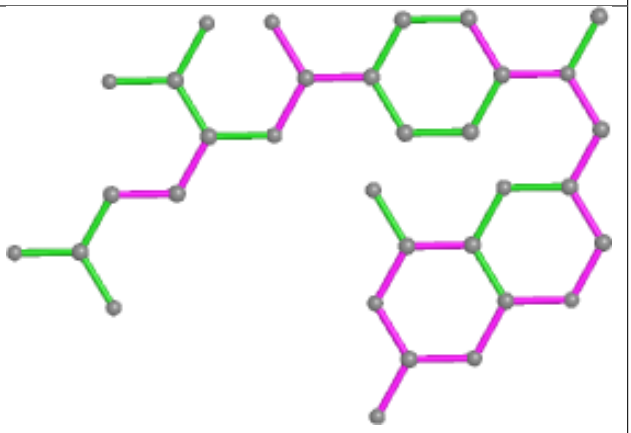


Rings

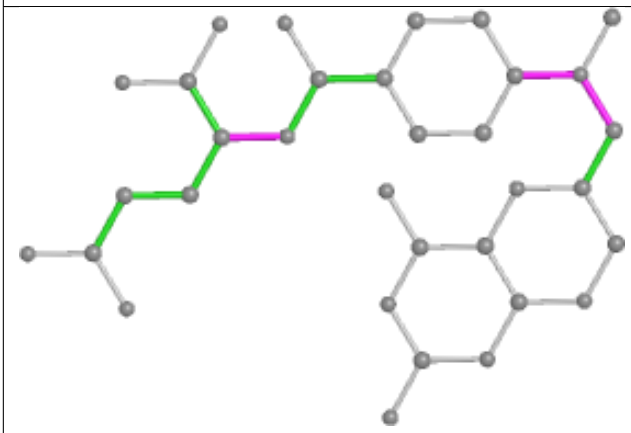
Ligand MTX C 613



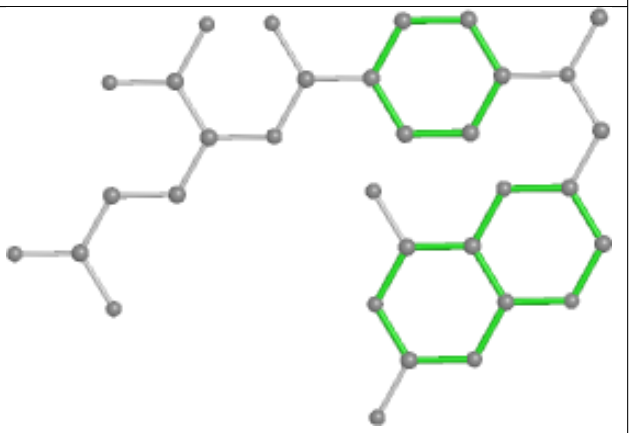
Bond lengths



Bond angles

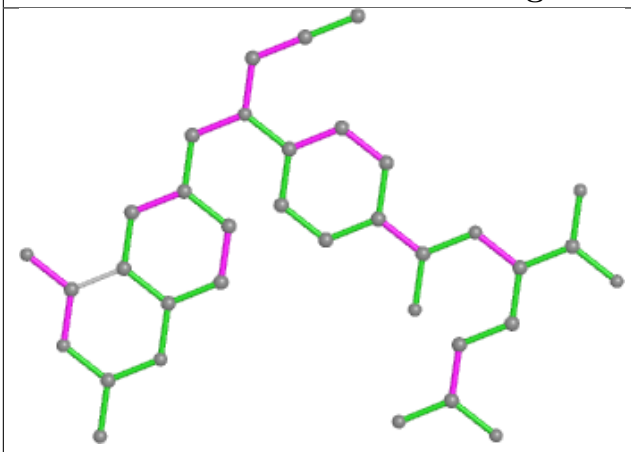


Torsions

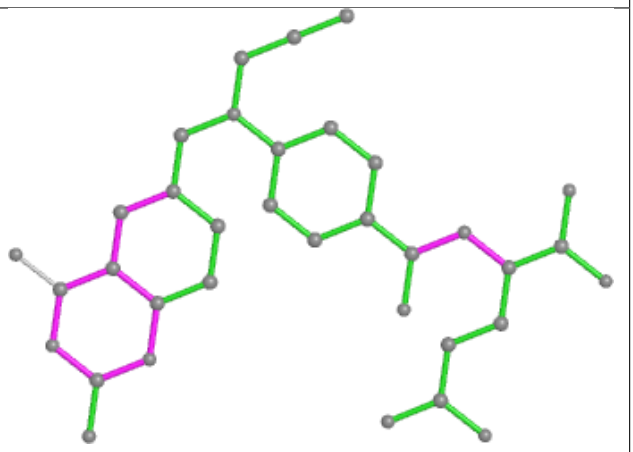


Rings

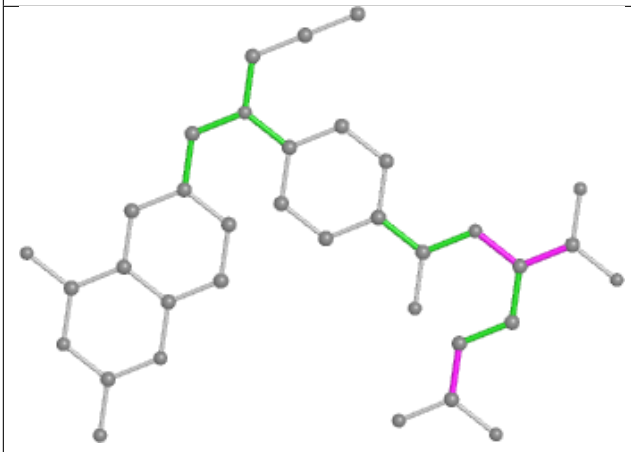
Ligand CB3 A 604



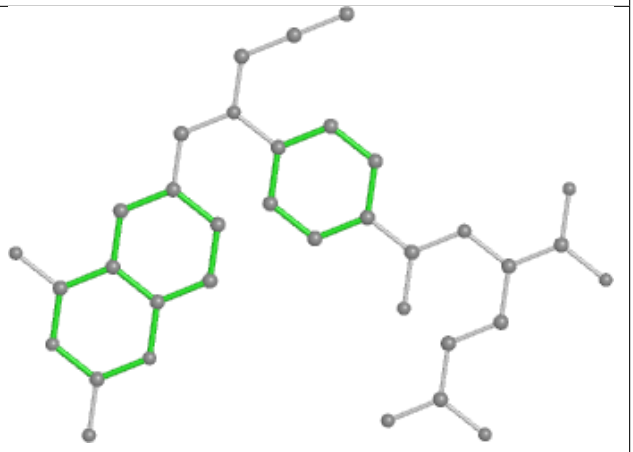
Bond lengths



Bond angles

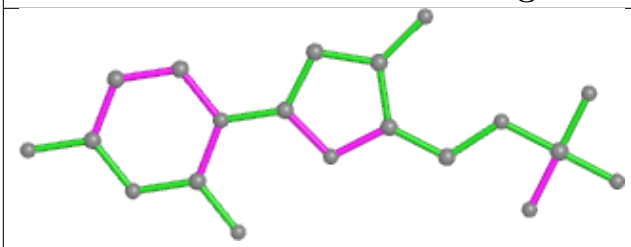


Torsions

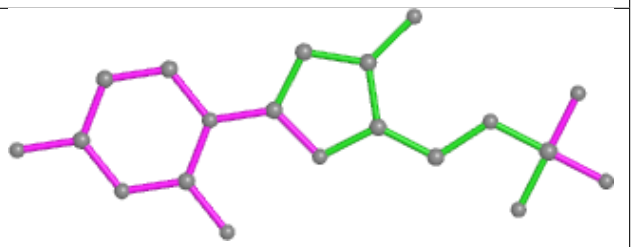


Rings

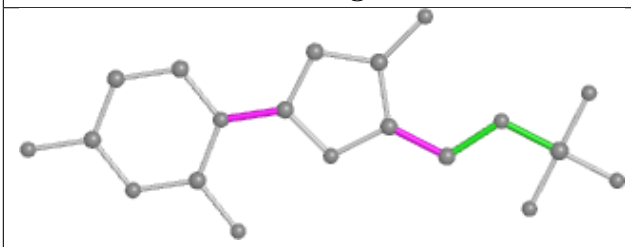
Ligand UMP A 603



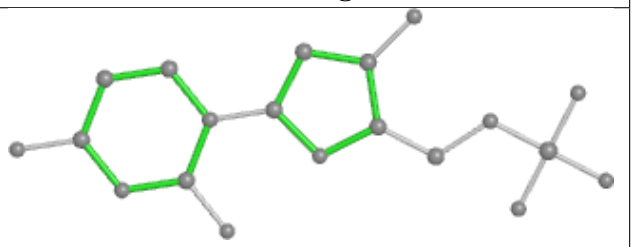
Bond lengths



Bond angles

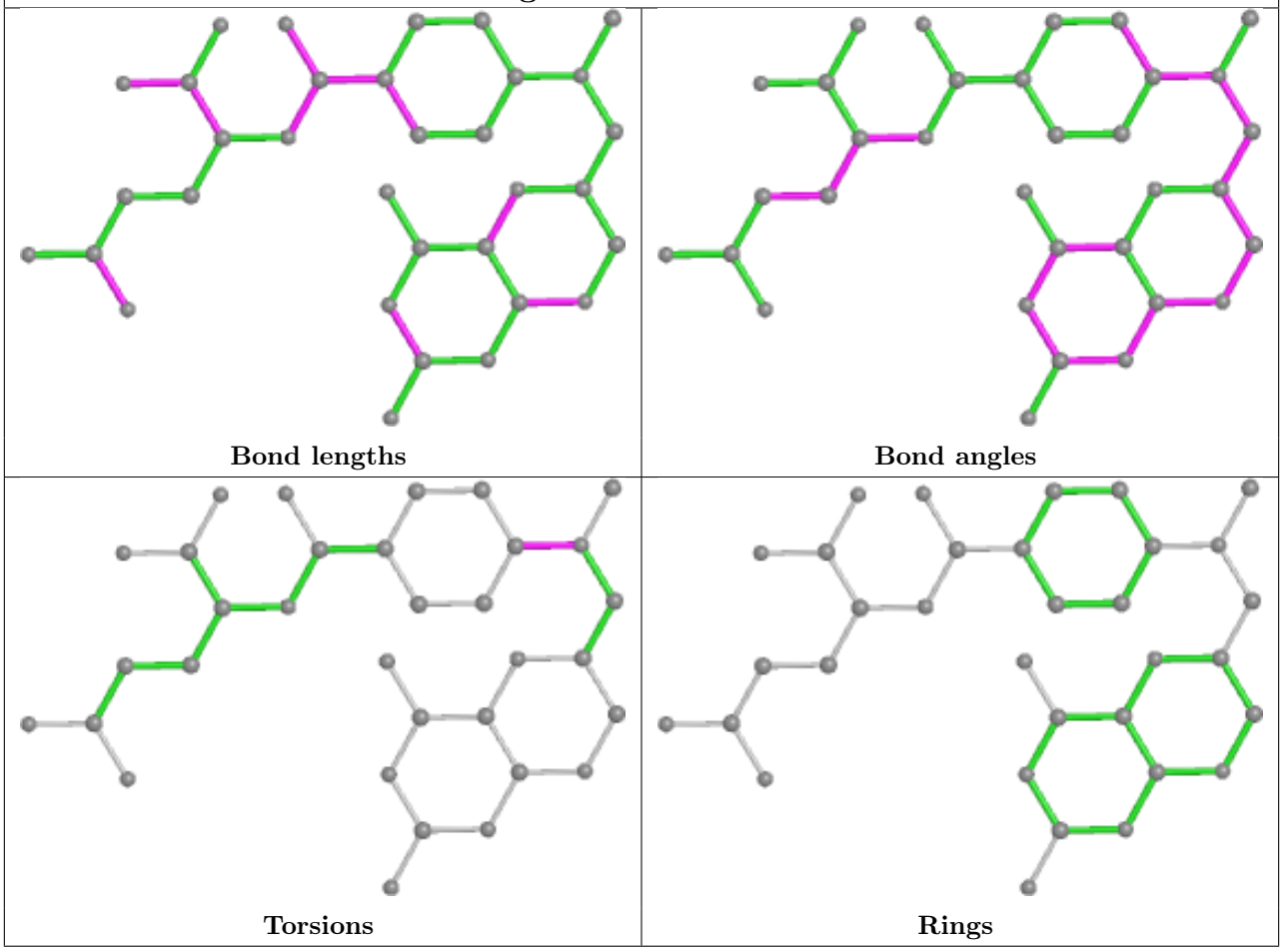


Torsions

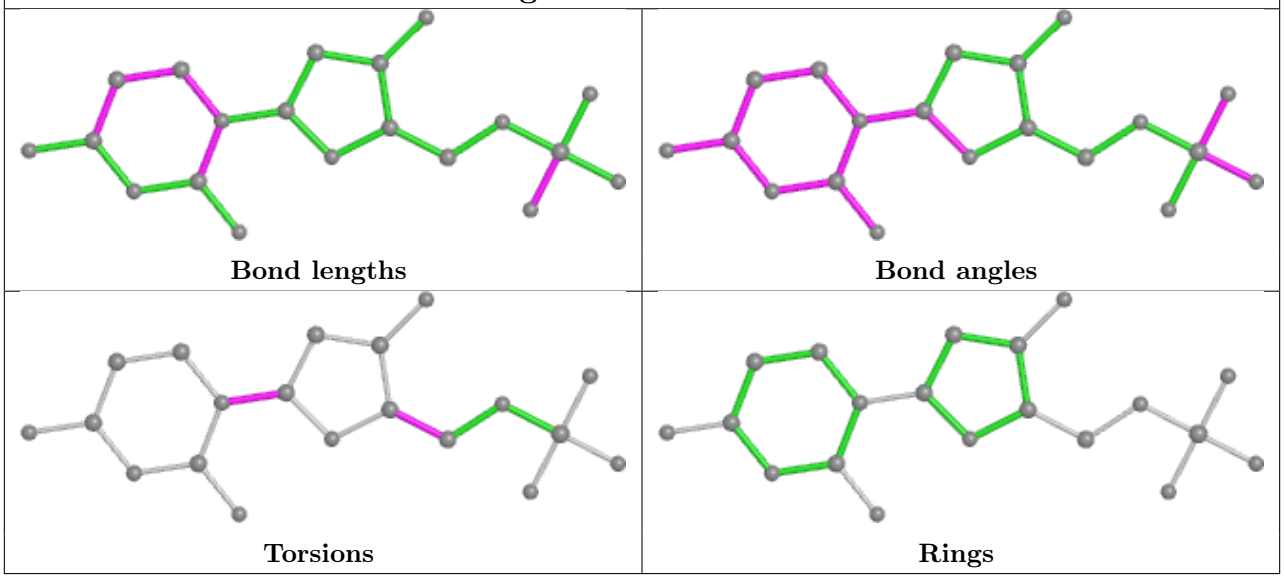


Rings

Ligand MTX B 609



Ligand UMP B 607



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, 95^{th} 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%)	-0.15	15 (2%)	50 51	19, 38, 67, 100	0
1	B	510/521 (97%)	-0.13	15 (2%)	51 52	22, 39, 75, 129	0
1	C	510/521 (97%)	0.37	38 (7%)	14 12	33, 54, 98, 126	0
1	D	505/521 (96%)	0.67	50 (9%)	7 5	41, 73, 101, 126	0
All	All	2033/2084 (97%)	0.19	118 (5%)	23 22	19, 50, 94, 129	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	GLN	9.6
