



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:48 PM UTC

PDB ID : 5Z2C / pdb_00005z2c
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

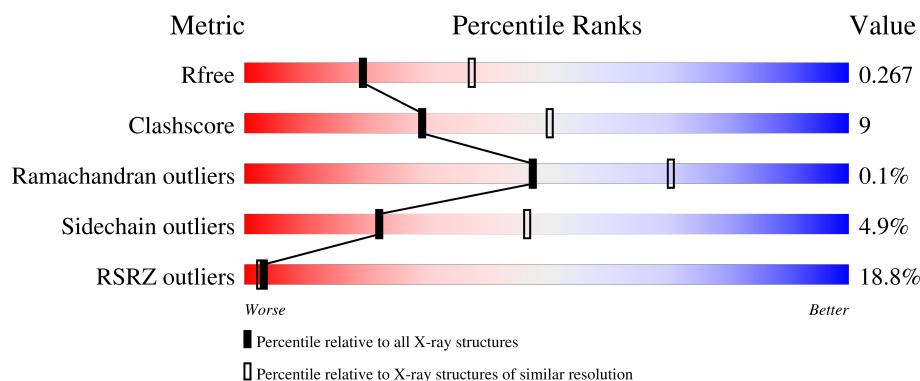
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	

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Mol	Chain	Length	Quality of chain
1	F	446	6% 82% 14%
1	G	446	30% 75% 19%
1	H	446	51% 70% 22% 5%
1	I	446	28% 70% 18% 9%

2 Entry composition

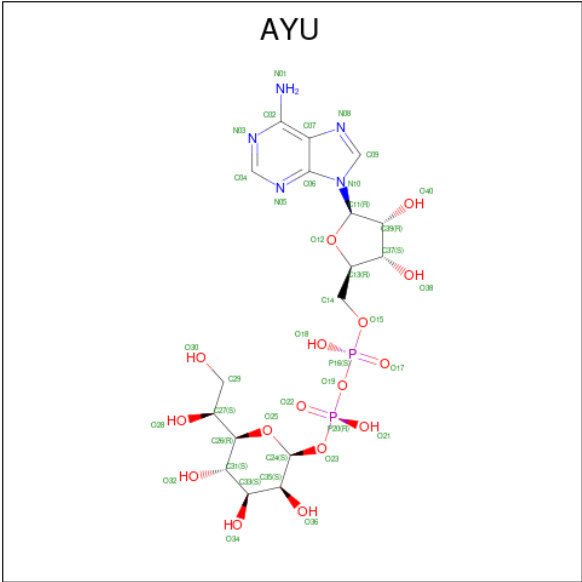
There are 2 unique types of molecules in this entry. The entry contains 30546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

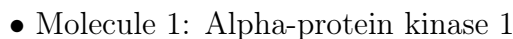
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3469	2203	597	654	15			
1	B	445	Total	C	N	O	S	0	0	0
			3469	2203	597	654	15			
1	C	427	Total	C	N	O	S	0	0	0
			3324	2115	572	622	15			
1	D	434	Total	C	N	O	S	0	0	0
			3388	2156	583	634	15			
1	E	433	Total	C	N	O	S	0	0	0
			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			

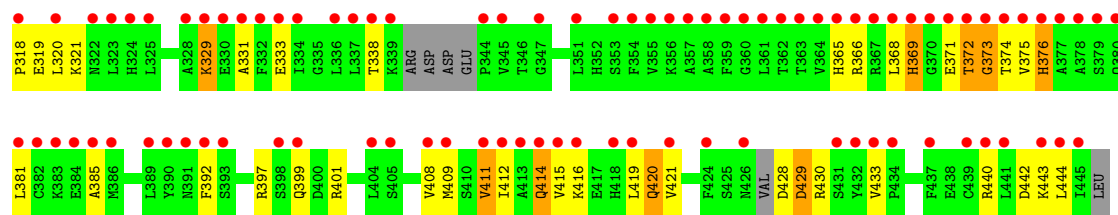
- Molecule 2 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2S,3S,4S,5S,6R)-6-[(1S)-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl] hydrogen phosphate (CCD ID: AYU) (formula: C₁₇H₂₇N₅O₁₆P₂).



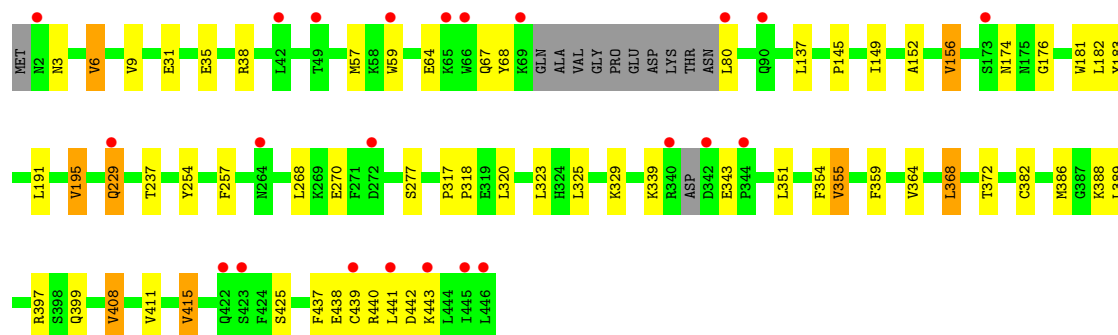
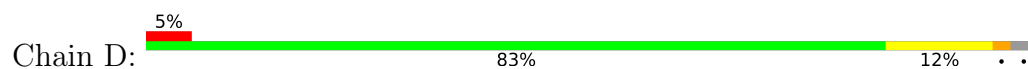
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	B	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	C	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	D	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	E	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	F	1	Total	C	N	O	P	0	0
			40	17	5	16	2		
2	G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

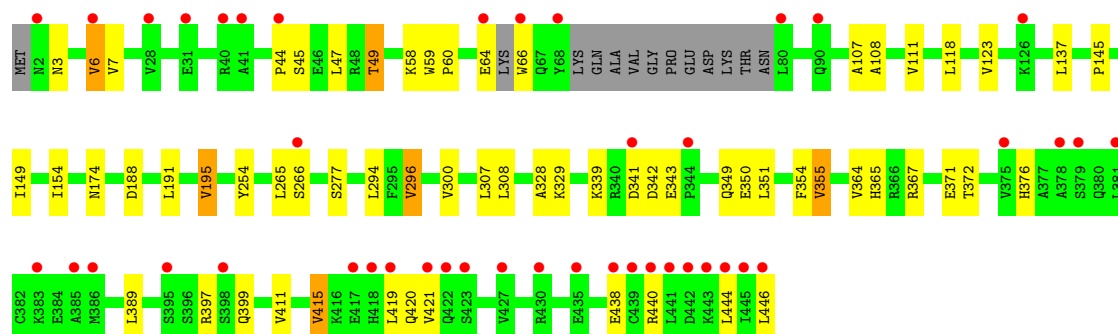
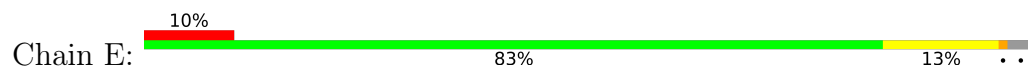




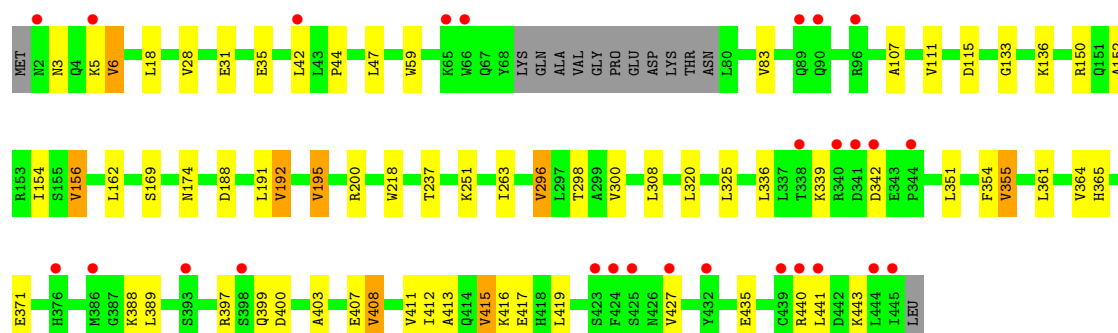
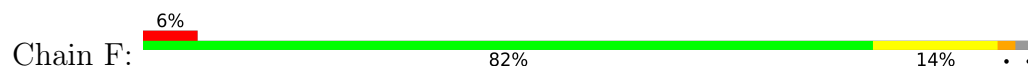
- Molecule 1: Alpha-protein kinase 1



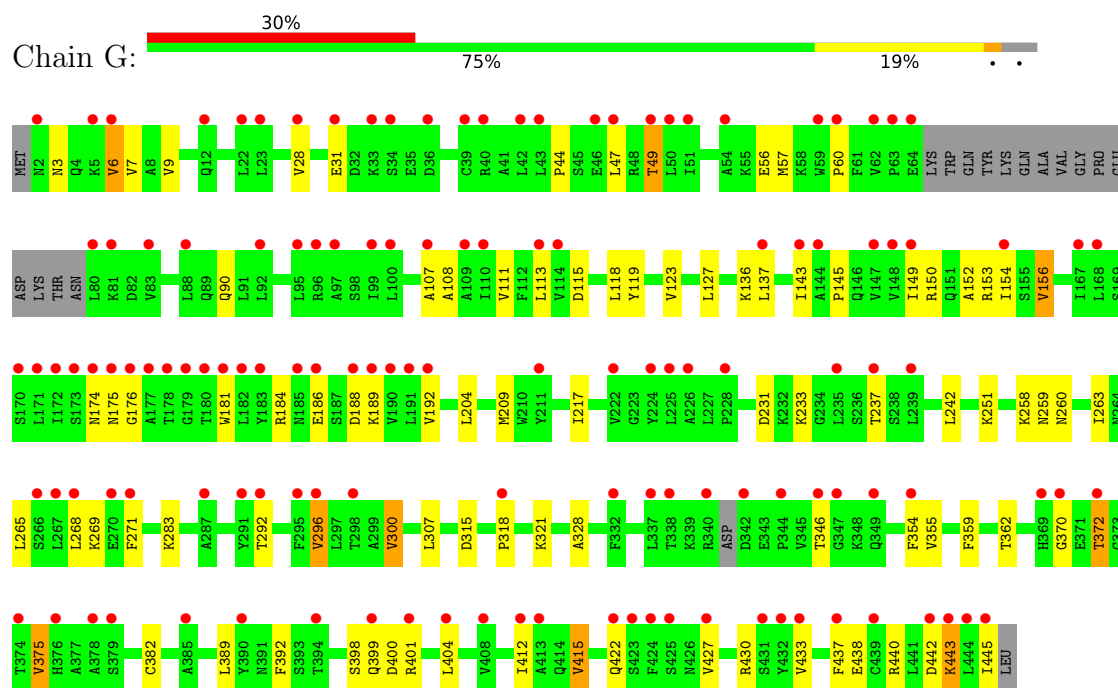
- Molecule 1: Alpha-protein kinase 1



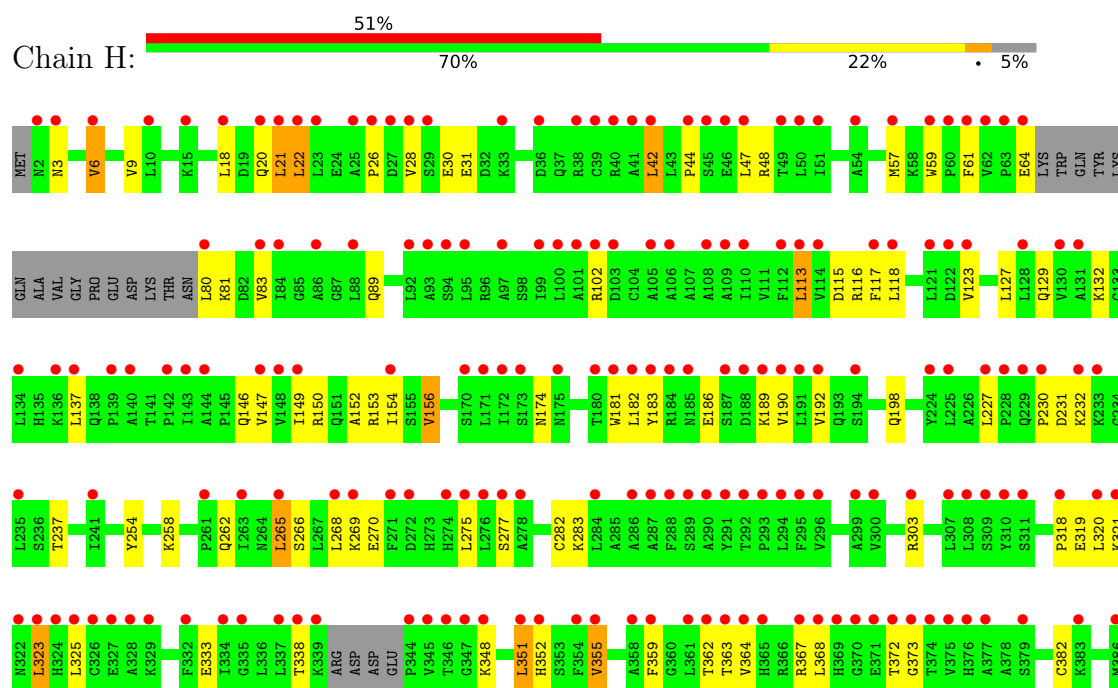
- Molecule 1: Alpha-protein kinase 1



- Molecule 1: Alpha-protein kinase 1

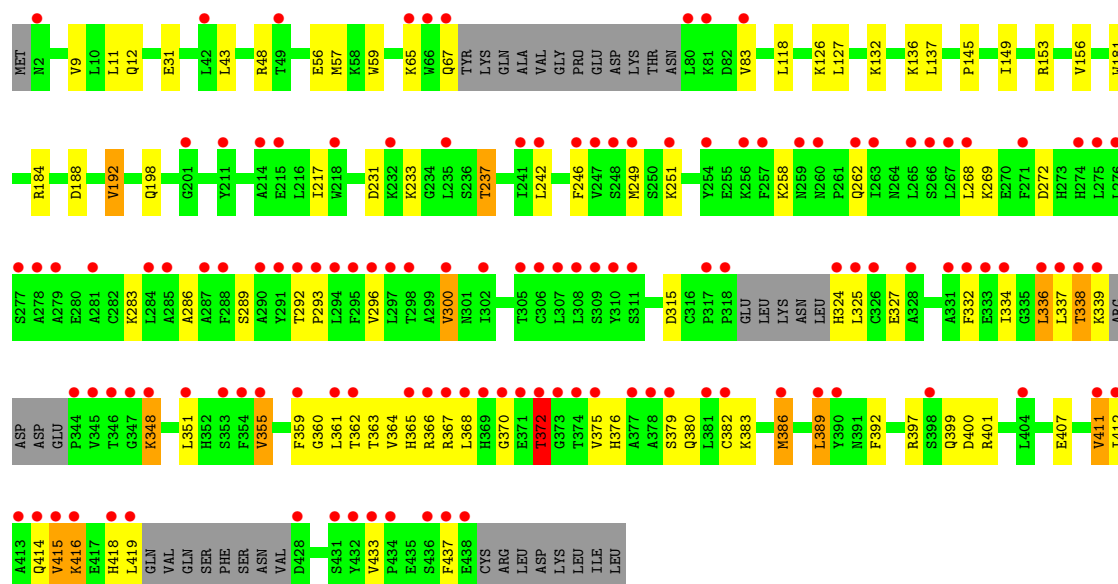


- Molecule 1: Alpha-protein kinase 1



- 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) 93.0 (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 0.246 , 0.267	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 , 41.4	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

5.1 Standard geometry

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	0.21	0/3528	0.36	0/4774
1	B	0.22	0/3528	0.38	0/4774
1	C	0.25	0/3378	0.45	2/4565 (0.0%)
1	D	0.26	0/3444	0.39	0/4656
1	E	0.20	0/3434	0.37	0/4645
1	F	0.18	0/3436	0.34	0/4648
1	G	0.19	0/3380	0.35	0/4570
1	H	0.16	0/3336	0.36	0/4508
1	I	0.28	0/3220	0.42	2/4352 (0.0%)
All	All	0.22	0/30684	0.38	4/41492 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	372	THR	CA-C-N	-5.25	114.12	119.94
1	I	372	THR	C-N-CA	-5.25	114.12	119.94
1	C	420	GLN	N-CA-C	5.01	118.51	111.74
1	C	372	THR	N-CA-C	-5.00	102.45	109.96

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	3469	0	3541	44	0
1	B	3469	0	3541	30	0
1	C	3324	0	3402	82	0
1	D	3388	0	3467	53	0
1	E	3378	0	3445	36	0
1	F	3379	0	3448	40	0
1	G	3327	0	3403	60	1
1	H	3284	0	3366	98	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	3	0
2	H	40	0	0	3	0
2	I	40	0	0	4	0
All	All	30546	0	30849	527	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 9.

