



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 12:28 AM EDT

PDB ID : 5Z2C
Title : Crystal structure of ALPK-1 N-terminal domain in complex with ADP-heptose
Authors : Ding, J.; She, Y.; Shao, F.
Deposited on : 2018-01-02
Resolution : 2.59 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:

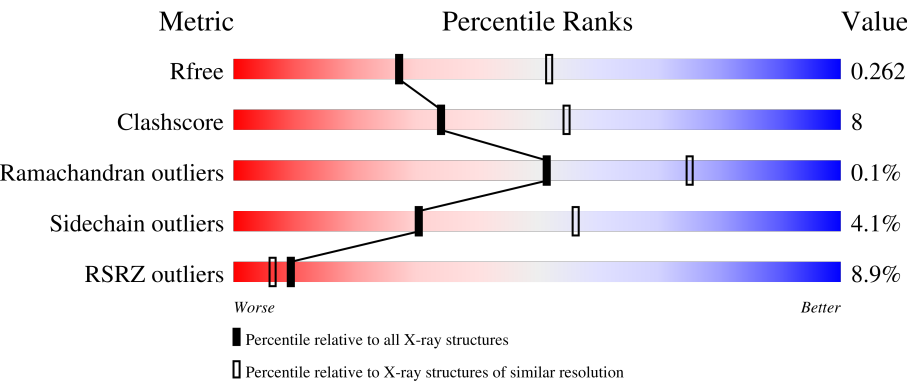
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 2.59 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	
1	B	446	
1	C	446	
1	D	446	
1	E	446	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	446	<div><div></div><div>5%</div><div>83%</div><div>13%</div><div></div><div></div></div>
1	G	446	<div><div></div><div>12%</div><div>76%</div><div>17%</div><div></div><div></div></div>
1	H	446	<div><div></div><div>20%</div><div>73%</div><div>20%</div><div></div><div>5%</div></div>
1	I	446	<div><div></div><div>17%</div><div>71%</div><div>19%</div><div></div><div>9%</div></div>

2 Entry composition

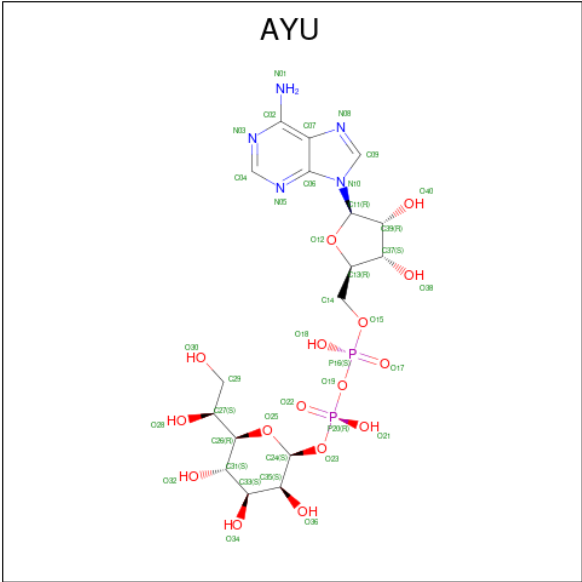
There are 2 unique types of molecules in this entry. The entry contains 30546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

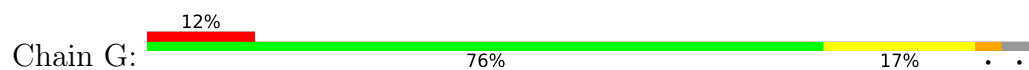
- Molecule 1 is a protein called Alpha-protein kinase 1.

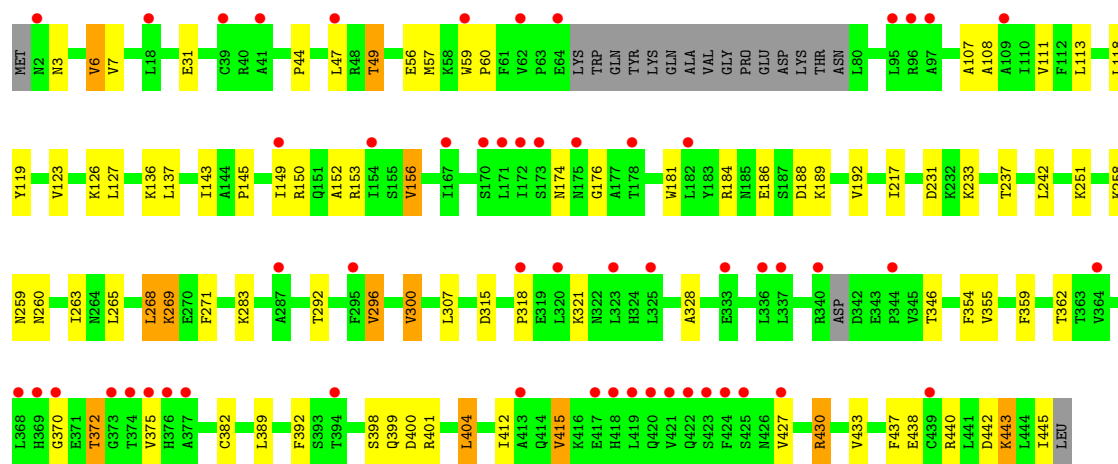
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3469	2203	597	654	15			
1	B	445	Total	C	N	O	S	0	0	0
			3469	2203	597	654	15			
1	C	427	Total	C	N	O	S	0	0	0
			3324	2115	572	622	15			
1	D	434	Total	C	N	O	S	0	0	0
			3388	2156	583	634	15			
1	E	433	Total	C	N	O	S	0	0	0
			3378	2148	580	635	15			
1	F	433	Total	C	N	O	S	0	0	0
			3379	2148	581	635	15			
1	G	428	Total	C	N	O	S	0	0	0
			3327	2113	573	626	15			
1	H	423	Total	C	N	O	S	0	0	0
			3284	2089	565	615	15			
1	I	408	Total	C	N	O	S	0	0	0
			3168	2017	544	593	14			

- Molecule 2 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2S,3S,4S,5S,6R)-6-[(1S)-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl] hydrogen phosphate (three-letter code: AYU) (formula: C₁₇H₂₇N₅O₁₆P₂).

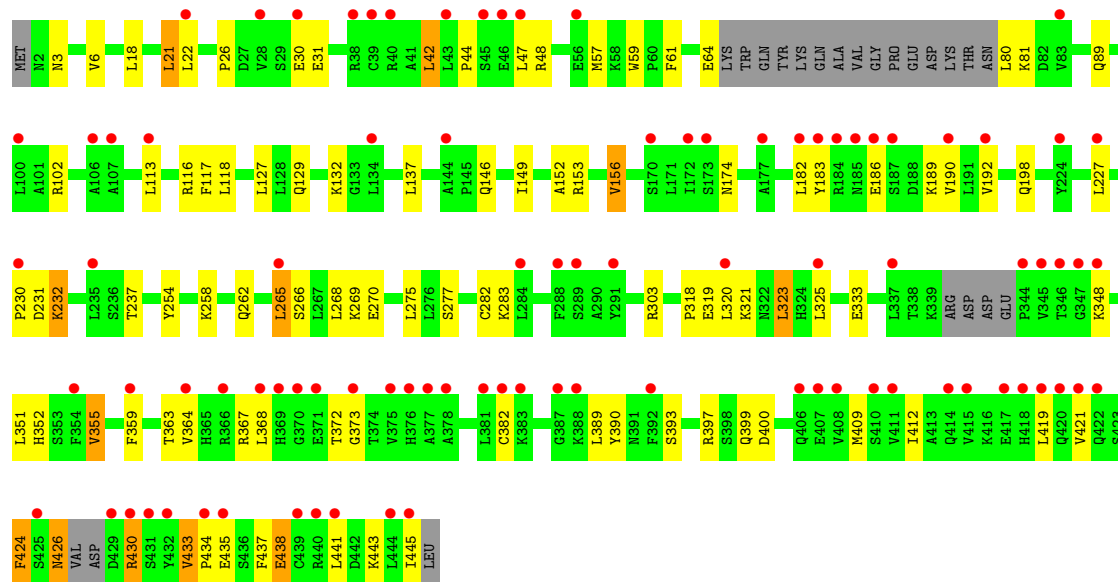


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	B	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	C	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	D	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	E	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	F	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	G	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	H	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	I	1	Total	C	N	O	P	0	0
			40	17	5	16	2		

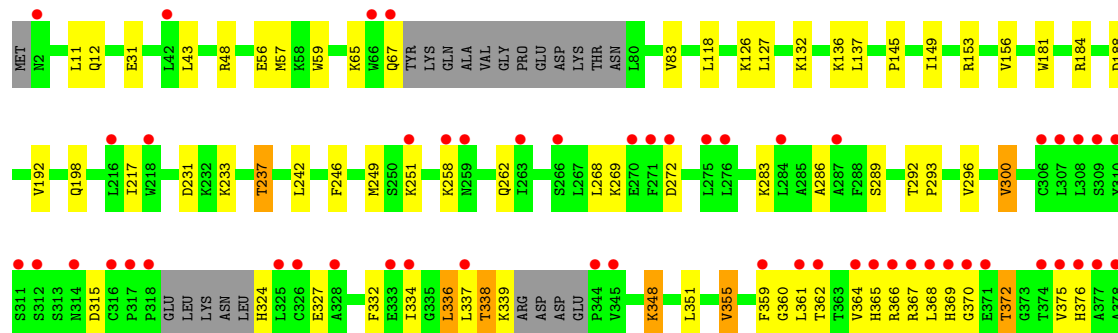


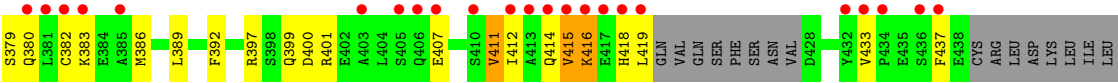


• Molecule 1: Alpha-protein kinase 1



• Molecule 1: Alpha-protein kinase 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.26Å 214.39Å 173.15Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	48.89 – 2.59 48.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.89-2.59) 93.1 (48.89-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.242 , 0.263 0.243 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30546	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AYU

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	0.30	0/3528	0.44	0/4774
1	B	0.30	0/3528	0.46	0/4774
1	C	0.30	0/3378	0.48	0/4565
1	D	0.33	0/3444	0.44	0/4656
1	E	0.29	0/3434	0.44	0/4645
1	F	0.29	0/3436	0.43	0/4648
1	G	0.27	0/3380	0.42	0/4570
1	H	0.26	0/3336	0.44	0/4508
1	I	0.29	0/3220	0.44	0/4352
All	All	0.29	0/30684	0.44	0/41492

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3469	0	3541	44	0
1	B	3469	0	3541	29	0
1	C	3324	0	3402	82	0
1	D	3388	0	3467	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3378	0	3445	36	0
1	F	3379	0	3448	38	0
1	G	3327	0	3403	56	1
1	H	3284	0	3366	97	0
1	I	3168	0	3236	105	1
2	A	40	0	0	1	0
2	B	40	0	0	2	0
2	C	40	0	0	2	0
2	D	40	0	0	1	0
2	E	40	0	0	0	0
2	F	40	0	0	0	0
2	G	40	0	0	4	0
2	H	40	0	0	3	0
2	I	40	0	0	4	0
All	All	30546	0	30849	514	1

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 8.

