



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:45 AM UTC

PDB ID : 1IL2 / pdb_00001il2
Title : Crystal Structure of the E. coli Aspartyl-tRNA Synthetase:Yeast tRNAasp:aspartyl-Adenylate Complex
Authors : Moulinier, L.; Eiler, S.; Eriani, G.; Gangloff, J.; Thierry, J.C.; Gabriel, K.; McClain, W.H.; Moras, D.
Deposited on : 2001-05-07
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

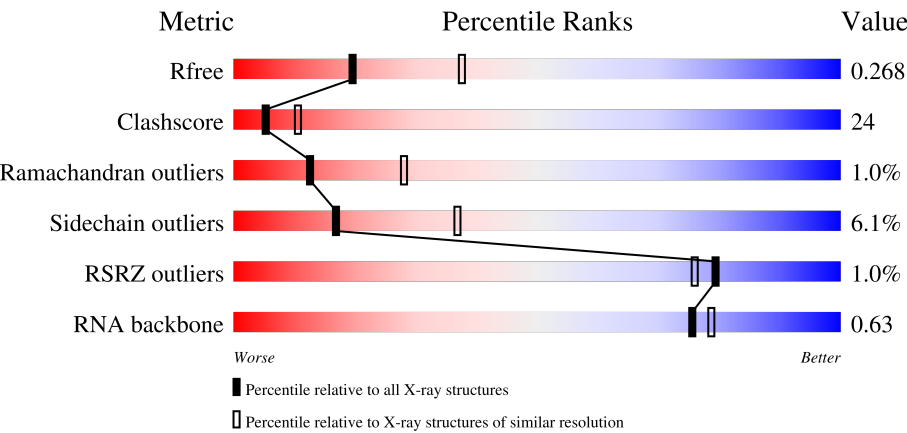
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	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)
RNA backbone	3983	1014 (2.84-2.36)

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	C	75	
1	D	75	
2	A	590	

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Mol	Chain	Length	Quality of chain
2	B	590	% 53% 41% . ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	701	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12753 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 RNA chain called ASPARTYL TRANSFER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1601	715	280	531	75			
1	D	70	Total	C	N	O	P	0	0	0
			1496	668	262	496	70			

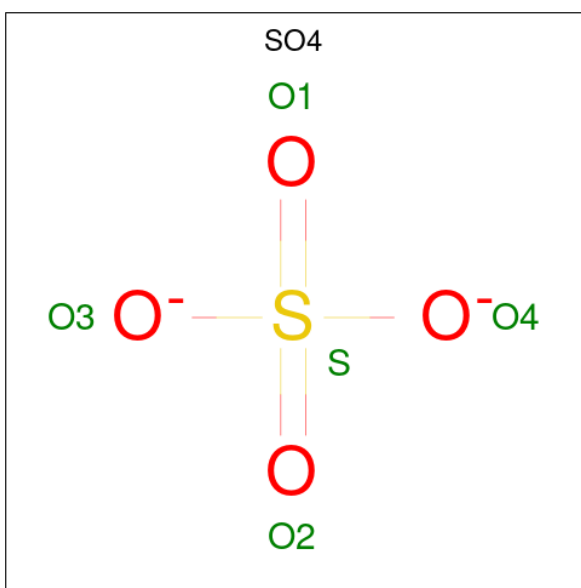
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	913	PSU	U	modified residue	GB 176417
C	916	H2U	U	modified residue	GB 176417
C	919	H2U	U	modified residue	GB 176417
C	932	PSU	U	modified residue	GB 176417
C	937	1MG	G	modified residue	GB 176417
C	949	5MC	C	modified residue	GB 176417
C	954	5MU	U	modified residue	GB 176417
C	955	PSU	U	modified residue	GB 176417
D	1913	PSU	U	modified residue	GB 176417
D	1916	H2U	U	modified residue	GB 176417
D	1919	H2U	U	modified residue	GB 176417
D	1932	PSU	U	modified residue	GB 176417
D	1937	1MG	G	modified residue	GB 176417
D	1949	5MC	C	modified residue	GB 176417
D	1954	5MU	U	modified residue	GB 176417
D	1955	PSU	U	modified residue	GB 176417

- Molecule 2 is a protein called ASPARTYL-TRNA SYNTHETASE.

