Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 05:09 PM EDT

PDB ID	:	3IRN
Title	:	Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase COMPLEXED WITH NADPH AND Cycloguanil
Authors	:	Chitnumsub, P.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on	:	2009-08-24
Resolution	:	2.60 Å(reported)

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

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

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

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

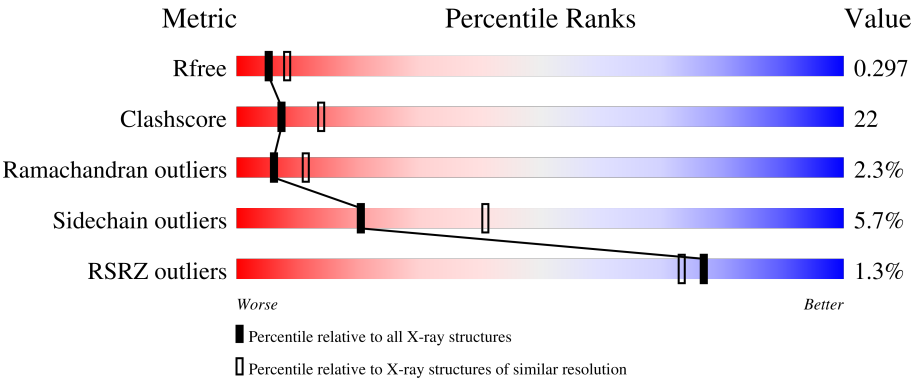
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	62% 34%
1	B	521	53% 41% 5%
1	C	521	60% 36%
1	D	521	55% 38%

2 Entry composition (i)

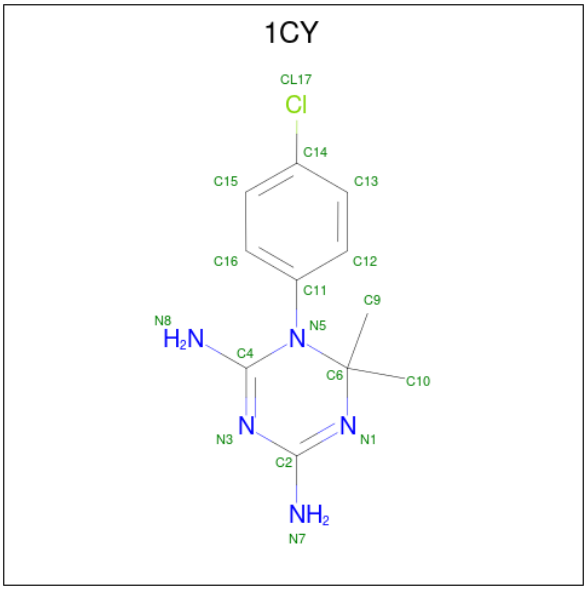
There are 5 unique types of molecules in this entry. The entry contains 16901 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4107	2605	726	757	19			
1	B	516	Total	C	N	O	S	0	0	0
			4110	2608	727	756	19			
1	C	516	Total	C	N	O	S	0	0	0
			4107	2605	726	757	19			
1	D	513	Total	C	N	O	S	0	0	0
			4087	2594	723	752	18			

- Molecule 2 is 1-(4-chlorophenyl)-6,6-dimethyl-1,6-dihydro-1,3,5-triazine-2,4-diamine (three-letter code: 1CY) (formula: $C_{11}H_{14}ClN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	B	1	Total	C	Cl	N	0	0
			17	11	1	5		

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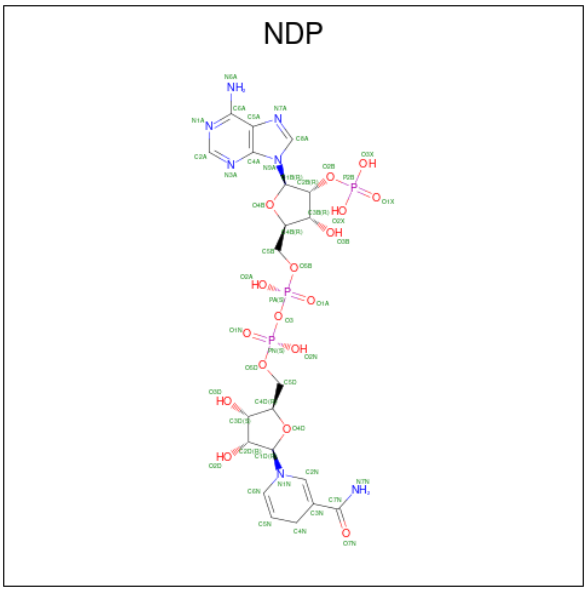
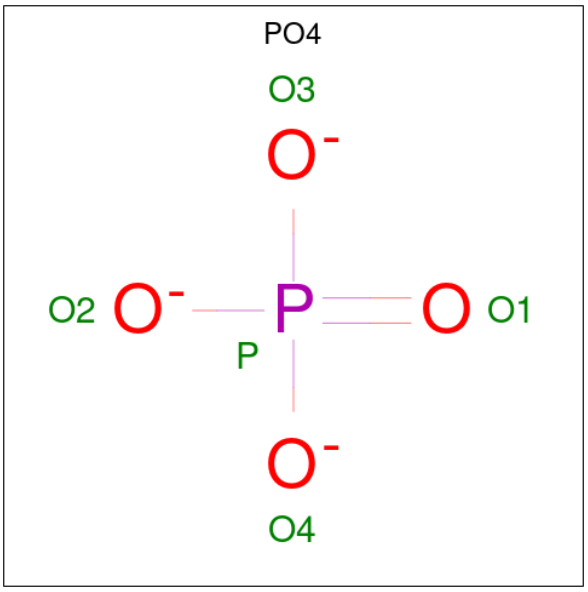
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	D	1	Total	C	Cl	N	0	0
			17	11	1	5		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

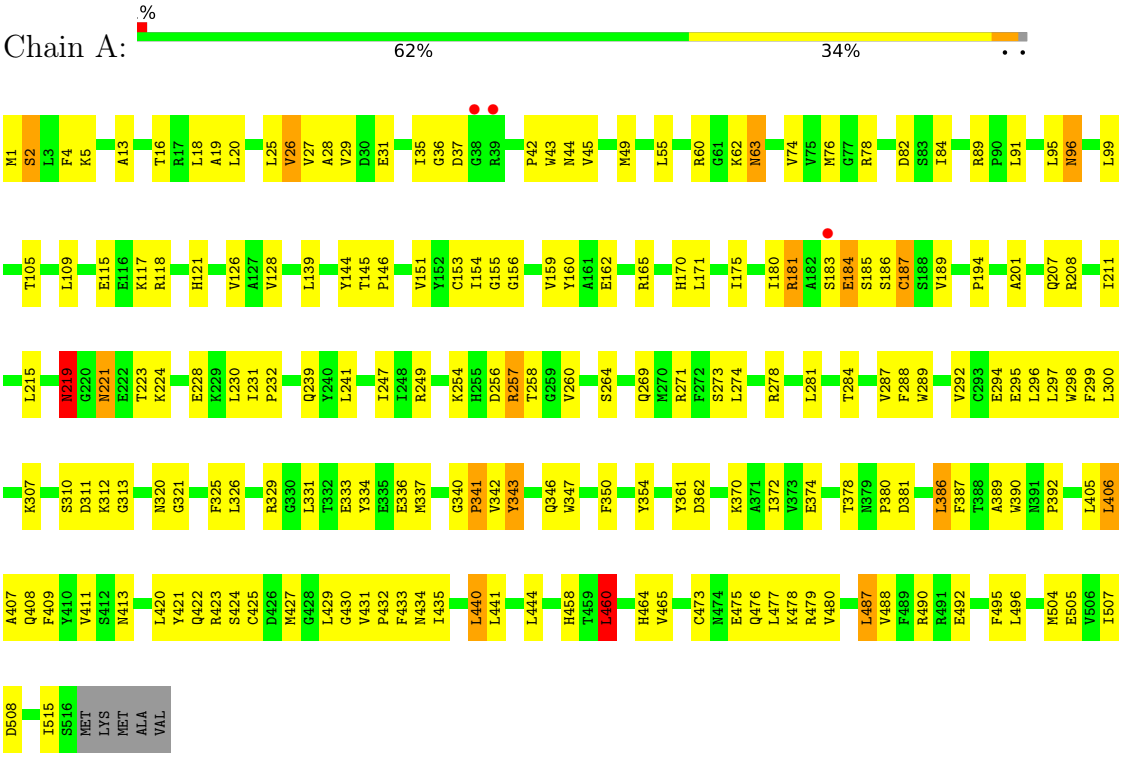
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	58	Total O 58 58	0	0
5	B	49	Total O 49 49	0	0
5	C	60	Total O 60 60	0	0
5	D	43	Total O 43 43	0	0

3 Residue-property plots (i)

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

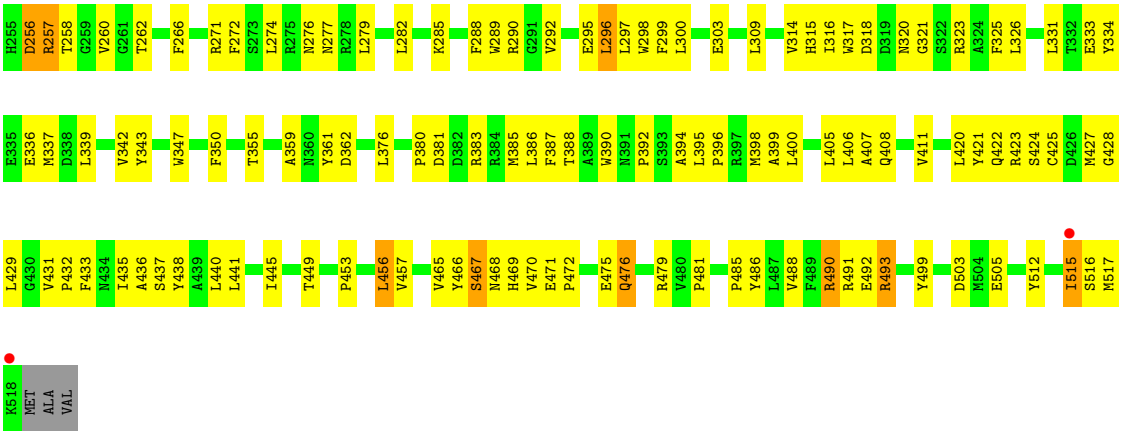
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain A:

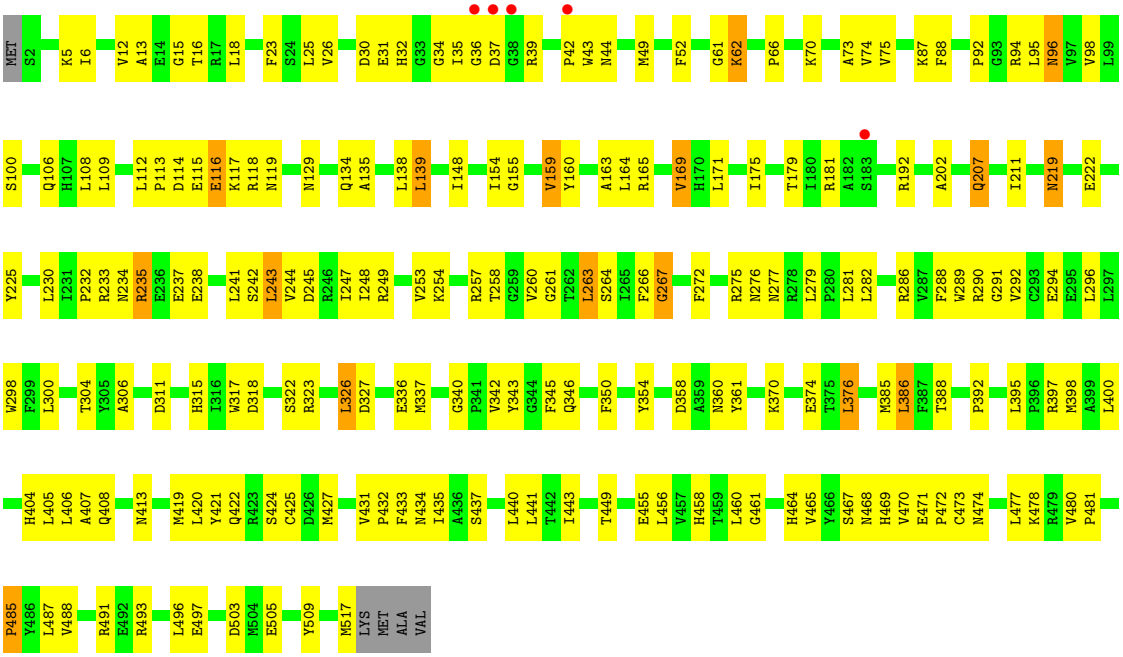


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

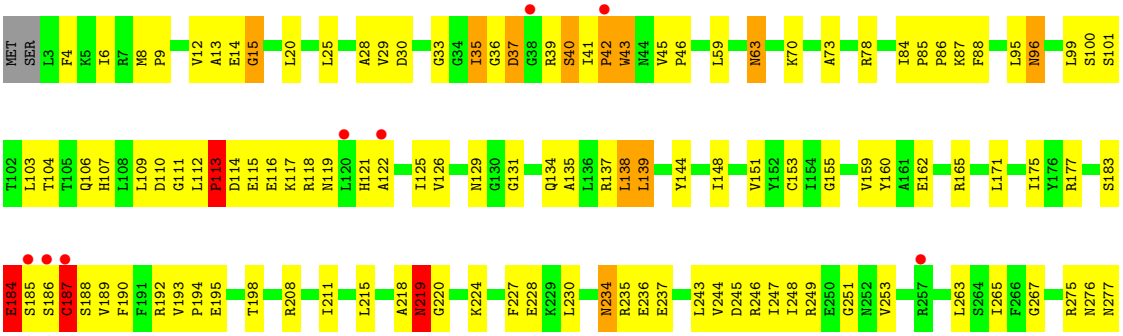
Chain B:

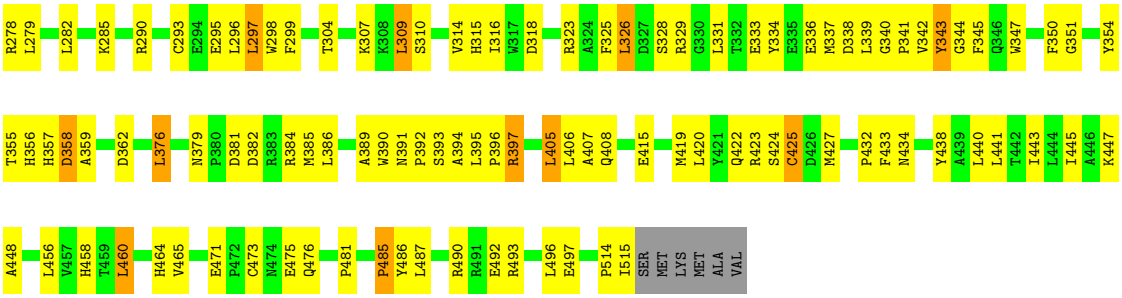


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase




R278 L279 L282 K285 R290 C293 E294 E295 L296 L297 W298 F299 T304 K307 K308 L309 S310 V314 H315 I316 W317 D318 R323 A324 F325 L326 D327 S328 R329 G330 L331 T332 E333 Y334 E335 E336 M337 D338 L339 G340 P341 V342 Y343 G344 F345 Q346 W347 F350 G351 Y354
T355 H356 H357 D358 A359 D362 L376 N379 P380 D381 D382 R383 R384 M385 L386 A389 W390 N391 P392 S393 A394 L395 P396 R397 L405 L406 A407 Q408 E415 M419 L420 Y421 Q422 R423 S424 C425 D426 M427 P432 F433 N434 Y438 A439 L440 L441 T442 I443 L444 I445 A446 K447
A448 L456 V457 H458 T459 L460 H464 V465 E471 P472 C473 N474 E475 Q476 P481 P485 Y486 L487 R490 R491 E492 R493 L496 E497 P514 I515 SER MET LYS MET ALA VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.34Å 165.59Å 84.85Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	44.48 – 2.60 44.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.9 (44.48-2.60) 93.8 (44.39-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.230 , 0.299 0.228 , 0.297	Depositor DCC
R_{free} test set	3003 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 7.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.086 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16901	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: 1CY, PO4, 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	0.40	0/4207	0.68	2/5708 (0.0%)
1	B	0.39	0/4210	0.68	0/5711
1	C	0.40	0/4207	0.68	0/5708
1	D	0.40	0/4187	0.68	1/5682 (0.0%)
All	All	0.40	0/16811	0.68	3/22809 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	GLY	N-CA-C	-5.86	98.45	113.10
1	A	460	LEU	CA-CB-CG	5.25	127.37	115.30
1	D	465	VAL	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4107	0	4063	167	0
1	B	4110	0	4068	222	0
1	C	4107	0	4060	167	0
1	D	4087	0	4041	210	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	17	0	14	1	0
2	B	17	0	14	1	0
2	C	17	0	14	0	0
2	D	17	0	14	0	0
3	A	48	0	26	2	0
3	B	48	0	26	7	0
3	C	48	0	26	3	0
3	D	48	0	26	3	0
4	A	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	58	0	0	0	0
5	B	49	0	0	3	0
5	C	60	0	0	3	0
5	D	43	0	0	3	0
All	All	16901	0	16392	736	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (736) 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:B:490:ARG:HH11	1:B:490:ARG:HB3	1.24	0.99
1:B:181:ARG:HG3	1:B:224:LYS:HB2	1.42	0.97
1:C:300:LEU:HD13	1:C:496:LEU:HD11	1.48	0.95
1:D:114:ASP:HB3	1:D:117:LYS:HB2	1.48	0.95
1:A:181:ARG:HH11	1:A:181:ARG:HB3	1.33	0.93
1:B:112:LEU:HB3	1:B:117:LYS:HE3	1.52	0.91
1:D:117:LYS:HE2	1:D:121:HIS:NE2	1.86	0.91
1:A:1:MET:HB2	1:A:5:LYS:HG3	1.52	0.91
1:A:146:PRO:HB3	1:A:505:GLU:HG2	1.54	0.90
1:B:257:ARG:H	1:B:257:ARG:HD3	1.37	0.90
1:D:397:ARG:HG2	1:D:397:ARG:HH11	1.35	0.90
1:C:279:LEU:HD23	1:C:281:LEU:HG	1.53	0.88
1:D:114:ASP:HB3	1:D:117:LYS:CB	2.04	0.87
1:D:40:SER:C	1:D:42:PRO:HD3	1.97	0.85
1:B:285:LYS:HD2	1:B:476:GLN:HE21	1.41	0.84
1:B:490:ARG:HB3	1:B:490:ARG:NH1	1.94	0.83
1:D:278:ARG:NH1	5:D:1080:HOH:O	2.11	0.82
1:B:219:ASN:ND2	1:B:221:ASN:H	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ARG:HE	1:D:193:VAL:H	1.30	0.80
1:A:62:LYS:O	1:A:63:ASN:HB2	1.78	0.80
1:B:155:GLY:HA3	3:B:702:NDP:H5N	1.65	0.79
1:B:101:SER:HA	1:B:129:ASN:OD1	1.82	0.79
1:B:386:LEU:HD12	1:B:406:LEU:HD11	1.63	0.79
1:B:285:LYS:HD2	1:B:476:GLN:NE2	1.98	0.78
1:D:20:LEU:HB2	1:D:171:LEU:HD13	1.67	0.77
1:B:285:LYS:HE3	1:B:515:ILE:HD11	1.66	0.76
1:A:281:LEU:HD22	1:A:287:VAL:HB	1.67	0.75
1:D:246:ARG:HA	1:D:249:ARG:HH12	1.50	0.75
1:D:177:ARG:HH12	1:D:192:ARG:NH2	1.84	0.75
1:A:479:ARG:HH12	1:A:515:ILE:HG12	1.52	0.75
1:C:234:ASN:O	1:C:238:GLU:HG3	1.86	0.75
1:C:254:LYS:HD3	1:D:381:ASP:CG	2.07	0.75
1:C:253:VAL:HG22	1:C:263:LEU:HD22	1.69	0.75
1:D:112:LEU:HD12	1:D:113:PRO:HD2	1.70	0.74
1:B:239:GLN:HE22	1:B:271:ARG:H	1.36	0.73
1:C:96:ASN:N	1:C:96:ASN:HD22	1.86	0.73
1:C:471:GLU:HB2	1:C:472:PRO:HD3	1.70	0.73
1:A:1:MET:HB3	1:A:4:PHE:HB2	1.72	0.72
1:D:340:GLY:HA2	1:D:354:TYR:CE2	2.25	0.72
1:A:117:LYS:HG3	1:A:121:HIS:HD2	1.54	0.71
1:D:246:ARG:HA	1:D:249:ARG:NH1	2.06	0.71
1:A:257:ARG:H	1:A:257:ARG:HD3	1.54	0.71
1:A:300:LEU:HD21	1:A:441:LEU:CD1	2.21	0.71
1:B:492:GLU:O	1:B:493:ARG:HD2	1.90	0.70
1:A:254:LYS:HD3	1:B:381:ASP:OD1	1.91	0.70
1:D:192:ARG:HE	1:D:193:VAL:N	1.88	0.70
1:B:85:PRO:HB2	1:B:88:PHE:HD2	1.55	0.70
1:B:234:ASN:O	1:B:238:GLU:HG3	1.92	0.69
1:C:115:GLU:HG3	1:C:118:ARG:NH1	2.07	0.69
1:D:115:GLU:HA	1:D:118:ARG:NH1	2.07	0.69
1:A:117:LYS:HG3	1:A:121:HIS:CD2	2.28	0.68
1:A:239:GLN:HE22	1:A:271:ARG:H	1.40	0.68
1:B:33:GLY:O	1:B:190:PHE:HA	1.92	0.68
1:B:146:PRO:CB	1:B:505:GLU:HG2	2.22	0.68
1:B:104:THR:H	1:B:107:HIS:HB2	1.58	0.68
1:B:109:LEU:HD12	1:B:125:ILE:HD12	1.74	0.68
1:C:237:GLU:HG3	1:C:282:LEU:HD22	1.74	0.68
1:C:247:ILE:HG21	1:C:465:VAL:HG23	1.73	0.68
1:A:171:LEU:HD12	1:A:171:LEU:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:VAL:O	1:B:435:ILE:HG13	1.93	0.68
1:A:60:ARG:NH2	1:A:508:ASP:HA	2.09	0.67
1:D:355:THR:HG22	1:D:356:HIS:CD2	2.29	0.67
1:C:241:LEU:HD22	1:C:477:LEU:HD23	1.75	0.67
1:D:85:PRO:HG2	1:D:88:PHE:HB2	1.76	0.67
1:A:431:VAL:O	1:A:435:ILE:HG13	1.94	0.66
1:D:397:ARG:HH11	1:D:397:ARG:CG	2.08	0.66
1:C:244:VAL:O	1:C:248:ILE:HG13	1.96	0.66
1:C:37:ASP:OD2	1:C:42:PRO:HG3	1.96	0.66
1:B:146:PRO:HB3	1:B:505:GLU:HG2	1.78	0.66
1:C:264:SER:HB3	1:C:464:HIS:HB3	1.77	0.66
1:B:219:ASN:C	1:B:219:ASN:HD22	1.98	0.65
1:A:257:ARG:H	1:A:257:ARG:CD	2.08	0.65
1:A:37:ASP:HB2	1:A:42:PRO:HD3	1.78	0.65
1:C:31:GLU:OE2	1:C:181:ARG:HD2	1.96	0.65
1:D:395:LEU:HB2	1:D:396:PRO:HD3	1.78	0.65
1:B:376:LEU:HD23	1:B:449:THR:HG21	1.79	0.65
1:C:296:LEU:HD13	1:C:296:LEU:C	2.17	0.65
1:D:278:ARG:HG3	1:D:278:ARG:HH11	1.61	0.65
1:C:322:SER:O	1:C:326:LEU:HB2	1.96	0.65
1:D:234:ASN:C	1:D:234:ASN:HD22	2.00	0.65
1:B:296:LEU:HD11	1:B:441:LEU:HB2	1.78	0.64
1:C:425:CYS:SG	1:C:460:LEU:HD22	2.37	0.64
1:B:213:GLU:O	1:B:215:LEU:HD13	1.97	0.64
1:C:392:PRO:HD2	1:D:350:PHE:CZ	2.31	0.64
1:D:35:ILE:C	1:D:37:ASP:H	1.99	0.64
1:A:145:THR:HG23	1:A:507:ILE:HG21	1.80	0.64
1:B:285:LYS:HB2	1:B:476:GLN:NE2	2.13	0.64
1:D:110:ASP:HA	1:D:118:ARG:HE	1.62	0.64
1:D:96:ASN:N	1:D:96:ASN:HD22	1.95	0.64
1:C:254:LYS:HD3	1:D:381:ASP:OD2	1.98	0.63
1:C:350:PHE:CE1	1:D:392:PRO:HD2	2.34	0.63
1:A:29:VAL:HG12	1:A:35:ILE:HG22	1.80	0.63
1:D:441:LEU:O	1:D:445:ILE:HG12	1.98	0.63
1:A:181:ARG:HB3	1:A:181:ARG:NH1	2.11	0.63
1:A:479:ARG:NH1	1:A:515:ILE:HG12	2.14	0.63
1:B:84:ILE:HG22	1:B:89:ARG:HG2	1.81	0.63
1:D:298:TRP:CD1	1:D:309:LEU:HD13	2.33	0.63
1:A:31:GLU:OE2	1:A:181:ARG:HD2	1.98	0.63
1:D:276:ASN:O	1:D:277:ASN:HB2	1.98	0.62
1:D:351:GLY:HA2	5:D:1157:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ASP:O	1:B:118:ARG:HG3	1.99	0.62
1:C:135:ALA:O	1:C:139:LEU:HB2	1.97	0.62
1:A:96:ASN:N	1:A:96:ASN:HD22	1.94	0.62
1:A:406:LEU:HB3	1:A:421:TYR:HB3	1.82	0.62
1:B:86:PRO:HA	1:B:89:ARG:HG3	1.81	0.62
1:D:117:LYS:C	1:D:119:ASN:H	2.03	0.62
1:A:406:LEU:HD23	1:A:421:TYR:HB2	1.82	0.62
1:D:424:SER:OG	1:D:464:HIS:HE1	1.82	0.62
1:C:164:LEU:HA	1:C:169:VAL:HG13	1.81	0.61
1:D:379:ASN:ND2	1:D:382:ASP:HB2	2.15	0.61
1:A:473:CYS:O	1:A:477:LEU:HG	2.00	0.61
1:A:381:ASP:CG	1:B:254:LYS:HD3	2.21	0.61
1:D:20:LEU:CD2	1:D:137:ARG:HG3	2.31	0.61
1:A:269:GLN:HA	1:A:458:HIS:O	1.99	0.61
1:D:41:ILE:HD12	1:D:41:ILE:N	2.16	0.61
1:D:195:GLU:HB3	1:D:198:THR:HG21	1.82	0.61
1:D:386:LEU:HB3	1:D:408:GLN:HA	1.83	0.61
1:D:14:GLU:HG3	1:D:15:GLY:H	1.66	0.60
1:C:12:VAL:HG13	1:C:13:ALA:N	2.16	0.60
1:D:192:ARG:NE	1:D:192:ARG:HA	2.16	0.60
1:C:253:VAL:HG22	1:C:263:LEU:CD2	2.31	0.60
1:C:272:PHE:CZ	1:C:435:ILE:HD13	2.36	0.60
1:A:478:LYS:HD3	1:C:478:LYS:NZ	2.16	0.60
1:A:490:ARG:HB2	1:A:490:ARG:HH11	1.65	0.60
1:B:87:LYS:HE3	1:B:88:PHE:CE2	2.36	0.60
1:D:8:MET:HE3	1:D:448:ALA:HA	1.84	0.60
1:A:370:LYS:O	1:A:374:GLU:HG2	2.02	0.60
1:B:471:GLU:HB2	1:B:472:PRO:HD3	1.83	0.60
1:C:424:SER:OG	1:C:464:HIS:HE1	1.84	0.60
1:D:234:ASN:HD21	1:D:236:GLU:HB2	1.67	0.59
1:B:315:HIS:HB3	1:B:318:ASP:OD1	2.03	0.59
1:B:427:MET:SD	1:B:431:VAL:HG21	2.43	0.59
1:C:155:GLY:HA3	3:C:703:NDP:H5N	1.84	0.59
1:D:20:LEU:HB2	1:D:171:LEU:CD1	2.32	0.59
1:D:420:LEU:HD23	1:D:458:HIS:CD2	2.38	0.59
1:D:39:ARG:HD2	1:D:186:SER:HB2	1.83	0.59
1:A:241:LEU:HD11	1:A:284:THR:HG21	1.85	0.59
1:C:61:GLY:O	1:C:62:LYS:O	2.20	0.59
1:C:400:LEU:HD11	1:D:384:ARG:HH22	1.67	0.59
1:D:314:VAL:HG12	1:D:316:ILE:HG12	1.84	0.59
1:B:219:ASN:ND2	1:B:219:ASN:C	2.54	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:PRO:HB2	1:D:185:SER:OG	2.02	0.58
1:D:135:ALA:O	1:D:139:LEU:HD22	2.03	0.58
1:B:257:ARG:HD3	1:B:257:ARG:N	2.13	0.58
1:A:45:VAL:HG21	1:A:180:ILE:HG12	1.84	0.58
1:B:274:LEU:O	1:B:453:PRO:HB2	2.03	0.58
1:C:192:ARG:HG2	1:C:192:ARG:HH11	1.68	0.58
1:C:247:ILE:HD12	1:C:427:MET:HG3	1.86	0.58
1:D:114:ASP:HB3	1:D:117:LYS:HB3	1.85	0.58
1:D:116:GLU:O	1:D:119:ASN:HB3	2.02	0.58
1:C:207:GLN:NE2	1:C:233:ARG:HD2	2.19	0.58
1:D:299:PHE:HB3	1:D:347:TRP:CZ3	2.37	0.58
1:A:300:LEU:HD21	1:A:441:LEU:HD13	1.85	0.58
1:B:20:LEU:HB2	1:B:171:LEU:HD13	1.85	0.58
1:D:131:GLY:H	1:D:134:GLN:NE2	2.02	0.58
1:A:254:LYS:HD3	1:B:381:ASP:CG	2.24	0.58
1:A:336:GLU:O	1:A:337:MET:HB2	2.02	0.58
1:A:350:PHE:CZ	1:B:392:PRO:HD2	2.38	0.58
1:A:381:ASP:OD1	1:B:254:LYS:HD3	2.04	0.58
1:A:387:PHE:CE1	1:A:407:ALA:HB3	2.38	0.58
1:B:359:ALA:HB3	1:B:361:TYR:CZ	2.39	0.58
1:A:422:GLN:HB3	1:A:425:CYS:SG	2.43	0.58
1:B:89:ARG:HB2	1:B:112:LEU:HD22	1.85	0.58
1:B:109:LEU:O	1:B:112:LEU:HG	2.03	0.58
1:B:376:LEU:HD13	1:B:385:MET:SD	2.44	0.58
1:A:288:PHE:O	1:A:292:VAL:HG23	2.04	0.58
1:B:296:LEU:CD1	1:B:441:LEU:HB2	2.33	0.58
1:B:336:GLU:O	1:B:337:MET:HB2	2.04	0.57
1:B:420:LEU:HD22	1:B:438:TYR:CD2	2.39	0.57
1:D:115:GLU:HG2	1:D:118:ARG:HH11	1.67	0.57
1:B:85:PRO:HB2	1:B:88:PHE:CD2	2.37	0.57
1:C:247:ILE:CD1	1:C:427:MET:HG3	2.34	0.57
1:D:8:MET:HE3	1:D:8:MET:HA	1.86	0.57
1:A:35:ILE:HG13	1:A:36:GLY:N	2.20	0.57
1:B:104:THR:HG22	1:B:106:GLN:H	1.69	0.57
1:B:256:ASP:OD2	1:B:260:VAL:HB	2.05	0.57
1:B:431:VAL:HB	1:B:432:PRO:HD3	1.86	0.57
1:D:331:LEU:HD13	1:D:334:TYR:CE2	2.39	0.57
1:A:300:LEU:HD21	1:A:441:LEU:HD11	1.85	0.57
1:B:298:TRP:HH2	1:B:339:LEU:HD12	1.70	0.57
1:C:491:ARG:HD2	1:C:503:ASP:OD2	2.04	0.57
1:A:1:MET:H3	1:A:5:LYS:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLU:O	1:A:298:TRP:HB3	2.05	0.57
1:B:115:GLU:HA	1:B:118:ARG:HB2	1.86	0.56
1:C:12:VAL:HG13	1:C:13:ALA:H	1.70	0.56
1:C:323:ARG:HG3	1:C:327:ASP:OD2	2.05	0.56
1:C:336:GLU:O	1:C:337:MET:HB2	2.05	0.56
1:A:208:ARG:NH2	1:C:263:LEU:HD13	2.20	0.56
1:A:247:ILE:HG21	1:A:465:VAL:HG23	1.87	0.56
1:C:279:LEU:HD13	1:C:487:LEU:HB2	1.87	0.56
1:A:31:GLU:HG3	1:A:181:ARG:HA	1.86	0.56
1:A:1:MET:HB2	1:A:5:LYS:CG	2.31	0.56
1:A:256:ASP:HB2	1:A:257:ARG:HH11	1.70	0.56
1:D:296:LEU:CD2	1:D:440:LEU:HG	2.36	0.56
1:B:4:PHE:CD1	1:B:362:ASP:HB3	2.41	0.56
1:B:469:HIS:C	1:B:472:PRO:HD2	2.25	0.56
1:B:420:LEU:HD12	1:B:421:TYR:N	2.21	0.56
1:B:192:ARG:HD3	1:C:413:ASN:OD1	2.06	0.56
1:D:331:LEU:HB3	1:D:334:TYR:CD2	2.40	0.56
1:C:35:ILE:O	3:C:703:NDP:N7N	2.39	0.56
1:D:497:GLU:N	1:D:497:GLU:OE2	2.38	0.56
1:D:28:ALA:HB3	3:D:704:NDP:O7N	2.06	0.55
1:A:37:ASP:CB	1:A:42:PRO:HD3	2.35	0.55
1:D:336:GLU:OE1	1:D:336:GLU:N	2.33	0.55
1:C:266:PHE:CE2	1:D:419:MET:HB2	2.41	0.55
1:D:376:LEU:HD13	1:D:385:MET:SD	2.45	0.55
1:B:113:PRO:O	1:B:118:ARG:HD2	2.07	0.55
1:D:8:MET:HE3	1:D:9:PRO:HD2	1.89	0.55
1:D:177:ARG:HH12	1:D:192:ARG:HH22	1.52	0.55
1:A:99:LEU:HD12	1:A:159:VAL:HG22	1.88	0.55
1:B:219:ASN:HD22	1:B:220:GLY:N	2.04	0.55