All (527) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:433:VAL:C	2.44	0.96
1:H:424:PHE:CZ	1:H:434:PRO:N	2.34	0.95
1:H:424:PHE:HZ	1:H:433:VAL:C	1.74	0.95
1:G:438:GLU:O	1:G:443:LYS:NZ	2.02	0.92
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:I:416:LYS:HZ2	1:I:416:LYS:HA	1.43	0.80
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:C:371:GLU:CD	1:C:376:HIS:CE1	2.61	0.79
1:C:372:THR:O	1:C:373:GLY:C	2.25	0.78
1:I:365:HIS:HE1	1:I:419:LEU:CB	1.94	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:I:416:LYS:NZ	1:I:416:LYS:HA	2.01	0.75
1:C:428:ASP:O	1:C:430:ARG:N	2.19	0.75
1:A:246:PHE:HA	1:A:249:MET:HE2	1.68	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:365:HIS:NE2	1:C:419:LEU:CD2	2.51	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:246:PHE:HA	1:I:249:MET:HE2	1.71	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: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:438:GLU:O	1:H:443:LYS:NZ	2.25	0.65
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:176:GLY:N	1:G:189:LYS:HZ3	1.96	0.63
1:I:366:ARG:O	1:I:370:GLY:N	2.32	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:371:GLU:CD	1:C:376:HIS:NE2	2.60	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:C:372:THR:O	1:C:374:THR:N	2.36	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:I:337:LEU:C	1:I:339:LYS:N	2.63	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:I:289:SER:OG	1:I:292:THR:OG1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:LYS:H	1:F:251:LYS:HD2	1.72	0.55
1:D:57:MET:HE2	1:D:182:LEU:H	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
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: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:I:337:LEU:C	1:I:339:LYS:H	2.14	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:C:176:GLY:O	1:C:183:TYR:OH	2.24	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:C:428:ASP:C	1:C:430:ARG:N	2.66	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:C:428:ASP:O	1:C:429:ASP:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:341:ASP:OD1	1:E:343:GLU:N	2.43	0.52
1:G:175:ASN:C	1:G:189:LYS:HZ3	2.18	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:379:SER:C	1:I:383:LYS:HZ3	2.18	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:I:283:LYS:HG3	1:I:437:PHE:CE1	2.46	0.50
1:C:368:LEU:C	1:C:369:HIS:ND1	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:329:LYS:NZ	1:C:333:GLU:OE1	2.44	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:D:57:MET:HE1	1:D:181:TRP:HA	1.93	0.50
1:B:191:LEU:O	1:B:195:VAL:HG23	2.12	0.49
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:A:388:LYS:HB2	1:A:408:VAL:HG23	1.95	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:C:258:LYS:NZ	1:C:272:ASP:OD1	2.45	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:C:311:SER:O	1:C:321:LYS:HD2	2.13	0.49
1:D:57:MET:CE	1:D:182:LEU:H	2.24	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:D:64:GLU:HB2	1:D:67:GLN:HB2	1.95	0.48
1:G:204:LEU:HD22	1:G:209:MET:HE3	1.95	0.48
1:H:146:GLN:O	1:H:149:ILE:HG13	2.13	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:337:LEU:O	1:I:338:THR:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:416:LYS:NZ	1:I:416:LYS:C	2.72	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
1:D:339:LYS:HD2	1:D:343:GLU:HG3	1.96	0.47
1:D:57:MET:HE3	1:D:181:TRP:CE3	2.49	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:D:437:PHE:O	1:D:438:GLU:C	2.57	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:D:176:GLY:O	1:D:183:TYR:OH	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:428:ASP:C	1:C:430:ARG:H	2.24	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:A:249:MET:HE1	1:A:254:TYR:HD1	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:I:386:MET:HE2	1:I:389:LEU:HD12	1.99	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: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: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:399:GLN:CD	1:F:399:GLN:H	2.26	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:F:115:ASP:CG	1:F:150:ARG:HE	2.26	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:66:TRP:CD1	1:C:66:TRP:H	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:ARG:HE	1:E:440:ARG:HB2	1.58	0.42
1:H:348:LYS:HZ1	1:H:389:LEU:HD11	1.83	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:E:307:LEU:HB2	1:E:328:ALA:HB2	2.01	0.42
1:G:115:ASP:CG	1:G:150:ARG:HE	2.27	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
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:H:57:MET:HE3	1:H:181:TRP:CE3	2.55	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:249:MET:HE3	1:A:254:TYR:HB2	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:B:115:ASP:CG	1:B:150:ARG:HE	2.28	0.42
1:C:118:LEU:HB3	1:C:123:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:422:GLN:CD	1:G:422:GLN:H	2.28	0.41
1:H:115:ASP:CG	1:H:150:ARG:HE	2.27	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:D:440:ARG:O	1:D:441:LEU:C	2.62	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
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:C:368:LEU:HB3	1:C:369:HIS:CE1	2.55	0.41
1:D:359:PHE:CE1	1:D:386:MET:HE2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:G:90:GLN:H	1:G:90:GLN:CD	2.26	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	443/446 (99%)	436 (98%)	7 (2%)	0	100	100
1	C	419/446 (94%)	413 (99%)	4 (1%)	2 (0%)	24	46
1	D	428/446 (96%)	420 (98%)	8 (2%)	0	100	100
1	E	427/446 (96%)	420 (98%)	6 (1%)	1 (0%)	43	66
1	F	429/446 (96%)	422 (98%)	7 (2%)	0	100	100
1	G	422/446 (95%)	413 (98%)	8 (2%)	1 (0%)	43	66
1	H	415/446 (93%)	406 (98%)	9 (2%)	0	100	100
1	I	398/446 (89%)	394 (99%)	3 (1%)	1 (0%)	36	58
All	All	3824/4014 (95%)	3761 (98%)	58 (2%)	5 (0%)	48	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	429	ASP
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%)	369 (97%)	13 (3%)	32	60
1	B	382/383 (100%)	368 (96%)	14 (4%)	30	57
1	C	366/383 (96%)	352 (96%)	14 (4%)	29	56
1	D	373/383 (97%)	358 (96%)	15 (4%)	28	55
1	E	372/383 (97%)	358 (96%)	14 (4%)	29	56
1	F	372/383 (97%)	353 (95%)	19 (5%)	21	45
1	G	367/383 (96%)	347 (95%)	20 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	362/383 (94%)	327 (90%)	35 (10%)	8	17
1	I	347/383 (91%)	329 (95%)	18 (5%)	21	44
All	All	3323/3447 (96%)	3161 (95%)	162 (5%)	22	47

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	42	LEU
1	A	83	VAL
1	A	154	ILE
1	A	195	VAL
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	408	VAL
1	A	415	VAL
1	B	6	VAL
1	B	59	TRP
1	B	69	LYS
1	B	81	LYS
1	B	154	ILE
1	B	156	VAL
1	B	195	VAL
1	B	296	VAL
1	B	323	LEU
1	B	340	ARG
1	B	372	THR
1	B	374	THR
1	B	427	VAL
1	B	442	ASP
1	C	9	VAL
1	C	156	VAL
1	C	195	VAL
1	C	296	VAL
1	C	298	THR
1	C	300	VAL
1	C	329	LYS

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Mol	Chain	Res	Type
1	C	338	THR
1	C	369	HIS
1	C	376	HIS
1	C	411	VAL
1	C	414	GLN
1	C	420	GLN
1	C	433	VAL
1	D	6	VAL
1	D	9	VAL
1	D	59	TRP
1	D	80	LEU
1	D	156	VAL
1	D	174	ASN
1	D	195	VAL
1	D	229	GLN
1	D	237	THR
1	D	355	VAL
1	D	368	LEU
1	D	372	THR
1	D	408	VAL
1	D	415	VAL
1	D	439	CYS
1	E	6	VAL
1	E	49	THR
1	E	154	ILE
1	E	174	ASN
1	E	195	VAL
1	E	296	VAL
1	E	308	LEU
1	E	349	GLN
1	E	355	VAL
1	E	371	GLU
1	E	372	THR
1	E	376	HIS
1	E	415	VAL
1	E	444	LEU
1	F	6	VAL
1	F	28	VAL
1	F	42	LEU
1	F	59	TRP
1	F	83	VAL
1	F	154	ILE

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Mol	Chain	Res	Type
1	F	156	VAL
1	F	162	LEU
1	F	174	ASN
1	F	192	VAL
1	F	195	VAL
1	F	237	THR
1	F	296	VAL
1	F	298	THR
1	F	308	LEU
1	F	355	VAL
1	F	371	GLU
1	F	408	VAL
1	F	415	VAL
1	G	6	VAL
1	G	9	VAL
1	G	28	VAL
1	G	49	THR
1	G	143	ILE
1	G	154	ILE
1	G	156	VAL
1	G	174	ASN
1	G	186	GLU
1	G	292	THR
1	G	296	VAL
1	G	300	VAL
1	G	346	THR
1	G	372	THR
1	G	375	VAL
1	G	415	VAL
1	G	427	VAL
1	G	433	VAL
1	G	442	ASP
1	G	443	LYS
1	H	6	VAL
1	H	9	VAL
1	H	18	LEU
1	H	20	GLN
1	H	21	LEU
1	H	22	LEU
1	H	28	VAL
1	H	30	GLU
1	H	42	LEU

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Mol	Chain	Res	Type
1	H	59	TRP
1	H	83	VAL
1	H	89	GLN
1	H	113	LEU
1	H	123	VAL
1	H	147	VAL
1	H	154	ILE
1	H	156	VAL
1	H	174	ASN
1	H	186	GLU
1	H	190	VAL
1	H	227	LEU
1	H	262	GLN
1	H	265	LEU
1	H	275	LEU
1	H	320	LEU
1	H	323	LEU
1	H	338	THR
1	H	351	LEU
1	H	355	VAL
1	H	362	THR
1	H	368	LEU
1	H	408	VAL
1	H	424	PHE
1	H	426	ASN
1	H	433	VAL
1	I	9	VAL
1	I	59	TRP
1	I	83	VAL
1	I	192	VAL
1	I	237	THR
1	I	300	VAL
1	I	325	LEU
1	I	336	LEU
1	I	348	LYS
1	I	355	VAL
1	I	363	THR
1	I	372	THR
1	I	386	MET
1	I	389	LEU
1	I	411	VAL
1	I	415	VAL

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Mol	Chain	Res	Type
1	I	416	LYS
1	I	433	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	322	ASN
1	B	129	GLN
1	B	151	GLN
1	B	365	HIS
1	C	2	ASN
1	C	3	ASN
1	C	264	ASN
1	C	376	HIS
1	C	414	GLN
1	D	90	GLN
1	D	174	ASN
1	D	264	ASN
1	D	365	HIS
1	D	376	HIS
1	D	420	GLN
1	E	3	ASN
1	E	264	ASN
1	E	426	ASN
1	F	129	GLN
1	F	135	HIS
1	F	391	ASN
1	G	3	ASN
1	G	202	GLN
1	G	264	ASN
1	H	146	GLN
1	H	426	ASN
1	I	202	GLN
1	I	352	HIS
1	I	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	I	501	-	42,43,43	3.00	22 (52%)	62,66,66	1.42	13 (20%)
2	AYU	B	501	-	42,43,43	2.52	17 (40%)	62,66,66	1.31	9 (14%)
2	AYU	G	501	-	42,43,43	2.88	19 (45%)	62,66,66	1.37	9 (14%)
2	AYU	D	501	-	42,43,43	2.51	19 (45%)	62,66,66	1.27	9 (14%)
2	AYU	E	501	-	42,43,43	2.84	19 (45%)	62,66,66	1.32	10 (16%)
2	AYU	F	501	-	42,43,43	2.59	19 (45%)	62,66,66	1.32	9 (14%)
2	AYU	H	501	-	42,43,43	3.06	22 (52%)	62,66,66	1.45	11 (17%)
2	AYU	A	501	-	42,43,43	2.72	18 (42%)	62,66,66	1.36	9 (14%)
2	AYU	C	501	-	42,43,43	2.80	21 (50%)	62,66,66	1.33	7 (11%)

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	I	501	-	-	2/27/63/63	0/4/4/4
2	AYU	B	501	-	-	2/27/63/63	0/4/4/4
2	AYU	G	501	-	-	2/27/63/63	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AYU	D	501	-	-	1/27/63/63	0/4/4/4
2	AYU	E	501	-	-	1/27/63/63	0/4/4/4
2	AYU	F	501	-	-	1/27/63/63	0/4/4/4
2	AYU	H	501	-	-	4/27/63/63	0/4/4/4
2	AYU	A	501	-	-	1/27/63/63	0/4/4/4
2	AYU	C	501	-	-	3/27/63/63	0/4/4/4