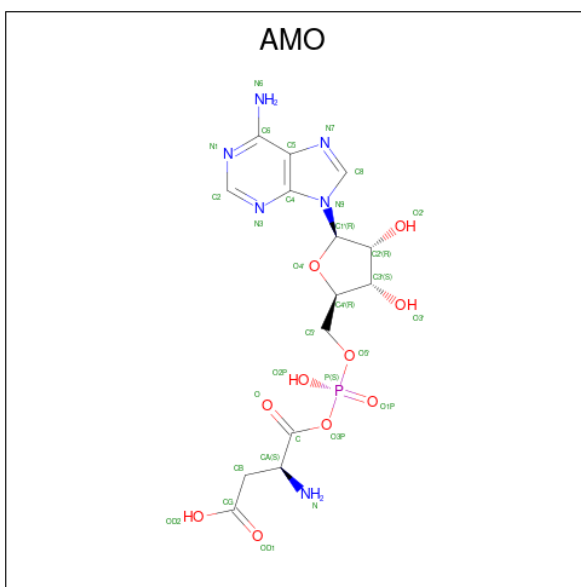
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	585	Total	C	N	O	S	0	0	0
			4591	2900	804	861	26			
2	B	585	Total	C	N	O	S	0	0	0
			4591	2900	804	861	26			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ASPARTYL-ADENOSINE-5'-MONOPHOSPHATE (CCD ID: AMO) (formula: C₁₄H₁₉N₆O₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	14	6	10	1		
4	B	1	Total	C	N	O	P	0	0
			31	14	6	10	1		

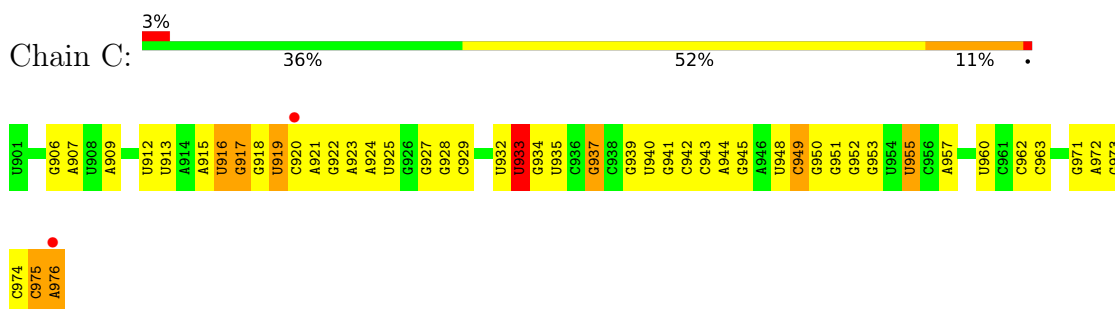
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	27	Total	O	0	0
			27	27		
5	D	33	Total	O	0	0
			33	33		
5	A	164	Total	O	0	0
			164	164		
5	B	178	Total	O	0	0
			178	178		