All (514) 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:H:424:PHE:HE1	1:H:434:PRO:CA	1.20	1.51
1:H:424:PHE:CE1	1:H:434:PRO:CG	1.94	1.51
1:I:366:ARG:CG	1:I:375:VAL:HG11	1.42	1.48
1:I:365:HIS:ND1	1:I:419:LEU:HD22	1.29	1.47
1:H:424:PHE:CE1	1:H:434:PRO:CA	2.03	1.41
1:H:424:PHE:CE1	1:H:434:PRO:HG3	1.56	1.37
1:I:366:ARG:HG3	1:I:375:VAL:CG1	1.61	1.29
1:H:424:PHE:CE1	1:H:434:PRO:N	2.03	1.27
1:H:424:PHE:CD1	1:H:434:PRO:HG3	1.68	1.27
1:H:426:ASN:ND2	1:H:435:GLU:CG	1.98	1.26
1:I:332:PHE:O	1:I:336:LEU:HD23	1.26	1.26
1:H:424:PHE:CE1	1:H:434:PRO:CB	2.21	1.23
1:H:424:PHE:CE1	1:H:434:PRO:CD	2.25	1.19
1:H:424:PHE:HE1	1:H:434:PRO:CB	1.52	1.19
1:H:424:PHE:HE1	1:H:434:PRO:N	1.38	1.18
1:I:372:THR:HG23	1:I:375:VAL:CG2	1.73	1.17
1:C:372:THR:HG22	1:C:375:VAL:HG13	1.18	1.16
1:I:365:HIS:CE1	1:I:419:LEU:HD22	1.84	1.12
1:I:365:HIS:HE1	1:I:419:LEU:HB3	1.09	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:365:HIS:ND1	1:I:419:LEU:CD2	2.11	1.10
1:I:372:THR:HG23	1:I:375:VAL:HG23	1.21	1.09
1:H:426:ASN:HD21	1:H:435:GLU:CA	1.66	1.08
1:G:440:ARG:O	1:G:443:LYS:HG3	1.54	1.08
1:I:366:ARG:HG2	1:I:375:VAL:HG11	1.30	1.08
1:H:426:ASN:HD21	1:H:435:GLU:N	1.52	1.06
1:H:426:ASN:ND2	1:H:435:GLU:HG2	1.69	1.05
1:C:371:GLU:HG2	1:C:376:HIS:CE1	1.93	1.04
1:H:426:ASN:ND2	1:H:435:GLU:HG3	1.65	1.03
1:H:426:ASN:ND2	1:H:435:GLU:N	2.06	1.03
1:I:366:ARG:CG	1:I:375:VAL:CG1	2.26	1.03
1:H:424:PHE:CE1	1:H:434:PRO:HA	1.91	1.02
1:I:366:ARG:HG3	1:I:375:VAL:HG11	1.06	1.01
1:H:426:ASN:HD22	1:H:435:GLU:HG3	1.21	1.01
1:C:372:THR:CG2	1:C:375:VAL:HG13	1.92	1.00
1:C:365:HIS:NE2	1:C:419:LEU:HD21	1.76	0.99
1:I:365:HIS:CE1	1:I:419:LEU:HB3	1.97	0.98
1:H:424:PHE:CZ	1:H:434:PRO:N	2.34	0.95
1:G:438:GLU:O	1:G:443:LYS:NZ	2.02	0.92
1:H:424:PHE:CZ	1:H:433:VAL:C	2.44	0.92
1:H:424:PHE:HZ	1:H:433:VAL:C	1.74	0.90
1:I:332:PHE:O	1:I:336:LEU:CD2	2.17	0.90
1:C:372:THR:HG22	1:C:375:VAL:CG1	2.00	0.89
1:H:424:PHE:CD1	1:H:434:PRO:CB	2.57	0.87
1:I:416:LYS:O	1:I:416:LYS:NZ	2.09	0.86
1:D:440:ARG:HB2	1:D:443:LYS:HB3	1.58	0.86
1:C:371:GLU:CG	1:C:376:HIS:CE1	2.59	0.84
1:D:440:ARG:O	1:D:443:LYS:HG2	1.78	0.83
1:H:424:PHE:CZ	1:H:434:PRO:CD	2.62	0.82
1:I:372:THR:CG2	1:I:375:VAL:HG23	2.08	0.82
1:C:365:HIS:CD2	1:C:419:LEU:HD21	2.15	0.81
1:H:424:PHE:HE1	1:H:434:PRO:CG	1.61	0.79
1:I:366:ARG:HG3	1:I:375:VAL:HG13	1.62	0.79
1:I:372:THR:HG23	1:I:375:VAL:HG21	1.65	0.79
1:I:365:HIS:HE1	1:I:419:LEU:CB	1.94	0.78
1:C:318:PRO:HB2	1:G:49:THR:HG23	1.66	0.77
1:I:337:LEU:O	1:I:339:LYS:N	2.16	0.77
1:C:371:GLU:HA	1:C:375:VAL:CG2	2.15	0.76
1:I:416:LYS:NZ	1:I:416:LYS:HA	2.01	0.76
1:C:381:LEU:CD1	1:C:415:VAL:HG12	2.16	0.75
1:H:426:ASN:HD21	1:H:435:GLU:CB	1.99	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:ASP:O	1:C:430:ARG:N	2.19	0.75
1:H:426:ASN:HD21	1:H:435:GLU:CG	1.80	0.75
1:H:424:PHE:CD1	1:H:434:PRO:CG	2.41	0.74
1:C:371:GLU:CD	1:C:376:HIS:CE1	2.61	0.74
1:C:372:THR:O	1:C:373:GLY:C	2.25	0.74
1:I:416:LYS:HA	1:I:416:LYS:HZ2	1.50	0.73
1:C:365:HIS:NE2	1:C:419:LEU:CD2	2.51	0.73
1:A:246:PHE:HA	1:A:249:MET:HE2	1.71	0.73
1:C:381:LEU:HD21	1:C:414:GLN:NE2	2.02	0.73
1:D:438:GLU:OE2	1:D:443:LYS:NZ	2.17	0.73
1:H:424:PHE:CD1	1:H:434:PRO:HB3	2.23	0.73
1:H:424:PHE:HE1	1:H:434:PRO:CD	1.82	0.72
1:I:365:HIS:CE1	1:I:419:LEU:HD13	2.24	0.72
1:I:366:ARG:HH11	1:I:375:VAL:CG1	2.02	0.72
1:H:426:ASN:ND2	1:H:435:GLU:H	1.88	0.71
1:C:381:LEU:HD12	1:C:415:VAL:HG12	1.71	0.71
1:I:372:THR:CG2	1:I:375:VAL:CG2	2.62	0.71
1:H:44:PRO:HD2	1:H:47:LEU:HD12	1.72	0.71
1:I:365:HIS:CE1	1:I:419:LEU:CD2	2.64	0.70
1:I:246:PHE:HA	1:I:249:MET:HE2	1.74	0.70
1:G:440:ARG:O	1:G:443:LYS:CG	2.38	0.70
1:E:438:GLU:OE1	1:E:440:ARG:NH2	2.25	0.69
1:C:366:ARG:HD3	1:C:371:GLU:HG2	1.75	0.69
1:I:258:LYS:NZ	1:I:272:ASP:OD2	2.25	0.69
1:C:269:LYS:NZ	1:F:342:ASP:OD2	2.25	0.68
1:A:251:LYS:NZ	1:A:315:ASP:OD1	2.25	0.68
1:I:365:HIS:CE1	1:I:419:LEU:CB	2.74	0.67
1:C:381:LEU:CD2	1:C:414:GLN:NE2	2.58	0.67
1:A:269:LYS:HD2	1:A:446:LEU:HD12	1.78	0.66
1:I:56:GLU:O	1:I:184:ARG:NH2	2.28	0.66
1:C:371:GLU:HA	1:C:375:VAL:HG21	1.77	0.66
1:C:198:GLN:NE2	2:C:501:AYU:O30	2.23	0.66
1:H:57:MET:HE1	1:H:182:LEU:H	1.61	0.66
1:H:348:LYS:NZ	1:H:348:LYS:O	2.29	0.65
1:G:56:GLU:O	1:G:184:ARG:NH2	2.22	0.65
1:I:289:SER:HG	1:I:292:THR:HG1	1.41	0.65
1:G:296:VAL:O	1:G:300:VAL:HG22	1.97	0.64
1:B:296:VAL:O	1:B:300:VAL:HG22	1.97	0.64
1:G:44:PRO:HD2	1:G:47:LEU:HD12	1.79	0.64
1:I:360:GLY:O	1:I:364:VAL:HG22	1.97	0.64
1:H:355:VAL:HG21	1:H:389:LEU:HD22	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLU:N	1:G:31:GLU:OE1	2.31	0.64
1:C:416:LYS:O	1:C:421:VAL:HG22	1.99	0.64
1:H:198:GLN:NE2	2:H:501:AYU:O30	2.28	0.64
1:E:419:LEU:O	1:E:421:VAL:N	2.30	0.63
1:G:354:PHE:HB3	1:G:412:ILE:HD13	1.80	0.63
1:H:22:LEU:HD23	1:H:137:LEU:HD23	1.80	0.63
1:I:324:HIS:ND1	1:I:327:GLU:OE1	2.19	0.63
1:F:440:ARG:HE	1:F:443:LYS:HD2	1.64	0.63
1:H:232:LYS:H	1:H:232:LYS:HD3	1.61	0.63
1:I:366:ARG:O	1:I:370:GLY:N	2.32	0.63
1:H:438:GLU:O	1:H:443:LYS:NZ	2.25	0.62
1:C:381:LEU:HD13	1:C:415:VAL:CG1	2.28	0.62
1:D:35:GLU:OE1	1:D:38:ARG:NH1	2.33	0.62
1:I:145:PRO:O	1:I:149:ILE:HG13	2.00	0.62
1:E:3:ASN:HB3	1:E:6:VAL:HG23	1.82	0.62
1:F:365:HIS:ND1	1:F:419:LEU:HD22	2.15	0.62
1:C:318:PRO:HA	1:C:321:LYS:HG3	1.81	0.62
1:I:361:LEU:O	1:I:364:VAL:HG23	1.99	0.62
1:A:397:ARG:NH1	1:F:400:ASP:OD1	2.33	0.61
1:E:44:PRO:HD2	1:E:47:LEU:HD12	1.82	0.61
1:H:266:SER:O	1:H:270:GLU:HB2	2.00	0.61
1:H:283:LYS:HG3	1:H:437:PHE:CD2	2.35	0.61
1:B:3:ASN:HB3	1:B:6:VAL:HG23	1.82	0.61
1:B:152:ALA:O	1:B:156:VAL:HG23	2.01	0.61
1:I:414:GLN:O	1:I:418:HIS:ND1	2.34	0.61
1:D:68:TYR:HB3	1:D:229:GLN:HG2	1.83	0.61
1:G:145:PRO:O	1:G:149:ILE:HG13	1.99	0.61
1:E:6:VAL:HG13	1:H:390:TYR:HB3	1.83	0.61
1:H:424:PHE:HD1	1:H:434:PRO:HB3	1.63	0.61
1:C:317:PRO:HG2	1:C:320:LEU:HD23	1.83	0.61
1:I:67:GLN:NE2	2:I:501:AYU:O34	2.33	0.61
1:E:145:PRO:O	1:E:149:ILE:HG13	2.01	0.60
1:I:296:VAL:O	1:I:300:VAL:HG22	2.01	0.60
1:F:296:VAL:O	1:F:300:VAL:HG22	2.00	0.60
1:D:3:ASN:HB3	1:D:6:VAL:HG23	1.84	0.60
1:H:254:TYR:OH	1:H:277:SER:OG	2.14	0.60
1:H:424:PHE:CZ	1:H:434:PRO:HD3	2.35	0.60
1:F:397:ARG:NH1	1:F:400:ASP:OD1	2.35	0.60
1:A:365:HIS:ND1	1:A:419:LEU:HD22	2.17	0.60
1:A:380:GLN:NE2	1:H:319:GLU:O	2.33	0.59
1:G:355:VAL:HG21	1:G:389:LEU:HD22	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:359:PHE:CE1	1:I:382:CYS:HB3	2.36	0.59
1:F:355:VAL:HG21	1:F:389:LEU:HD22	1.84	0.59
1:C:372:THR:O	1:C:374:THR:N	2.36	0.59
1:C:381:LEU:HD21	1:C:414:GLN:HE22	1.65	0.59
1:E:397:ARG:NH2	1:E:399:GLN:OE1	2.36	0.59
1:H:258:LYS:HA	1:H:268:LEU:HD11	1.83	0.59
1:I:365:HIS:ND1	1:I:419:LEU:HD13	2.17	0.59
1:I:362:THR:HB	1:I:366:ARG:HH12	1.68	0.59
1:C:440:ARG:HD2	1:C:442:ASP:H	1.68	0.59
1:A:390:TYR:HB3	1:B:6:VAL:HG13	1.85	0.59
1:E:365:HIS:ND1	1:E:419:LEU:HD22	2.18	0.59
1:I:365:HIS:CE1	1:I:419:LEU:CG	2.85	0.59
1:G:268:LEU:HD23	1:G:269:LYS:HE3	1.85	0.58
1:I:231:ASP:OD2	2:I:501:AYU:O34	2.21	0.58
1:C:385:ALA:HB1	1:C:408:VAL:HG23	1.86	0.58
1:I:251:LYS:NZ	1:I:315:ASP:OD2	2.35	0.58
1:E:45:SER:O	1:E:49:THR:OG1	2.21	0.58
1:H:118:LEU:HD12	1:H:127:LEU:HD22	1.85	0.58
1:C:44:PRO:HD2	1:C:47:LEU:HD12	1.84	0.58
1:I:258:LYS:HA	1:I:268:LEU:HD21	1.87	0.57
1:H:397:ARG:NH2	1:H:399:GLN:OE1	2.37	0.57
1:B:118:LEU:HD12	1:B:127:LEU:HD22	1.86	0.56
1:H:183:TYR:CD1	1:H:189:LYS:HE2	2.40	0.56
1:H:424:PHE:HZ	1:H:433:VAL:CA	2.17	0.56
1:A:441:LEU:HD12	1:D:323:LEU:HD13	1.88	0.56
1:C:145:PRO:O	1:C:149:ILE:HG13	2.06	0.56
1:D:440:ARG:HB2	1:D:443:LYS:CB	2.31	0.56
1:A:397:ARG:NH2	1:A:399:GLN:OE1	2.39	0.56
1:C:372:THR:N	1:C:375:VAL:HG22	2.21	0.56
1:B:266:SER:OG	1:B:443:LYS:O	2.11	0.56
1:C:381:LEU:HD13	1:C:415:VAL:HG13	1.88	0.56
1:A:333:GLU:HG2	1:A:421:VAL:HG12	1.87	0.55
1:F:191:LEU:O	1:F:195:VAL:HG23	2.06	0.55
1:I:258:LYS:HE3	1:I:269:LYS:HA	1.88	0.55
1:E:266:SER:HA	1:E:446:LEU:HD11	1.87	0.55
1:I:118:LEU:HD12	1:I:127:LEU:HD22	1.89	0.55
1:F:251:LYS:H	1:F:251:LYS:HD2	1.72	0.55
1:G:118:LEU:HD12	1:G:127:LEU:HD22	1.88	0.55
1:G:318:PRO:HA	1:G:321:LYS:HG3	1.88	0.55
1:I:188:ASP:O	1:I:192:VAL:HG23	2.06	0.55
1:C:333:GLU:HG2	1:C:421:VAL:HG12	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:ARG:NH2	1:D:442:ASP:HB2	2.22	0.55
1:B:329:LYS:HB2	1:B:364:VAL:HG11	1.87	0.55
1:C:56:GLU:O	1:C:184:ARG:NH2	2.28	0.55
1:C:371:GLU:CD	1:C:376:HIS:NE2	2.60	0.55
1:D:397:ARG:NH2	1:D:399:GLN:OE1	2.40	0.55
1:B:372:THR:OG1	1:B:373:GLY:N	2.40	0.54
1:D:440:ARG:CB	1:D:443:LYS:HB3	2.34	0.54
1:F:339:LYS:HB2	1:F:354:PHE:CZ	2.42	0.54
1:A:440:ARG:HH12	1:D:270:GLU:HG3	1.71	0.54
1:C:381:LEU:CD1	1:C:415:VAL:CG1	2.84	0.54
1:B:231:ASP:OD2	2:B:501:AYU:O34	2.26	0.54
1:D:145:PRO:O	1:D:149:ILE:HG13	2.07	0.54
1:I:397:ARG:NH2	1:I:399:GLN:OE1	2.41	0.54
1:D:351:LEU:O	1:D:355:VAL:HG23	2.08	0.54
1:E:351:LEU:O	1:E:355:VAL:HG23	2.06	0.54
1:E:254:TYR:HH	1:E:277:SER:HG	1.53	0.54
1:D:152:ALA:O	1:D:156:VAL:HG23	2.07	0.53
1:D:440:ARG:HB2	1:D:443:LYS:HD2	1.89	0.53
1:A:132:LYS:HE3	1:A:136:LYS:HE3	1.90	0.53
1:B:145:PRO:O	1:B:149:ILE:HG13	2.08	0.53
1:I:372:THR:CG2	1:I:375:VAL:HG21	2.34	0.53
1:D:31:GLU:O	1:D:35:GLU:HB2	2.08	0.53
1:F:188:ASP:O	1:F:192:VAL:HG23	2.08	0.53
1:G:231:ASP:OD2	2:G:501:AYU:O34	2.26	0.53
1:B:438:GLU:OE1	1:B:440:ARG:NH1	2.42	0.53
1:C:419:LEU:O	1:C:419:LEU:HD23	2.08	0.53
1:I:366:ARG:O	1:I:370:GLY:CA	2.55	0.53
1:G:430:ARG:H	1:G:430:ARG:HD2	1.73	0.53
1:H:434:PRO:HD2	1:H:437:PHE:CD1	2.43	0.53
1:C:381:LEU:CD2	1:C:414:GLN:HE21	2.21	0.53
1:F:351:LEU:O	1:F:355:VAL:HG23	2.09	0.53
1:C:152:ALA:O	1:C:156:VAL:HG23	2.08	0.53
1:I:366:ARG:HH11	1:I:375:VAL:HG13	1.74	0.53
1:G:251:LYS:NZ	1:G:315:ASP:OD1	2.36	0.53
1:I:43:LEU:O	1:I:48:ARG:NH1	2.40	0.53
1:I:365:HIS:ND1	1:I:419:LEU:CD1	2.72	0.53
1:A:381:LEU:HD23	1:H:323:LEU:HD11	1.91	0.52
1:D:57:MET:HE1	1:D:182:LEU:H	1.74	0.52
1:H:351:LEU:O	1:H:355:VAL:HG23	2.09	0.52
1:C:371:GLU:OE2	1:C:376:HIS:CE1	2.62	0.52
1:A:351:LEU:O	1:A:355:VAL:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:ASP:OD1	1:E:343:GLU:N	2.43	0.52
1:F:388:LYS:NZ	1:F:407:GLU:OE1	2.41	0.52
1:G:260:ASN:HB3	1:G:263:ILE:HD12	1.91	0.52
1:I:198:GLN:HE22	1:I:237:THR:HB	1.74	0.52
1:I:336:LEU:CD2	1:I:336:LEU:N	2.73	0.52
1:G:3:ASN:HB3	1:G:6:VAL:HG23	1.91	0.52
1:I:336:LEU:N	1:I:336:LEU:HD22	2.24	0.52
1:I:366:ARG:HH11	1:I:375:VAL:HG12	1.73	0.52
1:I:416:LYS:NZ	1:I:416:LYS:CA	2.72	0.52
1:I:416:LYS:HZ1	1:I:416:LYS:C	2.08	0.52
1:I:337:LEU:C	1:I:339:LYS:N	2.63	0.52
1:A:249:MET:HE3	1:A:254:TYR:HB2	1.91	0.52
1:C:397:ARG:NH2	1:C:399:GLN:OE1	2.43	0.52
1:F:152:ALA:O	1:F:156:VAL:HG23	2.09	0.52
1:I:336:LEU:CD2	1:I:336:LEU:H	2.23	0.52
1:C:372:THR:O	1:C:375:VAL:N	2.43	0.51
1:C:372:THR:O	1:C:375:VAL:HG22	2.11	0.51
1:H:348:LYS:HD3	1:H:393:SER:HB2	1.93	0.51
1:G:392:PHE:HB2	1:G:404:LEU:HD13	1.92	0.51
1:H:231:ASP:OD2	2:H:501:AYU:O34	2.29	0.51
1:B:390:TYR:HB3	1:F:6:VAL:HG13	1.92	0.51
1:C:191:LEU:O	1:C:195:VAL:HG23	2.11	0.51
1:D:339:LYS:HB2	1:D:354:PHE:CZ	2.45	0.51
1:F:325:LEU:HD22	1:F:364:VAL:HG23	1.92	0.51
1:D:254:TYR:OH	1:D:277:SER:OG	2.25	0.51
1:I:351:LEU:O	1:I:355:VAL:HG23	2.11	0.51
1:B:198:GLN:NE2	2:B:501:AYU:O30	2.40	0.51
1:H:333:GLU:HG2	1:H:421:VAL:HG12	1.93	0.51
1:I:365:HIS:CE1	1:I:419:LEU:CD1	2.93	0.51
1:B:367:ARG:NH2	1:F:35:GLU:OE1	2.41	0.51
1:D:191:LEU:O	1:D:195:VAL:HG23	2.11	0.51
1:E:191:LEU:O	1:E:195:VAL:HG23	2.11	0.51
1:D:57:MET:CE	1:D:182:LEU:H	2.24	0.51