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	AYU	P20-O23	8.94	1.86	1.59
2	E	501	AYU	P20-O23	8.89	1.86	1.59
2	G	501	AYU	P20-O23	8.70	1.85	1.59
2	C	501	AYU	P20-O23	8.24	1.84	1.59
2	A	501	AYU	P20-O23	8.16	1.84	1.59
2	I	501	AYU	P20-O23	8.09	1.83	1.59
2	B	501	AYU	P20-O23	8.01	1.83	1.59
2	F	501	AYU	P20-O23	7.62	1.82	1.59
2	D	501	AYU	P20-O23	7.30	1.81	1.59
2	H	501	AYU	P16-O19	6.99	1.67	1.59
2	I	501	AYU	P16-O19	6.85	1.66	1.59
2	H	501	AYU	P20-O19	6.20	1.66	1.59
2	G	501	AYU	P16-O19	5.93	1.65	1.59
2	I	501	AYU	P20-O19	5.74	1.65	1.59
2	I	501	AYU	P16-O15	5.62	1.81	1.59
2	H	501	AYU	P16-O15	5.61	1.81	1.59
2	E	501	AYU	P16-O19	5.60	1.65	1.59
2	G	501	AYU	C27-C26	5.48	1.64	1.52
2	A	501	AYU	C27-C26	5.48	1.64	1.52
2	H	501	AYU	C27-C26	5.46	1.64	1.52
2	G	501	AYU	P16-O15	5.40	1.80	1.59
2	I	501	AYU	C27-C26	5.38	1.64	1.52
2	E	501	AYU	C27-C26	5.34	1.63	1.52
2	C	501	AYU	P16-O19	5.25	1.65	1.59
2	F	501	AYU	P16-O15	5.25	1.80	1.59
2	B	501	AYU	C27-C26	5.12	1.63	1.52
2	E	501	AYU	P16-O15	5.11	1.79	1.59
2	G	501	AYU	P20-O19	5.03	1.64	1.59
2	A	501	AYU	P16-O15	4.98	1.78	1.59
2	D	501	AYU	C27-C26	4.90	1.63	1.52
2	A	501	AYU	P16-O19	4.77	1.64	1.59
2	C	501	AYU	P16-O15	4.77	1.78	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AYU	P20-O19	4.75	1.64	1.59
2	C	501	AYU	C27-C26	4.74	1.62	1.52
2	F	501	AYU	P16-O19	4.59	1.64	1.59
2	C	501	AYU	P20-O19	4.59	1.64	1.59
2	D	501	AYU	P16-O15	4.54	1.77	1.59
2	F	501	AYU	C27-C26	4.54	1.62	1.52
2	E	501	AYU	P20-O19	4.49	1.64	1.59
2	G	501	AYU	C29-C27	4.34	1.62	1.52
2	B	501	AYU	C31-C26	4.32	1.64	1.52
2	B	501	AYU	P16-O15	4.27	1.76	1.59
2	E	501	AYU	C29-C27	4.25	1.62	1.52
2	B	501	AYU	C29-C27	4.18	1.62	1.52
2	H	501	AYU	C31-C26	4.16	1.63	1.52
2	I	501	AYU	C29-C27	4.11	1.62	1.52
2	H	501	AYU	C29-C27	4.09	1.62	1.52
2	I	501	AYU	C09-N10	3.98	1.44	1.37
2	I	501	AYU	C11-N10	3.97	1.57	1.46
2	H	501	AYU	C09-N10	3.95	1.44	1.37
2	C	501	AYU	C09-N10	3.94	1.44	1.37
2	C	501	AYU	C11-N10	3.90	1.57	1.46
2	F	501	AYU	C29-C27	3.86	1.61	1.52
2	A	501	AYU	C29-C27	3.84	1.61	1.52
2	D	501	AYU	P16-O19	3.78	1.63	1.59
2	C	501	AYU	C29-C27	3.77	1.61	1.52
2	G	501	AYU	C09-N10	3.76	1.43	1.37
2	D	501	AYU	O25-C26	-3.69	1.38	1.44
2	F	501	AYU	C09-N10	3.68	1.43	1.37
2	G	501	AYU	C31-C26	3.63	1.62	1.52
2	D	501	AYU	C29-C27	3.61	1.61	1.52
2	D	501	AYU	C09-N10	3.60	1.43	1.37
2	E	501	AYU	C09-N10	3.59	1.43	1.37
2	E	501	AYU	O25-C26	-3.59	1.38	1.44
2	F	501	AYU	P20-O19	3.56	1.63	1.59
2	H	501	AYU	C11-N10	3.56	1.56	1.46
2	I	501	AYU	C31-C26	3.54	1.61	1.52
2	E	501	AYU	C31-C26	3.40	1.61	1.52
2	A	501	AYU	C09-N10	3.40	1.43	1.37
2	I	501	AYU	C04-N03	3.38	1.39	1.33
2	F	501	AYU	C31-C26	3.29	1.61	1.52
2	C	501	AYU	C31-C26	3.26	1.61	1.52
2	G	501	AYU	C04-N03	3.26	1.39	1.33
2	G	501	AYU	C11-N10	3.25	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AYU	C31-C26	3.24	1.61	1.52
2	H	501	AYU	C04-N03	3.22	1.39	1.33
2	C	501	AYU	O25-C26	-3.21	1.39	1.44
2	B	501	AYU	C04-N03	3.20	1.39	1.33
2	C	501	AYU	C04-N03	3.20	1.39	1.33
2	D	501	AYU	C31-C26	3.15	1.60	1.52
2	D	501	AYU	C04-N03	3.12	1.39	1.33
2	B	501	AYU	C09-N10	3.06	1.42	1.37
2	B	501	AYU	O28-C27	-3.02	1.37	1.43
2	I	501	AYU	C07-C06	3.02	1.44	1.39
2	D	501	AYU	C35-C33	2.99	1.60	1.52
2	E	501	AYU	C04-N03	2.98	1.39	1.33
2	A	501	AYU	C04-N03	2.96	1.39	1.33
2	F	501	AYU	C04-N03	2.96	1.39	1.33
2	F	501	AYU	O28-C27	-2.93	1.37	1.43
2	A	501	AYU	O28-C27	-2.90	1.37	1.43
2	H	501	AYU	C07-C06	2.90	1.44	1.39
2	E	501	AYU	C11-N10	2.87	1.54	1.46
2	C	501	AYU	C07-C06	2.86	1.44	1.39
2	C	501	AYU	C35-C33	2.86	1.59	1.52
2	D	501	AYU	C24-C35	2.83	1.60	1.52
2	D	501	AYU	C07-C06	2.81	1.44	1.39
2	B	501	AYU	O15-C14	-2.75	1.34	1.44
2	B	501	AYU	C11-N10	2.75	1.53	1.46
2	G	501	AYU	C07-C06	2.74	1.44	1.39
2	E	501	AYU	O15-C14	-2.71	1.34	1.44
2	I	501	AYU	O25-C26	-2.70	1.39	1.44
2	E	501	AYU	O28-C27	-2.68	1.37	1.43
2	C	501	AYU	C02-N01	2.66	1.41	1.34
2	B	501	AYU	O25-C26	-2.65	1.39	1.44
2	E	501	AYU	C24-C35	2.65	1.60	1.52
2	F	501	AYU	O15-C14	-2.62	1.34	1.44
2	A	501	AYU	C11-N10	2.61	1.53	1.46
2	F	501	AYU	C07-C06	2.61	1.43	1.39
2	A	501	AYU	C07-C06	2.61	1.43	1.39
2	A	501	AYU	C24-C35	2.60	1.60	1.52
2	D	501	AYU	O15-C14	-2.60	1.34	1.44
2	H	501	AYU	C02-N01	2.59	1.40	1.34
2	I	501	AYU	C02-N01	2.59	1.40	1.34
2	F	501	AYU	C11-N10	2.58	1.53	1.46
2	B	501	AYU	C24-C35	2.58	1.60	1.52
2	G	501	AYU	C02-N01	2.57	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	AYU	O25-C26	-2.56	1.40	1.44
2	H	501	AYU	C14-C13	2.56	1.59	1.51
2	C	501	AYU	C14-C13	2.56	1.59	1.51
2	I	501	AYU	C06-N10	2.55	1.43	1.37
2	A	501	AYU	O25-C26	-2.52	1.40	1.44
2	C	501	AYU	C06-N05	2.51	1.39	1.34
2	I	501	AYU	O15-C14	-2.50	1.35	1.44
2	I	501	AYU	C06-N05	2.49	1.39	1.34
2	H	501	AYU	O15-C14	-2.49	1.35	1.44
2	H	501	AYU	C06-N05	2.47	1.39	1.34
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	B	501	AYU	P16-O19	2.46	1.62	1.59
2	A	501	AYU	O15-C14	-2.46	1.35	1.44
2	A	501	AYU	C35-C33	2.44	1.58	1.52
2	A	501	AYU	C02-N01	2.41	1.40	1.34
2	D	501	AYU	C11-N10	2.41	1.53	1.46
2	E	501	AYU	C07-C06	2.41	1.43	1.39
2	E	501	AYU	C33-C31	2.40	1.58	1.52
2	G	501	AYU	C35-C33	2.38	1.58	1.52
2	I	501	AYU	C14-C13	2.38	1.58	1.51
2	D	501	AYU	O28-C27	-2.37	1.38	1.43
2	E	501	AYU	C06-N05	2.36	1.38	1.34
2	C	501	AYU	C24-C35	2.35	1.59	1.52
2	G	501	AYU	O25-C26	-2.34	1.40	1.44
2	G	501	AYU	C06-N05	2.33	1.38	1.34
2	C	501	AYU	O28-C27	-2.33	1.38	1.43
2	G	501	AYU	C33-C31	2.30	1.58	1.52
2	D	501	AYU	C02-N01	2.30	1.40	1.34
2	A	501	AYU	C14-C13	2.29	1.58	1.51
2	D	501	AYU	P20-O19	2.28	1.62	1.59
2	I	501	AYU	C24-C35	2.27	1.59	1.52
2	I	501	AYU	O28-C27	-2.25	1.38	1.43
2	G	501	AYU	O28-C27	-2.25	1.38	1.43
2	F	501	AYU	C02-N01	2.23	1.39	1.34
2	F	501	AYU	C24-C35	2.21	1.59	1.52
2	B	501	AYU	C35-C33	2.17	1.58	1.52
2	D	501	AYU	C06-N05	2.16	1.38	1.34
2	E	501	AYU	C35-C33	2.16	1.58	1.52
2	F	501	AYU	C35-C33	2.16	1.58	1.52
2	H	501	AYU	C06-N10	2.16	1.42	1.37
2	C	501	AYU	C06-N10	2.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	AYU	O25-C24	2.14	1.47	1.41
2	H	501	AYU	C24-C35	2.14	1.58	1.52
2	B	501	AYU	O25-C24	2.12	1.47	1.41
2	E	501	AYU	C02-N01	2.11	1.39	1.34
2	F	501	AYU	C06-N05	2.10	1.38	1.34
2	I	501	AYU	O25-C24	2.10	1.47	1.41
2	H	501	AYU	O25-C26	-2.09	1.40	1.44
2	D	501	AYU	O40-C39	-2.08	1.37	1.43
2	G	501	AYU	C24-C35	2.07	1.58	1.52
2	I	501	AYU	C35-C33	2.05	1.57	1.52
2	H	501	AYU	C35-C33	2.05	1.57	1.52
2	H	501	AYU	O28-C27	-2.05	1.39	1.43
2	B	501	AYU	O40-C39	-2.04	1.37	1.43
2	I	501	AYU	C07-C02	2.04	1.46	1.41
2	H	501	AYU	C07-C02	2.03	1.46	1.41
2	H	501	AYU	C09-N08	2.03	1.35	1.31
2	C	501	AYU	C07-C02	2.01	1.46	1.41
2	B	501	AYU	C07-C06	2.01	1.42	1.39

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AYU	C24-O25-C26	3.80	119.16	113.07
2	H	501	AYU	O25-C26-C31	3.64	113.08	107.94
2	H	501	AYU	C24-O25-C26	3.60	118.84	113.07
2	I	501	AYU	C24-O25-C26	3.41	118.53	113.07
2	I	501	AYU	C07-C06-N05	-3.30	122.18	126.72
2	A	501	AYU	C07-C06-N05	-3.23	122.27	126.72
2	B	501	AYU	O25-C26-C27	3.17	112.76	106.60
2	C	501	AYU	O23-P20-O22	-3.12	99.84	109.81
2	H	501	AYU	C07-C06-N05	-3.09	122.46	126.72
2	E	501	AYU	C07-C06-N05	-3.09	122.47	126.72
2	C	501	AYU	C07-C06-N05	-3.07	122.49	126.72
2	B	501	AYU	C07-C06-N05	-3.05	122.52	126.72
2	A	501	AYU	C06-C07-N08	-3.01	107.14	110.58
2	A	501	AYU	C07-C06-N10	2.97	109.05	105.81
2	I	501	AYU	C06-C07-N08	-2.96	107.20	110.58
2	H	501	AYU	C07-C06-N10	2.93	109.01	105.81
2	H	501	AYU	C06-C07-N08	-2.93	107.23	110.58
2	D	501	AYU	O23-P20-O22	-2.93	100.45	109.81
2	G	501	AYU	C07-C06-N05	-2.93	122.69	126.72
2	D	501	AYU	C07-C06-N05	-2.92	122.69	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	AYU	C07-C06-N10	2.92	108.99	105.81
2	F	501	AYU	C07-C06-N05	-2.91	122.71	126.72
2	C	501	AYU	C07-C06-N10	2.88	108.95	105.81
2	G	501	AYU	C07-C06-N10	2.85	108.92	105.81
2	G	501	AYU	C06-C07-N08	-2.83	107.34	110.58
2	I	501	AYU	C37-C39-C11	2.83	106.82	101.46
2	F	501	AYU	O21-P20-O19	2.81	114.87	107.27
2	C	501	AYU	C06-C07-N08	-2.80	107.39	110.58
2	G	501	AYU	O25-C26-C31	2.77	111.85	107.94
2	F	501	AYU	C06-C07-N08	-2.74	107.45	110.58
2	D	501	AYU	C06-C07-N08	-2.73	107.47	110.58
2	F	501	AYU	C07-C06-N10	2.70	108.76	105.81
2	E	501	AYU	C06-C07-N08	-2.69	107.50	110.58
2	B	501	AYU	C06-C07-N08	-2.69	107.50	110.58
2	D	501	AYU	C24-O25-C26	2.68	117.36	113.07
2	G	501	AYU	O25-C26-C27	2.67	111.80	106.60
2	F	501	AYU	O25-C26-C27	2.67	111.78	106.60
2	I	501	AYU	C07-N08-C09	2.64	107.60	103.45
2	H	501	AYU	O21-P20-O19	2.64	114.40	107.27
2	I	501	AYU	O21-P20-O19	2.61	114.34	107.27
2	G	501	AYU	O21-P20-O19	2.61	114.32	107.27
2	D	501	AYU	C07-C06-N10	2.59	108.64	105.81
2	F	501	AYU	O23-P20-O22	-2.55	101.65	109.81
2	A	501	AYU	C07-N08-C09	2.53	107.42	103.45
2	H	501	AYU	C07-N08-C09	2.52	107.41	103.45
2	H	501	AYU	C37-C39-C11	2.51	106.22	101.46
2	E	501	AYU	C07-N08-C09	2.51	107.40	103.45
2	G	501	AYU	O23-P20-O22	-2.50	101.80	109.81
2	B	501	AYU	C07-C06-N10	2.50	108.53	105.81
2	H	501	AYU	O23-P20-O22	-2.49	101.86	109.81
2	E	501	AYU	C07-C06-N10	2.48	108.51	105.81
2	C	501	AYU	C07-N08-C09	2.47	107.33	103.45
2	E	501	AYU	C24-O25-C26	2.47	117.03	113.07
2	C	501	AYU	C24-O25-C26	2.46	117.02	113.07
2	I	501	AYU	O23-P20-O22	-2.44	102.00	109.81
2	B	501	AYU	C07-N08-C09	2.42	107.25	103.45
2	A	501	AYU	O25-C26-C27	2.40	111.26	106.60
2	G	501	AYU	C07-N08-C09	2.40	107.22	103.45
2	G	501	AYU	C24-O25-C26	2.39	116.91	113.07
2	E	501	AYU	O21-P20-O19	2.39	113.74	107.27
2	F	501	AYU	C07-N08-C09	2.39	107.20	103.45
2	F	501	AYU	C24-O25-C26	2.38	116.89	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	AYU	O25-C26-C31	2.38	111.30	107.94
2	D	501	AYU	C07-N08-C09	2.30	107.06	103.45
2	E	501	AYU	O25-C26-C27	2.29	111.04	106.60
2	C	501	AYU	O25-C26-C31	2.28	111.17	107.94
2	I	501	AYU	C13-O12-C11	2.26	114.46	109.47
2	B	501	AYU	O21-P20-O19	2.26	113.37	107.27
2	B	501	AYU	O12-C11-C39	-2.24	101.82	106.62
2	A	501	AYU	O21-P20-O19	2.21	113.25	107.27
2	A	501	AYU	O12-C11-C39	-2.18	101.94	106.62
2	E	501	AYU	O23-P20-O22	-2.18	102.85	109.81
2	F	501	AYU	C37-C39-C11	2.17	105.56	101.46
2	I	501	AYU	O25-C26-C27	2.16	110.79	106.60
2	B	501	AYU	O25-C24-O23	2.12	114.14	111.36
2	I	501	AYU	C06-N10-C09	-2.11	103.52	105.74
2	B	501	AYU	C02-C07-C06	2.11	120.06	117.18
2	A	501	AYU	C02-C07-C06	2.11	120.05	117.18
2	E	501	AYU	C14-C13-C37	-2.11	107.63	115.21
2	D	501	AYU	C14-C13-C37	-2.09	107.70	115.21
2	H	501	AYU	O25-C24-C35	-2.05	106.15	110.37
2	I	501	AYU	C02-C07-C06	2.05	119.97	117.18
2	H	501	AYU	C13-O12-C11	2.04	113.98	109.47
2	D	501	AYU	C37-C39-C11	2.02	105.28	101.46
2	E	501	AYU	O12-C11-C39	-2.01	102.31	106.62
2	D	501	AYU	C02-C07-C06	2.00	119.91	117.18

There are no chirality outliers.