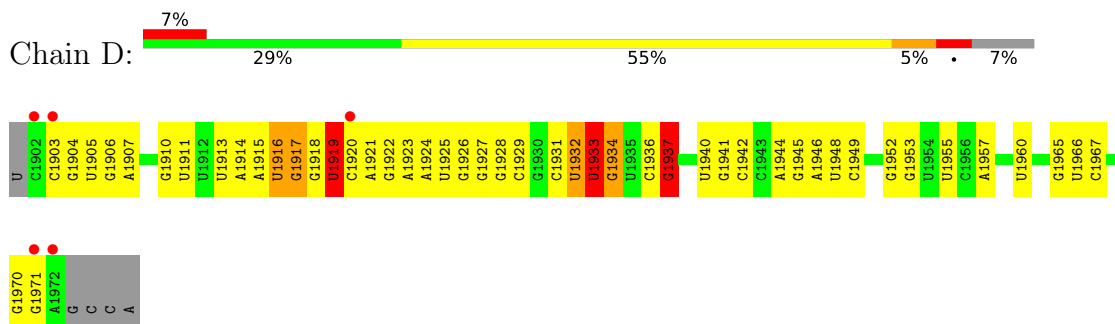
3 Residue-property plots

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

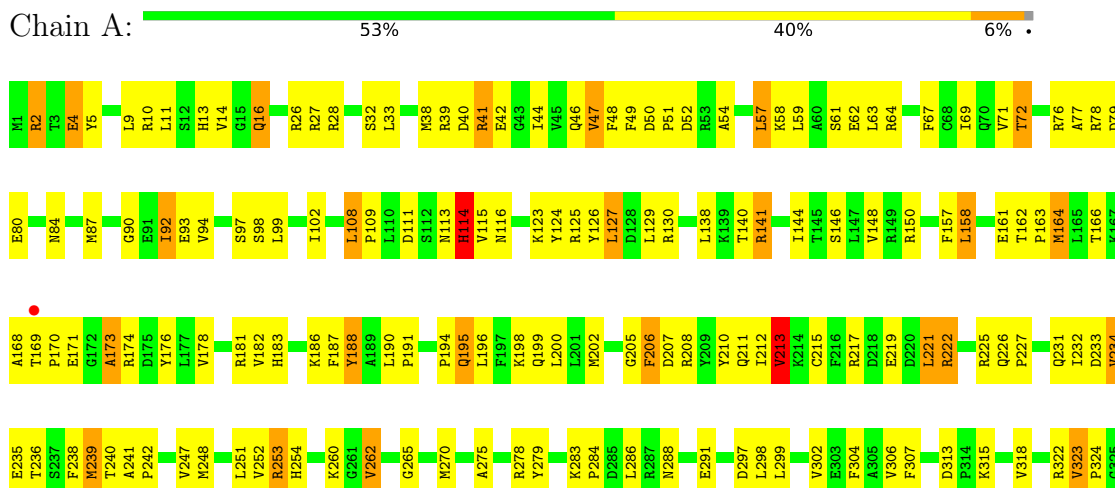
• Molecule 1: ASPARTYL TRANSFER RNA

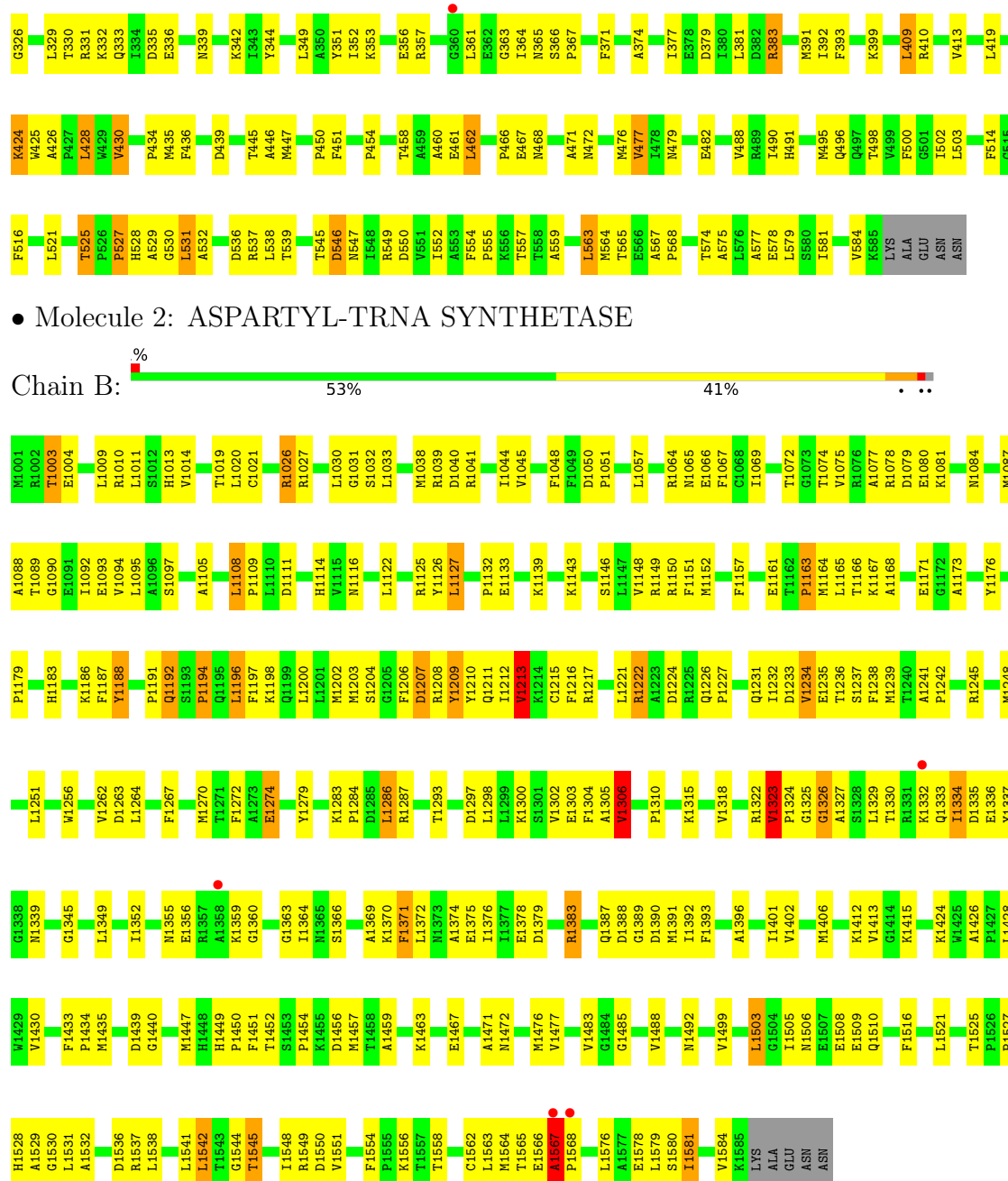


• Molecule 1: ASPARTYL TRANSFER RNA



• Molecule 2: ASPARTYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.80Å 222.80Å 80.80Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	11.50 – 2.60 11.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.1 (11.50-2.60) 87.7 (11.50-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	3.70	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.257 0.220 , 0.268	Depositor DCC
R_{free} test set	3668 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12753	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 5MU, H2U, AMO, 1MG, 5MC, PSU, SO4