1:D:175:ILE:HB	1:D:230:LEU:HB2	1.89	0.55
1:B:35:ILE:HG13	1:B:36:GLY:N	2.21	0.55
1:B:295:GLU:O	1:B:298:TRP:HB3	2.05	0.55
1:D:41:ILE:O	1:D:43:TRP:N	2.35	0.55
1:D:386:LEU:HB2	1:D:407:ALA:O	2.07	0.55
1:B:245:ASP:O	1:B:249:ARG:HB2	2.06	0.55
1:A:146:PRO:CB	1:A:505:GLU:HG2	2.32	0.54
1:B:491:ARG:HD3	1:B:493:ARG:NH1	2.22	0.54
1:D:397:ARG:HG2	1:D:397:ARG:NH1	2.15	0.54
1:A:31:GLU:OE2	1:A:181:ARG:NH1	2.40	0.54
1:A:420:LEU:HD12	1:A:421:TYR:H	1.73	0.54
1:B:37:ASP:C	1:B:39:ARG:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LYS:HG3	1:C:88:PHE:CD2	2.42	0.54
1:D:39:ARG:N	1:D:187:CYS:SG	2.81	0.54
1:D:114:ASP:OD1	1:D:116:GLU:HG2	2.08	0.54
1:D:138:LEU:HD22	1:D:144:TYR:CE2	2.42	0.54
1:B:289:TRP:HH2	1:B:440:LEU:HD13	1.71	0.54
1:B:331:LEU:HB3	1:B:334:TYR:CD2	2.43	0.54
1:D:331:LEU:HD13	1:D:334:TYR:HE2	1.73	0.54
1:A:299:PHE:HB3	1:A:347:TRP:CZ3	2.43	0.54
1:C:34:GLY:O	1:C:43:TRP:HH2	1.90	0.54
1:A:18:LEU:HD22	1:A:488:VAL:HG11	1.88	0.54
1:B:181:ARG:HG2	1:B:181:ARG:HH11	1.72	0.54
1:B:467:SER:O	1:B:470:VAL:HG23	2.07	0.54
1:C:164:LEU:HA	1:C:169:VAL:CG1	2.38	0.54
1:C:233:ARG:CZ	1:C:235:ARG:NH1	2.71	0.54
1:B:206:TRP:CH2	1:B:232:PRO:HG3	2.43	0.54
1:D:30:ASP:HB3	1:D:43:TRP:CH2	2.43	0.54
1:B:331:LEU:HD22	1:B:334:TYR:CE2	2.43	0.54
1:B:55:LEU:HD21	1:B:176:TYR:CD1	2.43	0.54
1:B:386:LEU:HB3	1:B:408:GLN:HG3	1.90	0.54
1:B:395:LEU:N	1:B:396:PRO:CD	2.71	0.53
1:B:491:ARG:HD3	1:B:493:ARG:HH12	1.73	0.53
1:B:236:GLU:O	1:B:239:GLN:HB2	2.09	0.53
1:D:99:LEU:HD12	1:D:159:VAL:HG22	1.91	0.53
1:D:116:GLU:HA	1:D:119:ASN:HB3	1.90	0.53
1:D:285:LYS:HD2	1:D:476:GLN:HE22	1.73	0.53
1:D:407:ALA:HA	1:D:419:MET:O	2.08	0.53
1:B:58:LYS:O	1:B:72:ASN:ND2	2.40	0.53
1:B:45:VAL:HG21	1:B:180:ILE:HD12	1.91	0.53
1:B:146:PRO:HG3	1:B:505:GLU:HG2	1.90	0.53
1:B:428:GLY:O	1:B:429:LEU:HD23	2.08	0.53
1:C:207:GLN:HE21	1:C:233:ARG:HD2	1.72	0.53
1:C:279:LEU:HD23	1:C:281:LEU:CG	2.34	0.53
1:B:235:ARG:HB2	5:B:1152:HOH:O	2.08	0.53
1:A:219:ASN:N	1:A:219:ASN:HD22	2.05	0.53
1:C:392:PRO:HD2	1:D:350:PHE:CE1	2.44	0.53
1:D:12:VAL:HG13	1:D:13:ALA:N	2.24	0.53
1:A:289:TRP:HH2	1:A:440:LEU:HG	1.74	0.53
1:B:405:LEU:HD12	1:B:406:LEU:HB2	1.90	0.53
1:C:296:LEU:HD21	1:C:441:LEU:HB2	1.90	0.53
1:C:473:CYS:O	1:C:477:LEU:HG	2.08	0.53
1:D:425:CYS:SG	1:D:460:LEU:HD13	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLY:HA2	1:A:354:TYR:CE2	2.44	0.53
1:B:156:GLY:HA3	3:B:702:NDP:O2A	2.09	0.53
1:B:314:VAL:HA	5:B:1183:HOH:O	2.09	0.53
1:C:282:LEU:HD12	1:C:432:PRO:HG3	1.91	0.53
1:C:406:LEU:HD22	1:D:406:LEU:HD21	1.91	0.53
1:D:307:LYS:HA	1:D:310:SER:OG	2.09	0.53
1:B:321:GLY:O	1:B:336:GLU:HG3	2.09	0.53
1:C:35:ILE:HG13	1:C:36:GLY:N	2.24	0.53
1:C:376:LEU:CD1	1:C:385:MET:SD	2.97	0.53
1:B:96:ASN:HD22	1:B:96:ASN:N	2.07	0.53
1:C:242:SER:O	1:C:245:ASP:HB3	2.08	0.53
1:C:315:HIS:HB3	1:C:318:ASP:OD1	2.09	0.53
1:C:388:THR:HB	1:C:406:LEU:HD12	1.91	0.53
1:D:357:HIS:O	1:D:359:ALA:N	2.42	0.53
1:C:248:ILE:HA	1:C:263:LEU:HD12	1.91	0.52
1:C:350:PHE:CZ	1:D:392:PRO:HD2	2.44	0.52
1:D:41:ILE:N	1:D:42:PRO:HD3	2.24	0.52
1:D:155:GLY:HA2	3:D:704:NDP:H5N	1.91	0.52
1:A:208:ARG:HD3	1:A:228:GLU:OE1	2.09	0.52
1:B:423:ARG:HG3	1:B:424:SER:N	2.24	0.52
1:D:36:GLY:N	1:D:43:TRP:CZ2	2.76	0.52
1:A:289:TRP:CH2	1:A:440:LEU:HG	2.44	0.52
1:B:342:VAL:HG12	1:B:398:MET:HB3	1.91	0.52
1:D:115:GLU:HA	1:D:118:ARG:HH11	1.72	0.52
1:A:43:TRP:CD1	1:A:43:TRP:O	2.63	0.52
1:B:90:PRO:HB2	1:B:96:ASN:CG	2.30	0.52
1:B:115:GLU:HA	1:B:118:ARG:HD3	1.91	0.52
1:D:293:CYS:O	1:D:297:LEU:HD22	2.09	0.52
1:A:60:ARG:HH22	1:A:508:ASP:HA	1.73	0.52
1:A:350:PHE:CE1	1:B:392:PRO:HD2	2.44	0.52
1:B:31:GLU:OE1	1:B:181:ARG:HD3	2.10	0.52
1:C:155:GLY:HA2	1:C:160:TYR:CZ	2.45	0.52
1:B:299:PHE:HB3	1:B:347:TRP:CZ3	2.45	0.52
1:B:469:HIS:O	1:B:472:PRO:HD2	2.09	0.52
1:C:376:LEU:HD13	1:C:385:MET:SD	2.49	0.52
1:B:296:LEU:HD22	1:B:440:LEU:HD23	1.92	0.52
1:A:162:GLU:HA	1:A:165:ARG:NH1	2.25	0.51
1:A:311:ASP:C	1:A:313:GLY:H	2.14	0.51
1:B:296:LEU:O	1:B:300:LEU:HD23	2.10	0.51
1:B:472:PRO:O	1:B:475:GLU:HB2	2.10	0.51
1:D:115:GLU:HA	1:D:118:ARG:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ASN:OD1	1:D:192:ARG:HD3	2.10	0.51
1:A:424:SER:OG	1:B:383:ARG:HD2	2.11	0.51
1:B:285:LYS:CE	1:B:515:ILE:HD11	2.37	0.51
1:B:380:PRO:HB2	1:B:411:VAL:HG11	1.93	0.51
1:B:490:ARG:HG2	1:B:503:ASP:O	2.10	0.51
1:C:155:GLY:CA	3:C:703:NDP:H5N	2.40	0.51
1:D:8:MET:CE	1:D:448:ALA:HA	2.40	0.51
1:D:59:LEU:HD13	1:D:70:LYS:HG3	1.91	0.51
1:A:16:THR:O	1:A:16:THR:HG22	2.10	0.51
1:B:86:PRO:HG3	1:B:89:ARG:NH1	2.26	0.51
1:B:288:PHE:O	1:B:292:VAL:HG23	2.11	0.51
1:D:20:LEU:HD23	1:D:137:ARG:HG3	1.92	0.51
1:A:208:ARG:HH21	1:C:263:LEU:HD13	1.75	0.51
1:B:282:LEU:HD12	1:B:432:PRO:HB3	1.92	0.51
1:D:434:ASN:N	1:D:434:ASN:HD22	2.08	0.51
1:A:256:ASP:OD2	1:A:260:VAL:HB	2.09	0.51
1:D:106:GLN:HA	1:D:109:LEU:HD23	1.92	0.51
1:D:347:TRP:HE1	1:D:389:ALA:HB2	1.75	0.51
1:B:37:ASP:OD2	1:B:42:PRO:HG2	2.11	0.51
1:B:206:TRP:CZ3	1:B:232:PRO:HG3	2.46	0.51
1:C:219:ASN:C	1:C:219:ASN:HD22	2.14	0.51
1:D:490:ARG:HB3	1:D:490:ARG:NH1	2.25	0.51
1:A:115:GLU:OE2	1:A:118:ARG:NE	2.42	0.51
1:A:374:GLU:O	1:A:378:THR:HG23	2.11	0.50
1:B:98:VAL:HB	1:B:108:LEU:HD21	1.92	0.50
1:A:62:LYS:O	1:A:63:ASN:CB	2.56	0.50
1:A:392:PRO:HD2	1:B:350:PHE:CZ	2.47	0.50
1:C:342:VAL:HG12	1:C:398:MET:HB3	1.92	0.50
1:A:19:ALA:O	1:A:20:LEU:HD23	2.11	0.50
1:D:40:SER:OG	1:D:41:ILE:N	2.44	0.50
1:D:336:GLU:O	1:D:337:MET:HB2	2.12	0.50
1:A:84:ILE:O	1:A:89:ARG:HD3	2.10	0.50
1:A:84:ILE:HD13	1:A:91:LEU:HD21	1.92	0.50
1:C:96:ASN:N	1:C:96:ASN:ND2	2.58	0.50
1:C:281:LEU:HD21	1:C:289:TRP:HE3	1.77	0.50
1:B:296:LEU:HG	1:B:300:LEU:HD23	1.94	0.50
1:B:386:LEU:HB2	1:B:407:ALA:O	2.11	0.50
1:C:431:VAL:O	1:C:435:ILE:HG13	2.12	0.50
1:D:355:THR:HG22	1:D:356:HIS:HD2	1.74	0.50
1:A:271:ARG:NH2	1:B:266:PHE:O	2.39	0.50
1:B:146:PRO:CG	1:B:505:GLU:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ILE:HB	1:C:230:LEU:HB2	1.92	0.50
1:C:407:ALA:HA	1:C:419:MET:O	2.12	0.50
1:B:276:ASN:C	1:B:277:ASN:HD22	2.15	0.50
1:C:420:LEU:HD23	1:C:458:HIS:CD2	2.47	0.50
1:A:37:ASP:HB2	1:A:42:PRO:CD	2.42	0.49
1:B:109:LEU:CD1	1:B:125:ILE:HD12	2.41	0.49
1:B:285:LYS:CB	1:B:476:GLN:NE2	2.75	0.49
1:B:292:VAL:HG13	1:B:437:SER:OG	2.12	0.49
1:D:195:GLU:HB3	1:D:198:THR:CG2	2.40	0.49
1:A:180:ILE:HG23	1:A:223:THR:HG21	1.93	0.49
1:D:357:HIS:CG	1:D:358:ASP:H	2.30	0.49
1:A:264:SER:HB3	1:A:464:HIS:HB3	1.94	0.49
1:D:110:ASP:HA	1:D:118:ARG:NE	2.28	0.49
1:C:406:LEU:HB3	1:C:421:TYR:HB3	1.94	0.49
1:B:207:GLN:O	1:B:230:LEU:HA	2.13	0.49
1:B:395:LEU:HB2	1:B:396:PRO:HD3	1.94	0.49
1:C:6:ILE:HD11	1:C:370:LYS:HB2	1.95	0.49
1:D:101:SER:HA	1:D:129:ASN:ND2	2.27	0.49
1:D:247:ILE:O	1:D:251:GLY:N	2.44	0.49
1:D:279:LEU:HD22	1:D:487:LEU:HB2	1.94	0.49
1:B:321:GLY:O	1:B:337:MET:HE2	2.13	0.49
1:A:183:SER:O	1:A:184:GLU:HB2	2.13	0.49
1:B:132:LEU:HB3	1:B:162:GLU:HG2	1.94	0.49
1:C:116:GLU:HA	1:C:119:ASN:HD22	1.78	0.49
1:D:25:LEU:HD23	1:D:25:LEU:C	2.33	0.49
1:C:92:PRO:O	1:C:94:ARG:NE	2.43	0.49
1:B:84:ILE:CG2	1:B:89:ARG:HG2	2.43	0.48
1:B:104:THR:HB	1:B:107:HIS:ND1	2.28	0.48
1:D:333:GLU:O	1:D:356:HIS:HE1	1.96	0.48
1:A:139:LEU:HD13	1:A:151:VAL:HG22	1.94	0.48
1:C:304:THR:HB	1:C:340:GLY:O	2.13	0.48
1:C:340:GLY:HA2	1:C:354:TYR:CE2	2.49	0.48
1:C:386:LEU:HB3	1:C:408:GLN:HA	1.94	0.48
1:A:331:LEU:HB3	1:A:334:TYR:CD2	2.48	0.48
1:C:100:SER:O	1:C:129:ASN:HA	2.13	0.48
1:C:397:ARG:HG3	1:C:397:ARG:HH11	1.78	0.48
1:A:372:ILE:HG21	1:A:409:PHE:CD1	2.49	0.48
1:B:233:ARG:NH1	1:D:249:ARG:NH2	2.61	0.48
1:B:515:ILE:O	1:B:517:MET:N	2.42	0.48
1:A:2:SER:H	1:A:5:LYS:HD3	1.77	0.48
1:B:388:THR:HB	1:B:406:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:VAL:HB	1:A:432:PRO:HD3	1.96	0.48
1:B:52:PHE:CE1	1:B:56:THR:HG21	2.48	0.48
1:D:138:LEU:HD22	1:D:144:TYR:HE2	1.77	0.48
1:D:325:PHE:O	1:D:328:SER:HB3	2.14	0.48
1:A:139:LEU:HD13	1:A:151:VAL:CG2	2.43	0.48
1:B:208:ARG:NH2	1:D:251:GLY:O	2.41	0.48
1:C:155:GLY:O	1:C:159:VAL:HG21	2.13	0.48
1:C:296:LEU:HD13	1:C:296:LEU:O	2.14	0.48
1:A:25:LEU:HD11	1:A:160:TYR:HD1	1.79	0.48
1:B:39:ARG:O	1:B:40:SER:HB2	2.12	0.48
1:C:165:ARG:C	1:C:169:VAL:HG22	2.34	0.48
1:C:467:SER:O	1:C:470:VAL:HG23	2.13	0.48
1:A:231:ILE:HB	1:A:232:PRO:HD2	1.96	0.48
1:B:27:VAL:HG22	1:B:28:ALA:N	2.27	0.48
1:C:192:ARG:HG2	1:C:192:ARG:NH1	2.26	0.48
1:D:295:GLU:OE1	1:D:433:PHE:HE2	1.97	0.48
1:D:423:ARG:HG3	1:D:423:ARG:HH11	1.78	0.48
1:B:422:GLN:HG2	1:B:425:CYS:SG	2.54	0.47
1:C:75:VAL:O	1:C:154:ILE:HG12	2.14	0.47
1:B:20:LEU:HB2	1:B:171:LEU:CD1	2.44	0.47
1:D:153:CYS:SG	1:D:159:VAL:HG12	2.54	0.47
1:D:234:ASN:C	1:D:234:ASN:ND2	2.67	0.47
1:C:422:GLN:HE22	1:C:434:ASN:ND2	2.10	0.47
1:D:290:ARG:HG2	1:D:290:ARG:HH11	1.79	0.47
1:A:208:ARG:HD2	1:A:211:ILE:HB	1.96	0.47
1:A:292:VAL:HA	1:A:433:PHE:CZ	2.50	0.47
1:C:345:PHE:HE2	1:C:361:TYR:CD2	2.31	0.47
1:C:346:GLN:O	1:C:350:PHE:HB2	2.13	0.47
1:A:36:GLY:O	1:A:187:CYS:HB3	2.14	0.47
1:A:76:MET:SD	1:A:154:ILE:HD11	2.54	0.47
1:B:285:LYS:CD	1:B:476:GLN:NE2	2.76	0.47
1:C:469:HIS:C	1:C:472:PRO:HD2	2.35	0.47
1:D:78:ARG:HE	1:D:103:LEU:HD11	1.79	0.47
1:D:338:ASP:OD2	1:D:354:TYR:OH	2.29	0.47
1:A:128:VAL:HG23	1:A:128:VAL:O	2.14	0.47
1:A:257:ARG:HD3	1:A:257:ARG:N	2.25	0.47
1:A:487:LEU:HD11	1:A:504:MET:HB2	1.96	0.47
1:B:12:VAL:HG13	1:B:13:ALA:N	2.29	0.47
1:D:253:VAL:HG22	1:D:263:LEU:CD2	2.43	0.47
1:A:296:LEU:HD21	1:A:441:LEU:HB2	1.96	0.47
1:B:192:ARG:HD3	1:C:413:ASN:CG	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:HD22	1:C:488:VAL:HG11	1.96	0.47
1:D:73:ALA:HB2	1:D:148:ILE:HG21	1.97	0.47
1:A:296:LEU:HD13	1:A:296:LEU:C	2.34	0.47
1:B:65:LYS:HD2	1:B:65:LYS:N	2.30	0.47
1:B:320:ASN:ND2	1:B:400:LEU:HD22	2.30	0.47
1:A:273:SER:O	1:A:274:LEU:HD23	2.15	0.47
1:A:478:LYS:HD3	1:C:478:LYS:HZ2	1.79	0.47
1:D:63:ASN:C	1:D:63:ASN:HD22	2.19	0.47
1:A:74:VAL:HB	1:A:154:ILE:CG2	2.44	0.46
1:B:37:ASP:OD2	1:B:42:PRO:CG	2.63	0.46
1:B:257:ARG:H	1:B:257:ARG:CD	2.14	0.46
1:C:386:LEU:HD12	1:C:406:LEU:HD11	1.96	0.46
1:A:2:SER:HA	1:A:495:PHE:CE2	2.50	0.46
1:A:109:LEU:O	1:A:118:ARG:HD3	2.15	0.46
1:C:405:LEU:HD12	1:C:406:LEU:HB2	1.96	0.46
1:D:42:PRO:CB	1:D:185:SER:OG	2.62	0.46
1:A:422:GLN:HE21	1:A:425:CYS:HA	1.80	0.46
1:C:15:GLY:HA3	5:C:1110:HOH:O	2.15	0.46
1:C:266:PHE:HA	1:C:461:GLY:O	2.15	0.46
1:D:341:PRO:HD3	1:D:354:TYR:CD2	2.50	0.46
1:D:405:LEU:HD12	1:D:406:LEU:HD23	1.97	0.46
1:D:496:LEU:HD12	1:D:496:LEU:O	2.15	0.46
1:A:460:LEU:HD23	1:A:460:LEU:N	2.30	0.46
1:B:233:ARG:NH1	1:D:249:ARG:HH21	2.13	0.46
1:D:237:GLU:HB3	1:D:481:PRO:HB3	1.98	0.46
1:A:13:ALA:HB2	1:A:492:GLU:HG3	1.96	0.46
1:B:3:LEU:HD23	1:B:3:LEU:O	2.16	0.46
1:B:152:TYR:O	1:B:154:ILE:HG23	2.16	0.46
1:B:169:VAL:C	1:B:171:LEU:H	2.19	0.46
1:B:323:ARG:NH2	1:B:326:LEU:HB3	2.31	0.46
1:C:30:ASP:OD2	1:C:32:HIS:N	2.49	0.46
1:D:183:SER:O	1:D:184:GLU:O	2.34	0.46
1:B:41:ILE:HD11	1:B:43:TRP:O	2.16	0.46
1:B:78:ARG:HG3	1:B:103:LEU:HD12	1.96	0.46
1:B:219:ASN:HD21	1:B:221:ASN:H	1.56	0.46
1:C:74:VAL:HG23	1:C:74:VAL:O	2.14	0.46
1:C:267:GLY:HA2	1:C:460:LEU:O	2.15	0.46
1:C:400:LEU:HD11	1:D:384:ARG:NH2	2.30	0.46
1:D:162:GLU:HG3	1:D:165:ARG:NH1	2.31	0.46
1:A:341:PRO:HB2	1:A:346:GLN:HE21	1.80	0.46
1:A:490:ARG:NH1	1:A:490:ARG:CB	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:1CY:H16	3:B:702:NDP:H42N	1.97	0.46
1:C:181:ARG:HB3	1:C:181:ARG:NH1	2.31	0.46
1:D:35:ILE:C	1:D:37:ASP:N	2.68	0.46
1:B:45:VAL:HG21	1:B:180:ILE:CD1	2.46	0.46
1:B:433:PHE:O	1:B:436:ALA:HB3	2.16	0.46
1:C:211:ILE:HG23	1:C:211:ILE:O	2.15	0.46
1:C:427:MET:SD	1:C:431:VAL:HG21	2.55	0.46