All (17) 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	C	501	AYU	C39-C11-N10-C09
2	D	501	AYU	C39-C11-N10-C09
2	E	501	AYU	C39-C11-N10-C09
2	H	501	AYU	C39-C11-N10-C09
2	A	501	AYU	C35-C24-O23-P20
2	G	501	AYU	C35-C24-O23-P20
2	H	501	AYU	O25-C26-C27-O28
2	H	501	AYU	C31-C26-C27-O28

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Mol	Chain	Res	Type	Atoms
2	C	501	AYU	O12-C11-N10-C09
2	G	501	AYU	C39-C11-N10-C09
2	I	501	AYU	C39-C11-N10-C09
2	B	501	AYU	P16-O19-P20-O21

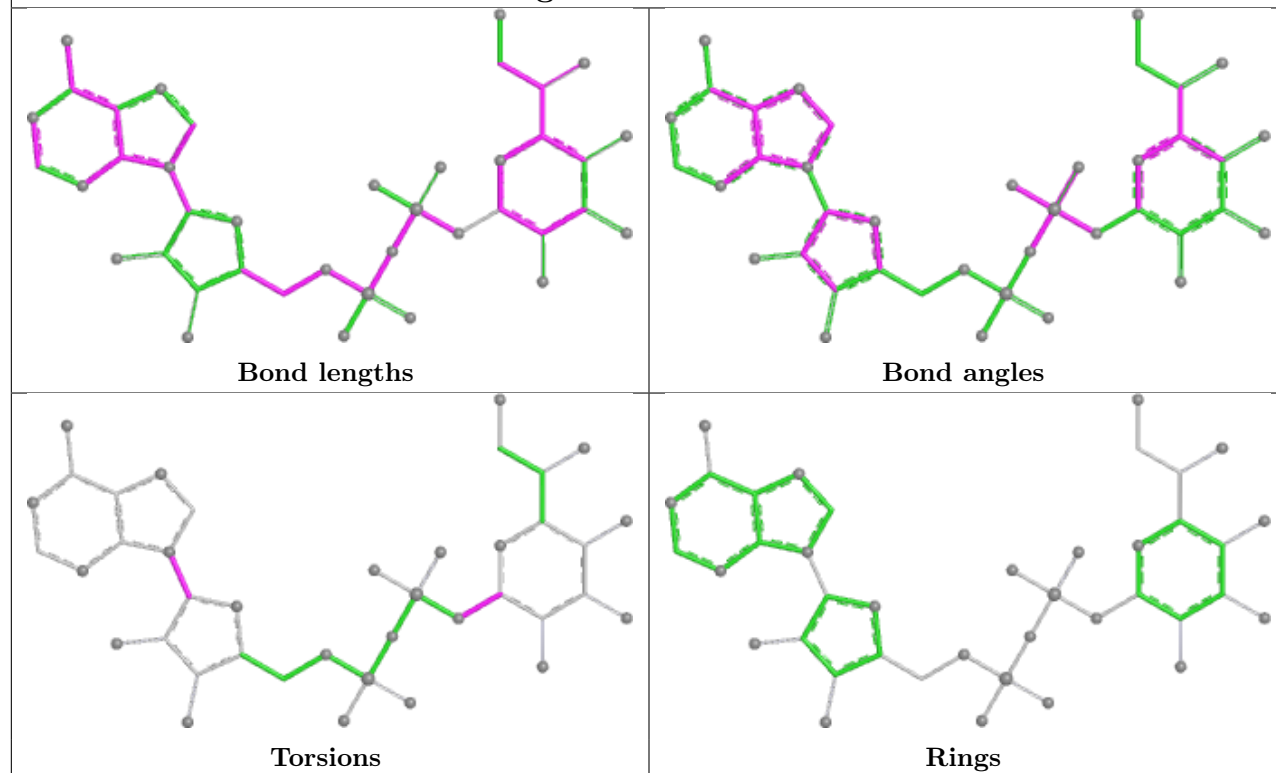
There are no ring outliers.

7 monomers are involved in 16 short contacts:

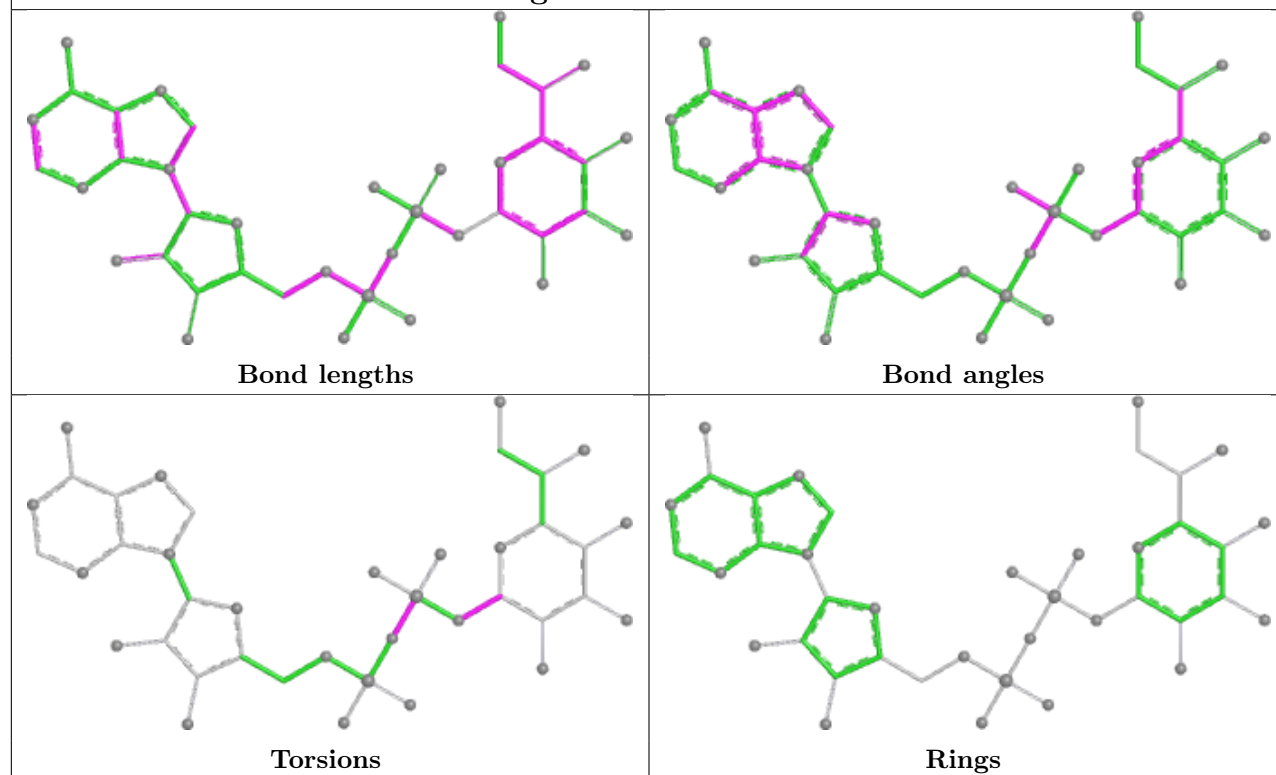
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	501	AYU	4	0
2	B	501	AYU	2	0
2	G	501	AYU	3	0
2	D	501	AYU	1	0
2	H	501	AYU	3	0
2	A	501	AYU	1	0
2	C	501	AYU	2	0

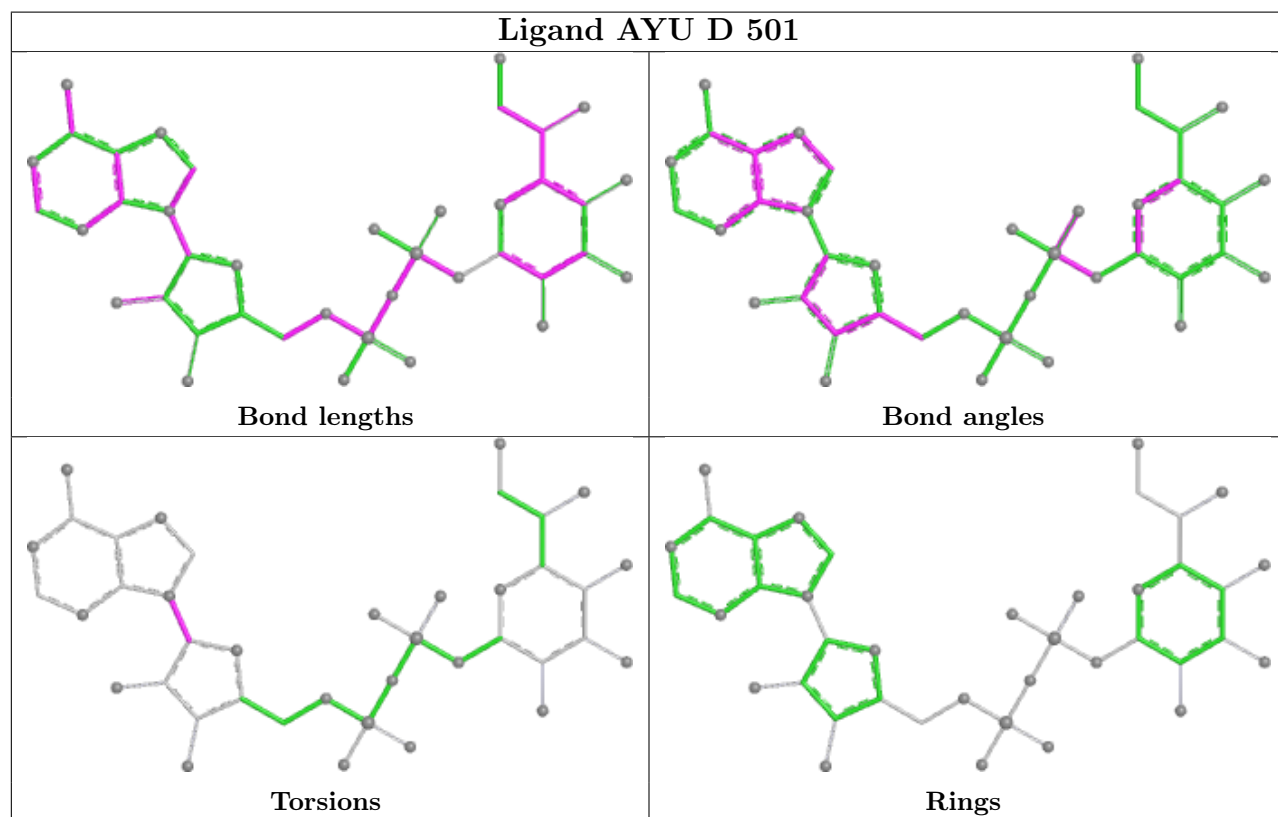
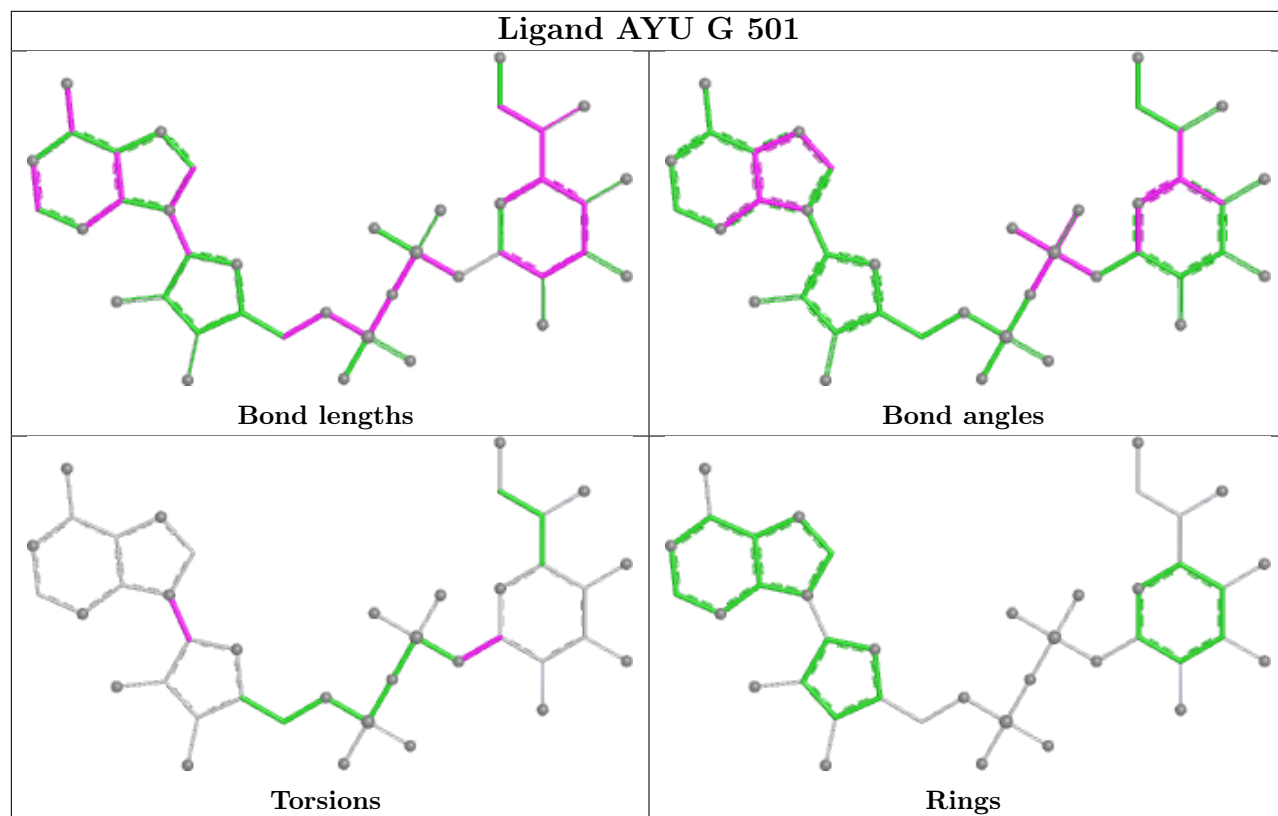
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