1:I:283:LYS:HG3	1:I:437:PHE:CE1	2.46	0.50
1:H:3:ASN:HB3	1:H:6:VAL:HG12	1.92	0.50
1:A:191:LEU:O	1:A:195:VAL:HG23	2.11	0.50
1:E:7:VAL:HG11	1:E:118:LEU:HD22	1.94	0.50
1:G:152:ALA:O	1:G:156:VAL:HG23	2.12	0.50
1:C:369:HIS:ND1	1:C:369:HIS:N	2.59	0.50
1:C:409:MET:O	1:C:412:ILE:HG13	2.12	0.50
1:B:191:LEU:O	1:B:195:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:GLU:OE1	1:C:319:GLU:N	2.45	0.49
1:H:258:LYS:HE3	1:H:269:LYS:HA	1.93	0.49
1:A:351:LEU:HG	1:A:408:VAL:HG11	1.94	0.49
1:I:286:ALA:HB1	1:I:296:VAL:HG23	1.94	0.49
1:H:438:GLU:HG2	1:H:443:LYS:NZ	2.28	0.49
1:I:289:SER:OG	1:I:292:THR:OG1	2.16	0.49
1:A:388:LYS:HB2	1:A:408:VAL:HG23	1.95	0.49
1:C:329:LYS:NZ	1:C:333:GLU:OE1	2.44	0.49
1:D:57:MET:CE	1:D:181:TRP:HA	2.42	0.49
1:I:132:LYS:HE2	1:I:136:LYS:HE3	1.94	0.49
1:D:440:ARG:H	1:D:443:LYS:CD	2.25	0.49
1:H:81:LYS:NZ	1:H:116:ARG:HB3	2.27	0.49
1:I:337:LEU:C	1:I:339:LYS:H	2.14	0.49
1:C:311:SER:O	1:C:321:LYS:HD2	2.13	0.49
1:D:325:LEU:HB3	1:D:368:LEU:HD21	1.93	0.49
1:G:217:ILE:HG21	1:G:242:LEU:HB2	1.95	0.49
1:D:355:VAL:HG21	1:D:389:LEU:HD22	1.94	0.49
1:H:31:GLU:OE1	1:I:367:ARG:NH1	2.43	0.49
1:A:427:VAL:HG11	1:D:440:ARG:HD2	1.95	0.48
1:B:77:LYS:NZ	1:B:428:ASP:OD1	2.42	0.48
1:B:258:LYS:HA	1:B:268:LEU:HD22	1.96	0.48
1:C:428:ASP:C	1:C:430:ARG:N	2.66	0.48
1:D:64:GLU:HB2	1:D:67:GLN:HB2	1.95	0.48
1:H:146:GLN:O	1:H:149:ILE:HG13	2.13	0.48
1:C:428:ASP:O	1:C:429:ASP:C	2.52	0.48
1:F:169:SER:OG	1:F:200:ARG:NH2	2.47	0.48
1:G:283:LYS:HG3	1:G:437:PHE:CE1	2.48	0.48
1:G:398:SER:OG	1:G:399:GLN:OE1	2.32	0.48
1:H:348:LYS:NZ	1:H:352:HIS:HB2	2.29	0.48
1:H:348:LYS:NZ	1:H:389:LEU:HD11	2.27	0.48
1:I:361:LEU:HA	1:I:364:VAL:CG2	2.44	0.48
1:I:380:GLN:OE1	1:I:380:GLN:HA	2.11	0.48
1:A:296:VAL:O	1:A:300:VAL:HG22	2.14	0.48
1:H:283:LYS:HG3	1:H:437:PHE:CE2	2.47	0.48
1:H:57:MET:CE	1:H:182:LEU:H	2.26	0.48
1:H:325:LEU:HD22	1:H:364:VAL:HG23	1.95	0.48
1:H:434:PRO:HD2	1:H:437:PHE:HD1	1.79	0.48
1:I:217:ILE:HG21	1:I:242:LEU:HB2	1.95	0.48
1:G:149:ILE:O	1:G:153:ARG:HG3	2.14	0.47
1:C:412:ILE:HA	1:C:415:VAL:HG22	1.95	0.47
1:F:218:TRP:CD2	1:F:263:ILE:HG23	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:LYS:HD2	1:D:343:GLU:HG3	1.96	0.47
1:C:258:LYS:HZ3	1:C:272:ASP:HA	1.80	0.47
1:E:58:LYS:HE3	1:E:59:TRP:CZ3	2.49	0.47
1:I:153:ARG:O	1:I:156:VAL:HG22	2.15	0.47
1:I:293:PRO:HA	1:I:296:VAL:HG12	1.95	0.47
1:H:64:GLU:HG2	1:H:80:LEU:HD22	1.95	0.47
1:I:376:HIS:O	1:I:380:GLN:HG2	2.14	0.47
1:H:81:LYS:HZ2	1:H:117:PHE:N	2.13	0.47
1:D:440:ARG:HB2	1:D:443:LYS:CG	2.45	0.47
1:A:231:ASP:OD2	2:A:501:AYU:O34	2.32	0.47
1:E:329:LYS:HB2	1:E:364:VAL:HG11	1.96	0.47
1:H:152:ALA:O	1:H:156:VAL:HG23	2.14	0.47
1:I:379:SER:C	1:I:383:LYS:HZ3	2.18	0.47
1:C:366:ARG:HD3	1:C:371:GLU:CG	2.43	0.47
1:D:440:ARG:NH2	1:D:442:ASP:OD1	2.47	0.47
1:F:361:LEU:HA	1:F:364:VAL:HG12	1.96	0.47
1:H:430:ARG:HD3	1:H:430:ARG:H	1.79	0.47
1:C:251:LYS:HE3	1:C:273:HIS:NE2	2.30	0.47
1:B:366:ARG:NH1	1:B:371:GLU:OE2	2.42	0.46
1:G:283:LYS:HG3	1:G:437:PHE:CD1	2.50	0.46
1:I:283:LYS:HG3	1:I:437:PHE:CD1	2.50	0.46
1:D:359:PHE:CE1	1:D:382:CYS:HB3	2.50	0.46
1:G:108:ALA:O	1:G:111:VAL:HG22	2.15	0.46
1:G:189:LYS:O	1:G:192:VAL:HG22	2.15	0.46
1:C:288:PHE:HZ	1:C:444:LEU:HD21	1.81	0.46
1:C:371:GLU:HG2	1:C:376:HIS:HE1	1.68	0.46
1:D:388:LYS:HB2	1:D:408:VAL:HG23	1.98	0.46
1:G:359:PHE:CE1	1:G:382:CYS:HB3	2.50	0.46
1:I:407:GLU:O	1:I:411:VAL:HG12	2.16	0.46
1:B:260:ASN:HB3	1:B:263:ILE:HD12	1.98	0.46
1:G:258:LYS:HA	1:G:268:LEU:HD21	1.98	0.46
1:I:57:MET:HG2	1:I:181:TRP:CZ3	2.50	0.46
1:I:367:ARG:HA	1:I:367:ARG:HD3	1.62	0.46
1:G:233:LYS:O	1:G:237:THR:HG23	2.15	0.46
1:I:365:HIS:ND1	1:I:419:LEU:CG	2.77	0.46
1:I:366:ARG:CD	1:I:375:VAL:CG1	2.91	0.46
1:C:57:MET:HG2	1:C:181:TRP:CH2	2.50	0.46
1:G:233:LYS:NZ	2:G:501:AYU:O36	2.46	0.46
1:H:318:PRO:HA	1:H:321:LYS:HG3	1.98	0.46
1:A:288:PHE:CZ	1:A:441:LEU:HD23	2.50	0.46
1:C:258:LYS:NZ	1:C:272:ASP:OD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ARG:O	1:C:443:LYS:HG2	2.16	0.46
1:E:108:ALA:O	1:E:111:VAL:HG22	2.14	0.46
1:F:427:VAL:HG23	1:F:435:GLU:OE1	2.16	0.46
1:G:237:THR:HG22	2:G:501:AYU:C07	2.46	0.46
1:C:368:LEU:C	1:C:369:HIS:ND1	2.69	0.46
1:D:351:LEU:HG	1:D:408:VAL:HG11	1.98	0.46
1:G:119:TYR:CD1	1:G:150:ARG:HD2	2.51	0.45
1:B:254:TYR:OH	1:B:277:SER:OG	2.21	0.45
1:I:361:LEU:O	1:I:364:VAL:CG2	2.64	0.45
1:A:355:VAL:HG21	1:A:389:LEU:HD22	1.97	0.45
1:A:445:ILE:HD13	1:D:320:LEU:HD21	1.97	0.45
1:H:21:LEU:HD12	1:H:137:LEU:HD11	1.99	0.45
1:H:149:ILE:O	1:H:153:ARG:HG3	2.16	0.45
1:H:283:LYS:HG3	1:H:437:PHE:HD2	1.78	0.45
1:H:424:PHE:O	1:H:424:PHE:CD2	2.69	0.45
1:B:38:ARG:O	1:B:42:LEU:HG	2.17	0.45
1:B:149:ILE:O	1:B:153:ARG:HG3	2.16	0.45
1:F:411:VAL:O	1:F:415:VAL:HG23	2.17	0.45
1:H:237:THR:HG22	2:H:501:AYU:C07	2.46	0.45
1:B:408:VAL:O	1:B:412:ILE:HG12	2.17	0.45
1:G:389:LEU:O	1:G:392:PHE:HB3	2.17	0.45
1:E:265:LEU:HD23	1:E:265:LEU:HA	1.90	0.44
1:E:294:LEU:HD13	1:E:350:GLU:HG3	1.99	0.44
1:A:75:GLU:HB2	1:D:425:SER:HB3	1.99	0.44
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.87	0.44
1:H:426:ASN:HD21	1:H:435:GLU:HA	1.71	0.44
1:A:257:PHE:CE2	1:A:268:LEU:HD11	2.52	0.44
1:A:369:HIS:O	1:A:372:THR:HG22	2.17	0.44
1:I:137:LEU:HD23	1:I:137:LEU:HA	1.83	0.44
1:C:411:VAL:HA	1:C:414:GLN:HG3	1.99	0.44
1:E:64:GLU:O	1:E:66:TRP:N	2.51	0.44
1:F:31:GLU:O	1:F:35:GLU:HG2	2.18	0.44
1:A:440:ARG:HH12	1:D:270:GLU:CG	2.30	0.44
1:F:403:ALA:O	1:F:407:GLU:HG3	2.17	0.44
1:F:408:VAL:O	1:F:412:ILE:HG12	2.18	0.44
1:G:258:LYS:NZ	1:G:271:PHE:O	2.44	0.44
1:A:372:THR:OG1	1:A:374:THR:HG22	2.18	0.44
1:D:67:GLN:NE2	2:D:501:AYU:O34	2.51	0.44
1:F:339:LYS:HD2	1:F:339:LYS:HA	1.82	0.44
1:A:411:VAL:O	1:A:415:VAL:HG23	2.17	0.44
1:A:427:VAL:HG11	1:D:440:ARG:CD	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:LEU:HD13	1:F:133:GLY:HA3	2.00	0.44
1:F:336:LEU:HB3	1:F:416:LYS:HD3	1.99	0.44
1:G:400:ASP:O	1:G:404:LEU:HG	2.17	0.44
1:H:348:LYS:HZ1	1:H:389:LEU:HD11	1.82	0.44
1:I:368:LEU:HD23	1:I:368:LEU:HA	1.74	0.44
1:E:355:VAL:HG21	1:E:389:LEU:HD22	2.00	0.43
1:E:419:LEU:O	1:E:421:VAL:HG23	2.18	0.43
1:G:401:ARG:HA	1:G:404:LEU:HD11	2.00	0.43
1:B:119:TYR:CD1	1:B:150:ARG:HD2	2.54	0.43
1:E:397:ARG:NH1	1:H:400:ASP:OD1	2.51	0.43
1:H:129:GLN:HA	1:H:132:LYS:HG2	2.00	0.43
1:I:337:LEU:O	1:I:338:THR:C	2.57	0.43
1:C:381:LEU:O	1:C:411:VAL:HG21	2.17	0.43
1:E:137:LEU:HD23	1:E:137:LEU:HA	1.84	0.43
1:G:176:GLY:N	1:G:189:LYS:HZ3	2.16	0.43
1:G:307:LEU:HB2	1:G:328:ALA:HB2	1.99	0.43
1:F:3:ASN:HB3	1:F:6:VAL:HG23	2.01	0.43
1:F:441:LEU:HD12	1:F:441:LEU:H	1.82	0.43
1:H:282:CYS:HB2	1:H:303:ARG:HB2	2.00	0.43
1:G:7:VAL:HG11	1:G:118:LEU:HD22	2.00	0.43
1:A:339:LYS:HB2	1:A:354:PHE:CZ	2.53	0.43
1:I:289:SER:OG	1:I:289:SER:O	2.36	0.43
1:A:397:ARG:O	1:A:401:ARG:HG3	2.18	0.43
1:A:440:ARG:HB2	1:A:443:LYS:HE2	1.99	0.43
1:C:176:GLY:O	1:C:183:TYR:OH	2.24	0.43
1:C:392:PHE:CE2	1:C:401:ARG:HB3	2.53	0.43
1:F:320:LEU:HD21	1:G:445:ILE:HD13	2.01	0.43
1:E:3:ASN:HB3	1:E:6:VAL:CG2	2.49	0.43
1:C:286:ALA:HB1	1:C:296:VAL:HG22	2.00	0.43
1:D:3:ASN:HB3	1:D:6:VAL:CG2	2.49	0.43
1:F:413:ALA:O	1:F:417:GLU:HG2	2.18	0.43
1:G:412:ILE:HA	1:G:415:VAL:HG23	2.01	0.43
1:E:440:ARG:HE	1:E:440:ARG:HB2	1.58	0.42
1:E:107:ALA:O	1:E:111:VAL:HG13	2.19	0.42
1:I:324:HIS:HA	1:I:327:GLU:OE1	2.19	0.42
1:A:266:SER:HA	1:A:446:LEU:HG	2.01	0.42
1:D:437:PHE:O	1:D:438:GLU:C	2.57	0.42
1:E:307:LEU:HB2	1:E:328:ALA:HB2	2.01	0.42
1:I:65:LYS:HB2	1:I:65:LYS:HE2	1.70	0.42
1:B:394:THR:HB	1:F:5:LYS:HD2	2.01	0.42
1:D:317:PRO:HA	1:D:318:PRO:HD3	1.95	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:LYS:HB2	1:D:364:VAL:HG11	2.01	0.42
1:E:118:LEU:HB3	1:E:123:VAL:HG23	2.01	0.42
1:H:44:PRO:O	1:H:48:ARG:HG3	2.19	0.42
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.88	0.42
1:C:300:VAL:HG22	1:C:331:ALA:HB1	2.02	0.42
1:H:409:MET:O	1:H:412:ILE:HG13	2.19	0.42
1:I:411:VAL:O	1:I:415:VAL:HG13	2.20	0.42
1:C:273:HIS:HD1	1:C:310:TYR:HD2	1.66	0.42
1:C:372:THR:HG23	1:C:374:THR:OG1	2.19	0.42
1:F:440:ARG:HH21	1:F:443:LYS:HE2	1.85	0.42
1:G:57:MET:HG2	1:G:181:TRP:CH2	2.55	0.42
1:I:12:GLN:HG3	1:I:126:LYS:HD3	2.01	0.42
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.90	0.42
1:H:113:LEU:HD13	1:H:113:LEU:HA	1.87	0.42
1:H:372:THR:OG1	1:H:373:GLY:N	2.53	0.42
1:I:366:ARG:O	1:I:370:GLY:HA2	2.20	0.42
1:A:352:HIS:ND1	1:A:389:LEU:HD21	2.34	0.42
1:E:296:VAL:O	1:E:300:VAL:HG22	2.19	0.42
1:F:107:ALA:O	1:F:111:VAL:HG23	2.18	0.42
1:F:339:LYS:HB2	1:F:354:PHE:HZ	1.84	0.42
1:H:42:LEU:HD22	1:H:42:LEU:HA	1.86	0.42
1:H:419:LEU:HD23	1:H:419:LEU:HA	1.85	0.42
1:I:361:LEU:HG	1:I:419:LEU:HD13	2.02	0.42
1:D:411:VAL:O	1:D:415:VAL:HG23	2.20	0.42
1:G:118:LEU:HB3	1:G:123:VAL:HG23	2.01	0.42
1:G:237:THR:HG22	2:G:501:AYU:C06	2.49	0.42
1:A:440:ARG:O	1:A:443:LYS:HG2	2.19	0.42
1:C:118:LEU:HB3	1:C:123:VAL:HG23	2.01	0.42
1:C:411:VAL:O	1:C:415:VAL:HG13	2.20	0.42
1:F:44:PRO:HD2	1:F:47:LEU:HD12	2.02	0.42
1:G:113:LEU:HD23	1:G:113:LEU:HA	1.86	0.42
1:B:77:LYS:HD3	1:B:430:ARG:HB2	2.02	0.41
1:C:231:ASP:OD2	2:C:501:AYU:O34	2.38	0.41
1:E:341:ASP:OD1	1:E:342:ASP:N	2.53	0.41
1:G:265:LEU:HD23	1:G:265:LEU:HA	1.86	0.41
1:A:79:ASN:OD1	1:A:292:THR:HG23	2.19	0.41
1:B:419:LEU:HD23	1:B:419:LEU:HA	1.89	0.41
1:C:408:VAL:HA	1:C:411:VAL:HG13	2.01	0.41
1:E:411:VAL:O	1:E:415:VAL:HG23	2.20	0.41
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.88	0.41
1:E:367:ARG:NH2	1:I:31:GLU:OE1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:233:LYS:HE2	2:I:501:AYU:N08	2.36	0.41
1:C:296:VAL:O	1:C:300:VAL:HB	2.21	0.41
1:F:136:LYS:HE3	1:F:136:LYS:HB3	1.89	0.41
1:G:359:PHE:HA	1:G:362:THR:HG22	2.02	0.41
1:H:230:PRO:HG2	1:H:441:LEU:HD22	2.03	0.41
1:H:363:THR:O	1:H:367:ARG:HG2	2.21	0.41
1:H:445:ILE:H	1:H:445:ILE:HG13	1.79	0.41
1:I:412:ILE:O	1:I:415:VAL:HG22	2.21	0.41
1:C:155:SER:HB2	1:C:164:ALA:HB2	2.03	0.41
1:D:257:PHE:CD2	1:D:268:LEU:HD11	2.56	0.41
1:D:339:LYS:HA	1:D:339:LYS:HD3	1.82	0.41
1:G:107:ALA:O	1:G:111:VAL:HG13	2.20	0.41
1:G:137:LEU:HD23	1:G:137:LEU:HA	1.84	0.41
1:I:392:PHE:CE2	1:I:401:ARG:HB3	2.55	0.41
1:A:11:LEU:HD11	1:A:118:LEU:HD13	2.03	0.41
1:A:39:CYS:HA	1:A:42:LEU:HD23	2.03	0.41
1:A:249:MET:HE1	1:A:254:TYR:HD1	1.86	0.41
1:C:368:LEU:HB3	1:C:369:HIS:CE1	2.55	0.41
1:I:237:THR:HG23	2:I:501:AYU:C06	2.51	0.41
1:A:57:MET:HG2	1:A:181:TRP:CZ3	2.56	0.41
1:B:366:ARG:HD2	1:B:367:ARG:HH12	1.86	0.41
1:C:43:LEU:O	1:C:48:ARG:NH1	2.46	0.41
1:C:381:LEU:HD22	1:C:414:GLN:NE2	2.35	0.41
1:E:339:LYS:HB2	1:E:354:PHE:CZ	2.56	0.41
1:G:258:LYS:HB2	1:G:258:LYS:HE3	1.79	0.41
1:G:392:PHE:CE2	1:G:401:ARG:HB3	2.55	0.41
1:H:61:PHE:CE2	1:H:192:VAL:HG12	2.56	0.41
1:H:61:PHE:HE2	1:H:192:VAL:HG12	1.86	0.41
1:I:11:LEU:HD11	1:I:118:LEU:HD13	2.03	0.41
1:I:416:LYS:HA	1:I:416:LYS:HD2	1.60	0.41
1:C:428:ASP:C	1:C:430:ARG:H	2.24	0.41
1:E:60:PRO:HG3	1:E:188:ASP:HB3	2.03	0.41
1:G:372:THR:O	1:G:375:VAL:HG22	2.21	0.41
1:H:359:PHE:CE1	1:H:382:CYS:HB3	2.56	0.41
1:I:348:LYS:HG3	1:I:392:PHE:CE1	2.56	0.40
1:I:397:ARG:HD3	1:I:400:ASP:OD2	2.22	0.40
1:C:372:THR:O	1:C:372:THR:HG23	2.21	0.40
1:G:136:LYS:HD3	1:G:136:LYS:HA	1.88	0.40
1:H:265:LEU:HD12	1:H:265:LEU:HA	1.98	0.40
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.85	0.40
1:I:334:ILE:O	1:I:338:THR:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:ARG:N	1:D:443:LYS:HD2	2.37	0.40
1:G:60:PRO:HG3	1:G:188:ASP:HB3	2.03	0.40
1:H:26:PRO:HG3	1:H:102:ARG:CZ	2.52	0.40