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	C	0.40	0/1604	0.59	3/2500 (0.1%)
1	D	0.41	0/1487	0.59	1/2318 (0.0%)
2	A	0.49	1/4677 (0.0%)	1.08	26/6320 (0.4%)
2	B	0.47	0/4677	1.08	28/6320 (0.4%)
All	All	0.46	1/12445 (0.0%)	0.97	58/17458 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	239	MET	SD-CE	-6.05	1.64	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	206	PHE	N-CA-C	-10.66	94.78	110.23
2	B	1323	VAL	N-CA-C	9.19	116.64	107.55
2	B	1232	ILE	N-CA-C	-8.70	93.65	106.88
2	A	213	VAL	CB-CA-C	-7.60	99.96	110.90
2	A	232	ILE	N-CA-C	-7.46	95.55	106.88
2	A	554	PHE	CA-C-N	7.41	127.32	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	554	PHE	C-N-CA	7.41	127.32	120.21
2	B	1192	GLN	N-CA-C	-7.25	104.31	113.01
2	B	1554	PHE	CA-C-N	7.07	126.99	120.21
2	B	1554	PHE	C-N-CA	7.07	126.99	120.21
2	B	1449	HIS	CA-C-N	6.90	128.47	119.84
2	B	1449	HIS	C-N-CA	6.90	128.47	119.84
2	A	424	LYS	N-CA-C	6.88	118.94	109.18
2	A	190	LEU	N-CA-C	-6.78	101.52	109.93
2	A	90	GLY	N-CA-C	6.64	120.94	112.83
2	A	221	LEU	N-CA-C	6.62	119.49	110.35
2	B	1108	LEU	CA-C-N	6.48	126.61	119.87
2	B	1108	LEU	C-N-CA	6.48	126.61	119.87
2	B	1287	ARG	N-CA-C	-6.47	104.42	112.90
2	A	166	THR	N-CA-C	6.46	116.52	108.19
2	B	1207	ASP	N-CA-C	6.37	119.03	111.33
2	A	213	VAL	N-CA-C	6.21	118.68	108.99
2	A	188	TYR	N-CA-C	-6.07	100.52	109.81
2	B	1072	THR	N-CA-C	-6.03	99.88	109.59
1	C	976	A	C2'-C3'-O3'	-6.00	100.50	109.50
2	B	1334	ILE	N-CA-C	-5.98	105.02	110.82
1	C	933	U	N1-C1'-C2'	5.95	120.92	112.00
1	C	975	C	C2'-C3'-O3'	-5.94	104.79	113.70
2	B	1163	PRO	N-CA-C	5.92	121.66	111.77
2	A	114	HIS	N-CA-C	5.89	117.36	108.46
2	B	1213	VAL	N-CA-C	5.84	117.84	108.85
2	A	2	ARG	N-CA-C	-5.84	101.88	110.52
2	B	1097	SER	N-CA-C	-5.84	106.80	114.04
2	B	1567	ALA	CA-C-N	-5.82	112.57	119.84
2	B	1567	ALA	C-N-CA	-5.82	112.57	119.84
2	A	546	ASP	N-CA-C	-5.75	104.10	113.19
1	D	1933	U	N1-C1'-C2'	5.52	120.28	112.00
2	B	1069	ILE	N-CA-C	5.49	116.61	108.65
2	B	1194	PRO	N-CA-C	-5.44	108.45	114.92
2	A	472	ASN	N-CA-C	-5.40	103.85	110.65
2	A	527	PRO	N-CA-C	-5.40	101.75	110.55
2	A	108	LEU	CA-C-N	5.40	126.11	120.12
2	A	108	LEU	C-N-CA	5.40	126.11	120.12
2	B	1003	THR	N-CA-C	-5.34	106.26	114.16
2	B	1424	LYS	N-CA-C	5.30	117.66	110.35
2	B	1041	ARG	N-CA-C	5.26	117.76	111.71
2	A	575	ALA	N-CA-C	-5.26	105.44	111.07
2	A	191	PRO	N-CA-C	5.24	118.72	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1191	PRO	N-CA-C	5.24	119.43	110.95
2	A	212	ILE	N-CA-C	-5.22	98.95	106.88
2	B	1143	LYS	N-CA-C	-5.14	105.85	111.82
2	B	1168	ALA	N-CA-C	5.14	116.93	110.24
2	B	1176	TYR	N-CA-C	-5.12	101.62	109.76
2	A	173	ALA	N-CA-C	5.11	116.53	110.19
2	B	1188	TYR	N-CA-C	-5.08	102.55	110.42
2	A	164	MET	N-CA-C	-5.05	106.81	113.12
2	A	430	VAL	N-CA-C	-5.04	100.39	107.75
2	A	97	SER	N-CA-C	-5.01	107.12	114.39

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	918	G	Sidechain
1	C	933	U	Sidechain
1	D	1933	U	Sidechain