1	B	191	GLY	8.2
1	C	182	THR	7.1
1	D	257	ARG	6.9
1	C	256	ASN	6.8
1	D	256	ASN	6.7
1	B	192	GLN	6.0
1	C	257	ARG	5.4
1	B	521	VAL	5.3
1	B	190	ARG	5.2
1	C	258	THR	5.0
1	D	209	ILE	4.8
1	D	260	ILE	4.6
1	D	231	PHE	4.6
1	B	520	ALA	4.4
1	C	65	ARG	4.2
1	D	258	THR	4.0
1	C	194	LYS	4.0
1	B	179	GLU	3.9
1	A	521	VAL	3.8
1	C	3	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	102	MET	3.8
1	C	105	ASP	3.7
1	D	124	LYS	3.5
1	A	192	GLN	3.4
1	D	323	GLU	3.4
1	A	84	ALA	3.4
1	C	113	CYS	3.3
1	D	425	CYS	3.3
1	D	102	MET	3.3
1	B	422	GLN	3.2
1	D	422	GLN	3.2
1	A	257	ARG	3.2
1	D	155	LEU	3.0
1	D	402	CYS	3.0
1	C	102	MET	3.0
1	D	44	CYS	2.9
1	D	263	TYR	2.9
1	A	103	ASN	2.9
1	D	253	TYR	2.9
1	C	422	GLN	2.8
1	C	438	TYR	2.8
1	D	114	GLY	2.8
1	A	105	ASP	2.8
1	C	180	LYS	2.8
1	B	3	GLU	2.7
1	D	178	GLN	2.7
1	D	421	TYR	2.7
1	C	420	LEU	2.6
1	A	113	CYS	2.6
1	C	431	SER	2.6
1	D	420	LEU	2.6
1	C	82	ASP	2.6
1	D	404	VAL	2.6
1	D	424	SER	2.6
1	D	142	GLU	2.5
1	C	193	LEU	2.5
1	C	421	TYR	2.5
1	D	333	ARG	2.5
1	B	180	LYS	2.5
1	D	194	LYS	2.5
1	D	107	ILE	2.5
1	C	195	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	327	ARG	2.5
1	C	197	ASP	2.5
1	D	84	ALA	2.4
1	C	412	ASN	2.4
1	C	66	PRO	2.4
1	B	84	ALA	2.4
1	D	113	CYS	2.4
1	C	200	VAL	2.4
1	D	207	ALA	2.4
1	C	521	VAL	2.4