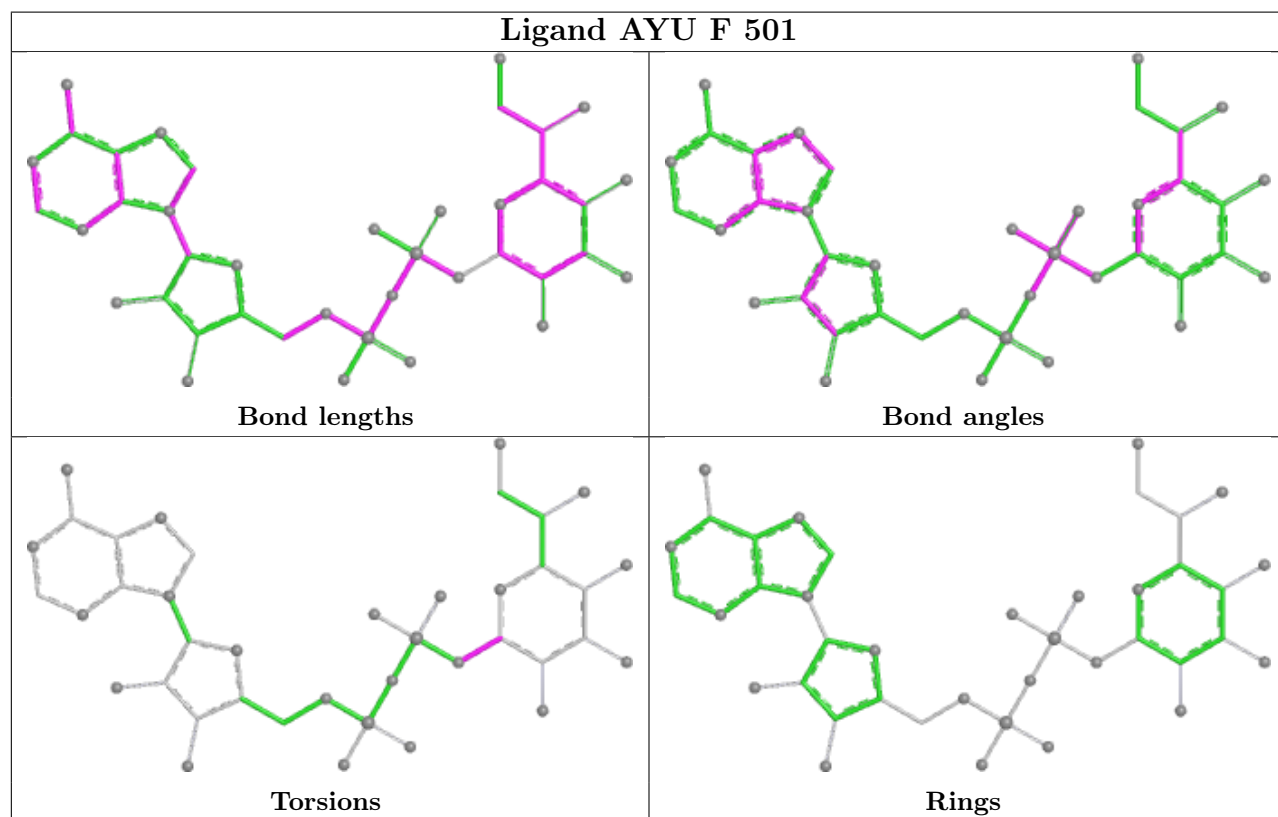
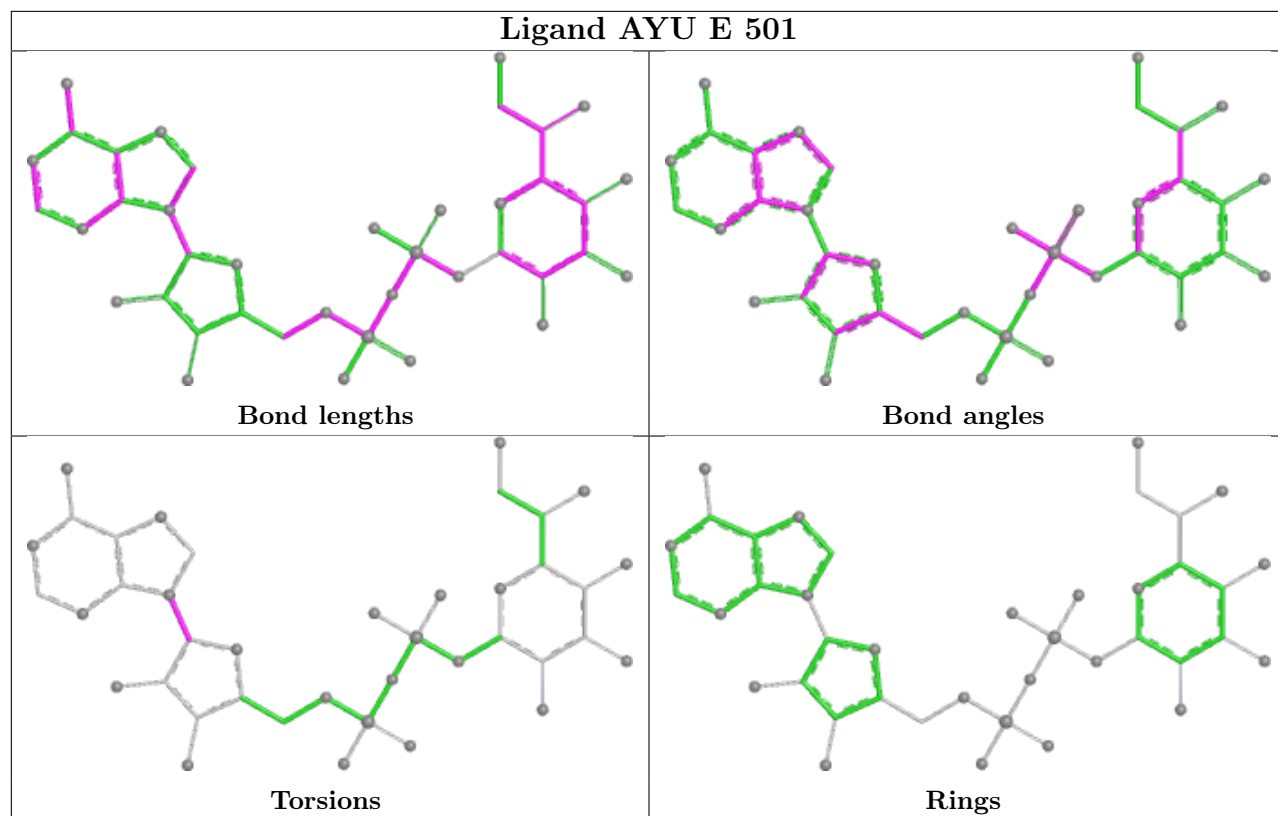
Ligand AYU I 501

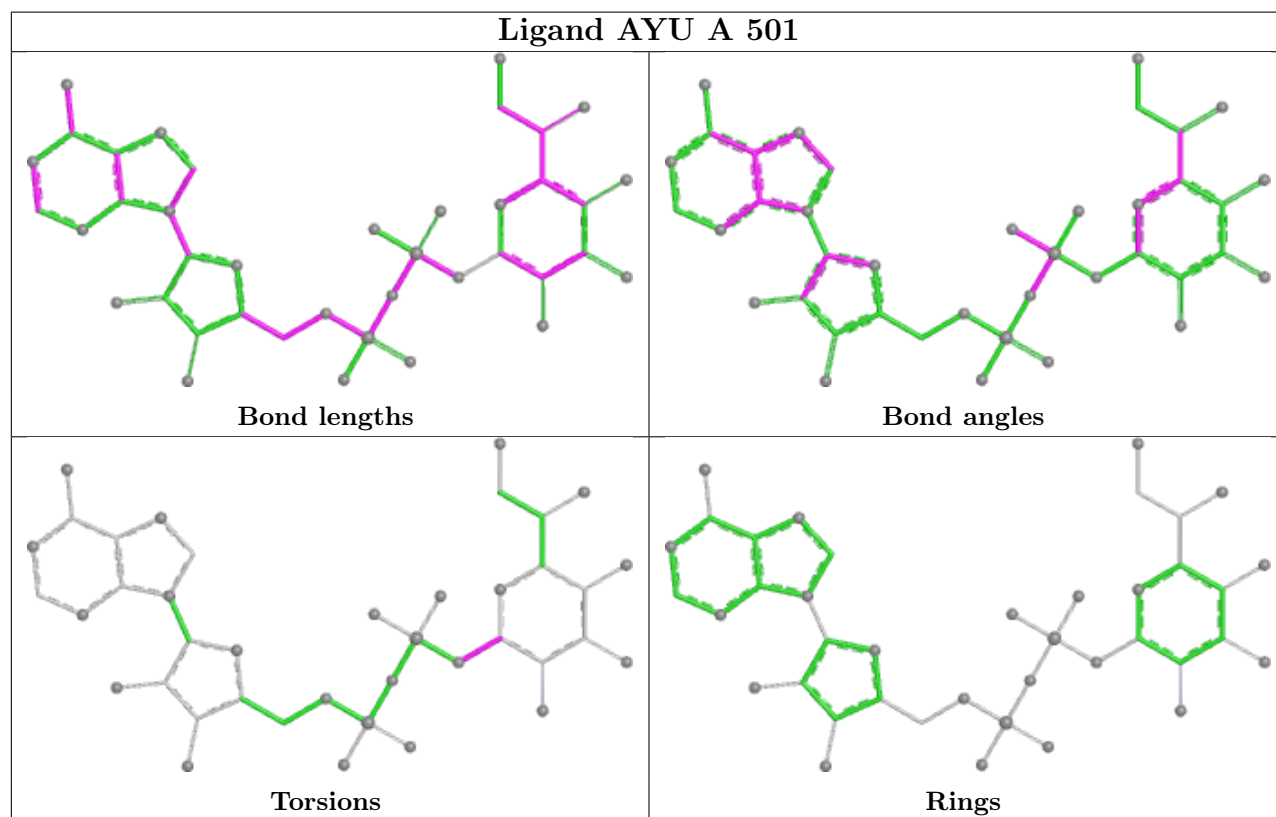
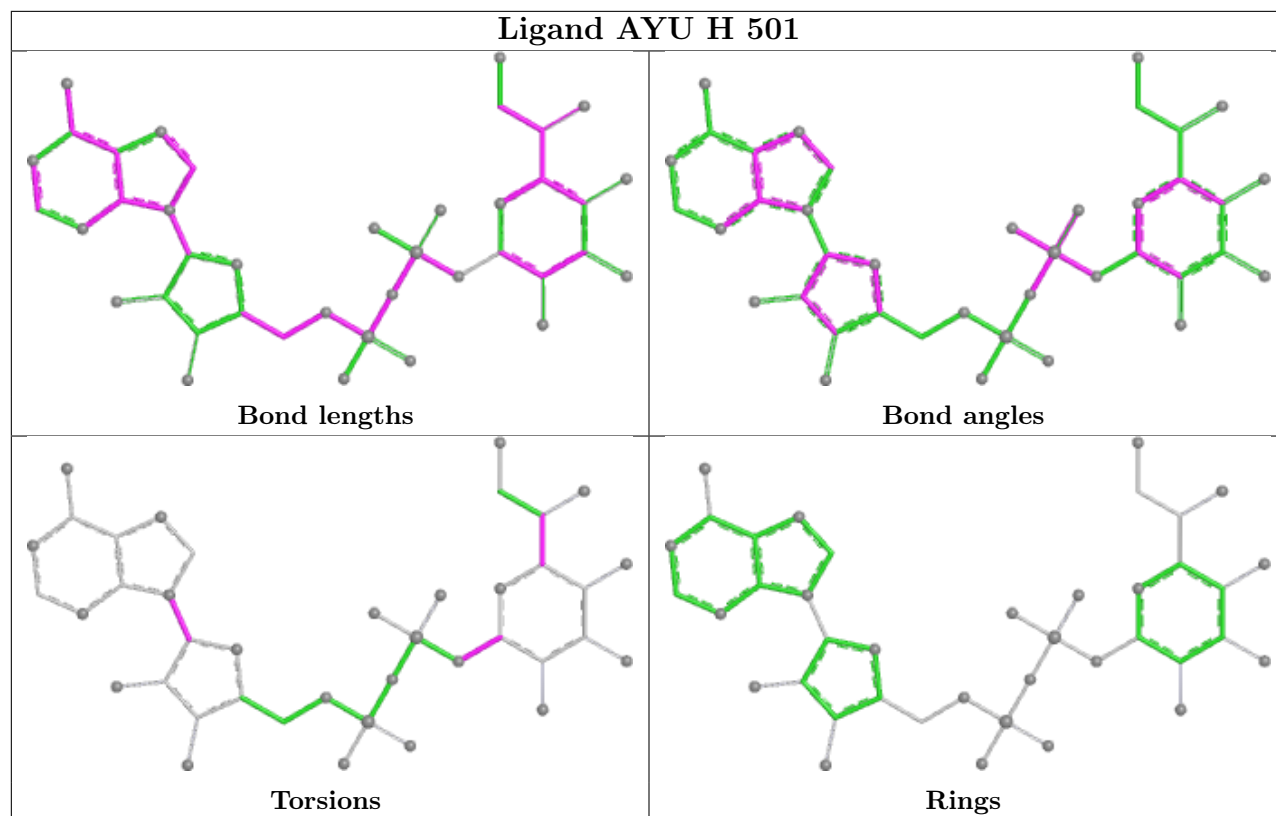


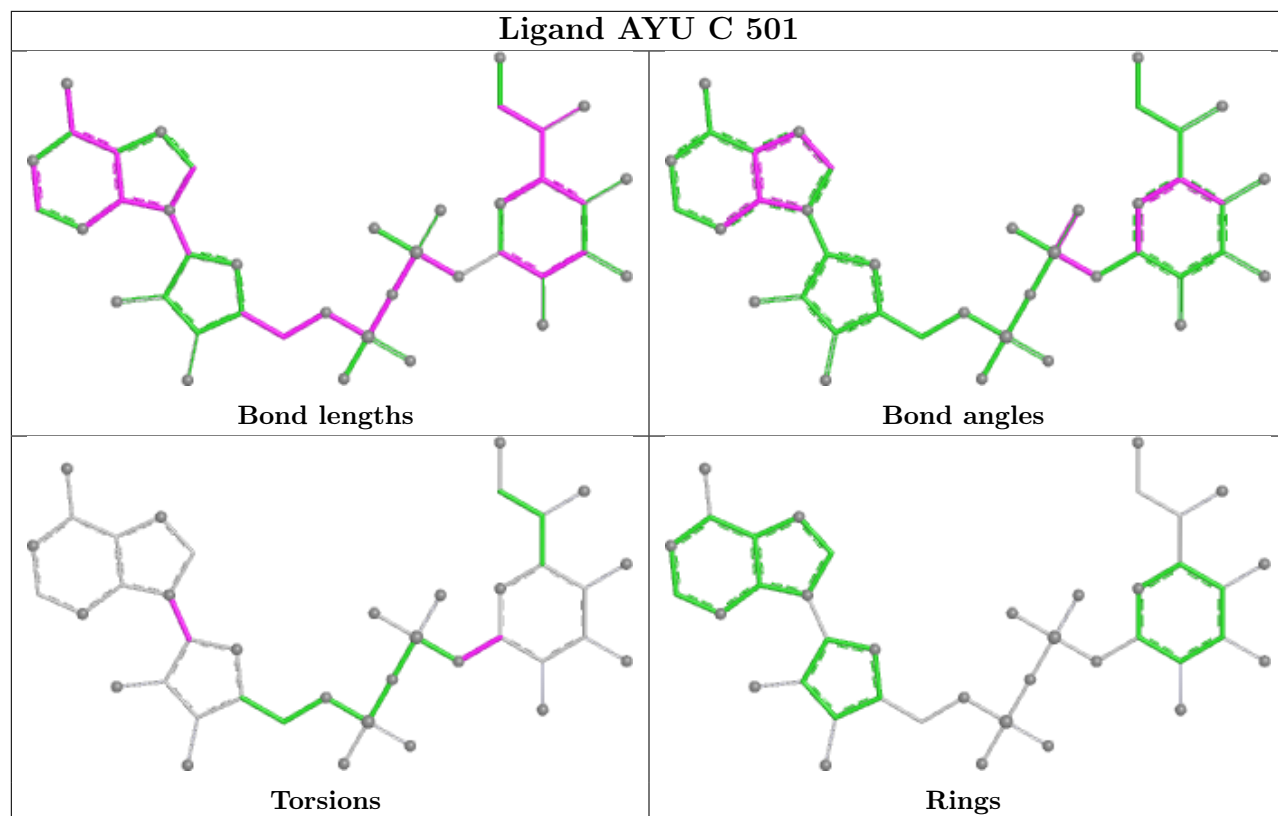
Ligand AYU B 501











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%)	0.34	20 (4%) 38 32	26, 41, 77, 119	0
1	B	445/446 (99%)	0.20	8 (1%) 67 63	25, 38, 67, 111	0
1	C	427/446 (95%)	1.30	124 (29%) 1 1	31, 59, 113, 138	0
1	D	434/446 (97%)	0.39	23 (5%) 32 26	26, 44, 74, 116	0
1	E	433/446 (97%)	0.68	43 (9%) 13 10	26, 48, 84, 116	0
1	F	433/446 (97%)	0.65	27 (6%) 26 21	26, 52, 83, 112	0
1	G	428/446 (95%)	1.62	132 (30%) 1 1	45, 70, 102, 126	0
1	H	423/446 (94%)	2.13	226 (53%) 0 0	51, 96, 128, 152	0
1	I	408/446 (91%)	1.52	127 (31%) 1 1	36, 78, 139, 180	0
All	All	3876/4014 (96%)	0.97	730 (18%) 3 2	25, 56, 114, 180	0