All (1) 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:G:259:ASN:O	1:I:262:GLN:NE2[2_11511]	2.17	0.03

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	443/446 (99%)	437 (99%)	6 (1%)	0	100	100
1	B	443/446 (99%)	436 (98%)	7 (2%)	0	100	100
1	C	419/446 (94%)	413 (99%)	4 (1%)	2 (0%)	29	52
1	D	428/446 (96%)	420 (98%)	8 (2%)	0	100	100
1	E	427/446 (96%)	420 (98%)	6 (1%)	1 (0%)	47	71
1	F	429/446 (96%)	422 (98%)	7 (2%)	0	100	100
1	G	422/446 (95%)	413 (98%)	8 (2%)	1 (0%)	47	71
1	H	415/446 (93%)	406 (98%)	9 (2%)	0	100	100
1	I	398/446 (89%)	394 (99%)	3 (1%)	1 (0%)	41	64
All	All	3824/4014 (95%)	3761 (98%)	58 (2%)	5 (0%)	51	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	429	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	420	GLN
1	I	338	THR
1	C	373	GLY
1	G	370	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/383 (100%)	371 (97%)	11 (3%)	42	68
1	B	382/383 (100%)	372 (97%)	10 (3%)	46	72
1	C	366/383 (96%)	348 (95%)	18 (5%)	25	48
1	D	373/383 (97%)	363 (97%)	10 (3%)	44	71
1	E	372/383 (97%)	360 (97%)	12 (3%)	39	65
1	F	372/383 (97%)	358 (96%)	14 (4%)	33	59
1	G	367/383 (96%)	345 (94%)	22 (6%)	19	39
1	H	362/383 (94%)	338 (93%)	24 (7%)	16	33
1	I	347/383 (91%)	332 (96%)	15 (4%)	29	54
All	All	3323/3447 (96%)	3187 (96%)	136 (4%)	30	56

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	59	TRP
1	A	126	LYS
1	A	292	THR
1	A	296	VAL
1	A	298	THR
1	A	342	ASP
1	A	355	VAL
1	A	372	THR
1	A	415	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	429	ASP
1	B	6	VAL
1	B	59	TRP
1	B	69	LYS
1	B	89	GLN
1	B	323	LEU
1	B	340	ARG
1	B	342	ASP
1	B	372	THR
1	B	374	THR
1	B	442	ASP
1	C	9	VAL
1	C	59	TRP
1	C	126	LYS
1	C	156	VAL
1	C	162	LEU
1	C	195	VAL
1	C	296	VAL
1	C	298	THR
1	C	300	VAL
1	C	329	LYS
1	C	338	THR
1	C	369	HIS
1	C	376	HIS
1	C	411	VAL
1	C	414	GLN
1	C	430	ARG
1	C	433	VAL
1	C	440	ARG
1	D	6	VAL
1	D	59	TRP
1	D	174	ASN
1	D	195	VAL
1	D	229	GLN
1	D	237	THR
1	D	355	VAL
1	D	372	THR
1	D	415	VAL
1	D	439	CYS
1	E	6	VAL
1	E	49	THR
1	E	59	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	126	LYS
1	E	174	ASN
1	E	195	VAL
1	E	296	VAL
1	E	355	VAL
1	E	372	THR
1	E	376	HIS
1	E	415	VAL
1	E	444	LEU
1	F	6	VAL
1	F	42	LEU
1	F	59	TRP
1	F	83	VAL
1	F	126	LYS
1	F	162	LEU
1	F	174	ASN
1	F	195	VAL
1	F	237	THR
1	F	296	VAL
1	F	298	THR
1	F	355	VAL
1	F	371	GLU
1	F	415	VAL
1	G	6	VAL
1	G	49	THR
1	G	59	TRP
1	G	126	LYS
1	G	143	ILE
1	G	156	VAL
1	G	174	ASN
1	G	186	GLU
1	G	268	LEU
1	G	269	LYS
1	G	292	THR
1	G	296	VAL
1	G	300	VAL
1	G	346	THR
1	G	372	THR
1	G	404	LEU
1	G	415	VAL
1	G	427	VAL
1	G	430	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	433	VAL
1	G	442	ASP
1	G	443	LYS
1	H	18	LEU
1	H	21	LEU
1	H	30	GLU
1	H	42	LEU
1	H	59	TRP
1	H	89	GLN
1	H	156	VAL
1	H	174	ASN
1	H	186	GLU
1	H	190	VAL
1	H	227	LEU
1	H	232	LYS
1	H	262	GLN
1	H	265	LEU
1	H	275	LEU
1	H	320	LEU
1	H	323	LEU
1	H	355	VAL
1	H	368	LEU
1	H	424	PHE
1	H	426	ASN
1	H	430	ARG
1	H	433	VAL
1	H	438	GLU
1	I	59	TRP
1	I	83	VAL
1	I	237	THR
1	I	300	VAL
1	I	336	LEU
1	I	348	LYS
1	I	355	VAL
1	I	369	HIS
1	I	372	THR
1	I	386	MET
1	I	389	LEU
1	I	411	VAL
1	I	415	VAL
1	I	416	LYS
1	I	433	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	322	ASN
1	C	376	HIS
1	C	414	GLN
1	D	174	ASN
1	H	426	ASN

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](#)

9 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	AYU	H	501	-	37,43,43	2.73	15 (40%)	47,66,66	1.68	8 (17%)
2	AYU	F	501	-	37,43,43	2.45	12 (32%)	47,66,66	1.47	8 (17%)
2	AYU	B	501	-	37,43,43	2.55	13 (35%)	47,66,66	1.36	5 (10%)
2	AYU	I	501	-	37,43,43	2.65	16 (43%)	47,66,66	1.59	7 (14%)
2	AYU	E	501	-	37,43,43	2.69	13 (35%)	47,66,66	1.49	7 (14%)
2	AYU	G	501	-	37,43,43	2.65	14 (37%)	47,66,66	1.55	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AYU	C	501	-	37,43,43	2.58	15 (40%)	47,66,66	1.51	8 (17%)
2	AYU	D	501	-	37,43,43	2.44	13 (35%)	47,66,66	1.46	7 (14%)
2	AYU	A	501	-	37,43,43	2.57	13 (35%)	47,66,66	1.52	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AYU	H	501	-	-	1/23/63/63	0/4/4/4
2	AYU	F	501	-	-	1/23/63/63	0/4/4/4
2	AYU	B	501	-	-	1/23/63/63	0/4/4/4
2	AYU	I	501	-	-	1/23/63/63	0/4/4/4
2	AYU	E	501	-	-	0/23/63/63	0/4/4/4
2	AYU	G	501	-	-	1/23/63/63	0/4/4/4
2	AYU	C	501	-	-	1/23/63/63	0/4/4/4
2	AYU	D	501	-	-	0/23/63/63	0/4/4/4
2	AYU	A	501	-	-	1/23/63/63	0/4/4/4

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	AYU	P20-O23	9.89	1.86	1.60
2	E	501	AYU	P20-O23	9.83	1.86	1.60
2	G	501	AYU	P20-O23	9.61	1.85	1.60
2	C	501	AYU	P20-O23	9.08	1.84	1.60
2	A	501	AYU	P20-O23	8.99	1.84	1.60
2	I	501	AYU	P20-O23	8.91	1.83	1.60
2	B	501	AYU	P20-O23	8.81	1.83	1.60
2	F	501	AYU	P20-O23	8.36	1.82	1.60
2	D	501	AYU	P20-O23	7.99	1.81	1.60
2	I	501	AYU	P16-O15	5.46	1.81	1.59
2	H	501	AYU	P16-O15	5.44	1.81	1.59
2	G	501	AYU	C27-C26	5.39	1.64	1.52
2	A	501	AYU	C27-C26	5.39	1.64	1.52
2	H	501	AYU	C27-C26	5.37	1.64	1.52
2	I	501	AYU	C27-C26	5.29	1.64	1.52
2	E	501	AYU	C27-C26	5.26	1.63	1.52
2	G	501	AYU	P16-O15	5.24	1.80	1.59
2	F	501	AYU	P16-O15	5.10	1.80	1.59
2	B	501	AYU	C27-C26	5.04	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	AYU	P16-O15	4.96	1.79	1.59
2	A	501	AYU	P16-O15	4.84	1.78	1.59
2	D	501	AYU	C27-C26	4.82	1.63	1.52
2	C	501	AYU	C27-C26	4.66	1.62	1.52
2	C	501	AYU	P16-O15	4.64	1.78	1.59
2	F	501	AYU	C27-C26	4.46	1.62	1.52
2	D	501	AYU	P16-O15	4.42	1.77	1.59
2	B	501	AYU	C31-C26	4.36	1.64	1.52
2	H	501	AYU	C31-C26	4.20	1.63	1.52
2	B	501	AYU	P16-O15	4.15	1.76	1.59
2	G	501	AYU	C29-C27	3.96	1.62	1.52
2	E	501	AYU	C29-C27	3.88	1.62	1.52
2	B	501	AYU	C29-C27	3.81	1.62	1.52
2	I	501	AYU	C29-C27	3.75	1.62	1.52
2	H	501	AYU	C29-C27	3.73	1.62	1.52
2	G	501	AYU	C31-C26	3.66	1.62	1.52
2	D	501	AYU	O25-C26	-3.64	1.38	1.44
2	I	501	AYU	C31-C26	3.57	1.61	1.52
2	E	501	AYU	O25-C26	-3.54	1.38	1.44
2	F	501	AYU	C29-C27	3.52	1.61	1.52
2	A	501	AYU	C29-C27	3.50	1.61	1.52
2	I	501	AYU	C39-C11	3.49	1.59	1.53
2	C	501	AYU	C29-C27	3.44	1.61	1.52
2	E	501	AYU	C31-C26	3.42	1.61	1.52
2	H	501	AYU	C39-C11	3.39	1.58	1.53
2	F	501	AYU	C31-C26	3.32	1.61	1.52
2	D	501	AYU	C29-C27	3.29	1.61	1.52
2	C	501	AYU	C31-C26	3.28	1.61	1.52
2	A	501	AYU	C31-C26	3.27	1.61	1.52
2	I	501	AYU	C04-N03	3.24	1.39	1.33
2	C	501	AYU	C39-C11	3.21	1.58	1.53
2	D	501	AYU	C31-C26	3.18	1.60	1.52
2	C	501	AYU	O25-C26	-3.17	1.39	1.44
2	G	501	AYU	C04-N03	3.13	1.39	1.33
2	H	501	AYU	C04-N03	3.09	1.39	1.33
2	B	501	AYU	C04-N03	3.07	1.39	1.33
2	C	501	AYU	C04-N03	3.07	1.39	1.33
2	D	501	AYU	C35-C33	3.05	1.60	1.52
2	B	501	AYU	O28-C27	-2.99	1.37	1.43
2	D	501	AYU	C04-N03	2.99	1.39	1.33
2	C	501	AYU	C35-C33	2.92	1.59	1.52
2	F	501	AYU	O28-C27	-2.90	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	AYU	C24-C35	2.89	1.60	1.52
2	A	501	AYU	O28-C27	-2.88	1.37	1.43
2	E	501	AYU	C04-N03	2.86	1.39	1.33
2	A	501	AYU	C04-N03	2.84	1.39	1.33
2	F	501	AYU	C04-N03	2.84	1.39	1.33
2	B	501	AYU	O15-C14	-2.75	1.34	1.44
2	E	501	AYU	O15-C14	-2.71	1.34	1.44
2	E	501	AYU	C24-C35	2.70	1.60	1.52
2	I	501	AYU	O25-C26	-2.67	1.39	1.44
2	E	501	AYU	O28-C27	-2.66	1.37	1.43
2	A	501	AYU	C24-C35	2.65	1.60	1.52
2	B	501	AYU	C24-C35	2.64	1.60	1.52
2	F	501	AYU	O15-C14	-2.63	1.34	1.44
2	B	501	AYU	O25-C26	-2.62	1.39	1.44
2	D	501	AYU	O15-C14	-2.60	1.34	1.44
2	A	501	AYU	C39-C11	2.55	1.57	1.53
2	F	501	AYU	O25-C26	-2.53	1.40	1.44
2	I	501	AYU	O15-C14	-2.50	1.35	1.44
2	C	501	AYU	C06-N05	2.50	1.39	1.35
2	H	501	AYU	O15-C14	-2.49	1.35	1.44
2	A	501	AYU	C35-C33	2.49	1.58	1.52
2	A	501	AYU	O25-C26	-2.49	1.40	1.44
2	I	501	AYU	C06-N05	2.49	1.39	1.35
2	C	501	AYU	O15-C14	-2.47	1.35	1.44
2	G	501	AYU	O15-C14	-2.47	1.35	1.44
2	A	501	AYU	O15-C14	-2.47	1.35	1.44
2	H	501	AYU	C14-C13	2.45	1.59	1.51
2	C	501	AYU	C14-C13	2.45	1.59	1.51
2	H	501	AYU	C06-N05	2.45	1.39	1.35
2	E	501	AYU	C33-C31	2.45	1.58	1.52
2	G	501	AYU	C35-C33	2.43	1.58	1.52
2	C	501	AYU	C24-C35	2.40	1.59	1.52
2	D	501	AYU	O28-C27	-2.35	1.38	1.43
2	G	501	AYU	C33-C31	2.35	1.58	1.52
2	I	501	AYU	C24-C35	2.32	1.59	1.52
2	G	501	AYU	O25-C26	-2.31	1.40	1.44
2	C	501	AYU	O28-C27	-2.31	1.38	1.43
2	E	501	AYU	C06-N05	2.30	1.38	1.35
2	I	501	AYU	C14-C13	2.28	1.58	1.51
2	I	501	AYU	C04-N05	2.28	1.35	1.32
2	G	501	AYU	C06-N05	2.26	1.38	1.35
2	F	501	AYU	C24-C35	2.25	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	AYU	O28-C27	-2.23	1.38	1.43
2	G	501	AYU	O28-C27	-2.23	1.38	1.43
2	B	501	AYU	C35-C33	2.22	1.58	1.52
2	E	501	AYU	C35-C33	2.21	1.58	1.52
2	F	501	AYU	C35-C33	2.21	1.58	1.52
2	D	501	AYU	O40-C39	-2.20	1.37	1.43
2	A	501	AYU	C14-C13	2.19	1.58	1.51
2	H	501	AYU	C24-C35	2.18	1.58	1.52
2	B	501	AYU	O40-C39	-2.16	1.37	1.43
2	F	501	AYU	O25-C24	2.15	1.47	1.41
2	B	501	AYU	O25-C24	2.14	1.47	1.41
2	G	501	AYU	C24-C35	2.12	1.58	1.52
2	I	501	AYU	O25-C24	2.12	1.47	1.41
2	I	501	AYU	C35-C33	2.10	1.57	1.52
2	H	501	AYU	C35-C33	2.10	1.57	1.52
2	C	501	AYU	C04-N05	2.09	1.35	1.32
2	H	501	AYU	O25-C26	-2.06	1.40	1.44
2	H	501	AYU	C04-N05	2.04	1.35	1.32
2	D	501	AYU	C06-N05	2.04	1.38	1.35
2	H	501	AYU	O28-C27	-2.04	1.39	1.43
2	G	501	AYU	C39-C11	2.03	1.56	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	AYU	C27-C26-C31	-4.58	106.43	114.03
2	G	501	AYU	C27-C26-C31	-4.50	106.56	114.03
2	I	501	AYU	C27-C26-C31	-4.50	106.56	114.03
2	E	501	AYU	O19-P20-O23	4.11	110.78	102.48
2	C	501	AYU	C27-C26-C31	-4.09	107.24	114.03
2	A	501	AYU	C27-C26-C31	-4.01	107.37	114.03
2	C	501	AYU	O19-P20-O23	3.92	110.40	102.48
2	F	501	AYU	C27-C26-C31	-3.91	107.55	114.03
2	H	501	AYU	O19-P20-O23	3.90	110.36	102.48
2	I	501	AYU	C37-C39-C11	3.88	106.82	100.98
2	I	501	AYU	O19-P20-O23	3.82	110.19	102.48
2	A	501	AYU	C24-O25-C26	3.78	119.16	113.06
2	H	501	AYU	O25-C26-C31	3.71	113.08	107.87
2	D	501	AYU	O19-P20-O23	3.69	109.93	102.48
2	D	501	AYU	C27-C26-C31	-3.64	108.00	114.03
2	H	501	AYU	C24-O25-C26	3.59	118.84	113.06
2	B	501	AYU	O12-C11-C39	-3.50	101.82	106.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	AYU	C37-C39-C11	3.48	106.22	100.98
2	A	501	AYU	O12-C11-C39	-3.41	101.94	106.93
2	I	501	AYU	C24-O25-C26	3.40	118.53	113.06
2	E	501	AYU	C27-C26-C31	-3.35	108.48	114.03
2	B	501	AYU	C27-C26-C31	-3.32	108.53	114.03
2	F	501	AYU	O19-P20-O23	3.25	109.04	102.48
2	G	501	AYU	O19-P20-O23	3.21	108.96	102.48
2	E	501	AYU	O12-C11-C39	-3.16	102.31	106.93
2	H	501	AYU	C07-C02-N01	3.12	125.09	120.35
2	A	501	AYU	C07-C02-N01	3.12	125.09	120.35
2	G	501	AYU	C07-C02-N01	3.08	125.03	120.35
2	A	501	AYU	O19-P20-O23	3.07	108.68	102.48
2	F	501	AYU	C37-C39-C11	3.05	105.56	100.98
2	C	501	AYU	C07-C02-N01	2.99	124.89	120.35
2	I	501	AYU	C07-C02-N01	2.99	124.89	120.35
2	G	501	AYU	O12-C11-C39	-2.97	102.59	106.93
2	D	501	AYU	C37-C39-C11	2.85	105.28	100.98
2	G	501	AYU	O25-C26-C31	2.84	111.85	107.87
2	F	501	AYU	C07-C02-N01	2.81	124.62	120.35
2	D	501	AYU	C07-C02-N01	2.80	124.61	120.35
2	E	501	AYU	C07-C02-N01	2.80	124.60	120.35
2	D	501	AYU	O12-C11-C39	-2.76	102.89	106.93
2	E	501	AYU	C37-C39-C11	2.70	105.04	100.98
2	D	501	AYU	C24-O25-C26	2.67	117.36	113.06
2	B	501	AYU	C07-C02-N01	2.60	124.30	120.35
2	F	501	AYU	O12-C11-C39	-2.59	103.14	106.93
2	C	501	AYU	O23-P20-O22	-2.57	99.84	109.47
2	C	501	AYU	C37-C39-C11	2.48	104.72	100.98
2	G	501	AYU	C37-C39-C11	2.48	104.72	100.98
2	C	501	AYU	O12-C11-C39	-2.47	103.32	106.93
2	E	501	AYU	C24-O25-C26	2.46	117.03	113.06
2	C	501	AYU	C24-O25-C26	2.46	117.02	113.06
2	I	501	AYU	O25-C26-C31	2.44	111.30	107.87
2	D	501	AYU	O23-P20-O22	-2.40	100.45	109.47
2	G	501	AYU	C24-O25-C26	2.39	116.91	113.06
2	F	501	AYU	C24-O25-C26	2.38	116.89	113.06
2	C	501	AYU	O25-C26-C31	2.35	111.17	107.87
2	B	501	AYU	O19-P20-O23	2.25	107.02	102.48
2	F	501	AYU	P20-O19-P16	-2.22	125.20	132.83
2	A	501	AYU	C06-C07-N08	-2.16	107.14	109.40
2	B	501	AYU	O25-C24-O23	2.12	114.14	111.36
2	I	501	AYU	C06-C07-N08	-2.11	107.20	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	AYU	O23-P20-O22	-2.08	101.65	109.47
2	H	501	AYU	C06-C07-N08	-2.08	107.23	109.40
2	G	501	AYU	O23-P20-O22	-2.04	101.80	109.47
2	H	501	AYU	O23-P20-O22	-2.03	101.86	109.47
2	E	501	AYU	C14-C13-C37	-2.01	107.63	115.18