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	C	1601	0	811	53	0
1	D	1496	0	757	32	0
2	A	4591	0	4590	262	0
2	B	4591	0	4587	252	0
3	B	5	0	0	0	0
3	C	5	0	0	2	0
4	A	31	0	17	1	0
4	B	31	0	17	1	0
5	A	164	0	0	11	0
5	B	178	0	0	8	0
5	C	27	0	0	2	0
5	D	33	0	0	0	0
All	All	12753	0	10779	560	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (560) 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)
2:A:236:THR:HB	2:A:239:MET:HE3	1.40	1.01
2:A:545:THR:HG22	2:A:547:ASN:H	1.23	0.99
2:B:1009:LEU:HA	2:B:1013:HIS:HD2	1.27	0.99
2:A:161:GLU:HA	2:A:211:GLN:NE2	1.80	0.96
2:A:547:ASN:OD1	2:A:549:ARG:HG2	1.66	0.95
2:A:72:THR:HG23	2:A:98:SER:HB3	1.52	0.91
2:A:260:LYS:HB2	2:A:262:VAL:HG12	1.53	0.90
2:A:248:MET:HE2	2:A:248:MET:HA	1.56	0.88
2:A:458:THR:HB	2:A:461:GLU:HG3	1.56	0.88
2:B:1241:ALA:HB3	2:B:1242:PRO:HD3	1.58	0.85
2:B:1531:LEU:HD13	2:B:1532:ALA:N	1.92	0.84
2:A:102:ILE:HG21	2:B:1527:PRO:HD3	1.60	0.84
2:B:1009:LEU:HA	2:B:1013:HIS:CD2	2.12	0.83
2:A:545:THR:HG22	2:A:546:ASP:H	1.43	0.83
2:A:236:THR:CB	2:A:239:MET:HE3	2.09	0.82
2:B:1111:ASP:H	2:B:1116:ASN:HD21	1.25	0.82
2:B:1336:GLU:HG3	2:B:1337:TYR:H	1.44	0.81
2:B:1356:GLU:HB3	2:B:1359:LYS:HD3	1.62	0.81
2:A:491:HIS:HD2	2:A:527:PRO:HA	1.47	0.80
2:B:1163:PRO:HG2	2:B:1166:THR:CG2	2.11	0.80
2:B:1567:ALA:HB3	2:B:1568:PRO:HD3	1.62	0.80
2:A:270:MET:HE1	2:A:284:PRO:HG3	1.64	0.79
2:B:1048:PHE:HE1	2:B:1050:ASP:HB3	1.47	0.79
2:B:1326:GLY:O	2:B:1329:LEU:HD13	1.83	0.78
2:A:183:HIS:HB3	2:A:186:LYS:HD2	1.67	0.77
2:B:1026:ARG:HE	2:B:1065:ASN:HD21	1.33	0.77
2:B:1248:MET:HE2	2:B:1248:MET:HA	1.65	0.77
2:A:72:THR:CG2	2:A:98:SER:HB3	2.15	0.77
2:B:1084:ASN:HB3	2:B:1087:MET:HE2	1.68	0.76
2:A:211:GLN:CD	2:A:213:VAL:HG13	2.09	0.76
2:A:458:THR:HG22	2:A:460:ALA:H	1.51	0.76
2:A:521:LEU:HA	2:A:525:THR:HG21	1.67	0.76
1:C:915:A:H2'	1:C:916:H2U:H62	1.68	0.76
2:A:352:ILE:HA	2:A:366:SER:HB3	1.67	0.75
2:A:48:PHE:CE1	2:A:50:ASP:HB3	2.22	0.75
2:A:330:THR:HG22	2:A:332:LYS:H	1.50	0.75
2:A:545:THR:HG22	2:A:546:ASP:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:27:ARG:HD3	2:A:63:LEU:O	1.89	0.73
2:B:1336:GLU:HG3	2:B:1337:TYR:N	2.03	0.72
2:B:1302:VAL:HG12	2:B:1304:PHE:H	1.54	0.72