1	A	258	THR	2.3
1	D	521	VAL	2.3
1	C	44	CYS	2.3
1	C	437	SER	2.3
1	D	137	ALA	2.3
1	D	259	GLY	2.3
1	C	255	GLU	2.3
1	D	105	ASP	2.3
1	B	256	ASN	2.3
1	A	179	GLU	2.3
1	C	373	GLU	2.3
1	D	3	GLU	2.3
1	B	258	THR	2.3
1	A	180	LYS	2.3
1	C	112	VAL	2.2
1	D	93	ASN	2.2
1	D	355	THR	2.2
1	D	326	GLU	2.2
1	D	403	HIS	2.2
1	D	79	LEU	2.2
1	D	134	THR	2.2
1	D	505	GLU	2.2
1	C	101	LEU	2.2
1	D	139	GLU	2.2
1	C	403	HIS	2.2
1	D	193	LEU	2.2
1	D	208	GLY	2.2
1	D	352	GLU	2.1
1	C	402	CYS	2.1
1	D	95	GLU	2.1
1	D	335	GLU	2.1
1	A	256	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	437	SER	2.1
1	C	46	SER	2.1
1	D	516	LYS	2.1
1	B	331	GLY	2.1
1	A	494	GLU	2.1
1	C	181	LYS	2.1
1	B	404	VAL	2.1
1	A	520	ALA	2.1
1	C	47	ASN	2.1
1	C	259	GLY	2.0
1	C	520	ALA	2.0
1	B	425	CYS	2.0
1	D	121	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
3	CB3	C	612	35/35	0.57	0.54	65,69,76,76	0
2	UMP	B	607	20/20	0.65	0.54	52,66,72,72	0
3	CB3	B	608	35/35	0.66	0.43	63,69,76,76	0
3	CB3	A	604	35/35	0.70	0.38	66,71,77,78	0
2	UMP	A	603	20/20	0.76	0.45	55,68,73,73	0
2	UMP	C	611	20/20	0.78	0.36	55,66,73,73	0
4	MTX	D	615	33/33	0.87	0.21	65,70,133,151	0
5	NDP	D	616	48/48	0.88	0.20	54,74,151,159	0
4	MTX	C	613	33/33	0.90	0.19	52,63,100,144	0
5	NDP	C	614	48/48	0.91	0.17	50,74,118,195	0