There are no chirality outliers.

All (7) torsion outliers are listed below:

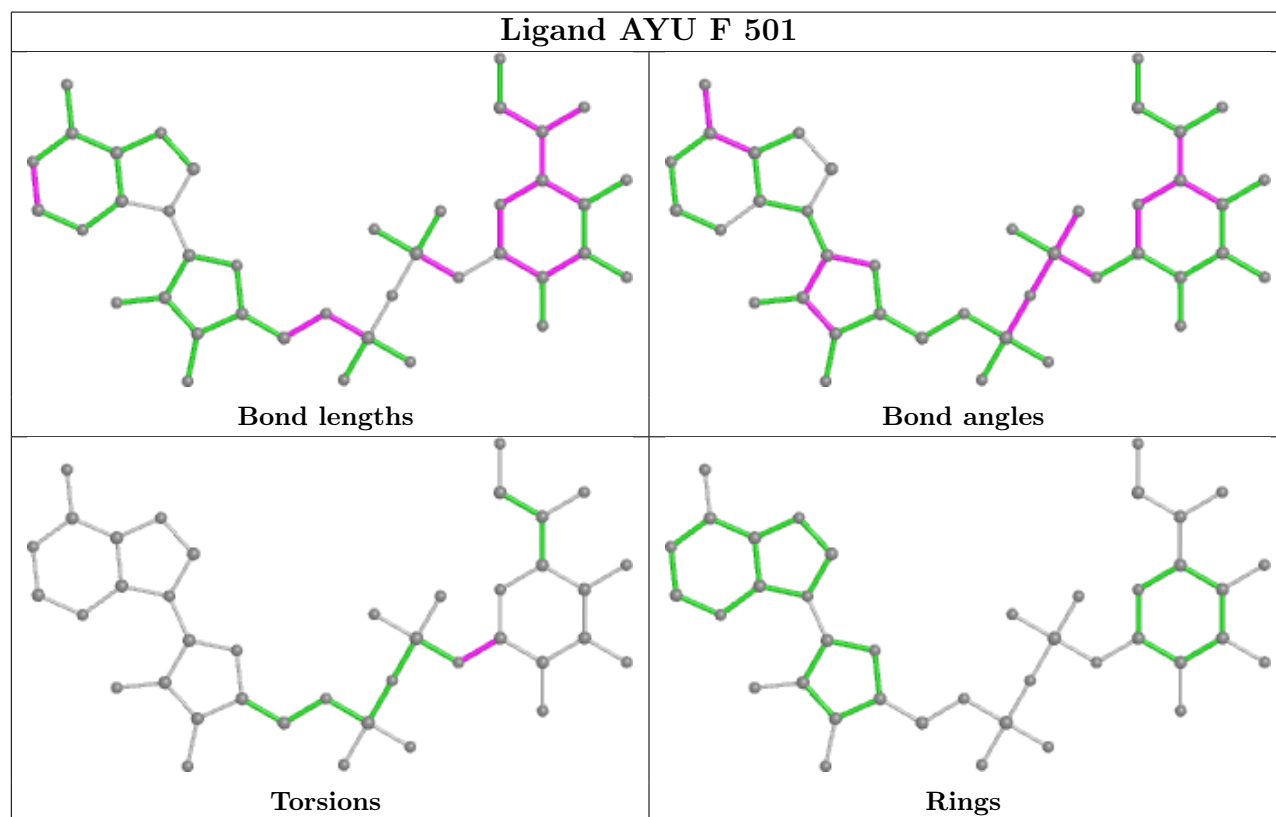
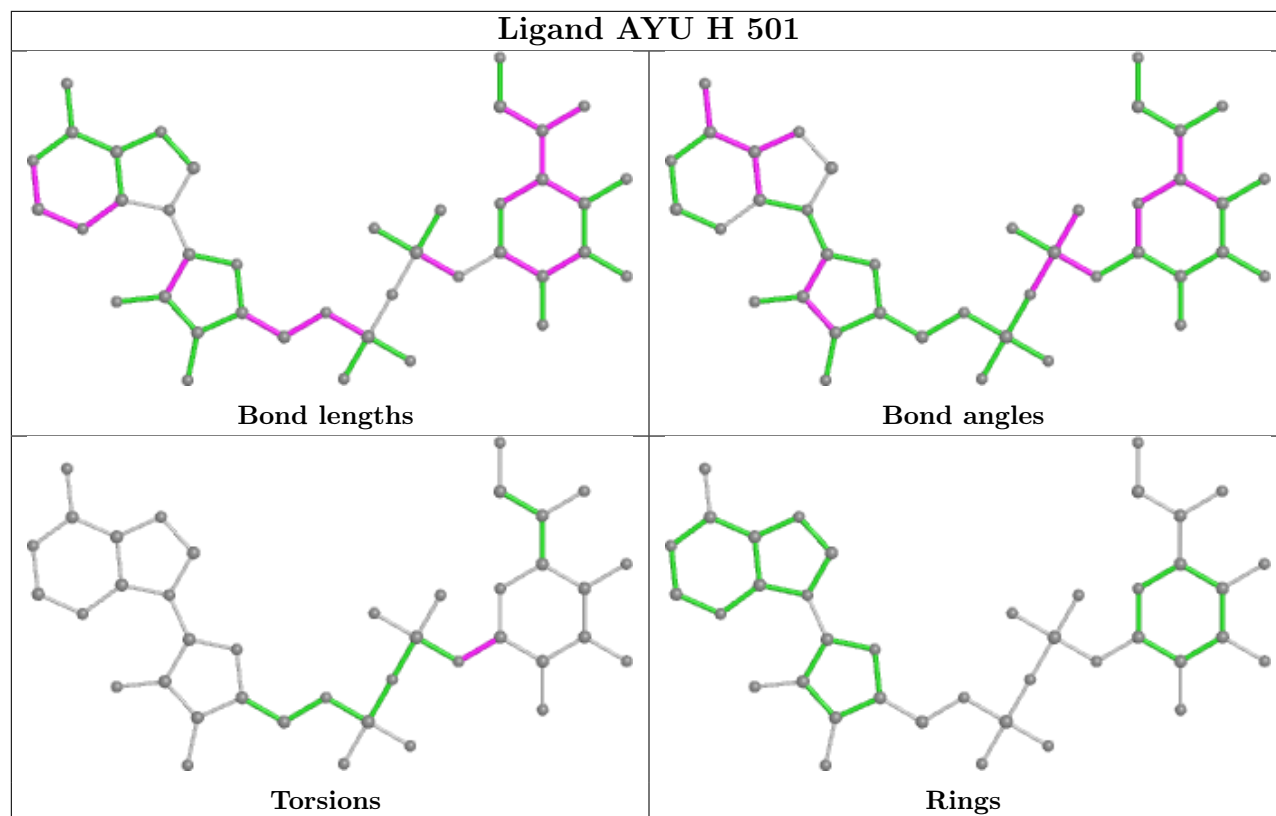
Mol	Chain	Res	Type	Atoms
2	B	501	AYU	C35-C24-O23-P20
2	F	501	AYU	C35-C24-O23-P20
2	H	501	AYU	C35-C24-O23-P20
2	C	501	AYU	C35-C24-O23-P20
2	I	501	AYU	C35-C24-O23-P20
2	A	501	AYU	C35-C24-O23-P20
2	G	501	AYU	C35-C24-O23-P20

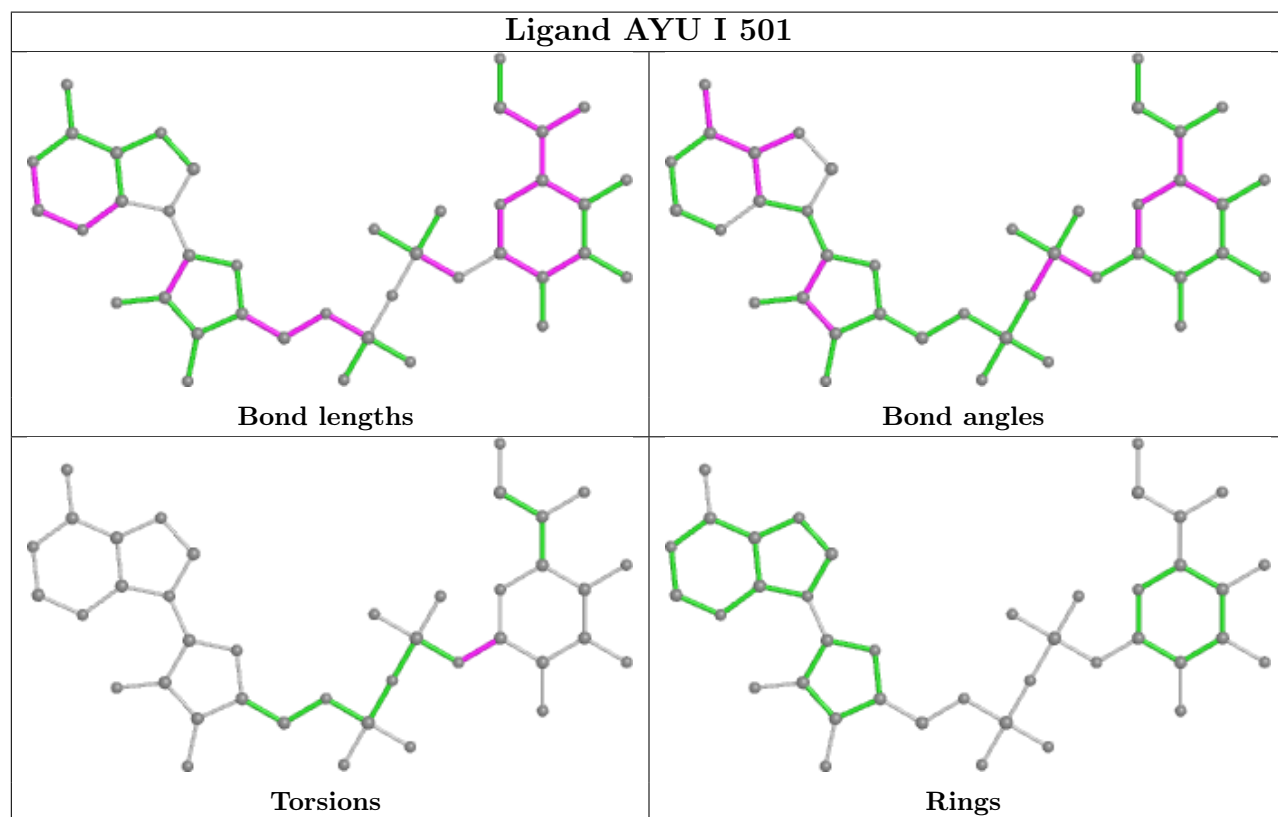
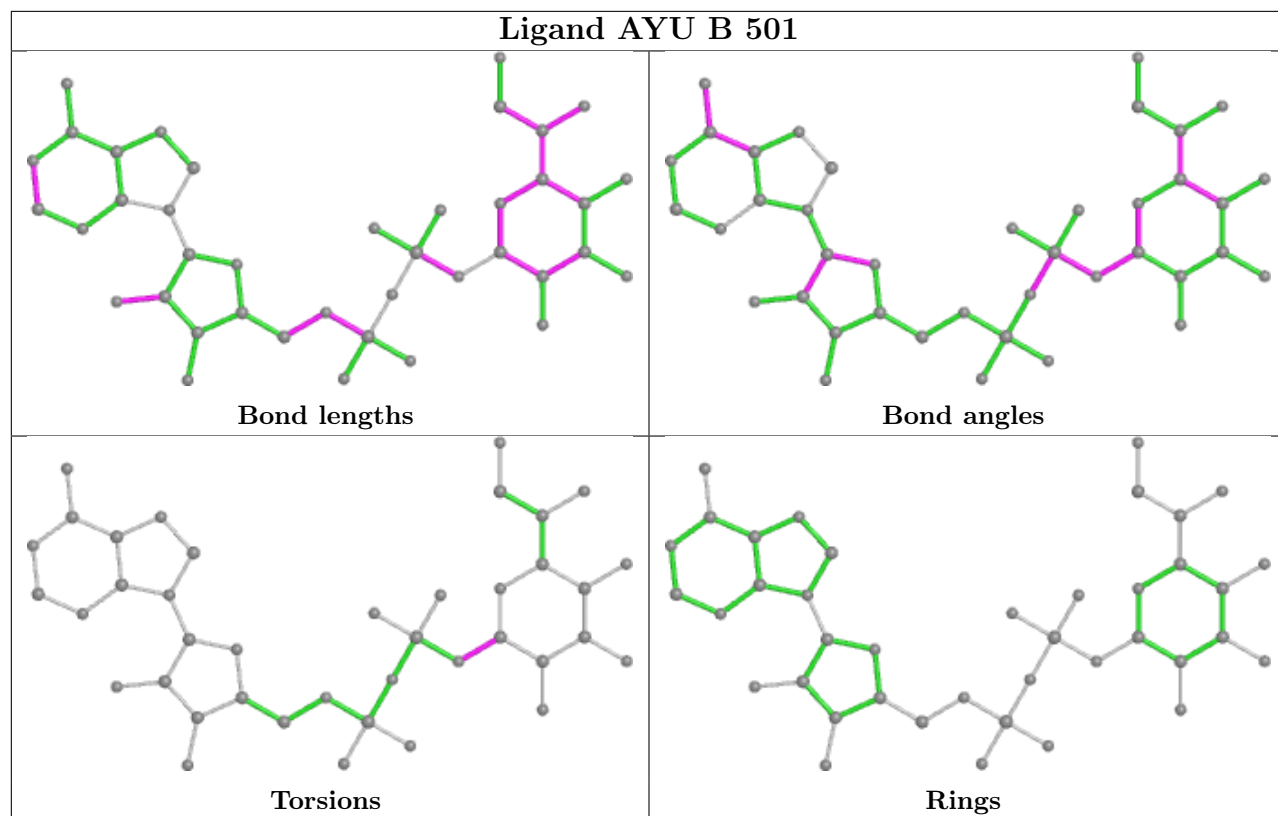
There are no ring outliers.