1:D:215:LEU:O	1:D:224:LYS:HA	2.15	0.46
1:D:490:ARG:HB3	1:D:490:ARG:CZ	2.46	0.46
1:A:427:MET:SD	1:A:431:VAL:HG21	2.56	0.45
1:C:294:GLU:O	1:C:298:TRP:HB2	2.16	0.45
1:D:282:LEU:HD12	1:D:432:PRO:HB3	1.98	0.45
1:B:165:ARG:C	1:B:169:VAL:HG22	2.36	0.45
1:B:205:GLU:HA	5:B:1041:HOH:O	2.16	0.45
1:D:315:HIS:HB3	1:D:318:ASP:OD1	2.15	0.45
1:A:180:ILE:HG23	1:A:223:THR:CG2	2.46	0.45
1:B:277:ASN:O	1:B:486:TYR:HA	2.16	0.45
1:B:316:ILE:HG13	1:B:317:TRP:CD1	2.52	0.45
1:D:298:TRP:HH2	1:D:339:LEU:HD12	1.80	0.45
1:B:169:VAL:C	1:B:171:LEU:N	2.68	0.45
1:C:163:ALA:O	1:C:169:VAL:HG13	2.17	0.45
1:C:164:LEU:CA	1:C:169:VAL:HG13	2.45	0.45
1:D:243:LEU:HD23	1:D:427:MET:HE1	1.99	0.45
1:A:380:PRO:HB2	1:A:411:VAL:HG11	1.98	0.45
1:B:153:CYS:SG	1:B:159:VAL:HG12	2.56	0.45
1:C:112:LEU:HB2	1:C:118:ARG:HG2	1.98	0.45
1:D:397:ARG:CG	1:D:397:ARG:NH1	2.72	0.45
1:A:476:GLN:HB2	1:A:515:ILE:CD1	2.47	0.45
1:B:68:PRO:HA	1:B:71:ARG:HD3	1.98	0.45
1:D:104:THR:O	1:D:107:HIS:HB2	2.16	0.45
1:D:285:LYS:HD2	1:D:476:GLN:NE2	2.31	0.45
1:D:386:LEU:CB	1:D:408:GLN:HA	2.45	0.45
1:C:292:VAL:HA	1:C:433:PHE:CZ	2.52	0.45
1:B:361:TYR:O	1:B:362:ASP:C	2.55	0.45
1:B:456:LEU:HD22	1:B:457:VAL:N	2.32	0.45
1:D:110:ASP:C	1:D:112:LEU:H	2.21	0.45
1:D:193:VAL:O	1:D:194:PRO:C	2.55	0.45
1:B:279:LEU:O	1:B:485:PRO:HD2	2.17	0.45
1:B:296:LEU:HD22	1:B:440:LEU:CG	2.47	0.45
1:C:39:ARG:O	1:C:39:ARG:HG2	2.15	0.45
1:C:179:THR:O	1:C:225:TYR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:TRP:HB2	5:C:1026:HOH:O	2.17	0.45
1:D:35:ILE:HG12	1:D:189:VAL:O	2.17	0.45
1:D:36:GLY:O	1:D:37:ASP:HB2	2.16	0.45
1:D:208:ARG:NH1	1:D:228:GLU:OE1	2.46	0.45
1:B:8:MET:HE2	1:B:12:VAL:HG23	1.99	0.44
1:B:78:ARG:HD3	3:B:702:NDP:O2X	2.17	0.44
1:B:262:THR:HG22	1:B:466:TYR:CD2	2.51	0.44
1:D:325:PHE:HA	1:D:328:SER:HB3	1.99	0.44
1:C:98:VAL:HB	1:C:108:LEU:HD21	1.99	0.44
1:C:219:ASN:C	1:C:219:ASN:ND2	2.71	0.44
1:C:266:PHE:CZ	1:D:419:MET:HB2	2.52	0.44
1:D:295:GLU:O	1:D:298:TRP:HB3	2.18	0.44
1:A:320:ASN:HA	1:A:325:PHE:CD2	2.53	0.44
1:B:35:ILE:O	3:B:702:NDP:N7N	2.50	0.44
1:B:233:ARG:CZ	1:B:235:ARG:NH1	2.80	0.44
1:A:74:VAL:HB	1:A:154:ILE:HG23	1.99	0.44
1:A:78:ARG:NH1	1:A:82:ASP:OD1	2.42	0.44
1:A:175:ILE:HB	1:A:230:LEU:HB2	2.00	0.44
1:C:52:PHE:CD1	1:C:52:PHE:C	2.91	0.44
1:C:275:ARG:HH12	1:C:455:GLU:CG	2.31	0.44
1:A:42:PRO:HG2	1:A:43:TRP:CE3	2.53	0.44
1:A:153:CYS:SG	1:A:159:VAL:HG12	2.58	0.44
1:B:8:MET:CE	1:B:12:VAL:HG23	2.48	0.44
1:B:30:ASP:O	1:B:32:HIS:N	2.51	0.44
1:C:279:LEU:HD13	1:C:487:LEU:HD22	1.98	0.44
1:C:279:LEU:CD1	1:C:487:LEU:HD22	2.48	0.44
1:D:45:VAL:HA	1:D:46:PRO:HD2	1.88	0.44
1:D:278:ARG:HH11	1:D:278:ARG:CG	2.27	0.44
1:A:341:PRO:HB2	1:A:346:GLN:NE2	2.33	0.44
1:B:441:LEU:O	1:B:445:ILE:HG12	2.17	0.44
1:D:304:THR:HG22	1:D:345:PHE:HB2	2.00	0.44
1:D:391:ASN:OD1	1:D:393:SER:HB2	2.17	0.44
1:D:395:LEU:N	1:D:396:PRO:CD	2.81	0.44
1:A:249:ARG:HE	1:A:249:ARG:HB2	1.62	0.44
1:B:296:LEU:O	1:B:299:PHE:HB2	2.18	0.44
1:C:31:GLU:HG3	1:C:181:ARG:HA	1.99	0.44
1:D:100:SER:O	1:D:129:ASN:HA	2.17	0.44
1:A:215:LEU:O	1:A:224:LYS:HA	2.17	0.43
1:A:321:GLY:O	1:A:337:MET:N	2.51	0.43
1:B:4:PHE:CE1	1:B:362:ASP:HB3	2.53	0.43
1:B:14:GLU:N	1:B:14:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LEU:HD22	1:B:440:LEU:CD2	2.48	0.43
1:C:386:LEU:N	1:C:386:LEU:HD23	2.33	0.43
1:B:164:LEU:HD13	1:B:192:ARG:O	2.18	0.43
1:C:254:LYS:O	1:C:261:GLY:HA2	2.18	0.43
1:A:420:LEU:HD12	1:A:421:TYR:N	2.33	0.43
1:B:104:THR:CG2	1:B:106:GLN:H	2.31	0.43
1:B:146:PRO:HG3	1:B:505:GLU:CG	2.47	0.43
1:B:296:LEU:HD22	1:B:440:LEU:HG	2.00	0.43
1:C:288:PHE:CD1	1:C:291:GLY:HA3	2.53	0.43
1:D:36:GLY:HA2	1:D:43:TRP:CZ2	2.53	0.43
1:A:258:THR:HB	1:A:260:VAL:HG23	2.00	0.43
1:B:155:GLY:HA2	1:B:160:TYR:CZ	2.52	0.43
1:B:479:ARG:HD3	1:B:512:TYR:CG	2.54	0.43
1:D:155:GLY:HA2	1:D:160:TYR:CZ	2.53	0.43
1:D:183:SER:O	1:D:184:GLU:C	2.57	0.43
1:D:394:ALA:O	1:D:395:LEU:C	2.56	0.43
1:A:27:VAL:HG22	1:A:28:ALA:N	2.33	0.43
1:A:256:ASP:CG	1:A:260:VAL:HB	2.39	0.43
1:B:256:ASP:HB3	1:B:258:THR:H	1.83	0.43
1:B:272:PHE:CZ	1:B:435:ILE:HD13	2.54	0.43
1:C:5:LYS:HB3	1:C:497:GLU:OE2	2.19	0.43
1:C:404:HIS:H	1:C:404:HIS:CD2	2.35	0.43
1:D:59:LEU:CD1	1:D:70:LYS:HG3	2.49	0.43
1:B:387:PHE:O	1:B:406:LEU:HD12	2.18	0.43
1:C:37:ASP:CG	1:C:42:PRO:HG3	2.39	0.43
1:D:422:GLN:NE2	1:D:425:CYS:HB3	2.33	0.43
1:A:155:GLY:HA2	1:A:160:TYR:CZ	2.54	0.43
1:A:36:GLY:HA3	3:A:701:NDP:H1D	2.01	0.43
1:A:207:GLN:NE2	1:A:480:VAL:HG11	2.34	0.43
1:A:430:GLY:O	1:A:434:ASN:ND2	2.52	0.43
1:B:99:LEU:HD12	1:B:159:VAL:HG22	2.00	0.43
1:B:104:THR:HG22	1:B:106:GLN:N	2.31	0.43
1:B:390:TRP:CE3	1:B:405:LEU:HD22	2.53	0.43
1:C:23:PHE:N	1:C:23:PHE:CD2	2.87	0.43
1:D:4:PHE:CE2	1:D:362:ASP:HB3	2.54	0.43
1:D:186:SER:C	1:D:187:CYS:SG	2.97	0.43
1:D:244:VAL:O	1:D:248:ILE:HG13	2.19	0.43
1:B:233:ARG:HD3	1:B:235:ARG:NE	2.34	0.43
1:D:40:SER:O	1:D:42:PRO:HD3	2.18	0.43
1:D:357:HIS:CG	1:D:358:ASP:N	2.87	0.43
1:A:43:TRP:CH2	1:A:187:CYS:SG	3.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LEU:O	1:C:247:ILE:HG13	2.19	0.42
1:D:29:VAL:HG22	1:D:33:GLY:C	2.39	0.42
1:D:125:ILE:HG22	1:D:126:VAL:N	2.34	0.42
1:A:25:LEU:HD11	1:A:160:TYR:CD1	2.54	0.42
1:A:115:GLU:OE2	1:A:118:ARG:NH1	2.50	0.42
1:A:289:TRP:CZ2	1:A:487:LEU:HD13	2.54	0.42
1:A:386:LEU:HD22	1:A:408:GLN:HG3	2.01	0.42
1:A:413:ASN:CG	1:D:192:ARG:HD3	2.40	0.42
1:A:423:ARG:HG3	1:A:424:SER:N	2.34	0.42
1:A:440:LEU:HD22	1:A:444:LEU:CD1	2.49	0.42
1:B:43:TRP:HH2	1:B:187:CYS:SG	2.42	0.42
1:B:420:LEU:HD12	1:B:421:TYR:H	1.84	0.42
1:C:376:LEU:HB3	1:C:449:THR:HG21	2.00	0.42
1:D:78:ARG:HG2	1:D:103:LEU:HD12	2.00	0.42
1:B:27:VAL:CG2	1:B:28:ALA:N	2.82	0.42
1:B:247:ILE:HG21	1:B:465:VAL:HG23	2.01	0.42
1:B:493:ARG:HB2	1:B:499:TYR:CE1	2.54	0.42
1:D:386:LEU:HD12	1:D:406:LEU:HD13	2.01	0.42
1:D:456:LEU:C	1:D:456:LEU:HD13	2.40	0.42
1:B:29:VAL:O	1:B:179:THR:HA	2.20	0.42
1:B:172:LEU:HD21	1:B:175:ILE:HD11	2.01	0.42
1:C:441:LEU:C	1:C:441:LEU:HD23	2.39	0.42
1:D:188:SER:HB2	1:D:190:PHE:CE1	2.54	0.42
1:A:422:GLN:HG2	1:A:424:SER:O	2.19	0.42
1:B:493:ARG:HB2	1:B:499:TYR:CZ	2.55	0.42
1:C:73:ALA:HB2	1:C:148:ILE:HD12	2.00	0.42
1:C:468:ASN:O	1:C:469:HIS:HD2	2.02	0.42
1:A:331:LEU:HD13	1:A:334:TYR:CE2	2.54	0.42
1:B:103:LEU:HB3	1:B:108:LEU:CD1	2.50	0.42
1:B:233:ARG:HE	1:B:235:ARG:HD3	1.84	0.42
1:C:472:PRO:HB2	1:C:517:MET:HG3	2.01	0.42
1:A:194:PRO:HB2	1:A:201:ALA:HA	2.01	0.42
1:A:490:ARG:HB2	1:A:490:ARG:NH1	2.33	0.42
1:B:35:ILE:HD11	1:B:189:VAL:HB	2.02	0.42
1:B:290:ARG:HG2	1:B:290:ARG:HH11	1.84	0.42
1:C:66:PRO:HA	1:C:70:LYS:O	2.20	0.42
1:D:390:TRP:HB2	1:D:405:LEU:HB2	2.02	0.42
1:A:256:ASP:HB2	1:A:257:ARG:HD3	2.01	0.42
1:A:390:TRP:HD1	1:B:388:THR:HG21	1.85	0.42
1:B:61:GLY:O	1:B:63:ASN:N	2.44	0.42
1:C:219:ASN:ND2	1:C:222:GLU:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:VAL:HG22	1:D:492:GLU:OE1	2.20	0.42
1:D:342:VAL:O	1:D:343:TYR:C	2.58	0.42
2:A:601:1CY:H16	3:A:701:NDP:H42N	2.01	0.42
1:C:114:ASP:OD2	1:C:117:LYS:HB2	2.19	0.42
1:C:164:LEU:C	1:C:169:VAL:HG13	2.40	0.42
1:C:258:THR:OG1	1:C:260:VAL:HG23	2.20	0.42
1:C:404:HIS:HB2	1:C:420:LEU:HD11	2.02	0.42
1:C:480:VAL:HA	1:C:481:PRO:HD3	1.84	0.42
1:D:117:LYS:C	1:D:119:ASN:N	2.71	0.42
1:D:475:GLU:OE2	1:D:515:ILE:HG12	2.20	0.42
1:A:170:HIS:C	1:A:171:LEU:HD12	2.40	0.42
1:B:25:LEU:C	1:B:25:LEU:HD23	2.40	0.42
1:B:74:VAL:O	1:B:74:VAL:HG12	2.20	0.42
1:C:249:ARG:NH1	1:C:249:ARG:HB2	2.35	0.42
1:C:276:ASN:O	1:C:277:ASN:HB2	2.19	0.42
1:A:139:LEU:O	1:A:144:TYR:HB2	2.19	0.41
1:B:4:PHE:CG	1:B:362:ASP:HB3	2.54	0.41
1:B:211:ILE:HG23	1:B:211:ILE:O	2.18	0.41
1:D:218:ALA:C	1:D:220:GLY:H	2.23	0.41
1:D:485:PRO:C	1:D:486:TYR:CD1	2.93	0.41
1:A:26:VAL:HG13	1:A:55:LEU:HD23	2.03	0.41
1:B:237:GLU:HB3	1:B:481:PRO:HB3	2.02	0.41
1:C:87:LYS:CD	1:C:88:PHE:CE2	3.03	0.41
1:D:6:ILE:HD12	1:D:496:LEU:HD23	2.02	0.41
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.90	0.41
1:A:76:MET:HB3	1:A:154:ILE:CG1	2.51	0.41
1:A:99:LEU:HD23	1:A:128:VAL:CG2	2.51	0.41
1:A:307:LYS:HA	1:A:310:SER:OG	2.21	0.41
1:C:279:LEU:HD21	1:C:289:TRP:CZ3	2.56	0.41
1:C:306:ALA:HB3	1:C:337:MET:HE3	2.01	0.41
1:D:85:PRO:O	1:D:87:LYS:N	2.54	0.41
1:D:355:THR:CG2	1:D:356:HIS:CD2	3.00	0.41
1:A:361:TYR:O	1:A:362:ASP:C	2.59	0.41
1:C:290:ARG:HD2	5:C:1133:HOH:O	2.19	0.41
1:C:485:PRO:HB3	1:C:509:TYR:HA	2.03	0.41
1:D:253:VAL:HG22	1:D:263:LEU:HD22	2.02	0.41
1:D:265:ILE:HD12	1:D:265:ILE:C	2.40	0.41
1:D:443:ILE:O	1:D:447:LYS:HG3	2.20	0.41
1:B:60:ARG:O	1:B:62:LYS:N	2.53	0.41
1:A:171:LEU:N	1:A:171:LEU:CD1	2.80	0.41
1:A:390:TRP:HB2	1:A:405:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLU:HB2	1:A:515:ILE:HG21	2.02	0.41
1:B:325:PHE:HE2	1:B:399:ALA:O	2.04	0.41
1:C:12:VAL:CG1	1:C:13:ALA:N	2.83	0.41
1:C:25:LEU:C	1:C:25:LEU:HD23	2.41	0.41
1:C:115:GLU:CG	1:C:118:ARG:NH1	2.81	0.41
1:C:281:LEU:HD21	1:C:289:TRP:CE3	2.55	0.41
1:D:73:ALA:HB3	1:D:151:VAL:HG22	2.01	0.41
1:D:116:GLU:CA	1:D:119:ASN:HB3	2.50	0.41
1:D:278:ARG:NH1	1:D:278:ARG:CG	2.84	0.41
1:D:422:GLN:NE2	5:D:1210:HOH:O	2.52	0.41
1:A:346:GLN:HB3	1:A:389:ALA:HA	2.01	0.41
1:B:18:LEU:HD22	1:B:488:VAL:HG11	2.03	0.41
1:C:115:GLU:C	1:C:117:LYS:N	2.74	0.41
1:C:134:GLN:OE1	1:C:134:GLN:N	2.53	0.41
1:C:437:SER:O	1:C:440:LEU:HB3	2.20	0.41
1:A:329:ARG:HA	1:A:329:ARG:HD2	1.76	0.41
1:B:38:GLY:HA2	3:B:702:NDP:H4D	2.03	0.41
1:B:155:GLY:CA	3:B:702:NDP:H5N	2.43	0.41
1:B:394:ALA:O	1:B:398:MET:HG3	2.21	0.41
1:C:232:PRO:O	1:C:233:ARG:C	2.59	0.41
1:C:296:LEU:C	1:C:296:LEU:CD1	2.86	0.41
1:C:443:ILE:HD12	1:C:487:LEU:HD23	2.03	0.41
1:D:155:GLY:CA	3:D:704:NDP:H5N	2.50	0.41
1:D:211:ILE:HA	1:D:227:PHE:O	2.20	0.41
1:D:323:ARG:HH21	1:D:326:LEU:HB3	1.86	0.41
1:A:208:ARG:HG2	1:A:230:LEU:CD2	2.51	0.41
1:B:43:TRP:CH2	1:B:187:CYS:SG	3.14	0.41
1:B:239:GLN:NE2	1:B:271:ARG:H	2.12	0.41
1:B:298:TRP:CD1	1:B:309:LEU:HD13	2.56	0.41
1:D:78:ARG:HB2	1:D:100:SER:HB2	2.03	0.41
1:D:84:ILE:O	1:D:85:PRO:C	2.58	0.41
1:D:85:PRO:O	1:D:88:PHE:N	2.51	0.41
1:A:181:ARG:HH11	1:A:181:ARG:CB	2.18	0.40
1:B:422:GLN:HG2	1:B:424:SER:O	2.21	0.40
1:C:272:PHE:CE2	1:C:435:ILE:HD13	2.56	0.40
1:C:281:LEU:O	1:C:282:LEU:C	2.60	0.40
1:D:234:ASN:ND2	1:D:236:GLU:HB2	2.35	0.40
1:D:275:ARG:NE	1:D:415:GLU:OE2	2.54	0.40
1:D:425:CYS:SG	1:D:460:LEU:CD1	3.09	0.40
1:A:257:ARG:CD	1:A:257:ARG:N	2.81	0.40
1:B:49:MET:HE2	1:B:49:MET:HB3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ALA:O	1:B:139:LEU:HD22	2.20	0.40
1:B:490:ARG:HG2	1:B:490:ARG:H	1.60	0.40
1:C:431:VAL:O	1:C:432:PRO:C	2.58	0.40
1:D:115:GLU:CG	1:D:118:ARG:HH11	2.34	0.40
1:D:219:ASN:C	1:D:219:ASN:HD22	2.23	0.40
1:D:420:LEU:HD13	1:D:438:TYR:CE1	2.56	0.40
1:B:428:GLY:C	1:B:429:LEU:HD23	2.42	0.40
1:C:386:LEU:HD22	1:C:408:GLN:HG3	2.02	0.40
1:D:116:GLU:C	1:D:119:ASN:HB3	2.42	0.40
1:D:245:ASP:O	1:D:249:ARG:HB2	2.21	0.40
1:A:105:THR:HG23	1:A:126:VAL:HA	2.03	0.40
1:A:342:VAL:O	1:A:343:TYR:C	2.60	0.40
1:B:37:ASP:HA	1:B:187:CYS:HA	2.04	0.40
1:B:172:LEU:HD11	1:B:174:ALA:O	2.21	0.40
1:C:323:ARG:HB2	1:C:336:GLU:OE2	2.21	0.40
1:A:221:ASN:OD1	1:A:221:ASN:N	2.54	0.40
1:A:294:GLU:OE2	1:A:312:LYS:HD3	2.21	0.40
1:B:245:ASP:OD2	1:B:249:ARG:NH1	2.47	0.40
1:C:233:ARG:CZ	1:C:235:ARG:HH12	2.34	0.40
1:C:286:ARG:HA	1:C:509:TYR:OH	2.22	0.40
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	514/521 (99%)	468 (91%)	37 (7%)	9 (2%)	8 16
1	B	514/521 (99%)	467 (91%)	36 (7%)	11 (2%)	7 13
1	C	514/521 (99%)	467 (91%)	39 (8%)	8 (2%)	9 19
1	D	511/521 (98%)	446 (87%)	45 (9%)	20 (4%)	3 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2053/2084 (98%)	1848 (90%)	157 (8%)	48 (2%)	6 11