All (730) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	445	ILE	7.2
1	C	445	ILE	6.5
1	H	42	LEU	6.5
1	C	419	LEU	6.4
1	C	362	THR	5.9
1	C	325	LEU	5.7
1	E	66	TRP	5.7
1	I	419	LEU	5.6
1	E	440	ARG	5.4
1	C	415	VAL	5.4
1	E	446	LEU	5.3
1	C	441	LEU	5.2
1	C	381	LEU	5.2
1	C	344	PRO	5.2
1	I	276	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	292	THR	5.0
1	I	318	PRO	5.0
1	D	439	CYS	4.9
1	C	377	ALA	4.8
1	I	339	LYS	4.8
1	I	325	LEU	4.8
1	I	324	HIS	4.7
1	C	370	GLY	4.7
1	C	323	LEU	4.7
1	C	373	GLY	4.7
1	H	290	ALA	4.7
1	I	374	THR	4.7
1	I	337	LEU	4.7
1	C	358	ALA	4.6
1	G	439	CYS	4.6
1	H	344	PRO	4.6
1	C	310	TYR	4.6
1	F	441	LEU	4.5
1	E	427	VAL	4.5
1	C	385	ALA	4.4
1	I	370	GLY	4.4
1	I	309	SER	4.4
1	I	344	PRO	4.4
1	F	445	ILE	4.4
1	H	426	ASN	4.3
1	C	413	ALA	4.3
1	C	418	HIS	4.3
1	G	59	TRP	4.3
1	H	339	LYS	4.3
1	H	22	LEU	4.3
1	E	439	CYS	4.3
1	E	423	SER	4.3
1	C	365	HIS	4.2
1	H	80	LEU	4.2
1	D	423	SER	4.2
1	I	66	TRP	4.2
1	I	418	HIS	4.2
1	H	288	PHE	4.2
1	I	2	ASN	4.2
1	C	359	PHE	4.2
1	G	171	LEU	4.2
1	H	368	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	172	ILE	4.1
1	I	433	VAL	4.1
1	C	361	LEU	4.1
1	H	345	VAL	4.1
1	I	355	VAL	4.1
1	H	172	ILE	4.1
1	H	28	VAL	4.1
1	I	336	LEU	4.1
1	I	287	ALA	4.0
1	E	2	ASN	4.0
1	D	66	TRP	4.0
1	G	64	GLU	4.0
1	I	366	ARG	4.0
1	G	370	GLY	4.0
1	H	289	SER	4.0
1	D	446	LEU	4.0
1	H	338	THR	4.0
1	I	368	LEU	4.0
1	G	143	ILE	4.0
1	I	437	PHE	4.0
1	I	311	SER	4.0
1	I	365	HIS	4.0
1	H	434	PRO	4.0
1	I	362	THR	3.9
1	H	354	PHE	3.9
1	I	332	PHE	3.9
1	H	84	ILE	3.9
1	I	369	HIS	3.9
1	D	443	LYS	3.9
1	G	176	GLY	3.9
1	B	341	ASP	3.9
1	H	99	ILE	3.9
1	I	334	ILE	3.9
1	C	412	ILE	3.9
1	A	439	CYS	3.9
1	C	437	PHE	3.8
1	D	422	GLN	3.8
1	G	173	SER	3.8
1	I	377	ALA	3.8
1	C	275	LEU	3.8
1	H	436	SER	3.8
1	B	439	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	332	PHE	3.8
1	G	445	ILE	3.8
1	C	308	LEU	3.8
1	G	182	LEU	3.8
1	H	113	LEU	3.8
1	C	374	THR	3.8
1	I	306	CYS	3.8
1	G	144	ALA	3.8
1	I	218	TRP	3.8
1	G	178	THR	3.7
1	I	415	VAL	3.7
1	H	430	ARG	3.7
1	H	424	PHE	3.7
1	H	419	LEU	3.7
1	I	310	TYR	3.7
1	H	180	THR	3.7
1	H	347	GLY	3.7
1	G	50	LEU	3.7
1	B	2	ASN	3.7
1	E	422	GLN	3.7
1	H	409	MET	3.7
1	G	427	VAL	3.7
1	C	329	LYS	3.7
1	E	443	LYS	3.6
1	C	369	HIS	3.6
1	G	179	GLY	3.6
1	G	340	ARG	3.6
1	H	370	GLY	3.6
1	E	441	LEU	3.6
1	E	444	LEU	3.5
1	I	308	LEU	3.5
1	C	364	VAL	3.5
1	H	303	ARG	3.5
1	A	377	ALA	3.5
1	H	181	TRP	3.5
1	F	424	PHE	3.5
1	H	437	PHE	3.5
1	E	430	ARG	3.5
1	C	363	THR	3.5
1	C	439	CYS	3.5
1	H	432	TYR	3.5
1	H	182	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	323	LEU	3.5
1	C	378	ALA	3.5
1	H	62	VAL	3.5
1	H	227	LEU	3.5
1	H	183	TYR	3.5
1	C	375	VAL	3.4
1	I	284	LEU	3.4
1	I	351	LEU	3.4
1	G	97	ALA	3.4
1	H	287	ALA	3.4
1	F	342	ASP	3.4
1	G	2	ASN	3.4
1	I	372	THR	3.4
1	G	80	LEU	3.4
1	C	351	LEU	3.4
1	H	325	LEU	3.4
1	C	434	PRO	3.4
1	H	170	SER	3.4
1	G	186	GLU	3.4
1	C	408	VAL	3.4
1	I	275	LEU	3.4
1	H	228	PRO	3.4
1	H	25	ALA	3.4
1	H	418	HIS	3.4
1	I	290	ALA	3.4
1	I	378	ALA	3.4
1	H	431	SER	3.4
1	H	375	VAL	3.3
1	H	408	VAL	3.3
1	G	167	ILE	3.3
1	I	412	ILE	3.3
1	G	39	CYS	3.3
1	C	80	LEU	3.3
1	C	368	LEU	3.3
1	H	23	LEU	3.3
1	H	100	LEU	3.3
1	H	320	LEU	3.3
1	G	148	VAL	3.3
1	H	106	ALA	3.3
1	I	328	ALA	3.3
1	H	269	LYS	3.3
1	H	443	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	137	LEU	3.3
1	C	376	HIS	3.3
1	I	274	HIS	3.3
1	I	347	GLY	3.3
1	I	373	GLY	3.3
1	H	144	ALA	3.3
1	I	281	ALA	3.3
1	C	311	SER	3.3
1	C	336	LEU	3.3
1	G	192	VAL	3.3
1	H	421	VAL	3.3
1	H	346	THR	3.3
1	I	346	THR	3.3
1	H	348	LYS	3.3
1	H	47	LEU	3.2
1	H	134	LEU	3.2
1	I	438	GLU	3.2
1	C	409	MET	3.2
1	C	354	PHE	3.2
1	H	425	SER	3.2
1	A	341	ASP	3.2
1	F	341	ASP	3.2
1	F	344	PRO	3.2
1	C	443	LYS	3.2
1	G	287	ALA	3.2
1	C	318	PRO	3.2
1	H	44	PRO	3.2
1	H	60	PRO	3.2
1	H	441	LEU	3.2
1	H	355	VAL	3.2
1	I	375	VAL	3.2
1	H	41	ALA	3.2
1	G	437	PHE	3.2
1	H	117	PHE	3.2
1	G	372	THR	3.2
1	H	101	ALA	3.1
1	C	366	ARG	3.1
1	I	359	PHE	3.1
1	I	42	LEU	3.1
1	C	421	VAL	3.1
1	D	445	ILE	3.1
1	C	357	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	359	PHE	3.1
1	F	66	TRP	3.1
1	H	139	PRO	3.1
1	G	95	LEU	3.1
1	H	284	LEU	3.1
1	G	62	VAL	3.1
1	C	299	ALA	3.1
1	I	331	ALA	3.1
1	H	444	LEU	3.1
1	D	340	ARG	3.1
1	F	89	GLN	3.1
1	H	365	HIS	3.1
1	H	318	PRO	3.1
1	G	424	PHE	3.1
1	I	268	LEU	3.1
1	H	440	ARG	3.1
1	A	375	VAL	3.1
1	I	298	THR	3.0
1	C	371	GLU	3.0
1	C	386	MET	3.0
1	G	42	LEU	3.0
1	C	431	SER	3.0
1	G	347	GLY	3.0
1	H	412	ILE	3.0
1	G	177	ALA	3.0
1	G	88	LEU	3.0
1	H	173	SER	3.0
1	H	185	ASN	3.0
1	H	149	ILE	3.0
1	C	389	LEU	3.0
1	H	265	LEU	3.0
1	C	424	PHE	3.0
1	F	425	SER	3.0
1	B	427	VAL	3.0
1	H	376	HIS	3.0
1	C	300	VAL	2.9
1	E	417	GLU	2.9
1	G	404	LEU	2.9
1	H	10	LEU	2.9
1	I	294	LEU	2.9
1	H	405	SER	2.9
1	H	328	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	67	GLN	2.9
1	G	175	ASN	2.9
1	G	99	ILE	2.9
1	H	143	ILE	2.9
1	C	269	LYS	2.9
1	C	328	ALA	2.9
1	H	286	ALA	2.9
1	H	118	LEU	2.9
1	G	291	TYR	2.9
1	B	425	SER	2.9
1	H	83	VAL	2.9
1	H	232	LYS	2.9
1	G	444	LEU	2.9
1	I	265	LEU	2.9
1	H	371	GLU	2.9
1	C	416	LYS	2.8
1	H	321	LYS	2.8
1	C	317	PRO	2.8
1	G	63	PRO	2.8
1	C	276	LEU	2.8
1	D	80	LEU	2.8
1	H	275	LEU	2.8
1	C	254	TYR	2.8
1	C	367	ARG	2.8
1	H	190	VAL	2.8
1	H	268	LEU	2.8
1	E	438	GLU	2.8
1	G	295	PHE	2.8
1	C	331	ALA	2.8
1	H	54	ALA	2.8
1	I	382	CYS	2.8
1	C	380	GLN	2.8
1	H	103	ASP	2.8
1	H	392	PHE	2.8
1	G	390	TYR	2.8
1	E	395	SER	2.8
1	F	398	SER	2.8
1	E	421	VAL	2.8
1	H	364	VAL	2.8
1	G	337	LEU	2.8
1	H	140	ALA	2.8
1	I	361	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	258	LYS	2.8
1	D	342	ASP	2.8
1	C	360	GLY	2.7
1	H	332	PHE	2.8
1	I	246	PHE	2.8
1	H	263	ILE	2.7
1	I	432	TYR	2.7
1	E	375	VAL	2.7
1	H	192	VAL	2.7
1	H	415	VAL	2.7
1	F	444	LEU	2.7
1	H	50	LEU	2.7
1	H	372	THR	2.7
1	I	256	LYS	2.7
1	G	342	ASP	2.7
1	H	373	GLY	2.7
1	I	271	PHE	2.7
1	G	412	ILE	2.7
1	H	293	PRO	2.7
1	G	170	SER	2.7
1	G	433	VAL	2.7
1	H	224	TYR	2.7
1	C	294	LEU	2.7
1	E	80	LEU	2.7
1	E	419	LEU	2.7
1	G	109	ALA	2.7
1	F	440	ARG	2.7
1	H	367	ARG	2.7
1	F	90	GLN	2.7
1	C	263	ILE	2.7
1	E	445	ILE	2.7
1	H	63	PRO	2.7
1	C	312	SER	2.7
1	C	268	LEU	2.7
1	C	383	LYS	2.7
1	C	432	TYR	2.7
1	E	386	MET	2.7
1	G	168	LEU	2.7
1	H	225	LEU	2.7
1	H	235	LEU	2.7
1	I	386	MET	2.7
1	I	390	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	394	THR	2.7
1	H	108	ALA	2.7
1	H	435	GLU	2.7
1	F	65	LYS	2.7
1	G	33	LYS	2.7
1	G	443	LYS	2.7
1	H	2	ASN	2.7
1	A	381	LEU	2.7
1	G	266	SER	2.7
1	H	40	ARG	2.7
1	H	92	LEU	2.7
1	H	337	LEU	2.7
1	H	401	ARG	2.7
1	H	64	GLU	2.7
1	H	291	TYR	2.7
1	D	90	GLN	2.7
1	D	344	PRO	2.6
1	H	322	ASN	2.6
1	C	307	LEU	2.6
1	G	191	LEU	2.6
1	H	88	LEU	2.6
1	H	114	VAL	2.6
1	C	353	SER	2.6
1	G	431	SER	2.6
1	I	398	SER	2.6
1	H	93	ALA	2.6
1	H	352	HIS	2.6
1	H	335	GLY	2.6
1	H	261	PRO	2.6
1	H	39	CYS	2.6
1	C	330	GLU	2.6
1	G	147	VAL	2.6
1	G	379	SER	2.6
1	H	311	SER	2.6
1	G	422	GLN	2.6
1	H	86	ALA	2.6
1	H	358	ALA	2.6
1	H	15	LYS	2.6
1	H	386	MET	2.6
1	I	302	ILE	2.6
1	C	320	LEU	2.6
1	H	18	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	333	GLU	2.6
1	H	411	VAL	2.6
1	I	413	ALA	2.6
1	G	224	TYR	2.6
1	B	440	ARG	2.6
1	I	317	PRO	2.6
1	I	434	PRO	2.6
1	H	295	PHE	2.6
1	C	265	LEU	2.6
1	E	64	GLU	2.6
1	G	113	LEU	2.6
1	G	268	LEU	2.6
1	I	80	LEU	2.6
1	I	307	LEU	2.6
1	I	381	LEU	2.6
1	H	300	VAL	2.6
1	I	411	VAL	2.6
1	C	313	SER	2.6
1	F	423	SER	2.6
1	G	34	SER	2.6
1	G	54	ALA	2.6
1	G	346	THR	2.6
1	C	356	LYS	2.6
1	D	65	LYS	2.6
1	E	68	TYR	2.6
1	G	318	PRO	2.5
1	G	442	ASP	2.5
1	G	149	ILE	2.5
1	C	271	PHE	2.5
1	C	444	LEU	2.5
1	H	351	LEU	2.5
1	G	190	VAL	2.5
1	G	385	ALA	2.5
1	C	372	THR	2.5
1	C	379	SER	2.5
1	I	326	CYS	2.5
1	H	49	THR	2.5
1	I	292	THR	2.5
1	F	432	TYR	2.5
1	I	254	TYR	2.5
1	D	272	ASP	2.5
1	H	307	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	288	PHE	2.5
1	C	399	GLN	2.5
1	H	296	VAL	2.5
1	H	433	VAL	2.5
1	G	107	ALA	2.5
1	C	306	CYS	2.5
1	G	180	THR	2.5
1	C	404	LEU	2.5
1	G	354	PHE	2.5
1	A	3	ASN	2.5
1	H	147	VAL	2.5
1	F	340	ARG	2.5
1	G	96	ARG	2.5
1	C	338	THR	2.5
1	I	436	SER	2.5
1	G	183	TYR	2.5
1	H	310	TYR	2.5
1	H	154	ILE	2.5
1	A	441	LEU	2.5
1	C	284	LEU	2.5
1	G	47	LEU	2.5
1	G	225	LEU	2.5
1	H	128	LEU	2.5
1	H	294	LEU	2.5
1	I	416	LYS	2.5
1	C	414	GLN	2.5
1	D	59	TRP	2.5
1	C	345	VAL	2.5
1	G	374	THR	2.5
1	I	353	SER	2.5
1	C	382	CYS	2.4
1	H	142	PRO	2.4
1	H	230	PRO	2.4
1	A	373	GLY	2.4
1	E	435	GLU	2.4
1	E	341	ASP	2.4
1	H	369	HIS	2.4
1	E	40	ARG	2.4
1	G	40	ARG	2.4
1	C	2	ASN	2.4
1	I	345	VAL	2.4
1	G	237	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	49	THR	2.4
1	E	398	SER	2.4
1	I	371	GLU	2.4
1	C	316	CYS	2.4
1	E	383	LYS	2.4
1	H	233	LYS	2.4
1	E	442	ASP	2.4
1	G	188	ASP	2.4
1	H	110	ILE	2.4
1	H	272	ASP	2.4
1	D	441	LEU	2.4
1	F	42	LEU	2.4
1	H	308	LEU	2.4
1	H	324	HIS	2.4
1	C	355	VAL	2.4
1	C	411	VAL	2.4
1	H	123	VAL	2.4
1	H	131	ALA	2.4
1	I	278	ALA	2.4
1	A	346	THR	2.4
1	C	384	GLU	2.4
1	E	379	SER	2.4
1	H	187	SER	2.4
1	H	383	LYS	2.4
1	I	215	GLU	2.4
1	G	43	LEU	2.4
1	H	38	ARG	2.4
1	C	211	TYR	2.4
1	G	114	VAL	2.4
1	G	226	ALA	2.4
1	H	329	LYS	2.4
1	I	348	LYS	2.4
1	C	347	GLY	2.4
1	H	51	ILE	2.4
1	E	418	HIS	2.4
1	G	92	LEU	2.4
1	H	27	ASP	2.4
1	I	267	LEU	2.4
1	I	291	TYR	2.4
1	I	354	PHE	2.4
1	G	408	VAL	2.4
1	C	3	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	377	ALA	2.4
1	G	31	GLU	2.4
1	C	292	THR	2.3
1	H	26	PRO	2.3
1	I	266	SER	2.3
1	G	51	ILE	2.3
1	G	36	ASP	2.3
1	H	36	ASP	2.3
1	I	297	LEU	2.3
1	C	433	VAL	2.3
1	A	2	ASN	2.3
1	D	264	ASN	2.3
1	E	378	ALA	2.3
1	D	229	GLN	2.3
1	H	399	GLN	2.3
1	H	191	LEU	2.3
1	I	242	LEU	2.3
1	C	295	PHE	2.3
1	H	327	GLU	2.3
1	H	105	ALA	2.3
1	H	362	THR	2.3
1	I	305	THR	2.3
1	F	393	SER	2.3
1	G	181	TRP	2.3
1	A	376	HIS	2.3
1	C	302	ILE	2.3
1	H	171	LEU	2.3
1	H	276	LEU	2.3
1	H	334	ILE	2.3
1	I	404	LEU	2.3
1	F	386	MET	2.3
1	A	383	LYS	2.3
1	A	438	GLU	2.3
1	I	83	VAL	2.3
1	I	296	VAL	2.3
1	G	60	PRO	2.3
1	H	97	ALA	2.3
1	C	440	ARG	2.3
1	H	102	ARG	2.3
1	I	414	GLN	2.3
1	H	389	LEU	2.3
1	H	33	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	148	VAL	2.3
1	G	401	ARG	2.3
1	G	432	TYR	2.3
1	H	184	ARG	2.3
1	I	259	ASN	2.2
1	H	363	THR	2.2
1	A	380	GLN	2.2
1	A	446	LEU	2.2
1	C	334	ILE	2.2
1	C	337	LEU	2.2
1	D	42	LEU	2.2
1	E	266	SER	2.2
1	H	29	SER	2.2
1	H	95	LEU	2.2
1	I	65	LYS	2.2
1	I	428	ASP	2.2
1	G	270	GLU	2.2
1	G	332	PHE	2.2
1	H	112	PHE	2.2
1	E	344	PRO	2.2
1	G	296	VAL	2.2
1	I	247	VAL	2.2
1	E	385	ALA	2.2
1	F	2	ASN	2.2
1	H	3	ASN	2.2
1	H	278	ALA	2.2
1	G	211	TYR	2.2
1	H	439	CYS	2.2
1	I	211	TYR	2.2
1	G	12	GLN	2.2
1	G	369	HIS	2.2
1	G	137	LEU	2.2
1	I	263	ILE	2.2
1	H	61	PHE	2.2
1	G	228	PRO	2.2
1	I	260	ASN	2.2
1	I	285	ALA	2.2
1	A	443	LYS	2.2
1	B	90	GLN	2.2
1	F	376	HIS	2.2
1	F	439	CYS	2.2
1	G	49	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	292	THR	2.2
1	H	326	CYS	2.2
1	H	406	GLN	2.2
1	G	235	LEU	2.2
1	H	361	LEU	2.2
1	D	173	SER	2.2
1	G	423	SER	2.2
1	G	425	SER	2.2
1	H	45	SER	2.2
1	I	248	SER	2.2
1	C	333	GLU	2.2
1	I	367	ARG	2.2
1	C	339	LYS	2.2
1	D	69	LYS	2.2
1	G	81	LYS	2.2
1	C	273	HIS	2.2
1	C	426	ASN	2.2
1	D	2	ASN	2.2
1	H	391	ASN	2.2
1	E	90	GLN	2.2
1	H	57	MET	2.2
1	H	21	LEU	2.2
1	H	121	LEU	2.2
1	H	387	GLY	2.2
1	G	110	ILE	2.2
1	A	425	SER	2.2
1	A	442	ASP	2.2
1	H	417	GLU	2.2
1	G	5	LYS	2.2
1	H	136	LYS	2.2
1	H	189	LYS	2.2
1	I	300	VAL	2.1
1	G	185	ASN	2.1
1	H	20	GLN	2.1
1	H	175	ASN	2.1
1	B	346	THR	2.1
1	E	381	LEU	2.1
1	G	154	ILE	2.1
1	H	46	GLU	2.1
1	C	309	SER	2.1
1	C	393	SER	2.1
1	C	398	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	194	SER	2.1
1	H	410	SER	2.1
1	I	379	SER	2.1
1	I	81	LYS	2.1
1	C	392	PHE	2.1
1	I	295	PHE	2.1
1	G	349	GLN	2.1
1	H	229	GLN	2.1
1	H	299	ALA	2.1
1	H	374	THR	2.1
1	I	235	LEU	2.1
1	I	389	LEU	2.1
1	I	241	ILE	2.1
1	G	46	GLU	2.1
1	H	122	ASP	2.1
1	H	423	SER	2.1
1	I	431	SER	2.1
1	G	344	PRO	2.1
1	H	6	VAL	2.1
1	I	262	GLN	2.1
1	C	290	ALA	2.1
1	E	41	ALA	2.1
1	G	378	ALA	2.1
1	C	391	ASN	2.1
1	G	174	ASN	2.1
1	G	23	LEU	2.1
1	G	239	LEU	2.1
1	H	404	LEU	2.1
1	I	201	GLY	2.1
1	F	5	LYS	2.1
1	G	189	LYS	2.1
1	H	94	SER	2.1
1	H	188	ASP	2.1
1	H	277	SER	2.1
1	H	379	SER	2.1
1	C	274	HIS	2.1
1	G	399	GLN	2.1
1	E	6	VAL	2.1
1	H	130	VAL	2.1
1	I	214	ALA	2.1
1	C	303	ARG	2.1
1	G	267	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	31	GLU	2.1
1	I	338	THR	2.1
1	H	241	ILE	2.1
1	I	251	LYS	2.1
1	H	429	ASP	2.1
1	I	293	PRO	2.1
1	A	418	HIS	2.1
1	C	324	HIS	2.1
1	G	376	HIS	2.1
1	H	422	GLN	2.0
1	F	427	VAL	2.0
1	G	6	VAL	2.0
1	G	28	VAL	2.0
1	G	83	VAL	2.0
1	H	271	PHE	2.0
1	F	96	ARG	2.0
1	I	279	ALA	2.0
1	G	22	LEU	2.0
1	G	100	LEU	2.0
1	A	59	TRP	2.0
1	C	201	GLY	2.0
1	H	59	TRP	2.0
1	E	126	LYS	2.0
1	E	44	PRO	2.0
1	H	309	SER	2.0
1	I	249	MET	2.0
1	H	274	HIS	2.0
1	E	28	VAL	2.0
1	G	222	VAL	2.0
1	G	271	PHE	2.0
1	I	257	PHE	2.0
1	G	413	ALA	2.0
1	H	109	ALA	2.0
1	C	322	ASN	2.0
1	I	232	LYS	2.0
1	C	305	THR	2.0
1	D	49	THR	2.0
1	F	338	THR	2.0
1	G	298	THR	2.0
1	G	338	THR	2.0
1	C	390	TYR	2.0
1	C	405	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	277	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