7 monomers are involved in 17 short contacts:

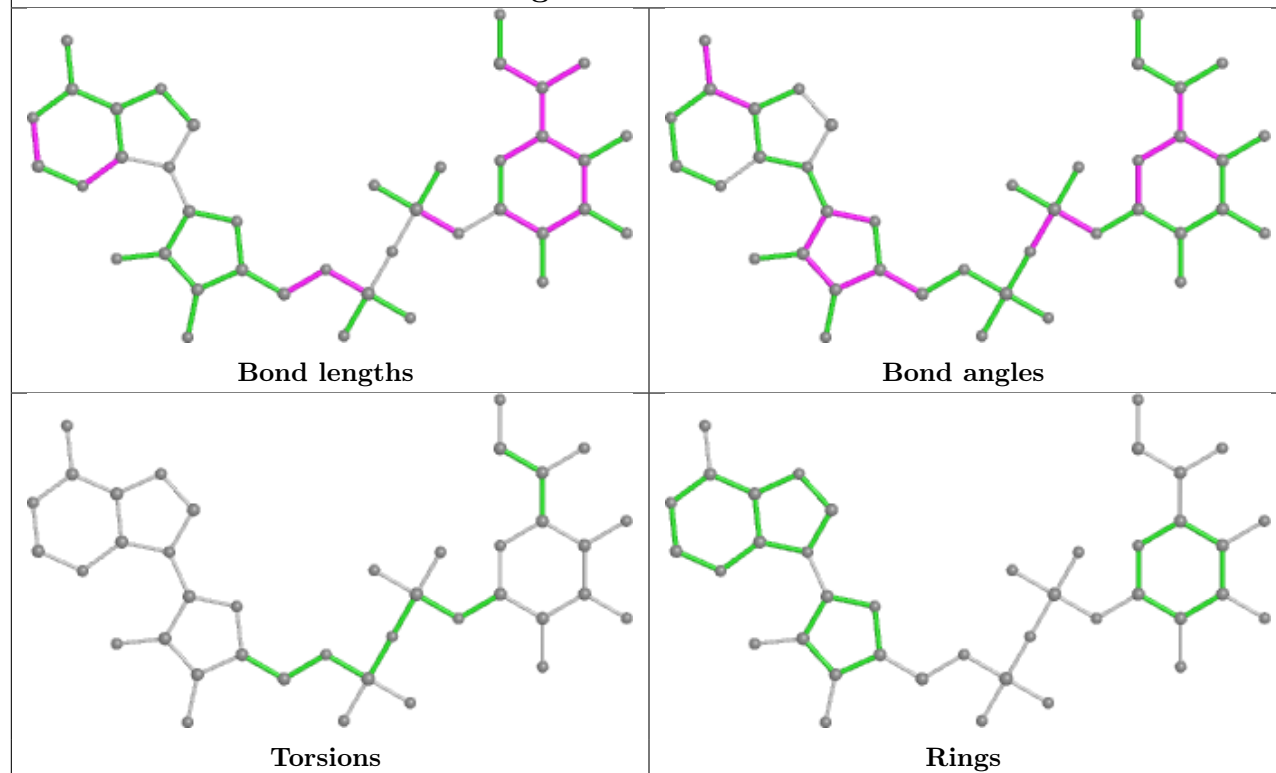
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	AYU	3	0
2	B	501	AYU	2	0
2	I	501	AYU	4	0
2	G	501	AYU	4	0
2	C	501	AYU	2	0
2	D	501	AYU	1	0
2	A	501	AYU	1	0

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

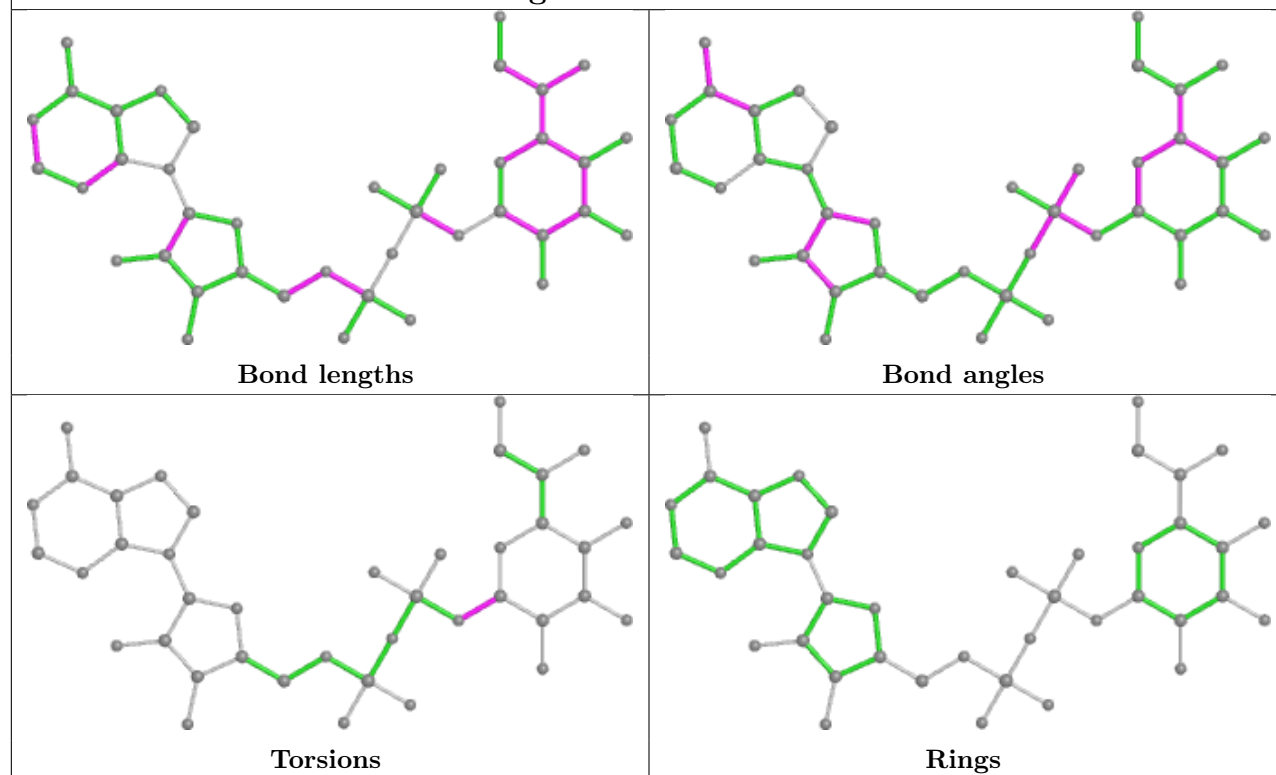


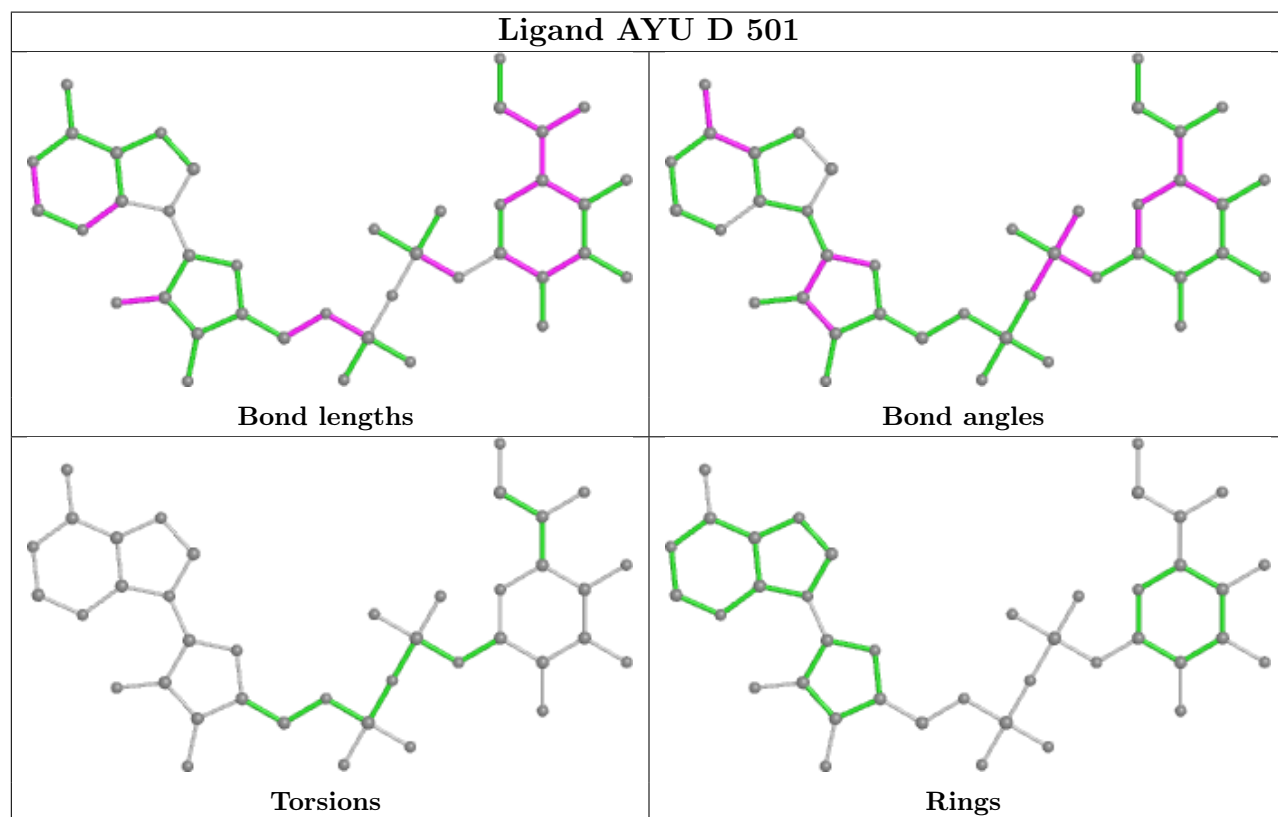
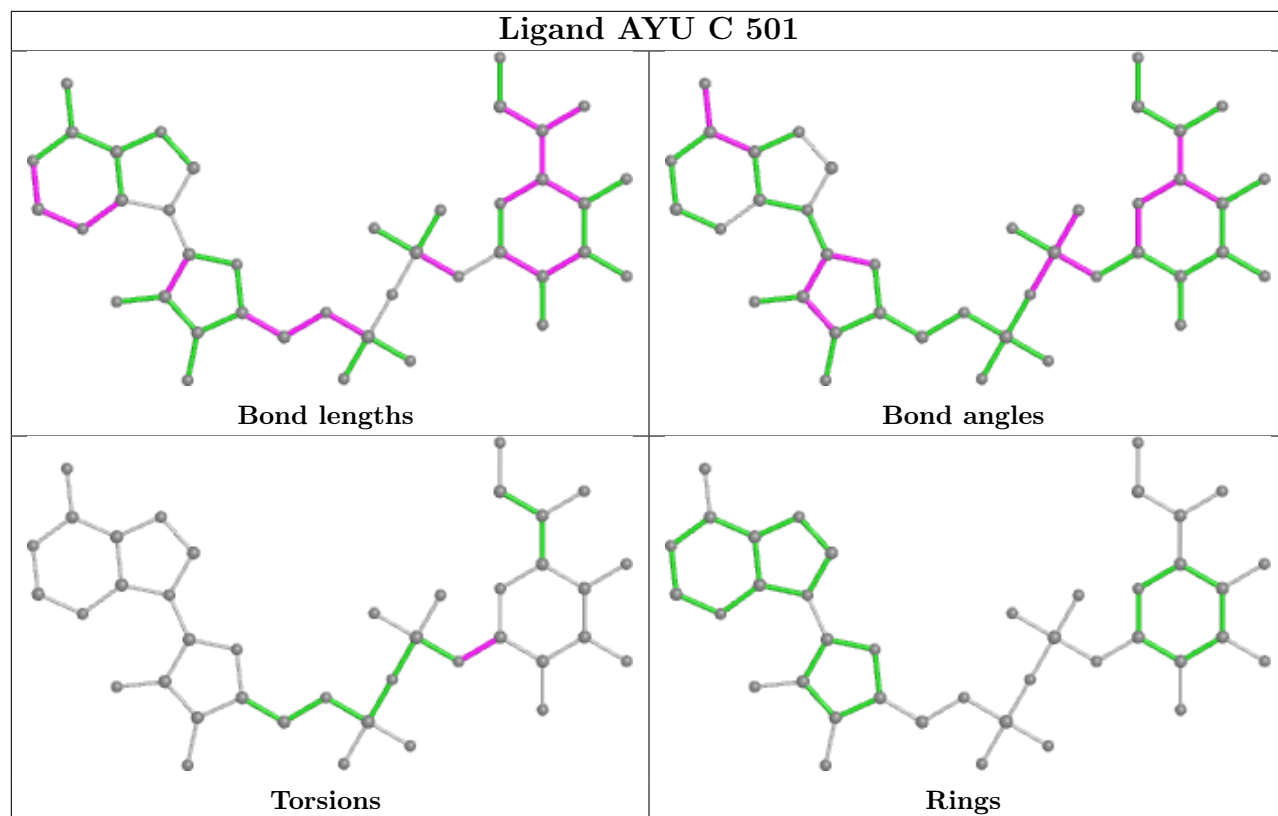


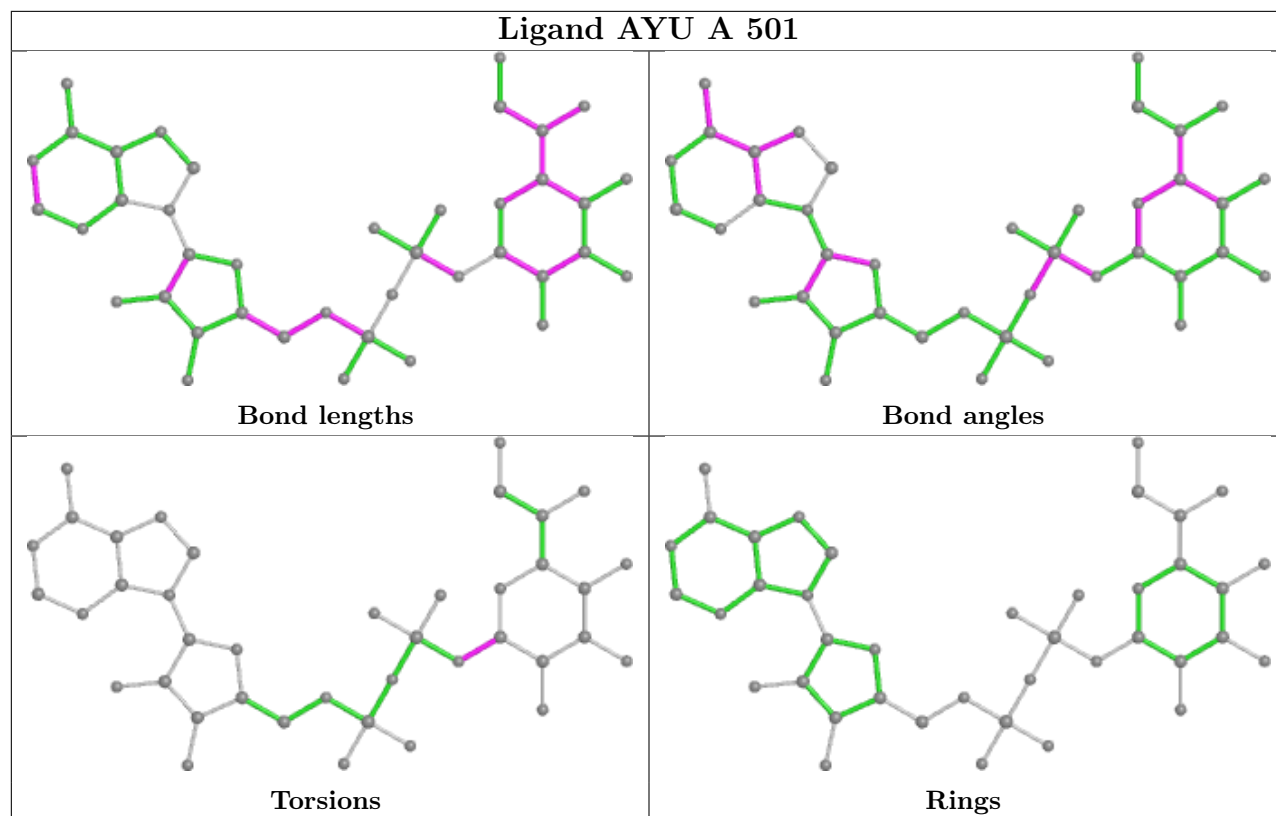
Ligand AYU E 501



Ligand AYU G 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	445/446 (99%)	0.31	6 (1%) 77 73	26, 41, 77, 119	0
1	B	445/446 (99%)	0.14	4 (0%) 84 82	25, 38, 67, 111	0
1	C	427/446 (95%)	0.76	50 (11%) 4 3	31, 59, 113, 138	0
1	D	434/446 (97%)	0.29	15 (3%) 44 36	26, 44, 74, 116	0
1	E	433/446 (97%)	0.52	26 (6%) 21 16	26, 48, 84, 116	0
1	F	433/446 (97%)	0.40	21 (4%) 30 24	26, 52, 83, 112	0
1	G	428/446 (95%)	0.91	55 (12%) 3 2	45, 70, 102, 126	0
1	H	423/446 (94%)	1.29	91 (21%) 0 0	51, 96, 128, 152	0
1	I	408/446 (91%)	1.02	76 (18%) 1 0	36, 78, 139, 180	0
All	All	3876/4014 (96%)	0.62	344 (8%) 9 6	25, 56, 114, 180	0