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	219	ASN
1	A	343	TYR
1	B	113	PRO
1	C	44	ASN
1	C	62	LYS
1	C	343	TYR
1	D	122	ALA
1	D	184	GLU
1	D	343	TYR
1	A	2	SER
1	A	63	ASN
1	A	186	SER
1	B	31	GLU
1	B	186	SER
1	B	188	SER
1	B	343	TYR
1	B	516	SER
1	D	15	GLY
1	D	37	ASP
1	D	43	TRP
1	D	187	CYS
1	D	358	ASP
1	C	113	PRO
1	D	113	PRO
1	A	187	CYS
1	B	63	ASN
1	C	311	ASP
1	D	111	GLY
1	D	219	ASN
1	D	514	PRO
1	C	202	ALA
1	D	40	SER
1	D	235	ARG
1	A	185	SER
1	B	40	SER
1	D	42	PRO

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Mol	Chain	Res	Type
1	D	86	PRO
1	D	485	PRO
1	C	267	GLY
1	A	341	PRO
1	B	46	PRO
1	B	61	GLY
1	C	485	PRO
1	D	267	GLY
1	D	344	GLY
1	B	38	GLY
1	D	35	ILE

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	442/446 (99%)	421 (95%)	21 (5%)	25 49
1	B	442/446 (99%)	414 (94%)	28 (6%)	18 36
1	C	442/446 (99%)	412 (93%)	30 (7%)	16 32
1	D	439/446 (98%)	417 (95%)	22 (5%)	24 47
All	All	1765/1784 (99%)	1664 (94%)	101 (6%)	20 41

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	44	ASN
1	A	49	MET
1	A	95	LEU
1	A	96	ASN
1	A	181	ARG
1	A	189	VAL
1	A	219	ASN
1	A	221	ASN
1	A	257	ARG

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Mol	Chain	Res	Type
1	A	278	ARG
1	A	297	LEU
1	A	326	LEU
1	A	333	GLU
1	A	386	LEU
1	A	406	LEU
1	A	429	LEU
1	A	440	LEU
1	A	460	LEU
1	A	487	LEU
1	A	496	LEU
1	B	14	GLU
1	B	37	ASP
1	B	40	SER
1	B	41	ILE
1	B	43	TRP
1	B	49	MET
1	B	74	VAL
1	B	95	LEU
1	B	104	THR
1	B	139	LEU
1	B	146	PRO
1	B	169	VAL
1	B	219	ASN
1	B	250	GLU
1	B	256	ASP
1	B	257	ARG
1	B	296	LEU
1	B	297	LEU
1	B	303	GLU
1	B	333	GLU
1	B	355	THR
1	B	456	LEU
1	B	467	SER
1	B	468	ASN
1	B	476	GLN
1	B	490	ARG
1	B	493	ARG
1	B	515	ILE
1	C	16	THR
1	C	26	VAL
1	C	49	MET

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Mol	Chain	Res	Type
1	C	95	LEU
1	C	96	ASN
1	C	106	GLN
1	C	109	LEU
1	C	116	GLU
1	C	138	LEU
1	C	139	LEU
1	C	159	VAL
1	C	169	VAL
1	C	171	LEU
1	C	207	GLN
1	C	219	ASN
1	C	235	ARG
1	C	243	LEU
1	C	257	ARG
1	C	263	LEU
1	C	326	LEU
1	C	358	ASP
1	C	360	ASN
1	C	374	GLU
1	C	376	LEU
1	C	386	LEU
1	C	395	LEU
1	C	456	LEU
1	C	474	ASN
1	C	493	ARG
1	C	505	GLU
1	D	63	ASN
1	D	95	LEU
1	D	96	ASN
1	D	113	PRO
1	D	138	LEU
1	D	139	LEU
1	D	184	GLU
1	D	187	CYS
1	D	219	ASN
1	D	234	ASN
1	D	297	LEU
1	D	309	LEU
1	D	326	LEU
1	D	329	ARG
1	D	376	LEU

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Mol	Chain	Res	Type
1	D	397	ARG
1	D	405	LEU
1	D	425	CYS
1	D	460	LEU
1	D	471	GLU
1	D	473	CYS
1	D	493	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	219	ASN
1	A	239	GLN
1	A	320	ASN
1	A	422	GLN
1	A	434	ASN
1	A	476	GLN
1	B	207	GLN
1	B	219	ASN
1	B	239	GLN
1	B	276	ASN
1	B	277	ASN
1	B	320	ASN
1	B	356	HIS
1	B	464	HIS
1	B	476	GLN
1	C	119	ASN
1	C	173	GLN
1	C	207	GLN
1	C	219	ASN
1	C	320	ASN
1	C	360	ASN
1	C	434	ASN
1	C	469	HIS
1	C	476	GLN
1	D	63	ASN
1	D	106	GLN
1	D	134	GLN
1	D	143	ASN
1	D	219	ASN
1	D	234	ASN

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Mol	Chain	Res	Type
1	D	239	GLN
1	D	276	ASN
1	D	277	ASN
1	D	356	HIS
1	D	379	ASN
1	D	434	ASN
1	D	458	HIS
1	D	464	HIS
1	D	474	ASN
1	D	476	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
4	PO4	C	804	-	4,4,4	2.44	1 (25%)	6,6,6	0.82	0
3	NDP	D	704	-	45,52,52	1.82	11 (24%)	53,80,80	1.55	11 (20%)
2	1CY	D	604	-	15,18,18	1.59	3 (20%)	15,27,27	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PO4	A	801	-	4,4,4	2.49	1 (25%)	6,6,6	0.89	0
3	NDP	B	702	-	45,52,52	1.72	10 (22%)	53,80,80	1.57	10 (18%)
4	PO4	D	803	-	4,4,4	2.51	1 (25%)	6,6,6	0.80	0
2	1CY	C	603	-	15,18,18	1.63	3 (20%)	15,27,27	0.84	0
3	NDP	A	701	-	45,52,52	1.75	12 (26%)	53,80,80	1.56	10 (18%)
4	PO4	A	802	-	4,4,4	2.42	1 (25%)	6,6,6	0.85	0
2	1CY	A	601	-	15,18,18	1.70	3 (20%)	15,27,27	0.60	0
2	1CY	B	602	-	15,18,18	1.60	3 (20%)	15,27,27	0.61	0
3	NDP	C	703	-	45,52,52	1.66	10 (22%)	53,80,80	1.55	10 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	D	704	-	-	11/30/77/77	0/5/5/5
2	1CY	D	604	-	-	0/4/23/23	0/2/2/2
3	NDP	B	702	-	-	9/30/77/77	0/5/5/5
2	1CY	C	603	-	-	0/4/23/23	0/2/2/2
3	NDP	A	701	-	-	2/30/77/77	0/5/5/5
2	1CY	A	601	-	-	0/4/23/23	0/2/2/2
2	1CY	B	602	-	-	0/4/23/23	0/2/2/2
3	NDP	C	703	-	-	7/30/77/77	0/5/5/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	803	PO4	P-O1	4.73	1.62	1.50
4	A	801	PO4	P-O1	4.71	1.61	1.50
4	C	804	PO4	P-O1	4.62	1.61	1.50
4	A	802	PO4	P-O1	4.60	1.61	1.50
3	B	702	NDP	C4N-C3N	-4.39	1.41	1.49
3	B	702	NDP	C4N-C5N	-4.35	1.37	1.48
3	C	703	NDP	C4N-C5N	-4.26	1.37	1.48
3	A	701	NDP	C4N-C3N	-4.24	1.41	1.49
3	D	704	NDP	C4N-C5N	-4.21	1.37	1.48
2	A	601	1CY	C2-N3	-4.20	1.27	1.36
3	B	702	NDP	C2N-C3N	4.15	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	603	1CY	C2-N3	-4.06	1.27	1.36
2	B	602	1CY	C2-N3	-4.03	1.27	1.36
3	D	704	NDP	C4N-C3N	-4.01	1.42	1.49
3	A	701	NDP	C4N-C5N	-3.90	1.38	1.48
3	C	703	NDP	C2N-C3N	3.86	1.45	1.34
2	D	604	1CY	C2-N3	-3.74	1.28	1.36
3	D	704	NDP	C2N-C3N	3.63	1.45	1.34
3	A	701	NDP	C2N-C3N	3.59	1.45	1.34
3	D	704	NDP	C3B-C2B	-3.56	1.45	1.52
3	C	703	NDP	C4N-C3N	-3.45	1.43	1.49
3	A	701	NDP	C4A-N3A	3.45	1.40	1.35
2	C	603	1CY	C4-N3	-3.34	1.27	1.34
2	A	601	1CY	C4-N3	-3.30	1.27	1.34
3	D	704	NDP	P2B-O2B	-3.22	1.53	1.59
3	D	704	NDP	C4A-N3A	3.18	1.40	1.35
3	D	704	NDP	C6N-C5N	3.17	1.39	1.33
2	D	604	1CY	C4-N3	-3.16	1.28	1.34
3	A	701	NDP	C6N-C5N	3.12	1.38	1.33
3	A	701	NDP	P2B-O2B	-3.10	1.53	1.59
3	C	703	NDP	C3B-C2B	-3.08	1.46	1.52
2	B	602	1CY	C4-N3	-3.08	1.28	1.34
3	D	704	NDP	C5D-C4D	2.83	1.60	1.51
2	B	602	1CY	C2-N1	-2.65	1.27	1.34
3	C	703	NDP	C6N-C5N	2.65	1.38	1.33
3	B	702	NDP	C3B-C2B	-2.64	1.47	1.52
2	D	604	1CY	C2-N1	-2.62	1.27	1.34
3	B	702	NDP	P2B-O2B	-2.62	1.54	1.59
3	C	703	NDP	O4B-C1B	2.61	1.44	1.41
2	A	601	1CY	C2-N1	-2.57	1.27	1.34
2	C	603	1CY	C2-N1	-2.56	1.27	1.34
3	B	702	NDP	C3B-C4B	-2.49	1.46	1.53
3	B	702	NDP	C6N-C5N	2.44	1.37	1.33
3	B	702	NDP	C4A-N3A	2.39	1.39	1.35
3	C	703	NDP	C6N-N1N	2.39	1.43	1.37
3	C	703	NDP	C4A-N3A	2.39	1.38	1.35
3	A	701	NDP	O4B-C1B	2.37	1.44	1.41
3	A	701	NDP	C3B-C2B	-2.35	1.47	1.52
3	D	704	NDP	C6N-N1N	2.29	1.43	1.37
3	B	702	NDP	C6N-N1N	2.28	1.43	1.37
3	D	704	NDP	C3B-C4B	-2.25	1.47	1.53
3	C	703	NDP	P2B-O2B	-2.24	1.55	1.59
3	A	701	NDP	PA-O1A	-2.22	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	704	NDP	PA-O1A	-2.21	1.43	1.50
3	A	701	NDP	C2A-N3A	2.17	1.35	1.32
3	C	703	NDP	C3B-C4B	-2.16	1.47	1.53
3	B	702	NDP	PA-O1A	-2.13	1.43	1.50
3	A	701	NDP	C3B-C4B	-2.07	1.47	1.53
3	A	701	NDP	C6N-N1N	2.06	1.42	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	NDP	C3N-C2N-N1N	-4.97	116.00	123.10
3	C	703	NDP	C3N-C2N-N1N	-4.96	116.02	123.10
3	A	701	NDP	C3N-C2N-N1N	-4.49	116.68	123.10
3	D	704	NDP	C1D-N1N-C2N	-4.45	113.71	121.11
3	D	704	NDP	C3N-C2N-N1N	-4.24	117.05	123.10
3	A	701	NDP	C1D-N1N-C2N	-4.23	114.08	121.11
3	C	703	NDP	C1D-N1N-C2N	-3.76	114.85	121.11
3	A	701	NDP	C3B-C2B-C1B	-3.38	96.53	102.89
3	C	703	NDP	C3B-C2B-C1B	-3.32	96.65	102.89
3	D	704	NDP	C3B-C2B-C1B	-3.16	96.95	102.89
3	B	702	NDP	C1D-N1N-C2N	-3.13	115.90	121.11
3	B	702	NDP	C3B-C2B-C1B	-2.91	97.41	102.89
3	B	702	NDP	O3B-C3B-C2B	2.87	119.31	111.17
3	B	702	NDP	O3B-C3B-C4B	2.82	119.19	111.05
3	D	704	NDP	O7N-C7N-N7N	-2.79	116.36	122.88
3	A	701	NDP	O3B-C3B-C2B	2.67	118.75	111.17
3	D	704	NDP	O3B-C3B-C4B	2.67	118.76	111.05
3	B	702	NDP	O7N-C7N-N7N	-2.66	116.66	122.88
3	C	703	NDP	O7N-C7N-N7N	-2.64	116.71	122.88
3	B	702	NDP	PN-O3-PA	2.61	141.79	132.83
3	C	703	NDP	O3B-C3B-C4B	2.61	118.60	111.05
3	A	701	NDP	O7N-C7N-N7N	-2.56	116.88	122.88
3	A	701	NDP	O3B-C3B-C4B	2.49	118.24	111.05
3	C	703	NDP	N3A-C2A-N1A	-2.49	124.79	128.68
3	A	701	NDP	N3A-C2A-N1A	-2.43	124.89	128.68
3	C	703	NDP	O3B-C3B-C2B	2.38	117.92	111.17
3	D	704	NDP	N3A-C2A-N1A	-2.34	125.02	128.68
3	B	702	NDP	N3A-C2A-N1A	-2.32	125.05	128.68
3	D	704	NDP	PN-O3-PA	2.29	140.69	132.83
3	A	701	NDP	C3D-C2D-C1D	-2.28	97.09	101.43
3	B	702	NDP	C2B-C3B-C4B	2.24	106.87	101.99
3	D	704	NDP	O3B-C3B-C2B	2.18	117.37	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	703	NDP	O2A-PA-O1A	2.17	122.96	112.24
3	A	701	NDP	O2N-PN-O1N	2.15	122.86	112.24
3	C	703	NDP	O2N-PN-O1N	2.11	122.69	112.24
3	D	704	NDP	O5D-PN-O1N	2.10	117.28	109.07
3	C	703	NDP	C2B-C3B-C4B	2.10	106.55	101.99
3	D	704	NDP	C3N-C7N-N7N	2.09	121.39	117.67
3	B	702	NDP	O2B-C2B-C3B	2.07	119.18	111.68
3	A	701	NDP	O2A-PA-O1A	2.02	122.21	112.24
3	D	704	NDP	O2A-PA-O1A	2.00	122.13	112.24