2:B:1415:LYS:HE3	5:B:2209:HOH:O	1.90	0.72
2:B:1562:CYS:HB3	2:B:1567:ALA:HB2	1.71	0.72
2:A:158:LEU:HD21	2:B:1139:LYS:HG2	1.71	0.71
2:B:1171:GLU:HG2	2:B:1217:ARG:NH2	2.06	0.70
1:C:933:U:H1'	2:A:33:LEU:HD13	1.74	0.70
2:A:298:LEU:HD21	2:A:379:ASP:HB3	1.73	0.70
2:B:1325:GLY:O	2:B:1327:ALA:N	2.25	0.70
2:A:10:ARG:H	2:A:13:HIS:CD2	2.10	0.69
2:B:1459:ALA:O	2:B:1463:LYS:HG2	1.91	0.69
2:B:1374:ALA:O	2:B:1378:GLU:HG3	1.92	0.69
2:A:426:ALA:H	2:A:479:ASN:ND2	1.90	0.69
2:A:426:ALA:H	2:A:479:ASN:HD21	1.40	0.69
2:A:48:PHE:HE1	2:A:50:ASP:HB3	1.55	0.69
2:B:1434:PRO:HG2	2:B:1447:MET:HG3	1.72	0.69
1:C:915:A:O2'	1:C:916:H2U:H5'	1.93	0.69
2:A:349:LEU:HD11	2:A:393:PHE:HB3	1.75	0.68
2:A:545:THR:HG22	2:A:547:ASN:N	2.01	0.68
2:A:557:THR:HG21	2:A:563:LEU:HD21	1.74	0.68
2:A:557:THR:CG2	2:A:563:LEU:HD21	2.23	0.68
2:B:1318:VAL:HG13	2:B:1396:ALA:HB2	1.75	0.68
2:A:41:ARG:HD2	5:A:2343:HOH:O	1.94	0.68
2:B:1322:ARG:HH21	2:B:1387:GLN:HG2	1.58	0.68
2:A:330:THR:HB	2:A:333:GLN:HG3	1.76	0.67
2:A:286:LEU:HD22	2:A:428:LEU:HD22	1.75	0.67
1:D:1903:C:O2'	1:D:1904:G:H5'	1.95	0.67
2:B:1352:ILE:HA	2:B:1366:SER:HB2	1.76	0.67
2:B:1499:VAL:O	2:B:1503:LEU:HD22	1.94	0.66
2:B:1077:ALA:HA	2:B:1092:ILE:HD13	1.78	0.66
2:A:545:THR:HG21	2:A:550:ASP:HB2	1.77	0.65
2:A:565:THR:HB	2:B:1167:LYS:HD2	1.78	0.65
2:B:1187:PHE:HZ	2:B:1581:ILE:HD11	1.62	0.65
2:A:270:MET:HE3	2:A:275:ALA:HB2	1.79	0.65
2:A:288:ASN:HB3	2:A:410:ARG:NH2	2.11	0.65
2:B:1364:ILE:C	2:B:1364:ILE:HD12	2.22	0.65
1:D:1970:G:O2'	1:D:1971:G:H5'	1.97	0.65
2:A:41:ARG:HH21	2:B:1208:ARG:H	1.43	0.65
2:B:1078:ARG:NH2	2:B:1087:MET:HE1	2.11	0.65
2:B:1163:PRO:HG2	2:B:1166:THR:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:ASP:HB2	2:A:51:PRO:HD2	1.77	0.65
2:A:260:LYS:HB2	2:A:262:VAL:CG1	2.25	0.64
2:B:1435:MET:HA	2:B:1471:ALA:HB2	1.80	0.64
2:A:351:TYR:O	2:A:366:SER:HB2	1.96	0.64
2:B:1084:ASN:CB	2:B:1087:MET:HE2	2.28	0.64
2:A:278:ARG:O	2:A:291:GLU:HB2	1.98	0.64
2:B:1202:MET:HE1	2:B:1207:ASP:O	1.98	0.63
2:A:202:MET:HE2	2:A:202:MET:HA	1.80	0.63
2:A:144:ILE:O	2:A:148:VAL:HG23	1.98	0.63
2:B:1078:ARG:HH22	2:B:1087:MET:HE1	1.63	0.63
2:A:162:THR:H	2:A:211:GLN:HE22	1.47	0.62
2:A:270:MET:CE	2:A:284:PRO:HG3	2.29	0.62