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	378	ALA	7.3
1	A	341	ASP	6.4
1	C	413	ALA	5.8
1	I	276	LEU	5.7
1	C	323	LEU	5.5
1	I	418	HIS	5.4
1	C	420	GLN	5.2
1	H	184	ARG	5.2
1	I	337	LEU	5.2
1	B	341	ASP	5.0
1	H	371	GLU	5.0
1	E	440	ARG	4.9
1	C	377	ALA	4.9
1	E	439	CYS	4.8
1	C	439	CYS	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	362	THR	4.8
1	H	417	GLU	4.7
1	I	415	VAL	4.7
1	H	347	GLY	4.7
1	H	45	SER	4.7
1	I	381	LEU	4.7
1	H	376	HIS	4.6
1	I	366	ARG	4.6
1	H	172	ILE	4.6
1	H	420	GLN	4.6
1	H	406	GLN	4.5
1	I	414	GLN	4.5
1	D	446	LEU	4.5
1	C	358	ALA	4.5
1	C	429	ASP	4.4
1	C	365	HIS	4.4
1	H	190	VAL	4.3
1	G	178	THR	4.3
1	I	417	GLU	4.3
1	H	230	PRO	4.2
1	C	418	HIS	4.2
1	I	362	THR	4.2
1	I	325	LEU	4.2
1	C	378	ALA	4.1
1	I	317	PRO	4.1
1	I	326	CYS	4.1
1	I	412	ILE	4.0
1	I	376	HIS	4.0
1	C	425	SER	4.0
1	H	429	ASP	4.0
1	G	369	HIS	4.0
1	H	227	LEU	4.0
1	H	445	ILE	4.0
1	H	30	GLU	4.0
1	C	421	VAL	4.0
1	H	419	LEU	4.0
1	H	288	PHE	3.9
1	H	291	TYR	3.9
1	H	441	LEU	3.9
1	I	434	PRO	3.9
1	I	380	GLN	3.9
1	E	66	TRP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	385	ALA	3.9
1	D	344	PRO	3.8
1	C	443	LYS	3.8
1	I	270	GLU	3.8
1	I	368	LEU	3.8
1	E	441	LEU	3.8
1	C	380	GLN	3.7
1	I	316	CYS	3.7
1	I	365	HIS	3.7
1	I	361	LEU	3.7
1	I	407	GLU	3.7
1	G	427	VAL	3.7
1	C	310	TYR	3.6
1	I	308	LEU	3.6
1	I	370	GLY	3.6
1	F	425	SER	3.6
1	D	342	ASP	3.6
1	H	182	LEU	3.6
1	I	367	ARG	3.6
1	I	310	TYR	3.5
1	I	311	SER	3.5
1	H	439	CYS	3.5
1	E	423	SER	3.5
1	A	320	LEU	3.5
1	G	173	SER	3.5
1	C	414	GLN	3.5
1	D	66	TRP	3.5
1	I	364	VAL	3.5
1	H	381	LEU	3.5
1	E	422	GLN	3.5
1	G	64	GLU	3.5
1	C	416	LYS	3.4
1	G	419	LEU	3.4
1	F	340	ARG	3.4
1	H	425	SER	3.4
1	I	318	PRO	3.4
1	G	375	VAL	3.4
1	G	439	CYS	3.4
1	C	326	CYS	3.4
1	E	427	VAL	3.4
1	F	429	ASP	3.4
1	C	337	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	170	SER	3.3
1	G	424	PHE	3.3
1	G	376	HIS	3.3
1	H	183	TYR	3.3
1	C	325	LEU	3.3
1	F	342	ASP	3.3
1	F	66	TRP	3.3
1	H	368	LEU	3.3
1	H	382	CYS	3.2
1	C	364	VAL	3.2
1	I	374	THR	3.2
1	E	381	LEU	3.2
1	I	334	ILE	3.2
1	H	432	TYR	3.2
1	H	56	GLU	3.2
1	E	430	ARG	3.2
1	G	96	ARG	3.2
1	H	440	ARG	3.1
1	C	424	PHE	3.1
1	H	185	ASN	3.1
1	I	307	LEU	3.1
1	I	271	PHE	3.1
1	C	373	GLY	3.1
1	I	433	VAL	3.1
1	E	68	TYR	3.1
1	G	62	VAL	3.1
1	H	345	VAL	3.1
1	G	422	GLN	3.0
1	G	2	ASN	3.0
1	F	341	ASP	3.0
1	H	370	GLY	3.0
1	E	41	ALA	3.0
1	G	318	PRO	3.0
1	C	445	ILE	3.0
1	A	446	LEU	3.0
1	G	97	ALA	3.0
1	H	107	ALA	3.0
1	H	113	LEU	3.0
1	I	67	GLN	3.0
1	H	187	SER	3.0
1	B	317	PRO	3.0
1	D	422	GLN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	434	PRO	3.0
1	C	359	PHE	2.9
1	H	354	PHE	2.9
1	I	416	LYS	2.9
1	H	344	PRO	2.9
1	I	405	SER	2.9
1	G	420	GLN	2.9
1	G	109	ALA	2.9
1	H	414	GLN	2.9
1	G	320	LEU	2.9
1	C	437	PHE	2.9
1	D	443	LYS	2.9
1	H	422	GLN	2.9
1	C	389	LEU	2.8
1	G	170	SER	2.8
1	I	266	SER	2.8
1	H	415	VAL	2.8
1	G	368	LEU	2.8
1	G	175	ASN	2.8
1	H	407	GLU	2.8
1	C	430	ARG	2.8
1	I	272	ASP	2.8
1	I	413	ALA	2.8
1	E	42	LEU	2.8
1	F	376	HIS	2.8
1	I	284	LEU	2.8
1	H	39	CYS	2.8
1	I	371	GLU	2.7
1	H	235	LEU	2.7
1	D	228	PRO	2.7
1	H	369	HIS	2.7
1	H	28	VAL	2.7
1	I	309	SER	2.7
1	D	441	LEU	2.7
1	G	182	LEU	2.7
1	H	444	LEU	2.7
1	I	42	LEU	2.7
1	I	218	TRP	2.7
1	H	375	VAL	2.7
1	H	378	ALA	2.7
1	C	368	LEU	2.7
1	H	22	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	369	HIS	2.7
1	C	375	VAL	2.7
1	C	381	LEU	2.7
1	G	59	TRP	2.7
1	D	439	CYS	2.7
1	I	312	SER	2.6
1	F	403	ALA	2.6
1	H	421	VAL	2.6
1	I	437	PHE	2.6
1	H	411	VAL	2.6
1	H	100	LEU	2.6
1	H	320	LEU	2.6
1	I	359	PHE	2.6
1	H	177	ALA	2.6
1	C	330	GLU	2.6
1	E	446	LEU	2.5
1	H	337	LEU	2.5
1	E	406	GLN	2.5
1	H	47	LEU	2.5
1	H	359	PHE	2.5
1	H	377	ALA	2.5
1	I	328	ALA	2.5
1	F	408	VAL	2.5
1	I	258	LYS	2.5
1	I	306	CYS	2.5
1	H	431	SER	2.5
1	E	371	GLU	2.5
1	H	346	THR	2.5
1	G	337	LEU	2.5
1	G	340	ARG	2.5
1	H	106	ALA	2.5
1	A	42	LEU	2.5
1	C	410	SER	2.5
1	I	377	ALA	2.5
1	G	418	HIS	2.5
1	I	251	LYS	2.5
1	G	287	ALA	2.5
1	G	344	PRO	2.5
1	C	251	LYS	2.4
1	F	415	VAL	2.4
1	H	364	VAL	2.4
1	I	383	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	289	SER	2.4
1	I	436	SER	2.4
1	H	392	PHE	2.4
1	G	423	SER	2.4
1	G	167	ILE	2.4
1	C	376	HIS	2.4
1	G	41	ALA	2.4
1	G	421	VAL	2.4
1	C	432	TYR	2.4
1	E	46	GLU	2.4
1	E	419	LEU	2.4
1	G	377	ALA	2.4
1	C	423	SER	2.4
1	G	47	LEU	2.4
1	H	83	VAL	2.4
1	B	2	ASN	2.4
1	C	320	LEU	2.4
1	C	406	GLN	2.4
1	I	275	LEU	2.4
1	I	2	ASN	2.4
1	G	39	CYS	2.4
1	I	314	ASN	2.3
1	H	430	ARG	2.3
1	E	341	ASP	2.3
1	I	344	PRO	2.3
1	H	144	ALA	2.3
1	H	383	LYS	2.3
1	F	423	SER	2.3
1	H	366	ARG	2.3
1	G	417	GLU	2.3
1	H	387	GLY	2.3
1	E	444	LEU	2.3
1	H	435	GLU	2.3
1	D	69	LYS	2.3
1	D	229	GLN	2.3
1	F	380	GLN	2.3
1	I	263	ILE	2.3
1	E	182	LEU	2.3
1	H	265	LEU	2.3
1	I	259	ASN	2.3
1	H	173	SER	2.3
1	H	373	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	394	THR	2.3
1	H	43	LEU	2.3
1	D	406	GLN	2.2
1	G	425	SER	2.2
1	H	38	ARG	2.2
1	G	336	LEU	2.2
1	I	419	LEU	2.2
1	D	423	SER	2.2
1	G	172	ILE	2.2
1	G	413	ALA	2.2
1	I	287	ALA	2.2
1	C	441	LEU	2.2
1	H	46	GLU	2.2
1	E	443	LYS	2.2
1	B	427	VAL	2.2
1	F	440	ARG	2.2
1	H	408	VAL	2.2
1	G	149	ILE	2.2
1	I	382	CYS	2.2
1	H	388	LYS	2.2
1	I	403	ALA	2.2
1	C	322	ASN	2.2
1	F	424	PHE	2.2
1	F	344	PRO	2.2
1	G	325	LEU	2.2
1	G	373	GLY	2.2
1	H	325	LEU	2.2
1	H	418	HIS	2.2
1	G	364	VAL	2.2
1	C	366	ARG	2.1
1	G	374	THR	2.1
1	C	268	LEU	2.1
1	F	389	LEU	2.1
1	G	95	LEU	2.1
1	I	369	HIS	2.1
1	H	192	VAL	2.1
1	H	186	GLU	2.1
1	E	90	GLN	2.1
1	H	40	ARG	2.1
1	G	18	LEU	2.1
1	F	89	GLN	2.1
1	G	154	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	66	TRP	2.1
1	H	348	LYS	2.1
1	E	415	VAL	2.1
1	F	430	ARG	2.1
1	H	224	TYR	2.1
1	A	439	CYS	2.1
1	G	171	LEU	2.1
1	E	83	VAL	2.1
1	I	345	VAL	2.1
1	I	375	VAL	2.1
1	D	442	ASP	2.1
1	C	392	PHE	2.1
1	F	351	LEU	2.1
1	I	385	ALA	2.0
1	I	432	TYR	2.0
1	C	42	LEU	2.0
1	H	134	LEU	2.0
1	I	406	GLN	2.0
1	E	385	ALA	2.0
1	G	333	GLU	2.0
1	I	333	GLU	2.0
1	H	410	SER	2.0
1	I	410	SER	2.0
1	A	368	LEU	2.0
1	E	47	LEU	2.0
1	F	441	LEU	2.0
1	G	323	LEU	2.0
1	G	370	GLY	2.0
1	C	374	THR	2.0
1	D	80	LEU	2.0
1	F	42	LEU	2.0
1	H	284	LEU	2.0
1	I	216	LEU	2.0
1	G	295	PHE	2.0
1	C	333	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

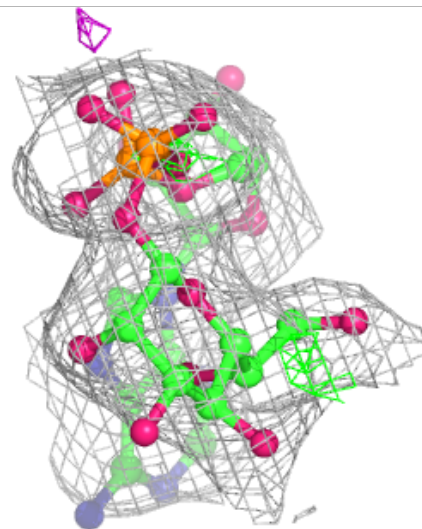
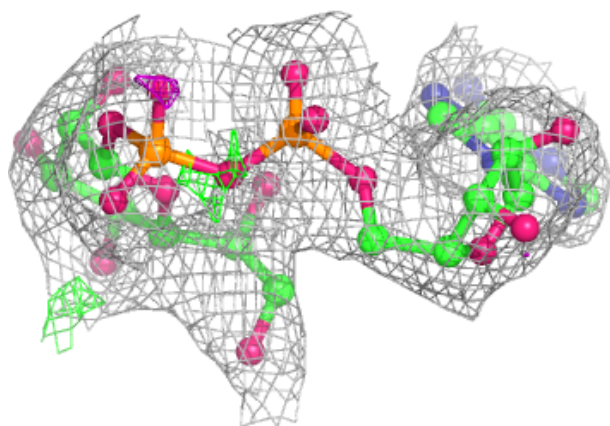
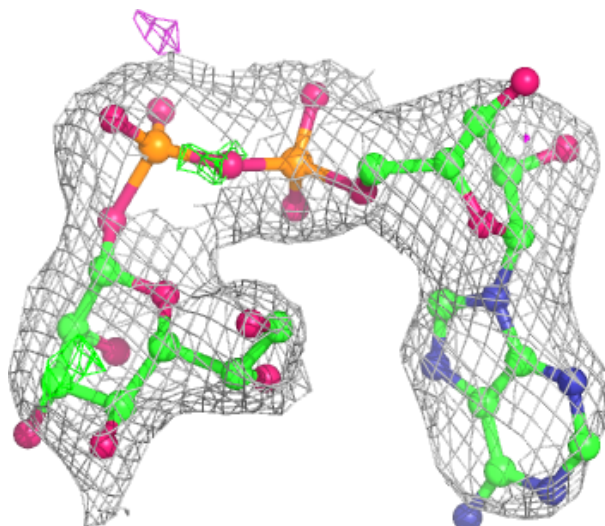
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AYU	H	501	40/40	0.92	0.19	79,86,90,94	0
2	AYU	G	501	40/40	0.94	0.18	52,58,65,71	0
2	AYU	C	501	40/40	0.95	0.19	32,43,57,63	0
2	AYU	I	501	40/40	0.95	0.18	57,70,86,99	0
2	AYU	F	501	40/40	0.96	0.16	34,40,43,50	0
2	AYU	A	501	40/40	0.96	0.20	26,30,37,43	0
2	AYU	D	501	40/40	0.97	0.17	25,31,35,45	0
2	AYU	E	501	40/40	0.97	0.17	30,36,40,53	0
2	AYU	B	501	40/40	0.97	0.17	19,28,33,35	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.