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	703	NDP	C5D-O5D-PN-O3
3	D	704	NDP	C2B-O2B-P2B-O1X
3	D	704	NDP	C2D-C1D-N1N-C6N
3	B	702	NDP	C3B-C4B-C5B-O5B
3	B	702	NDP	O4D-C4D-C5D-O5D
3	B	702	NDP	C3D-C4D-C5D-O5D
3	D	704	NDP	O4D-C4D-C5D-O5D
3	D	704	NDP	C2D-C1D-N1N-C2N
3	D	704	NDP	C3D-C4D-C5D-O5D
3	B	702	NDP	O4B-C4B-C5B-O5B
3	C	703	NDP	C2D-C1D-N1N-C2N
3	B	702	NDP	PA-O3-PN-O5D
3	D	704	NDP	O4D-C1D-N1N-C6N
3	D	704	NDP	C2B-O2B-P2B-O3X
3	A	701	NDP	O4D-C1D-N1N-C2N
3	C	703	NDP	C5D-O5D-PN-O1N
3	B	702	NDP	C2D-C1D-N1N-C2N
3	C	703	NDP	O4D-C1D-N1N-C2N
3	B	702	NDP	O4D-C1D-N1N-C2N
3	D	704	NDP	O4D-C1D-N1N-C2N
3	C	703	NDP	C2D-C1D-N1N-C6N
3	B	702	NDP	C2D-C1D-N1N-C6N
3	C	703	NDP	O4D-C1D-N1N-C6N
3	A	701	NDP	C2N-C3N-C7N-N7N
3	B	702	NDP	C2N-C3N-C7N-N7N
3	C	703	NDP	C2N-C3N-C7N-N7N
3	D	704	NDP	C5D-O5D-PN-O1N
3	D	704	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
3	D	704	NDP	C4D-C5D-O5D-PN

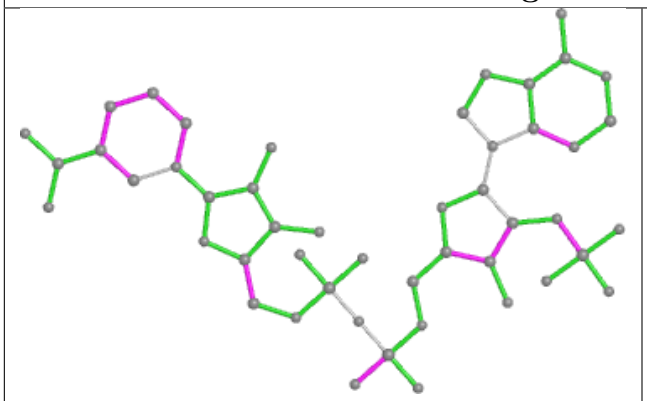
There are no ring outliers.

6 monomers are involved in 15 short contacts:

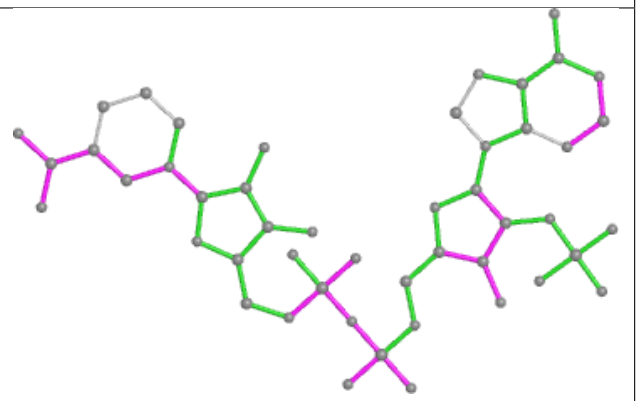
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	704	NDP	3	0
3	B	702	NDP	7	0
3	A	701	NDP	2	0
2	A	601	1CY	1	0
2	B	602	1CY	1	0
3	C	703	NDP	3	0

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.

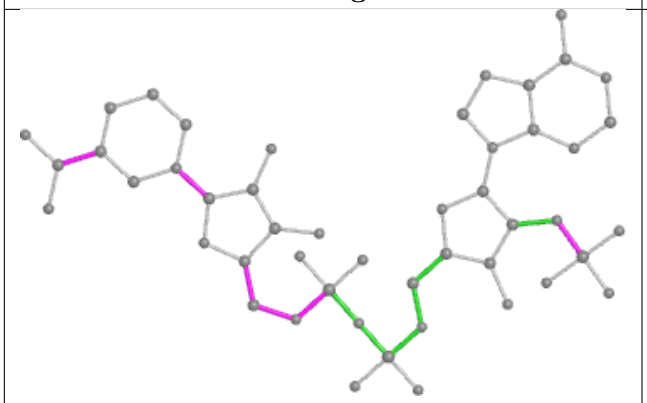
Ligand NDP D 704



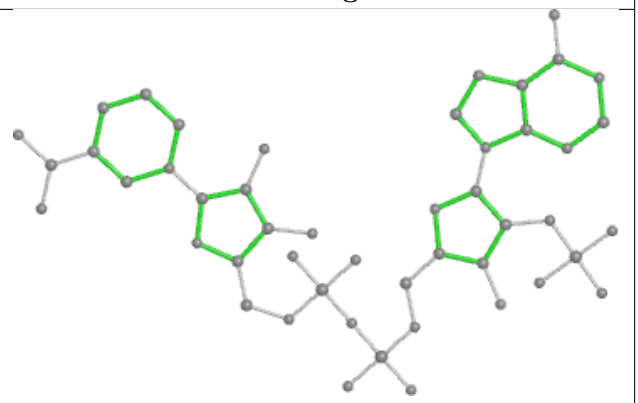
Bond lengths



Bond angles

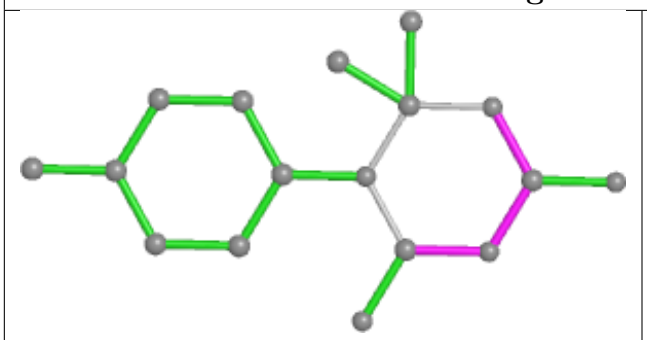


Torsions

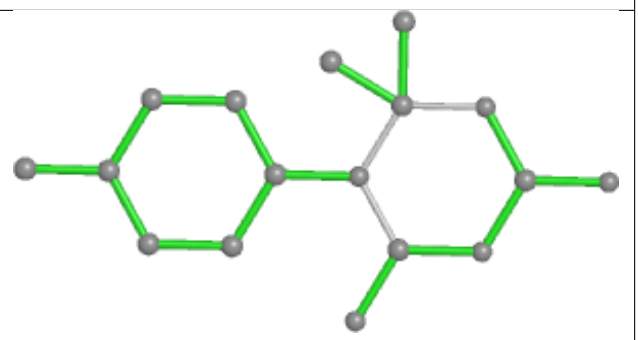


Rings

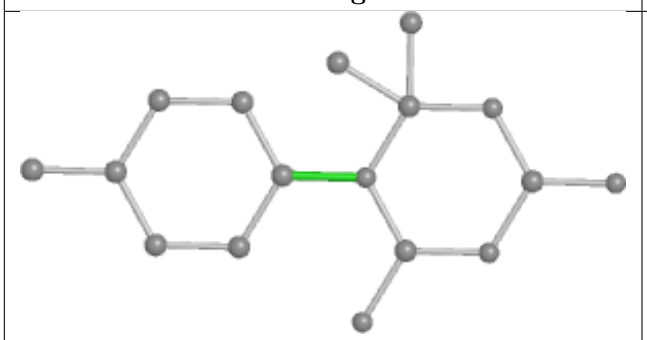
Ligand 1CY D 604



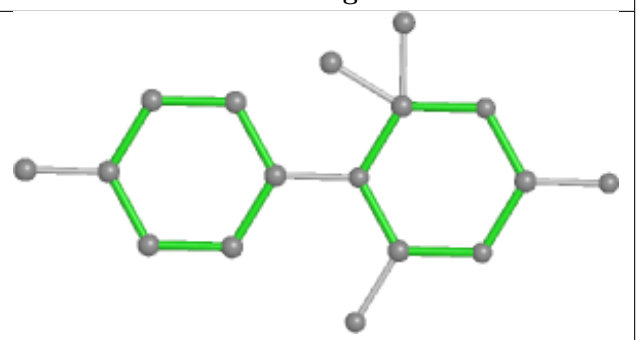
Bond lengths



Bond angles

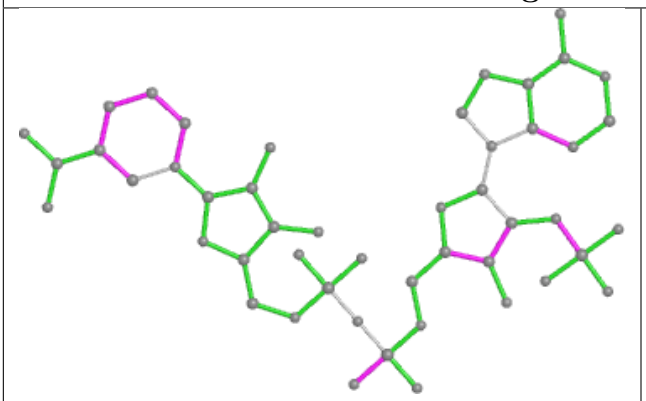


Torsions

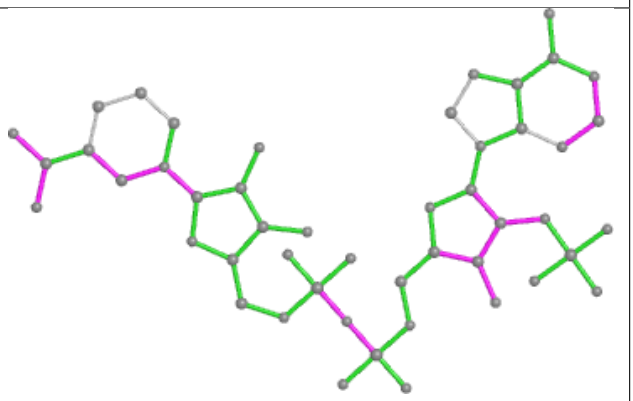


Rings

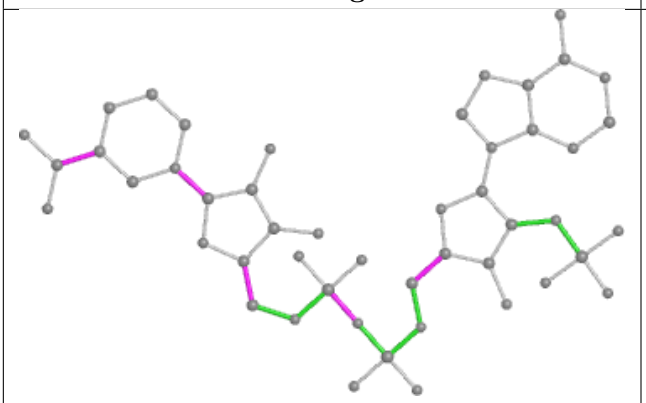
Ligand NDP B 702



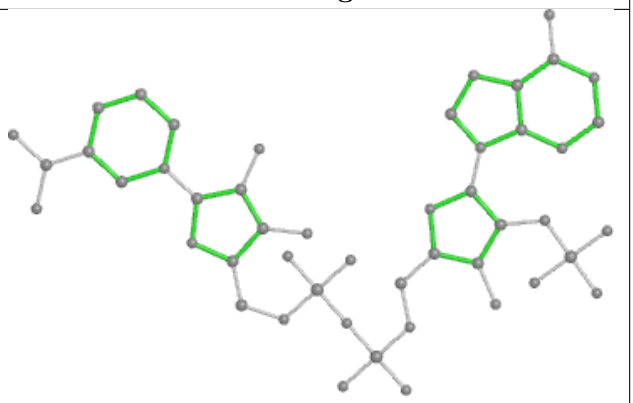
Bond lengths



Bond angles

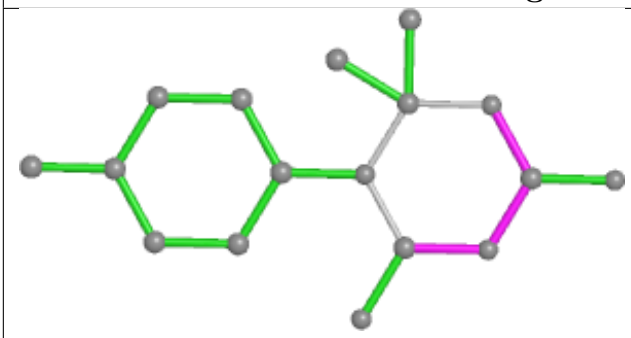


Torsions

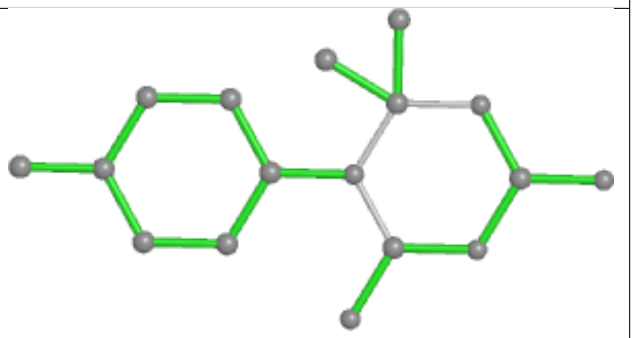


Rings

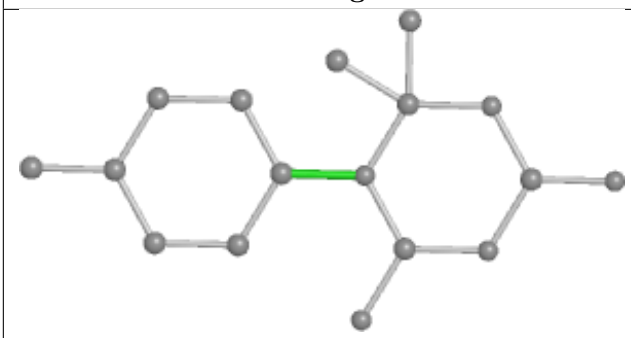
Ligand 1CY C 603



Bond lengths



Bond angles



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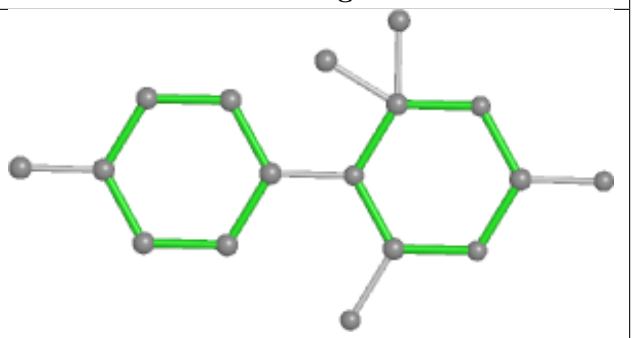
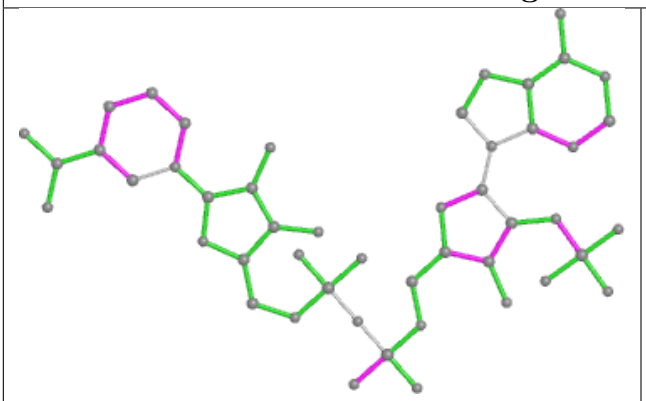
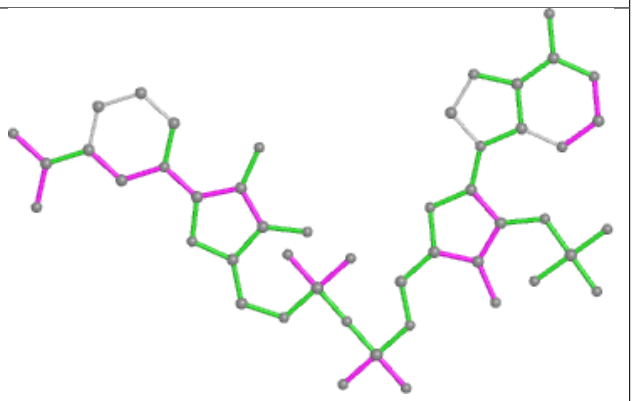