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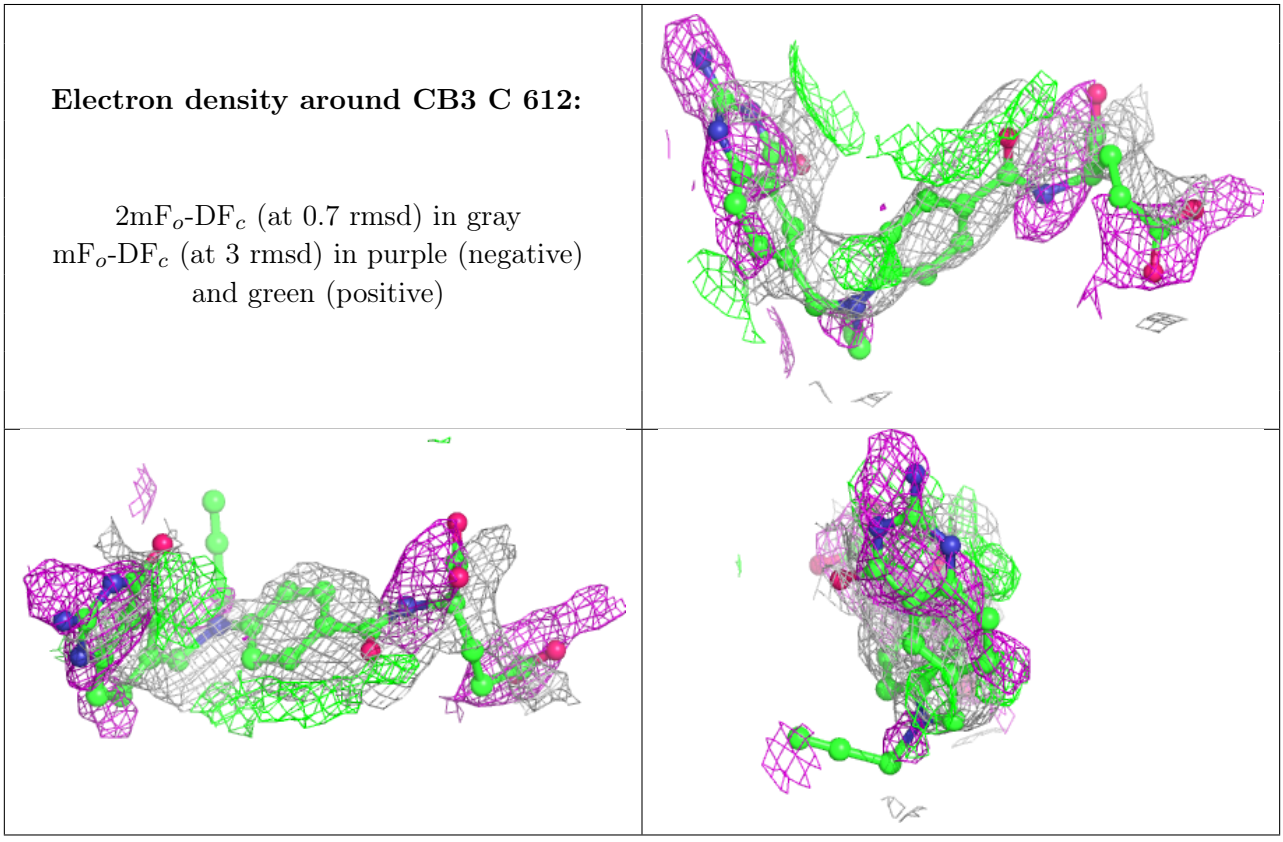
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MTX	A	605	33/33	0.94	0.18	28,40,56,79	0
4	MTX	B	609	33/33	0.95	0.14	27,38,51,73	0
5	NDP	A	606	48/48	0.97	0.14	27,38,50,69	0
5	NDP	B	610	48/48	0.98	0.11	24,33,46,49	0

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.

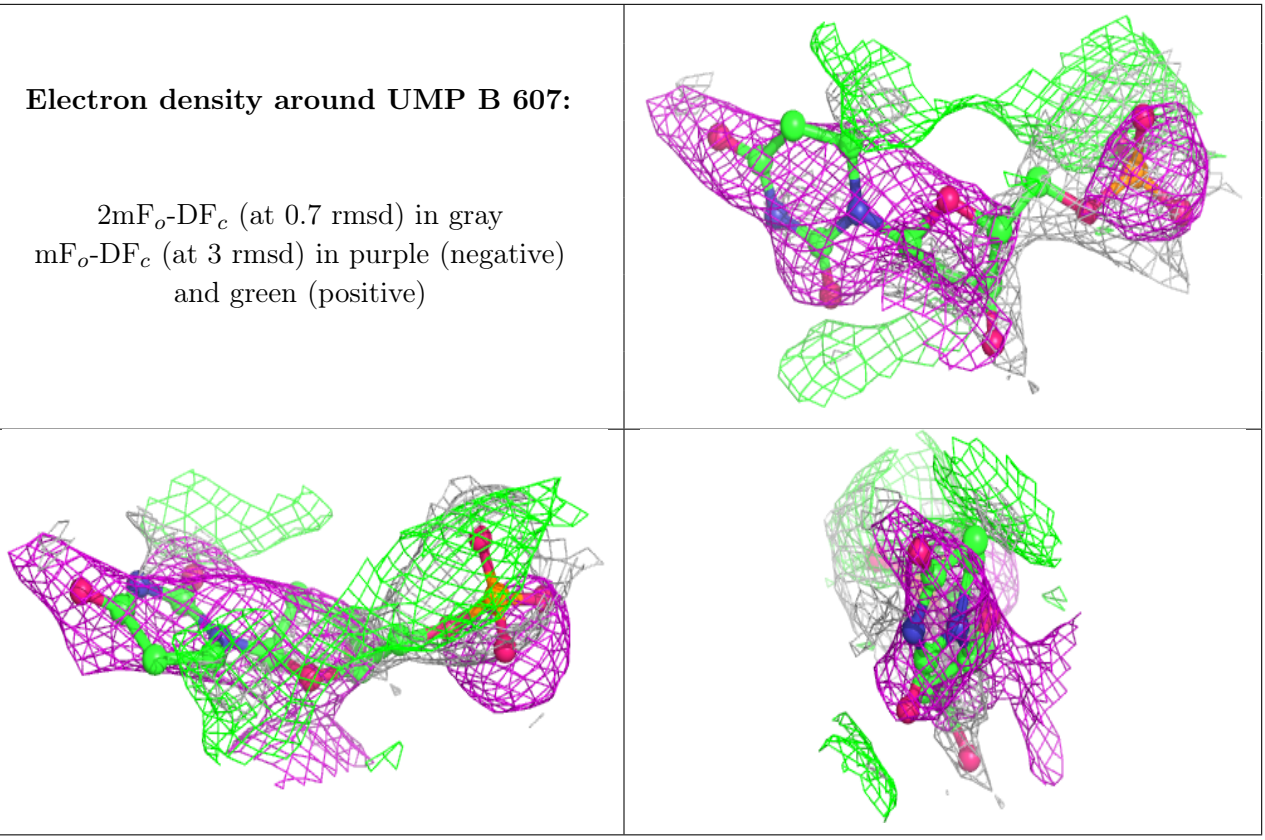
Electron density around CB3 C 612:

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



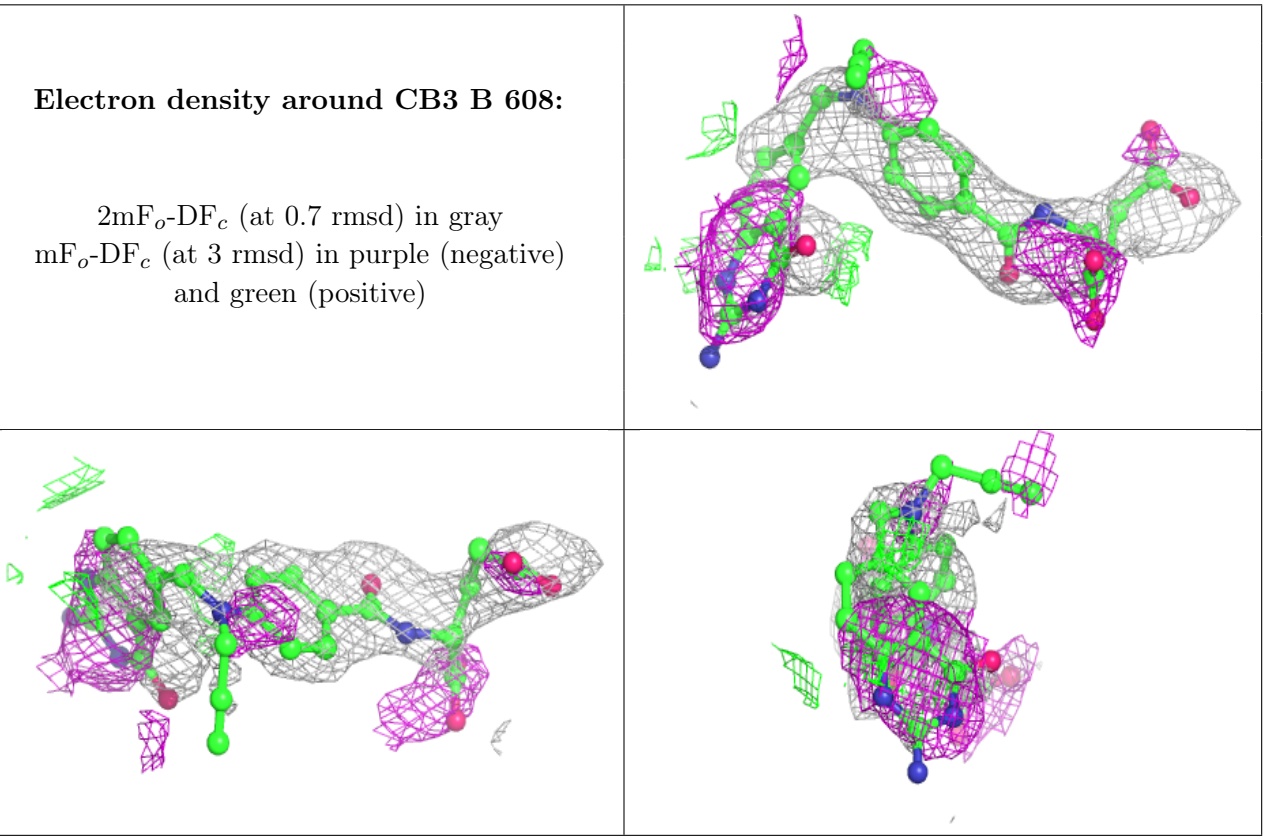
Electron density around UMP B 607:

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



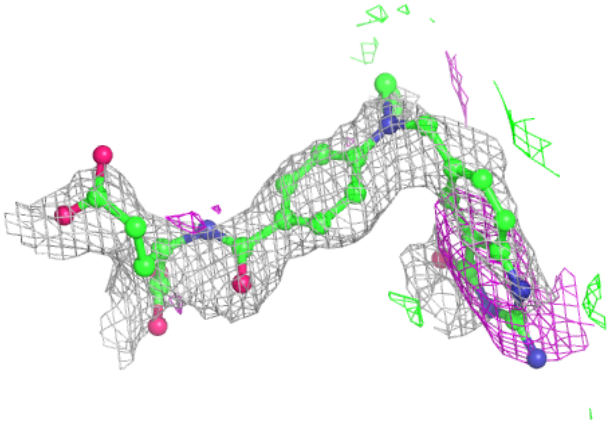
Electron density around CB3 B 608:

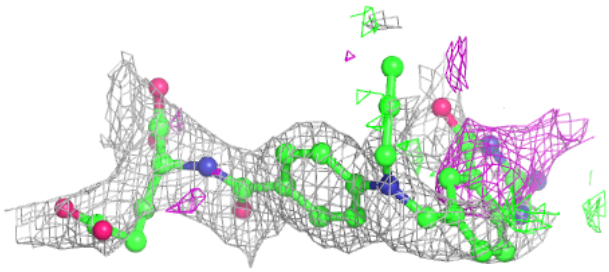
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

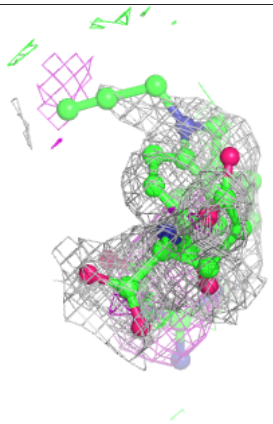


Electron density around CB3 A 604:

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

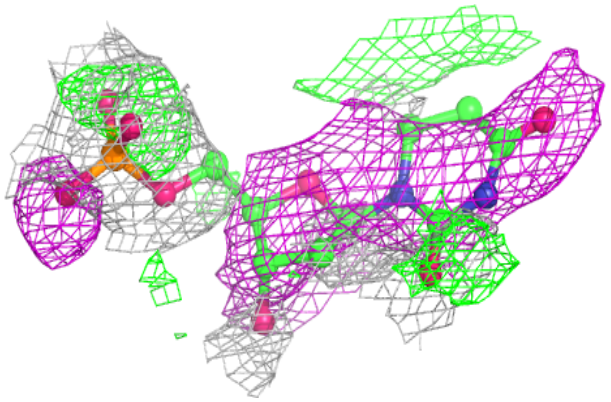


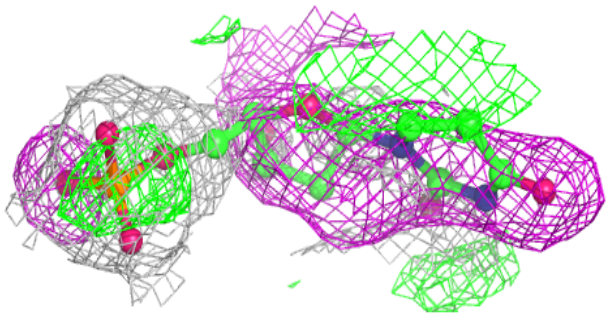


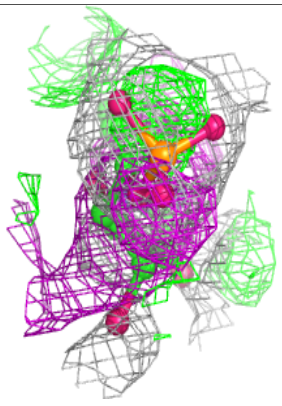


Electron density around UMP A 603:

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

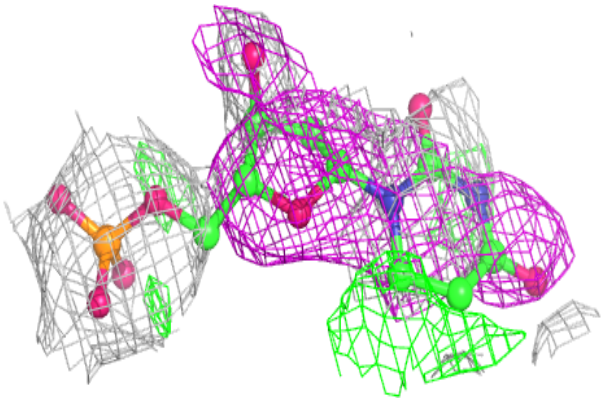


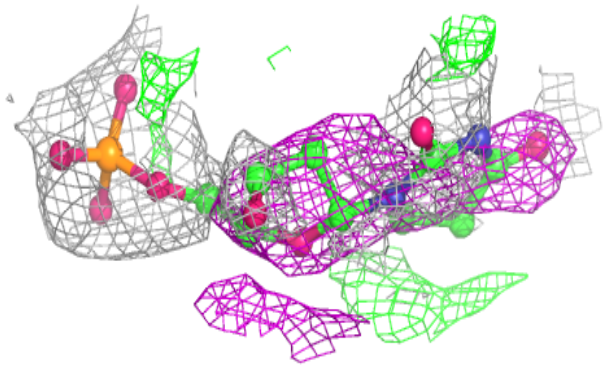


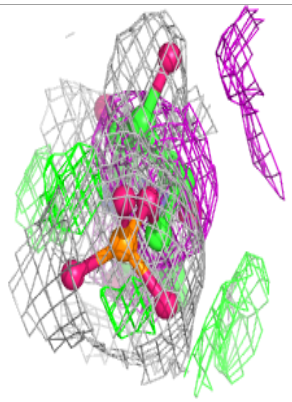


Electron density around UMP C 611:

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

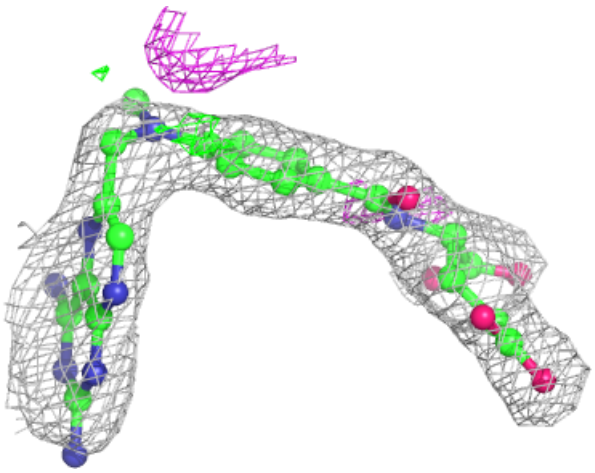


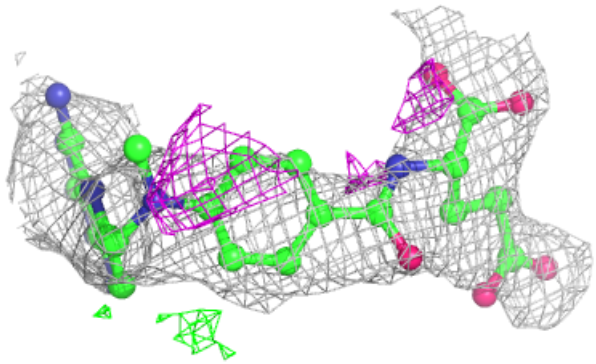


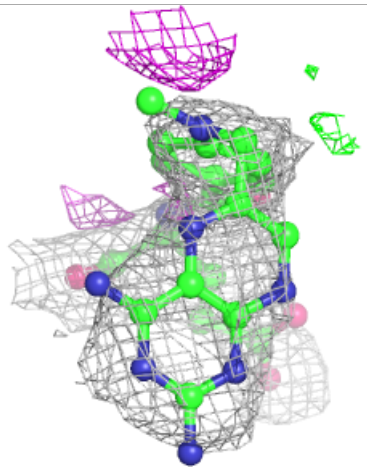


Electron density around MTX D 615:

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

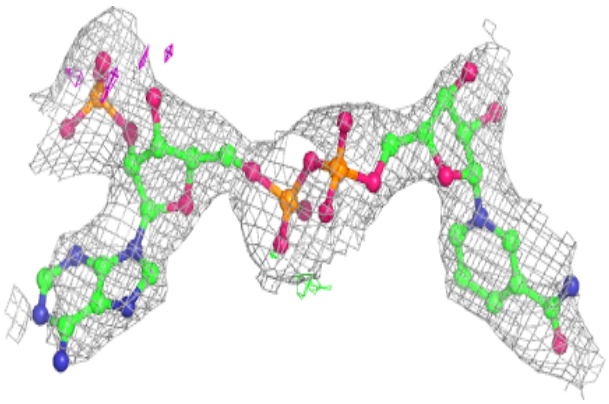


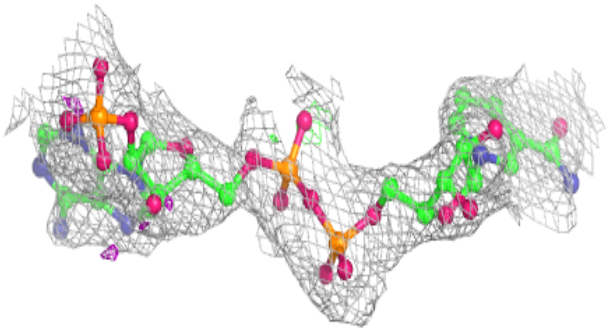


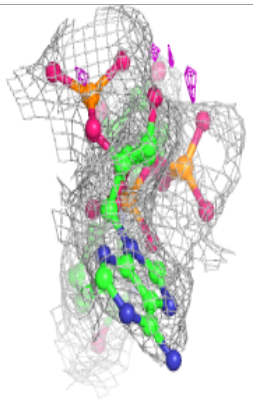


Electron density around NDP D 616:

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

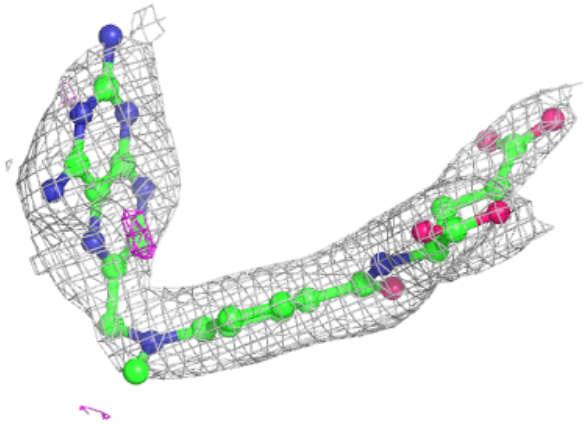


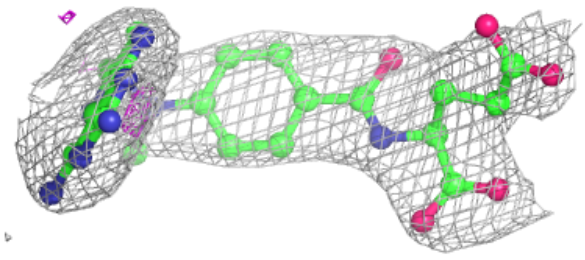


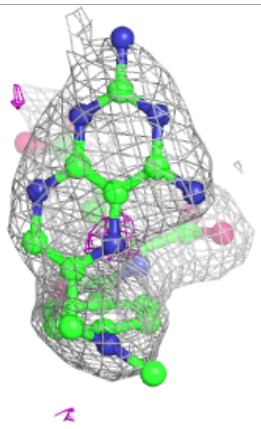


Electron density around MTX C 613:

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

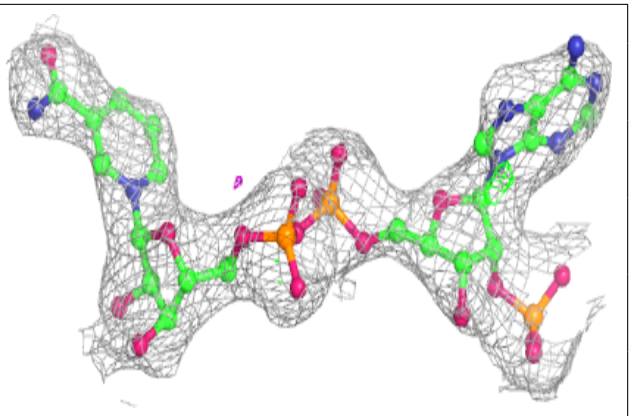


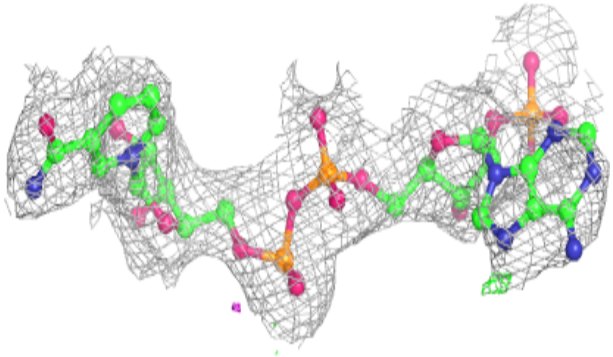


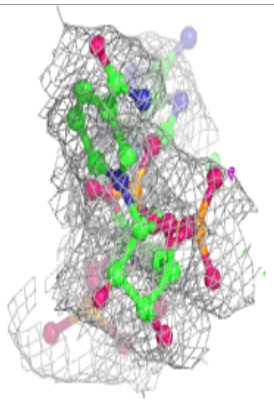


Electron density around NDP C 614:

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

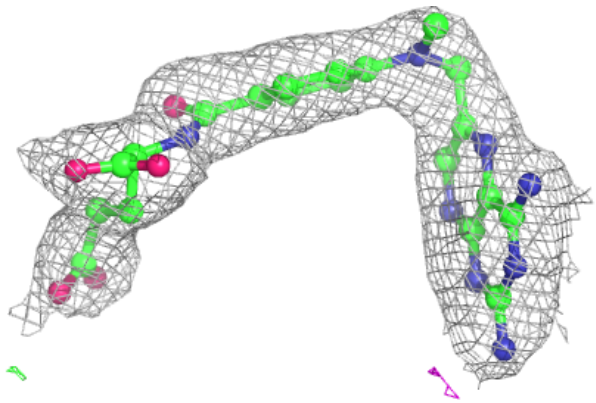


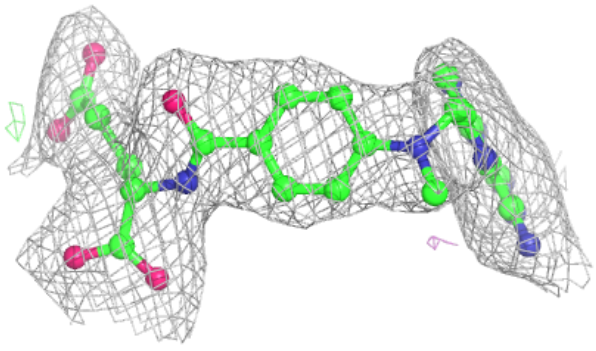


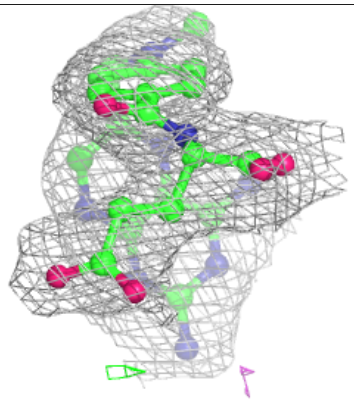


Electron density around MTX A 605:

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

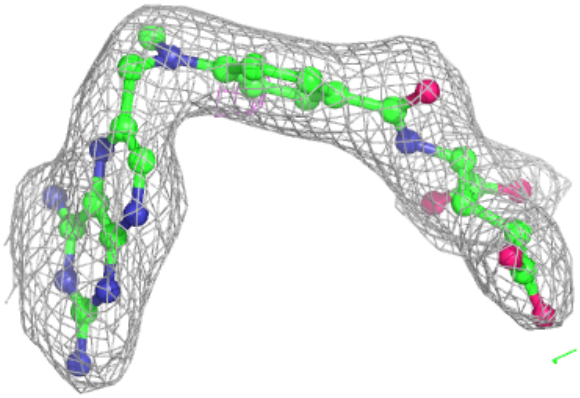


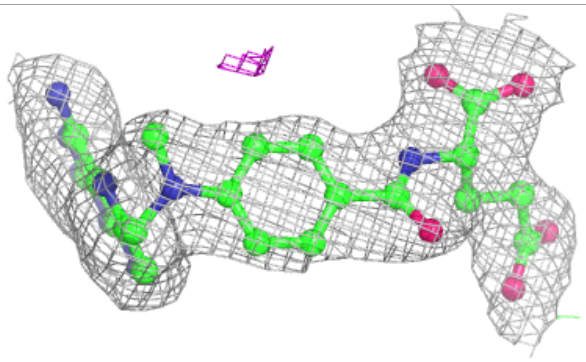


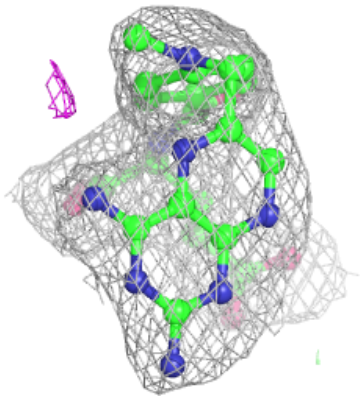


Electron density around MTX B 609:

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

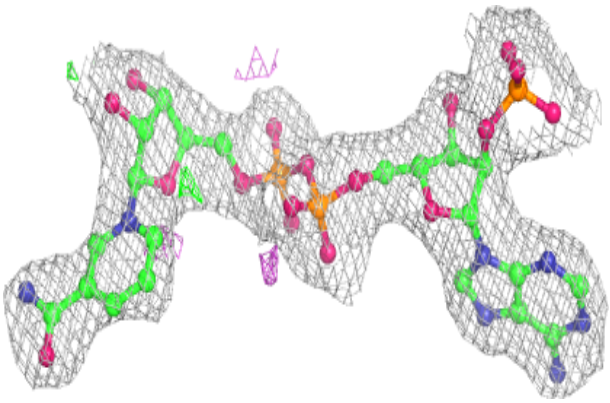


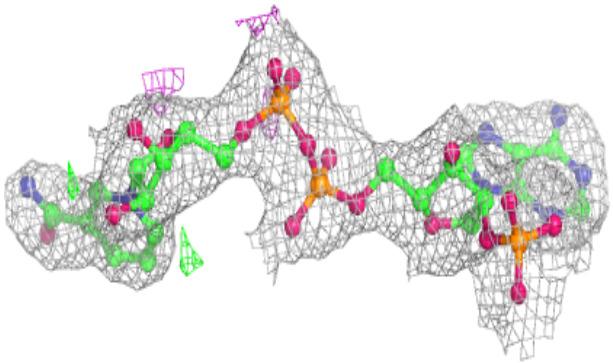




Electron density around NDP A 606:

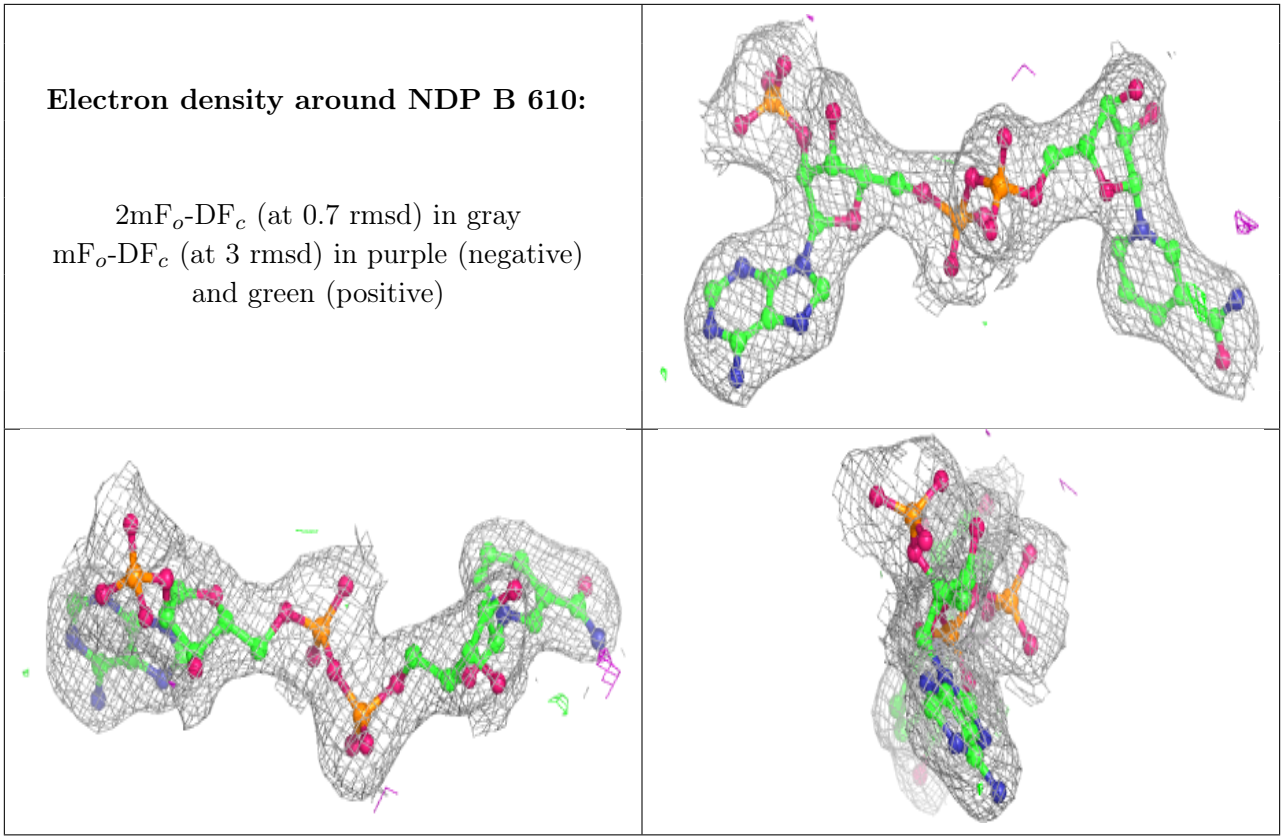
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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.