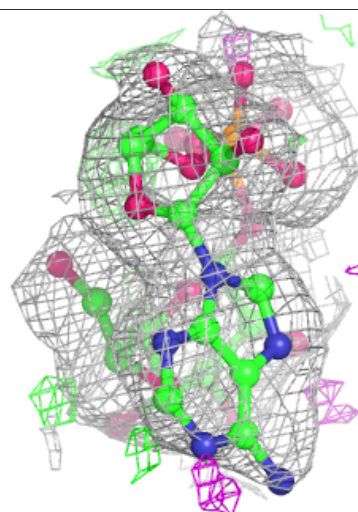
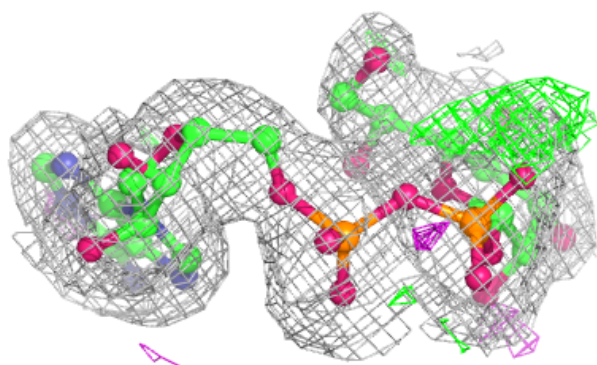
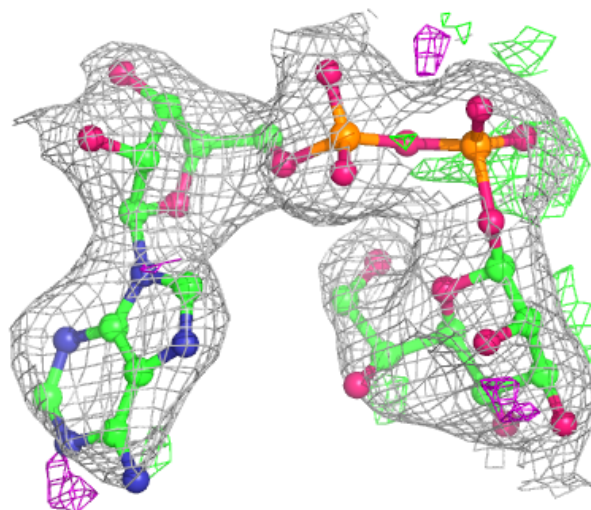
Electron density around AYU H 501:

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



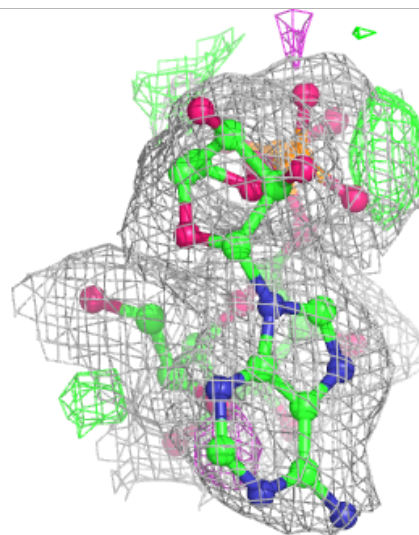
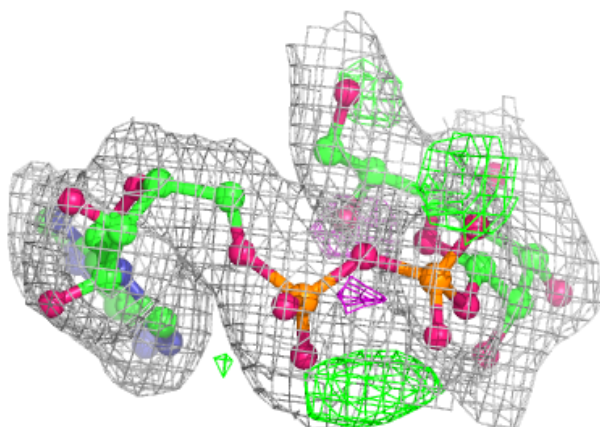
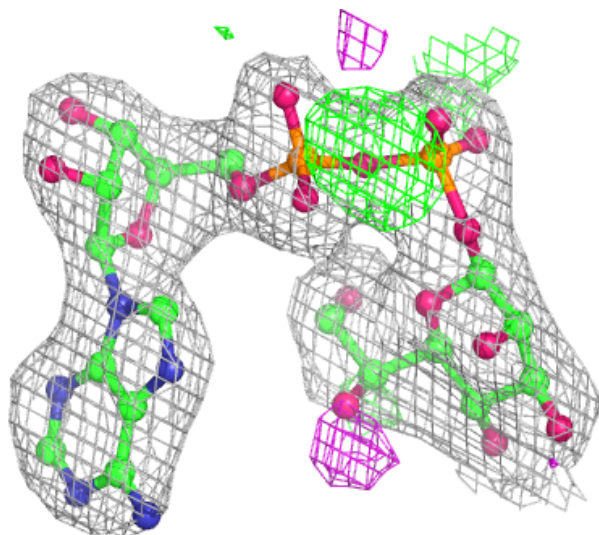
Electron density around AYU G 501:

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



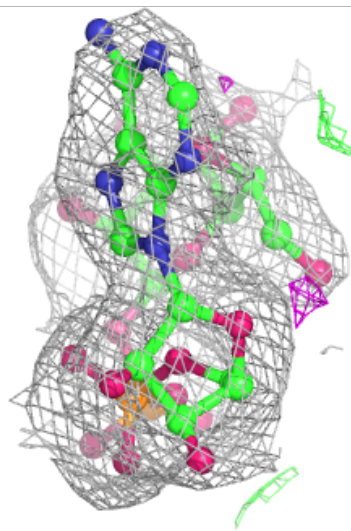
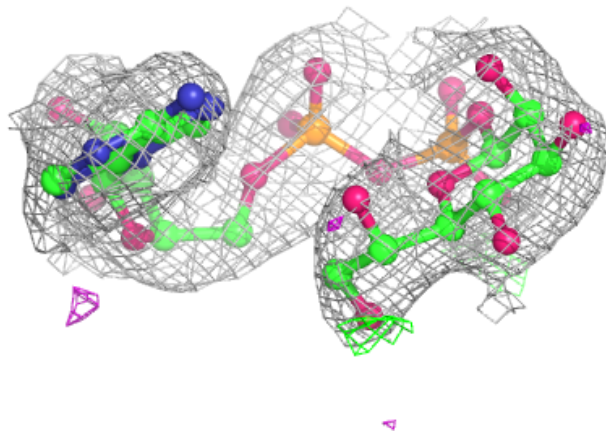
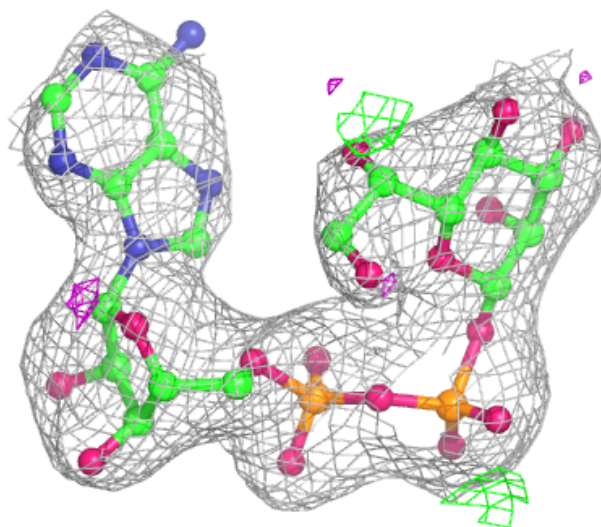
Electron density around AYU C 501:

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



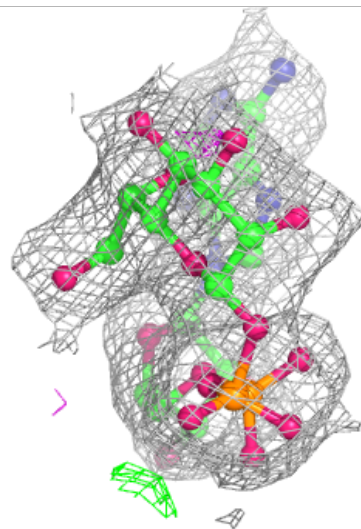
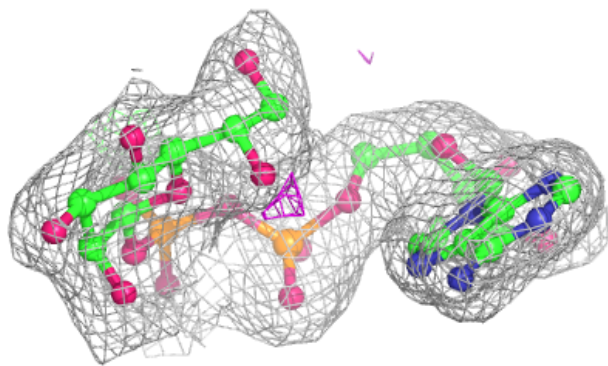
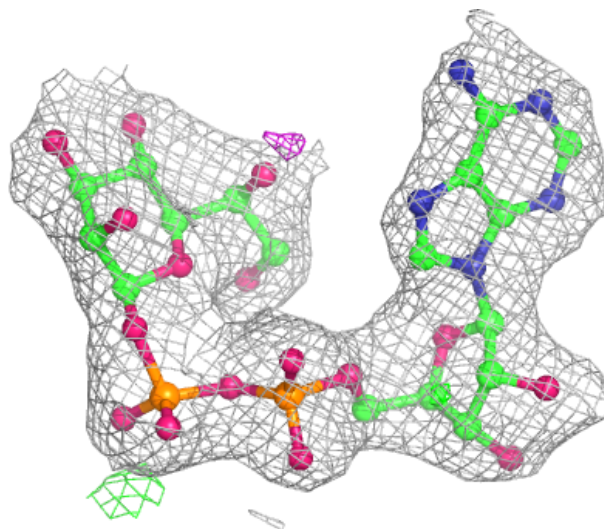
Electron density around AYU I 501:

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



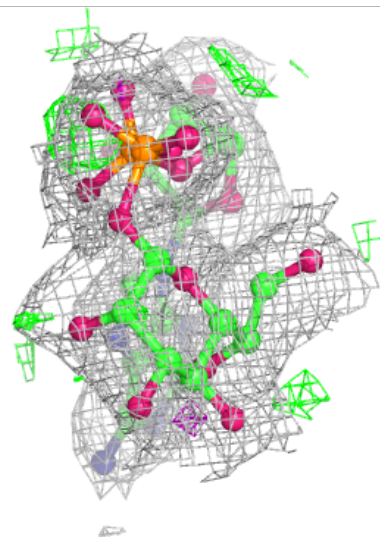
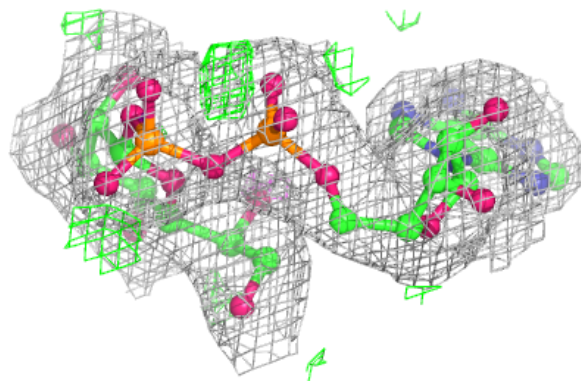
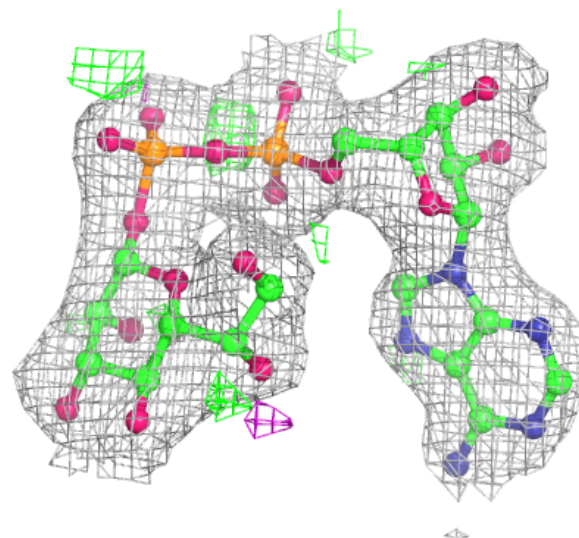
Electron density around AYU F 501:

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



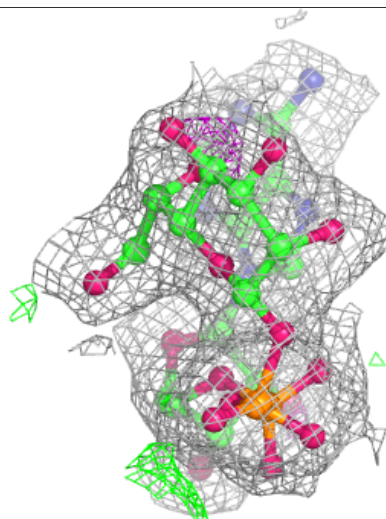
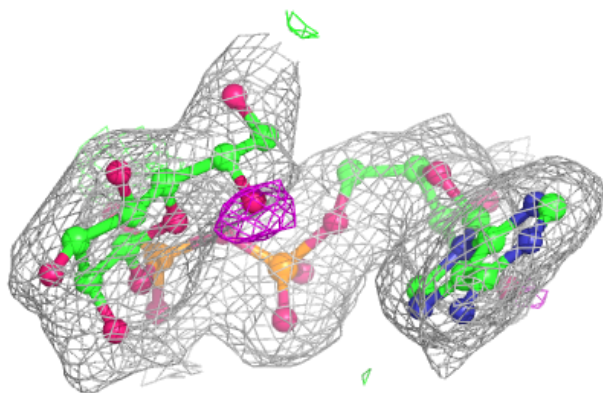
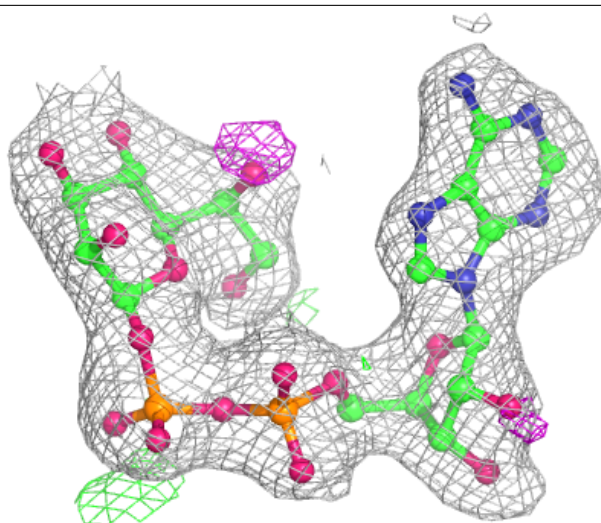
Electron density around AYU A 501:

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



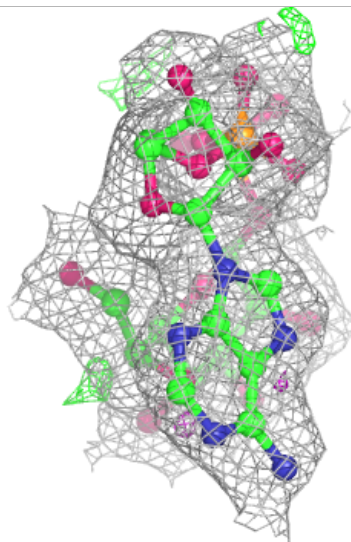
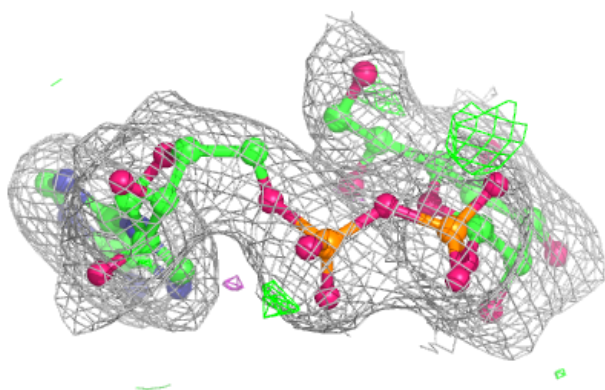
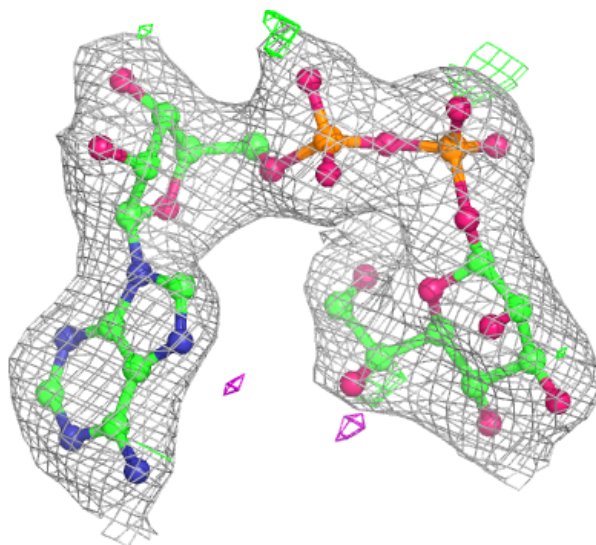
Electron density around AYU D 501:

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



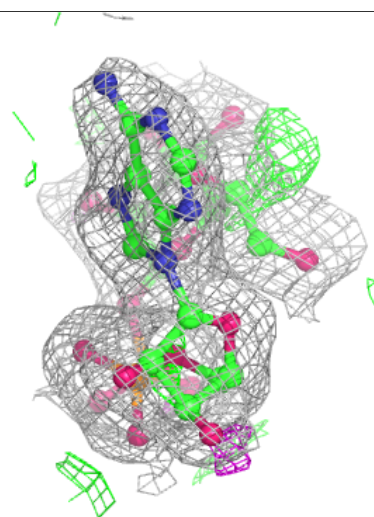
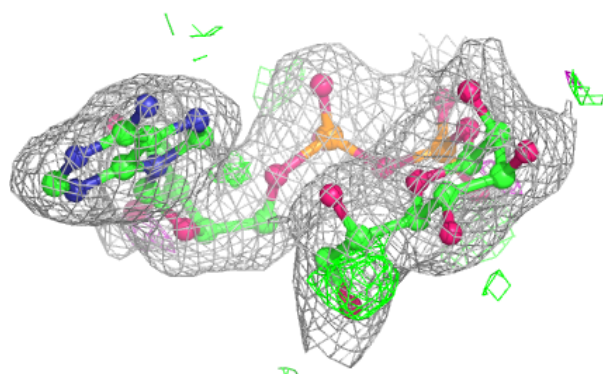
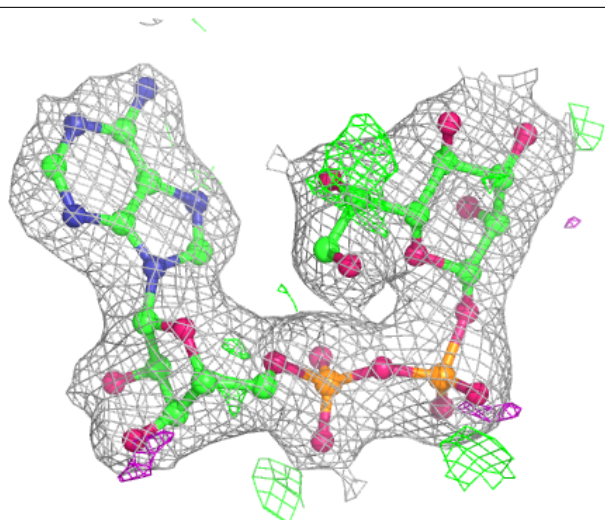
Electron density around AYU E 501:

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



Electron density around AYU B 501:

$2mF_o-DF_c$ (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.