Rings

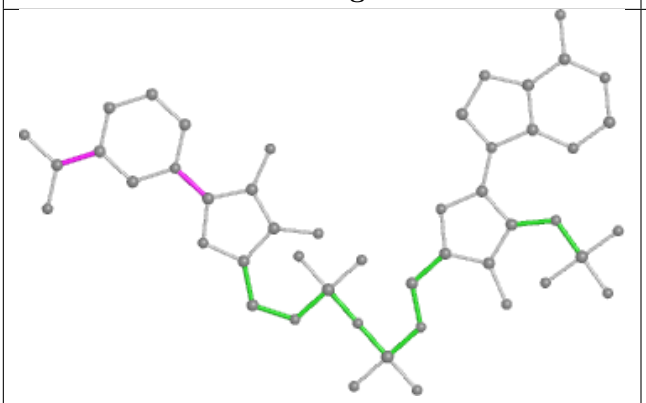
Ligand NDP A 701



Bond lengths



Bond angles



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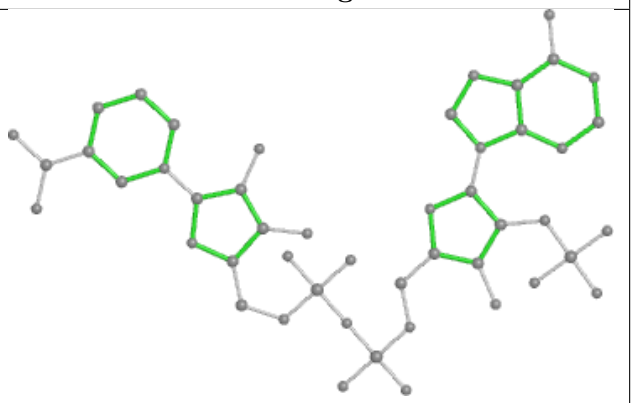
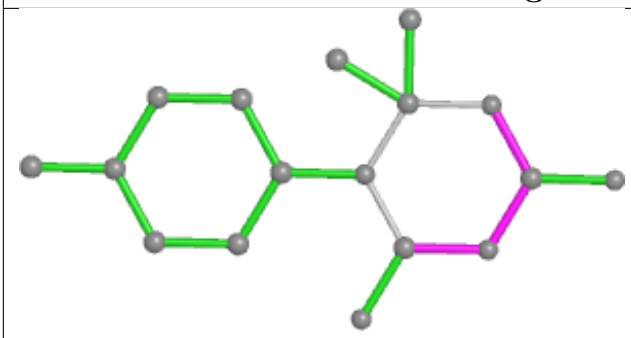
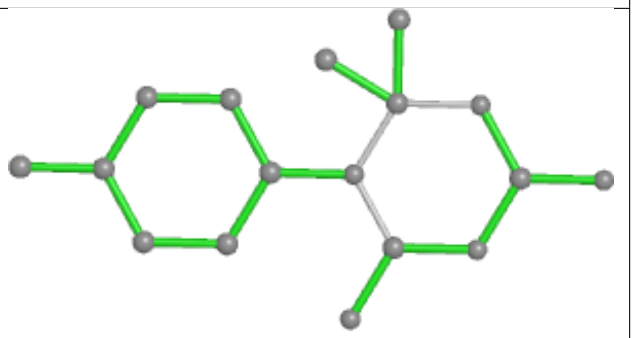


Rings

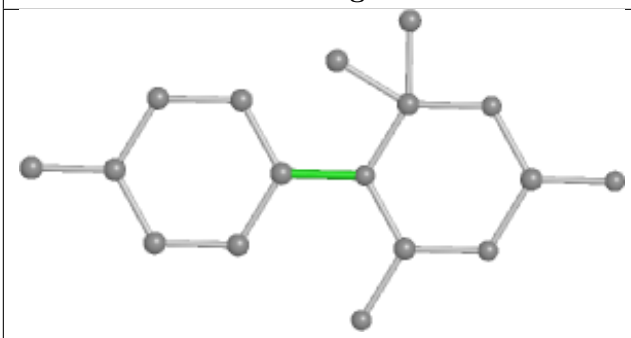
Ligand 1CY A 601



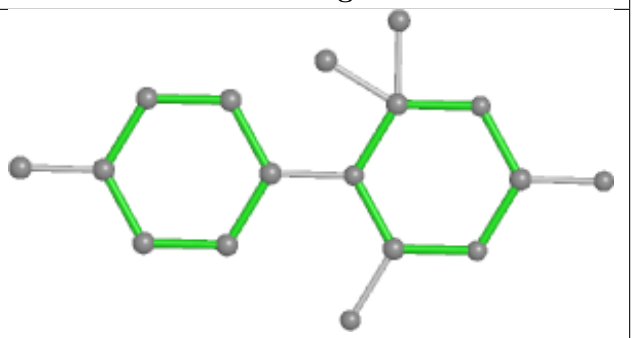
Bond lengths



Bond angles

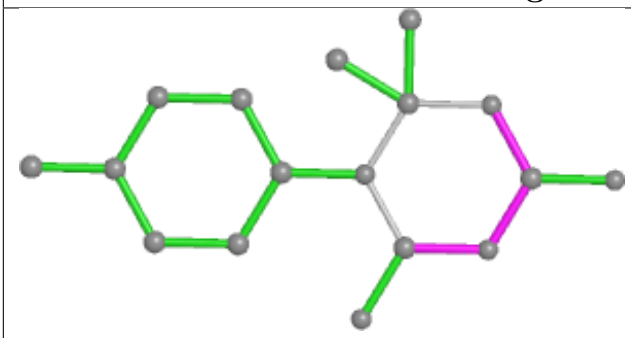


Torsions

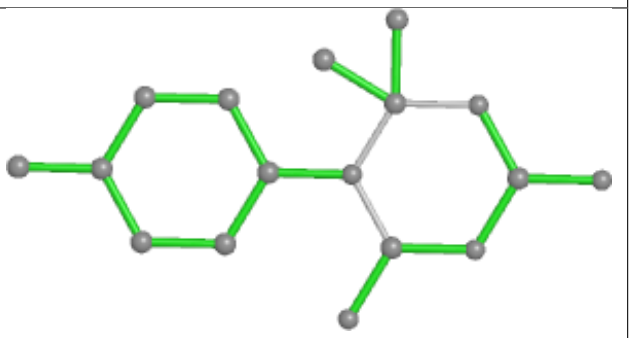


Rings

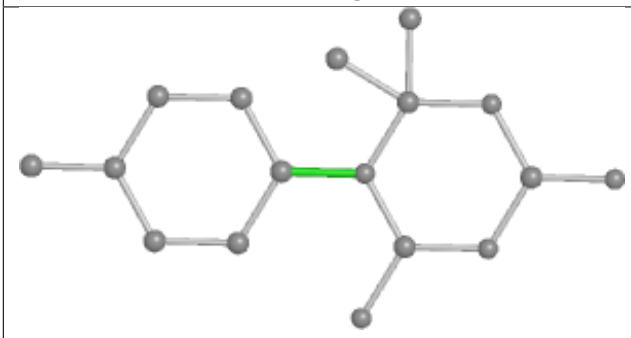
Ligand 1CY B 602



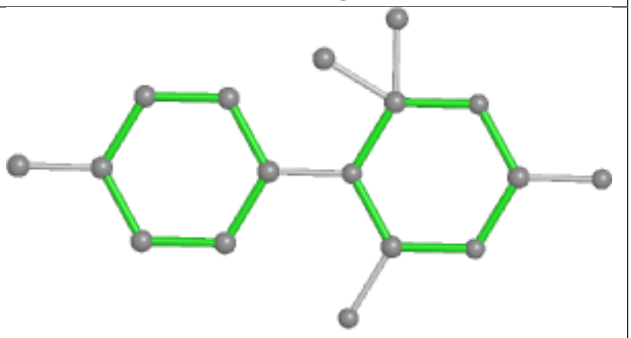
Bond lengths



Bond angles

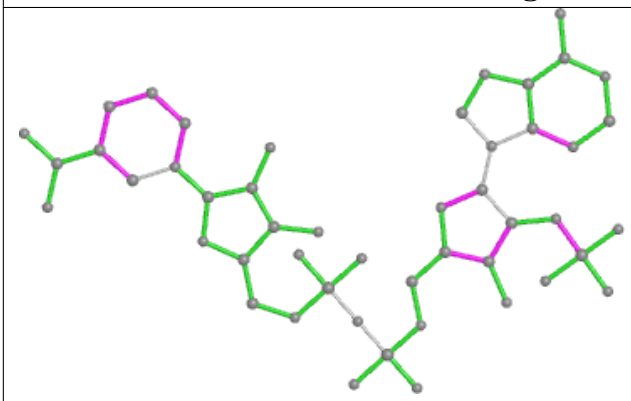


Torsions

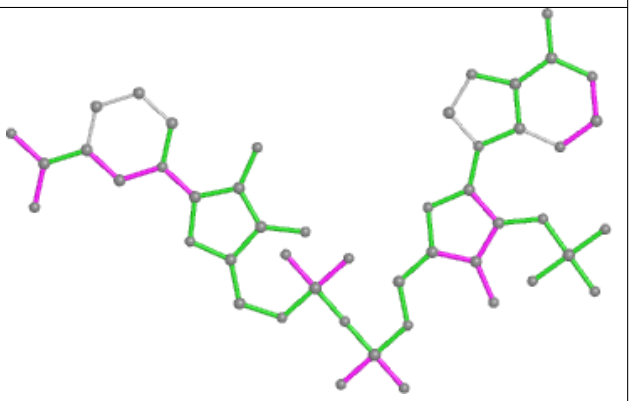


Rings

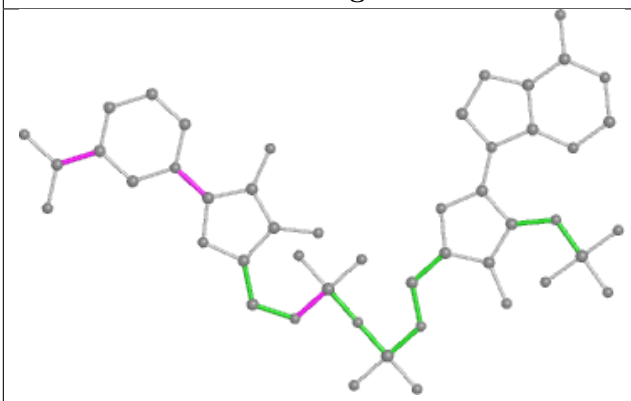
Ligand NDP C 703



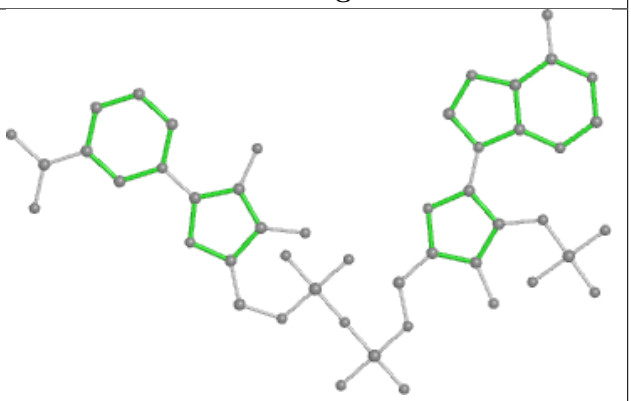
Bond lengths



Bond angles



Torsions



Rings

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	516/521 (99%)	-0.55	3 (0%) 89 88	13, 28, 56, 79	0
1	B	516/521 (99%)	-0.42	10 (1%) 66 62	12, 31, 70, 91	0
1	C	516/521 (99%)	-0.52	5 (0%) 82 80	11, 28, 65, 89	0
1	D	513/521 (98%)	-0.45	8 (1%) 72 68	13, 31, 67, 91	0
All	All	2061/2084 (98%)	-0.49	26 (1%) 77 73	11, 29, 65, 91	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	186	SER	6.8
1	D	38	GLY	5.9
1	C	37	ASP	4.8
1	B	42	PRO	4.8
1	B	186	SER	4.4
1	C	38	GLY	3.9
1	D	185	SER	3.5
1	B	518	LYS	3.4
1	C	36	GLY	3.2
1	B	183	SER	2.9
1	A	38	GLY	2.9
1	A	39	ARG	2.8
1	D	187	CYS	2.8
1	C	42	PRO	2.7
1	A	183	SER	2.7
1	C	183	SER	2.7
1	B	515	ILE	2.6
1	B	38	GLY	2.6
1	D	120	LEU	2.5
1	D	122	ALA	2.4
1	B	188	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	39	ARG	2.3
1	B	37	ASP	2.3
1	B	43	TRP	2.2
1	D	257	ARG	2.1
1	D	42	PRO	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)

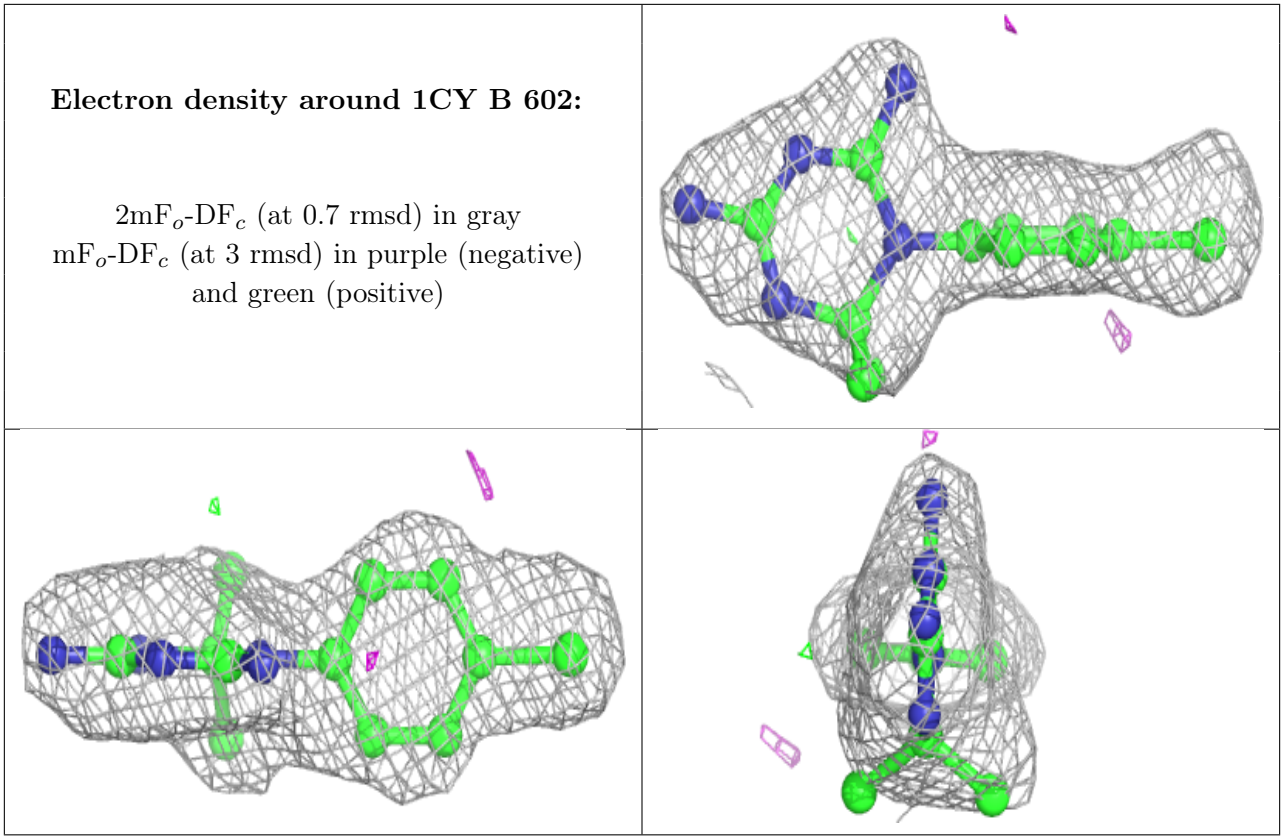
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	1CY	B	602	17/17	0.90	0.15	40,42,44,46	0
3	NDP	B	702	48/48	0.93	0.16	43,55,79,81	0
3	NDP	D	704	48/48	0.93	0.17	36,44,64,64	0
3	NDP	C	703	48/48	0.94	0.17	30,37,64,67	0
2	1CY	D	604	17/17	0.94	0.16	34,36,38,38	0
4	PO4	D	803	5/5	0.94	0.14	57,59,60,61	0
4	PO4	A	802	5/5	0.95	0.16	57,57,58,58	0
2	1CY	C	603	17/17	0.95	0.16	30,31,33,33	0
3	NDP	A	701	48/48	0.96	0.14	29,39,66,67	0
4	PO4	C	804	5/5	0.96	0.10	66,67,68,68	0
2	1CY	A	601	17/17	0.96	0.15	31,34,35,37	0
4	PO4	A	801	5/5	0.97	0.08	33,33,34,35	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.