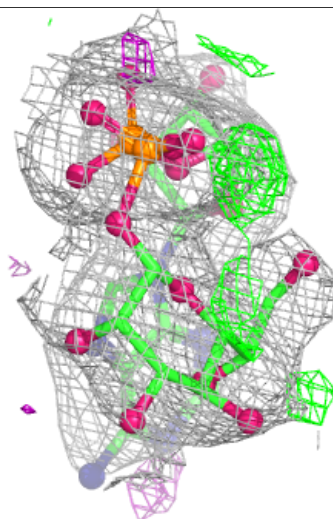
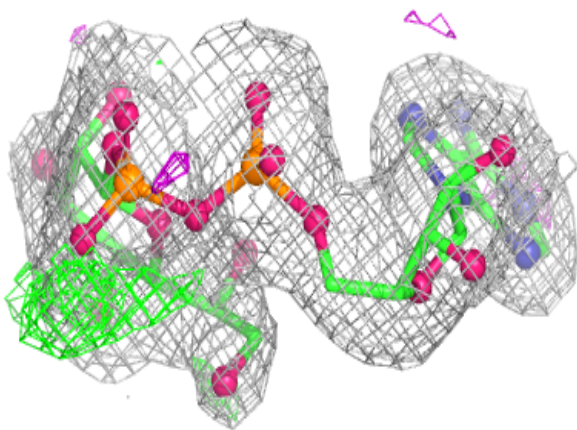
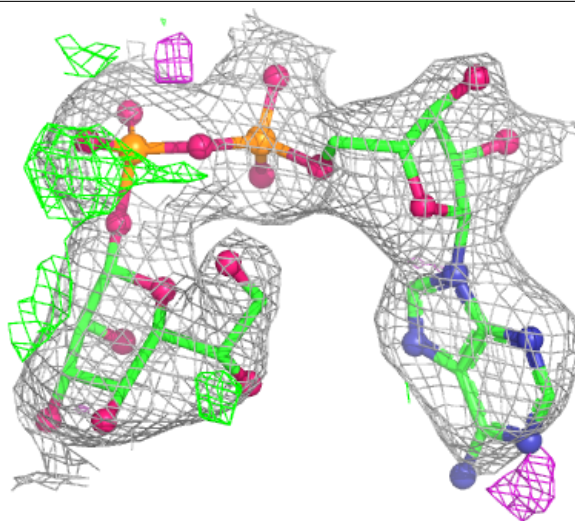
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AYU	G	501	40/40	0.90	0.12	52,58,65,71	0
2	AYU	H	501	40/40	0.90	0.14	79,86,90,94	0
2	AYU	C	501	40/40	0.93	0.10	32,43,57,63	0
2	AYU	I	501	40/40	0.93	0.11	57,70,86,99	0
2	AYU	F	501	40/40	0.95	0.08	34,40,43,50	0
2	AYU	A	501	40/40	0.95	0.09	26,30,37,43	0
2	AYU	D	501	40/40	0.96	0.08	25,31,35,45	0
2	AYU	E	501	40/40	0.96	0.07	30,36,40,53	0
2	AYU	B	501	40/40	0.96	0.08	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.

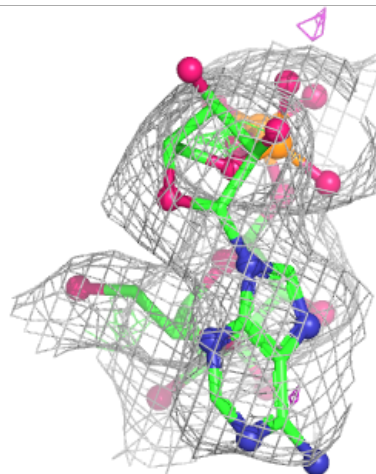
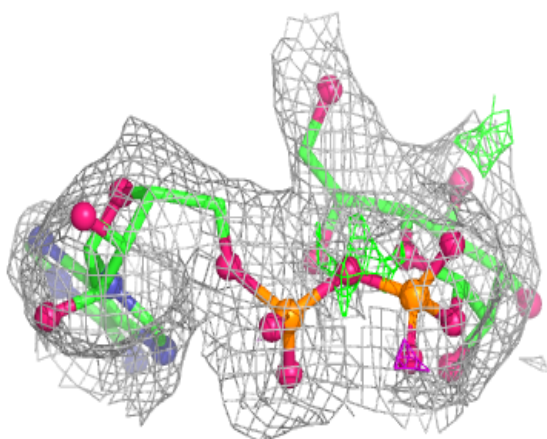
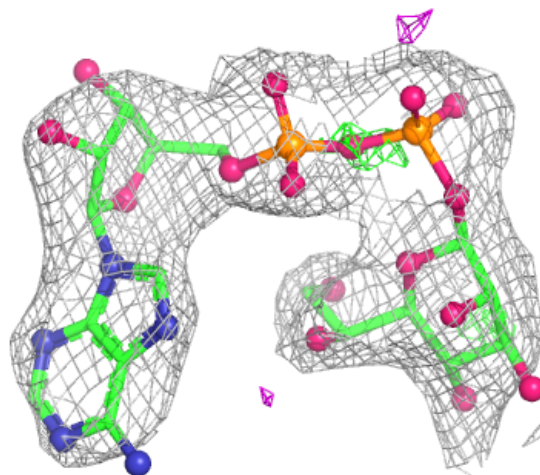
Electron density around AYU G 501:

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



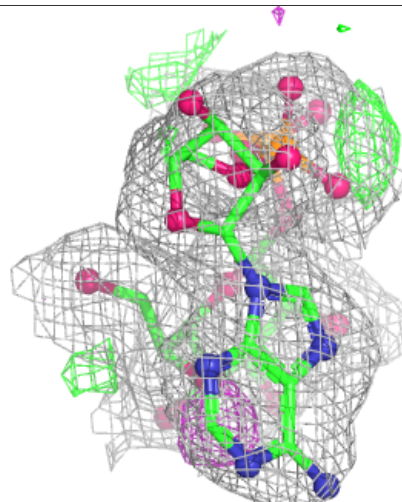
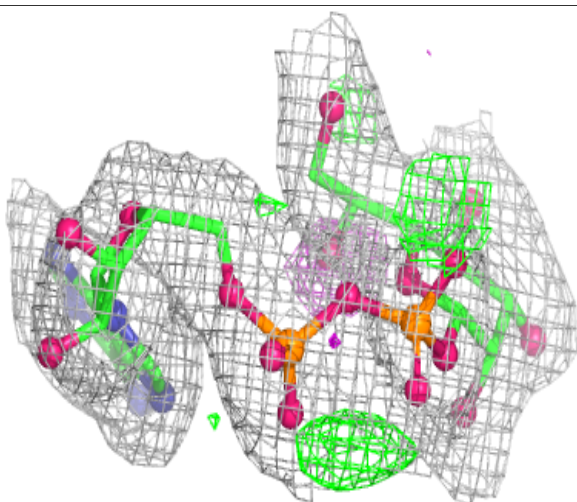
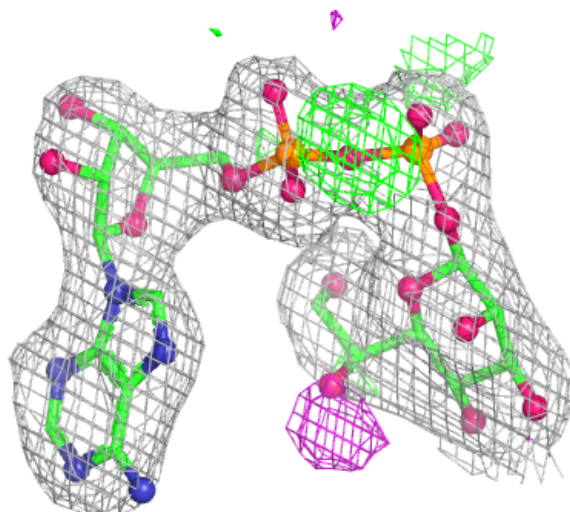
Electron density around AYU H 501:

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



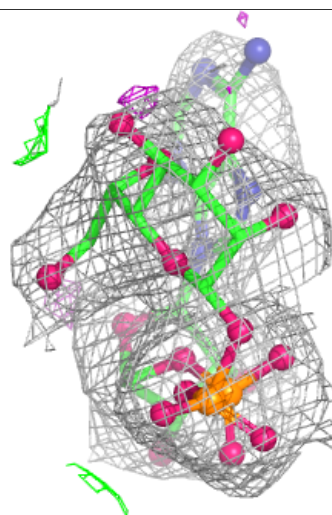
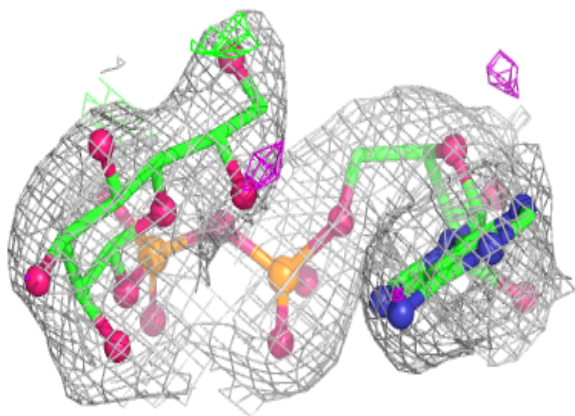
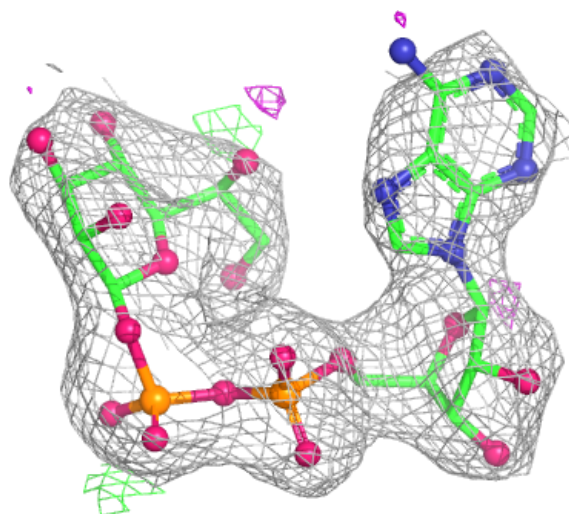
Electron density around AYU C 501:

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



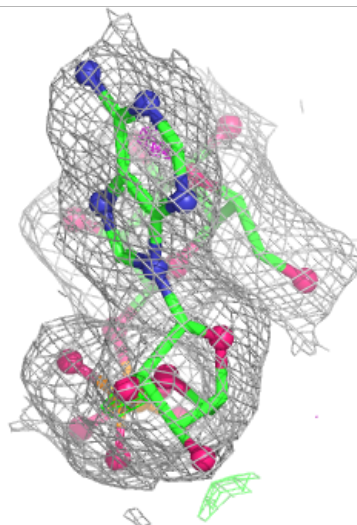
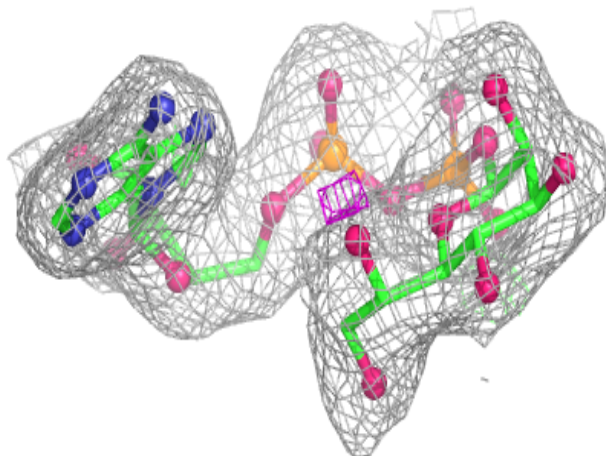
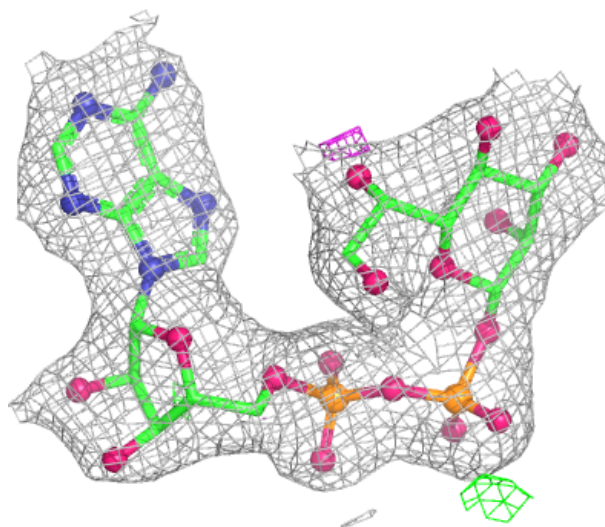
Electron density around AYU I 501:

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



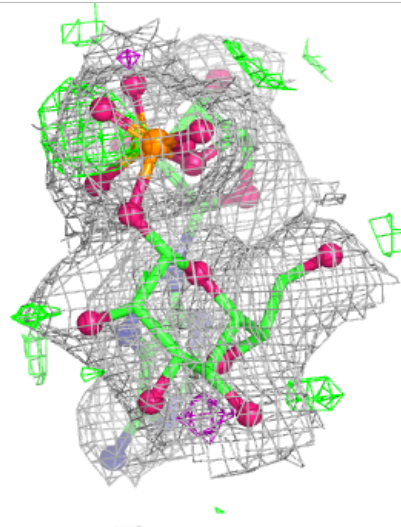
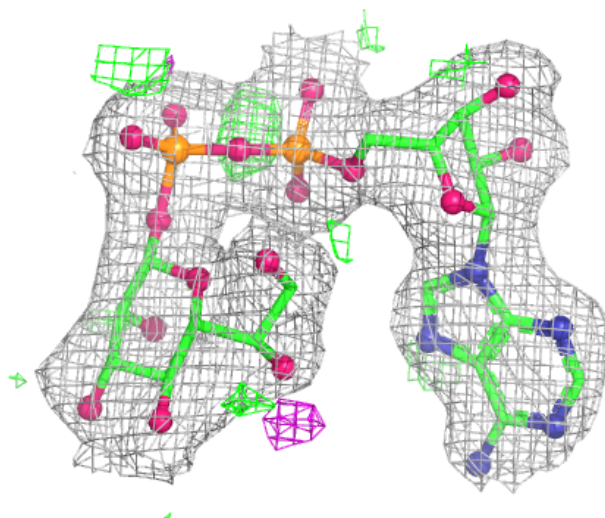
Electron density around AYU F 501:

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



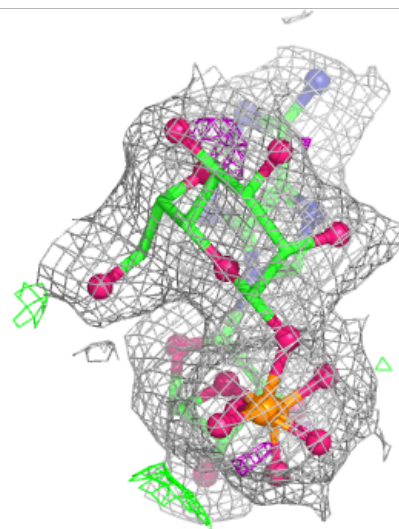
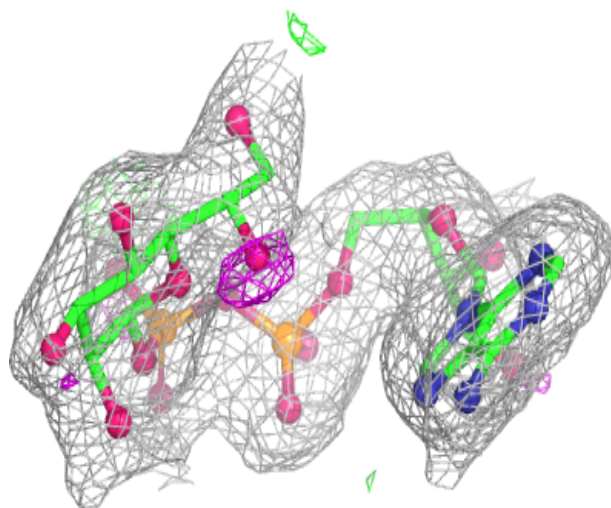
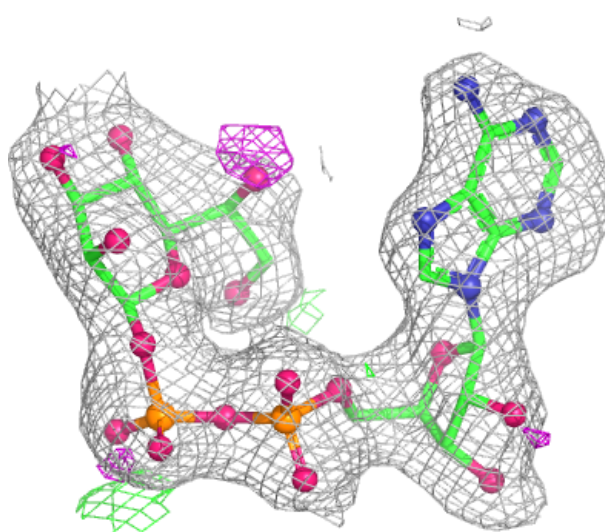
Electron density around AYU A 501:

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



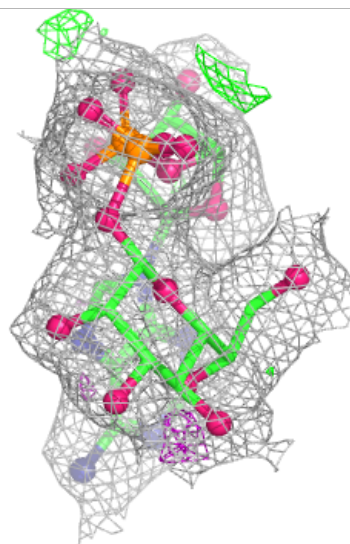
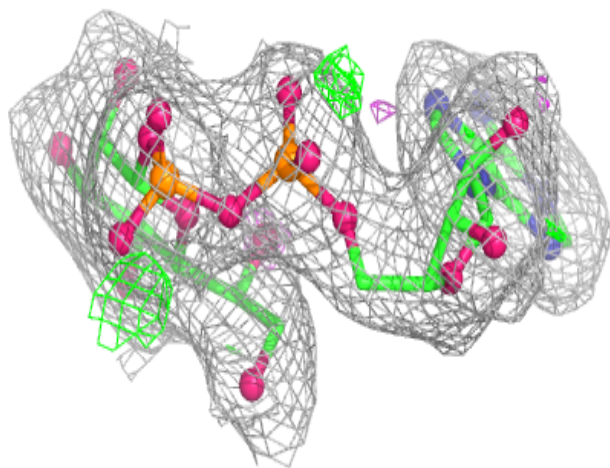
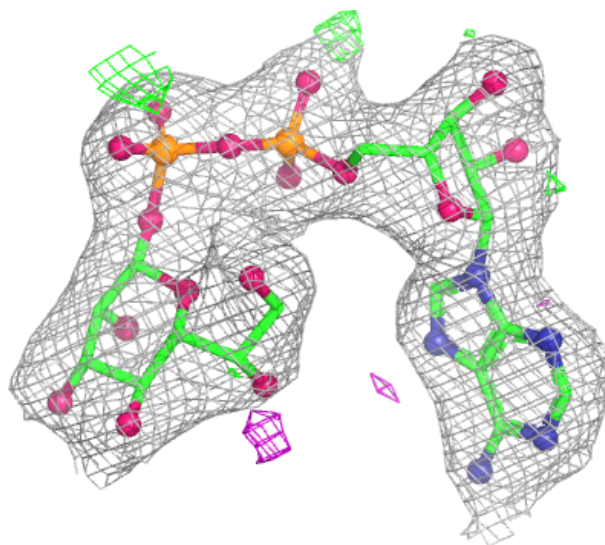
Electron density around AYU D 501:

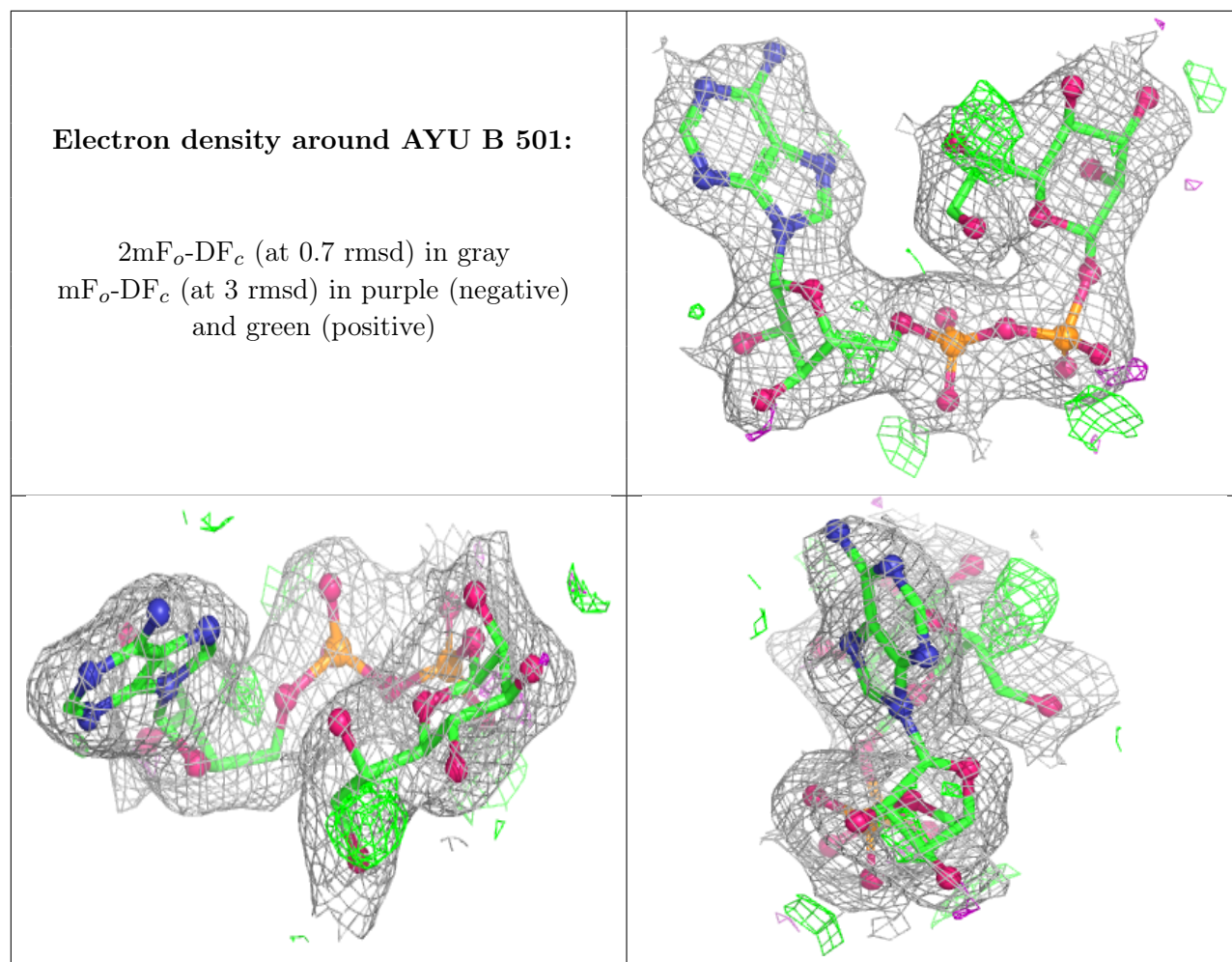
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.