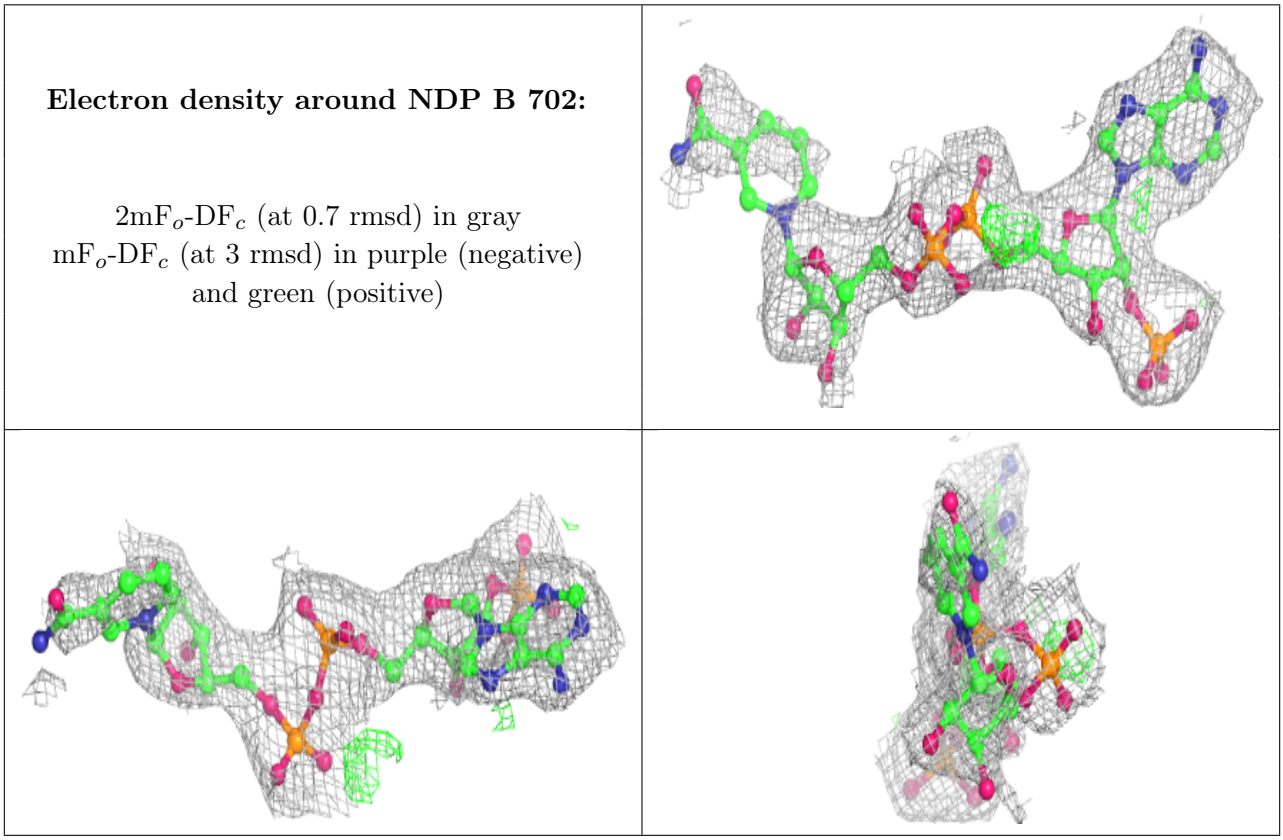
Electron density around 1CY B 602:

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



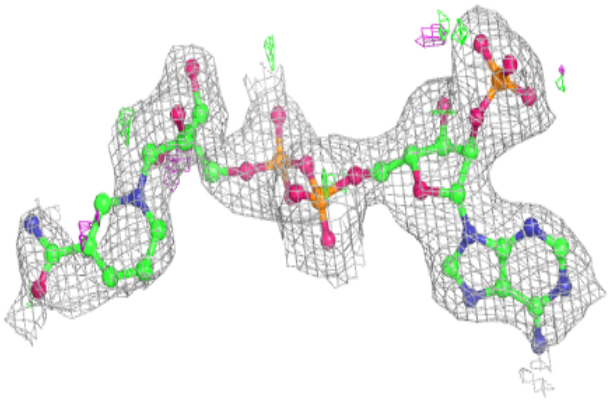
Electron density around NDP B 702:

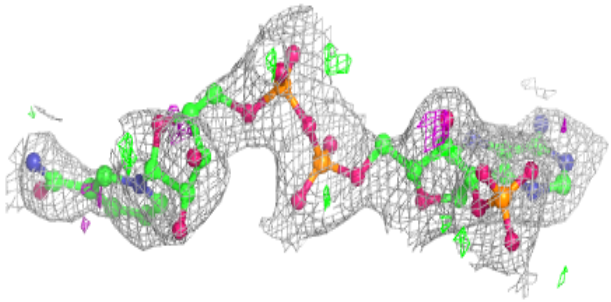
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

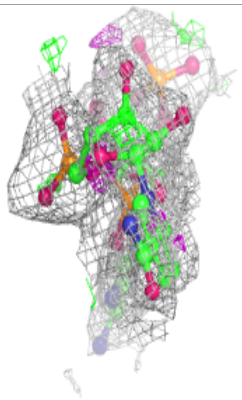


Electron density around NDP D 704:

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

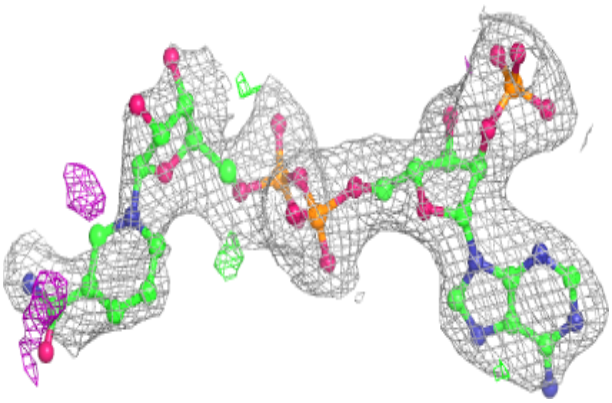


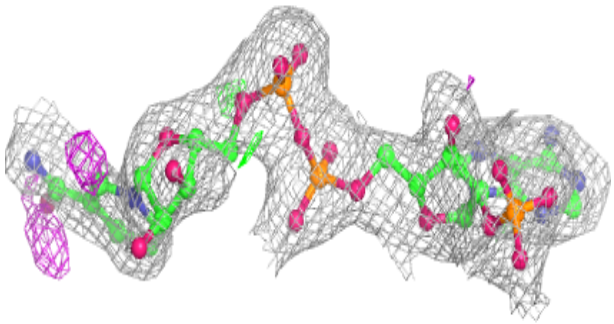


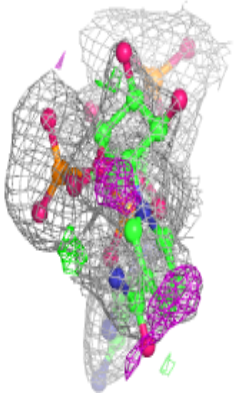


Electron density around NDP C 703:

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

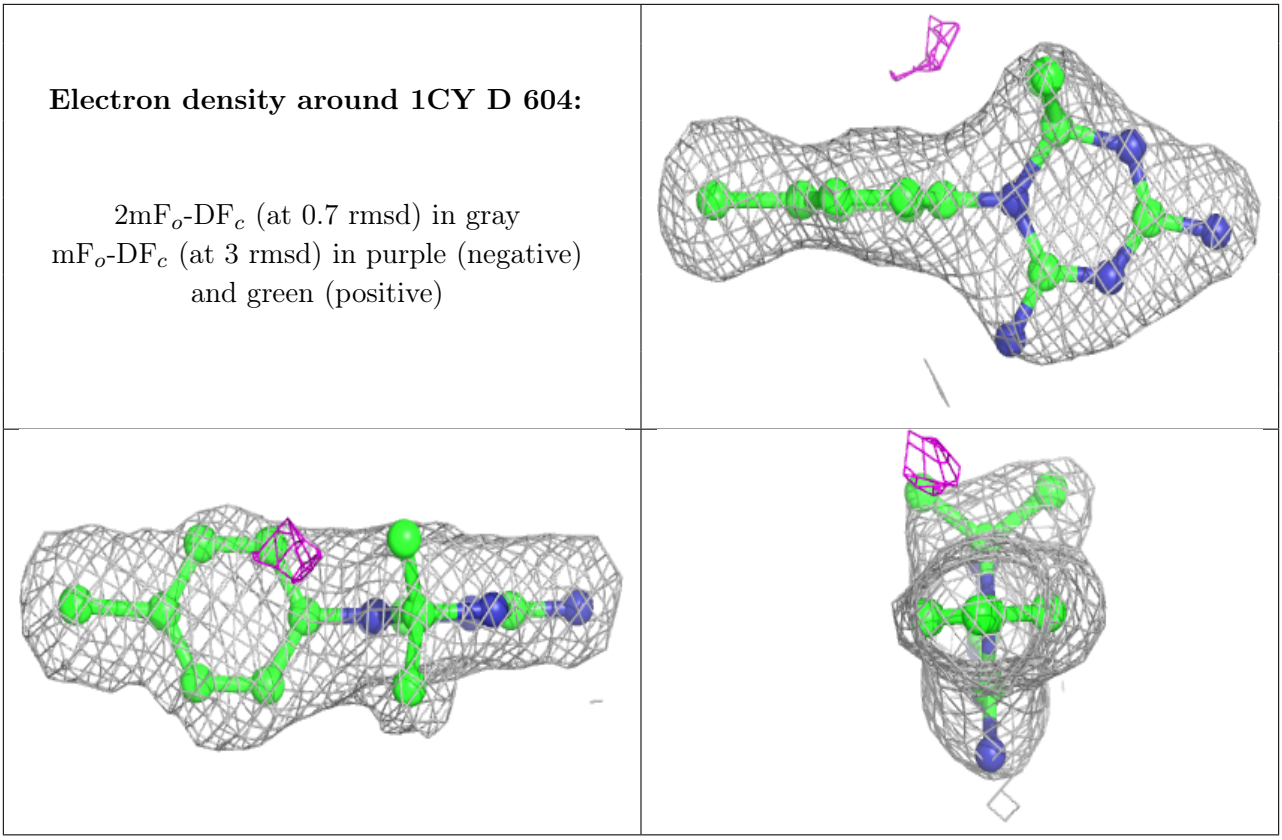






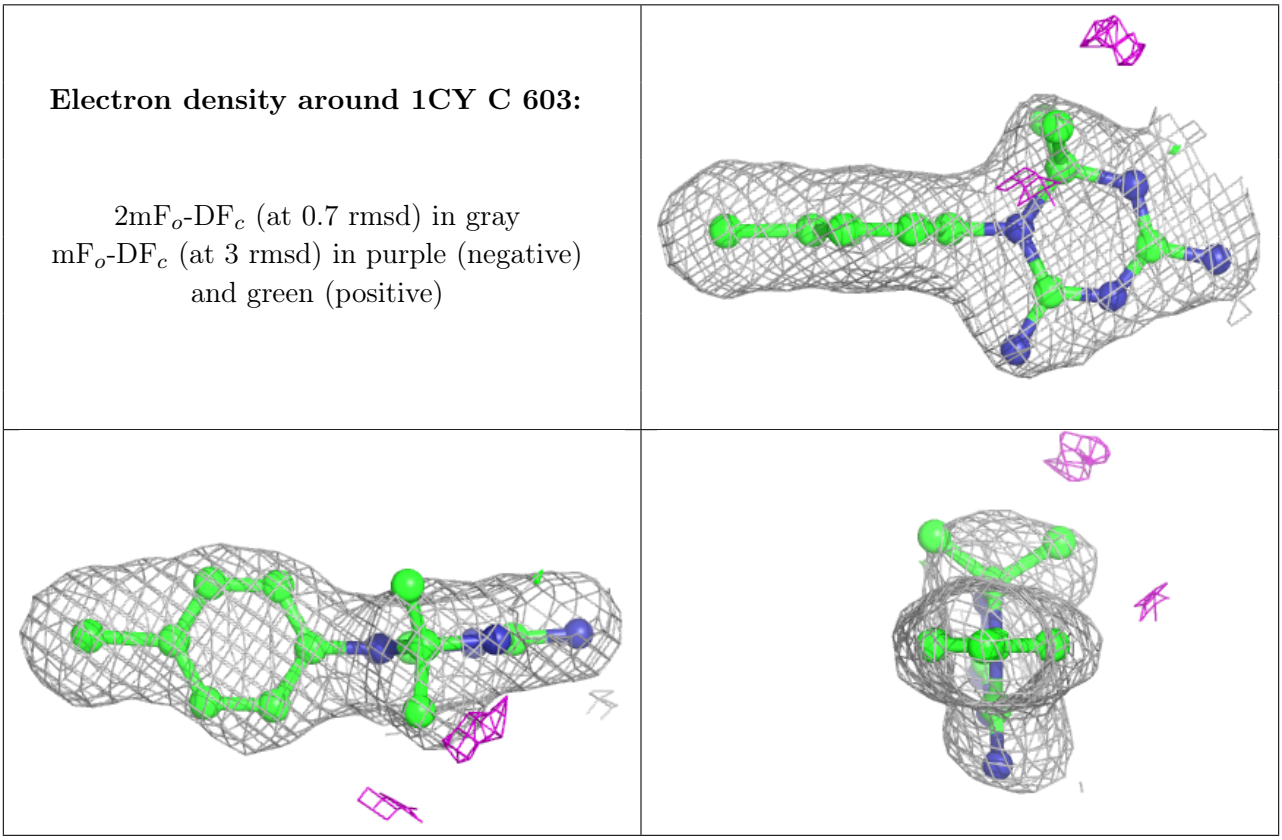
Electron density around 1CY D 604:

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



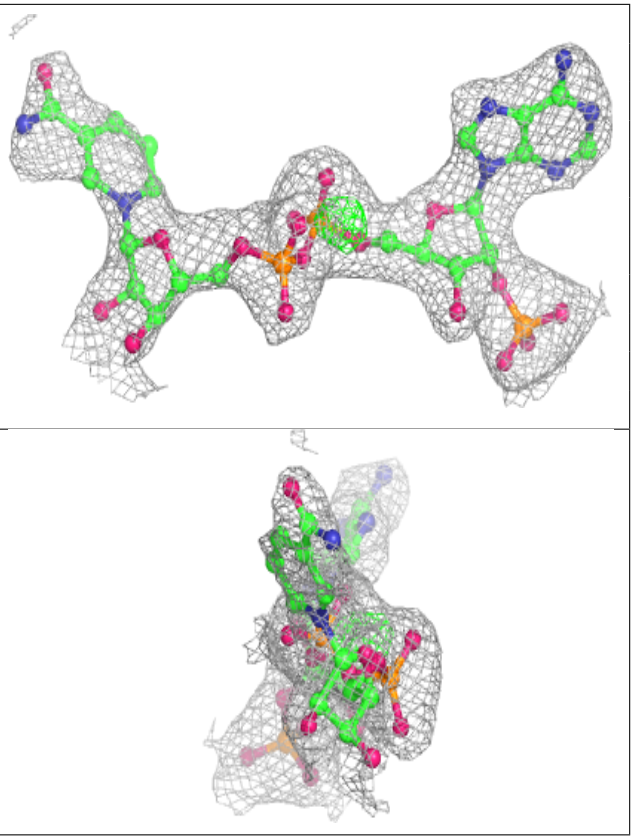
Electron density around 1CY C 603:

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



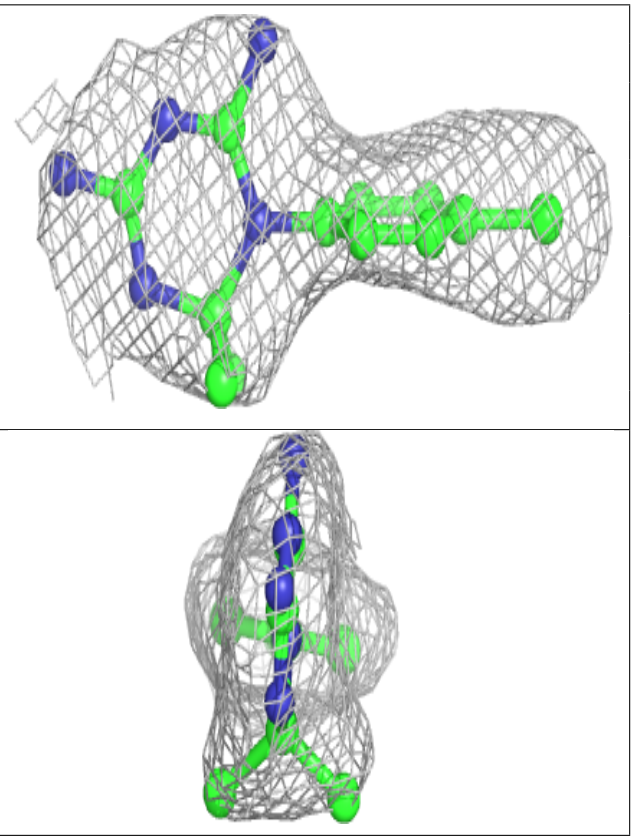
Electron density around NDP A 701:

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



Electron density around 1CY A 601:

$2mF_o$-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.