2:A:361:LEU:HD11	2:A:374:ALA:HB2	1.81	0.62
2:A:39:ARG:HB2	2:A:44:ILE:HG12	1.81	0.62
2:A:130:ARG:HG3	2:B:1204:SER:O	1.99	0.62
2:B:1531:LEU:HD13	2:B:1532:ALA:H	1.62	0.62
1:C:976:A:H3'	4:A:831:AMO:O1P	2.00	0.62
2:A:194:PRO:HG2	2:A:213:VAL:HG21	1.81	0.62
2:B:1026:ARG:NE	2:B:1065:ASN:HD21	1.96	0.62
2:B:1211:GLN:CD	2:B:1213:VAL:HG13	2.24	0.62
2:A:221:LEU:O	2:A:222:ARG:HD3	2.00	0.62
2:B:1164:MET:HE3	2:B:1216:PHE:CE1	2.34	0.62
2:A:236:THR:HB	2:A:239:MET:CE	2.23	0.62
2:B:1234:VAL:HG11	2:B:1248:MET:SD	2.40	0.61
2:A:322:ARG:NH1	2:A:324:PRO:HG3	2.14	0.61
2:A:462:LEU:HD22	2:A:502:ILE:CD1	2.30	0.61
1:D:1933:U:O4'	2:B:1032:SER:HB2	2.00	0.61
2:A:170:PRO:HG2	2:A:514:PHE:CZ	2.36	0.61
2:B:1485:GLY:C	2:B:1531:LEU:HD22	2.26	0.61
1:C:976:A:H5'	2:A:217:ARG:NH1	2.15	0.61
1:C:909:A:N3	1:C:945:G:H2'	2.16	0.60
2:A:531:LEU:C	2:A:531:LEU:HD23	2.26	0.60
2:A:568:PRO:HD3	2:B:1188:TYR:CE1	2.36	0.60
2:B:1375:GLU:HA	2:B:1378:GLU:OE1	2.01	0.60
2:A:196:LEU:HD21	2:A:451:PHE:CZ	2.37	0.60
2:A:326:GLY:O	2:A:329:LEU:HD13	2.01	0.60
2:B:1009:LEU:HD12	2:B:1045:VAL:HG21	1.83	0.60
1:C:976:A:N3	1:C:976:A:H2'	2.16	0.60
2:A:141:ARG:NH2	2:A:536:ASP:OD1	2.35	0.60
2:A:468:ASN:N	2:A:468:ASN:HD22	2.00	0.60
2:B:1187:PHE:CZ	2:B:1581:ILE:HD11	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1435:MET:HE1	2:B:1452:THR:O	2.02	0.60
2:A:304:PHE:HB2	2:A:371:PHE:HB3	1.84	0.60
2:A:323:VAL:CG2	2:A:326:GLY:HA3	2.32	0.60
2:A:64:ARG:HB2	2:A:67:PHE:CE2	2.37	0.59
2:A:364:ILE:HD12	2:A:364:ILE:C	2.27	0.59
1:D:1952:G:O2'	1:D:1953:G:H5'	2.02	0.59
2:A:46:GLN:NE2	2:A:78:ARG:NH1	2.51	0.59
2:B:1298:LEU:HD13	2:B:1383:ARG:NH2	2.16	0.59
2:B:1435:MET:HE2	2:B:1454:PRO:HG3	1.85	0.59
1:C:920:C:H2'	1:C:921:A:H5''	1.85	0.59
2:A:248:MET:HE2	2:A:248:MET:CA	2.31	0.59
2:B:1167:LYS:HD3	2:B:1516:PHE:CE2	2.37	0.59
2:A:126:TYR:CD1	2:A:127:LEU:HD22	2.37	0.59
2:A:221:LEU:HD12	2:A:221:LEU:N	2.17	0.59
2:A:409:LEU:CD2	2:A:413:VAL:HG23	2.33	0.59
2:A:111:ASP:HB3	2:A:114:HIS:NE2	2.17	0.59
2:A:435:MET:HE2	2:A:454:PRO:HG3	1.85	0.59
2:B:1272:PHE:CD2	2:B:1434:PRO:HD3	2.38	0.59
2:A:38:MET:HE3	2:A:69:ILE:HG13	1.84	0.58
2:B:1349:LEU:HD11	2:B:1393:PHE:HB3	1.85	0.58
2:A:235:GLU:OE2	2:A:530:GLY:HA3	2.03	0.58
2:B:1014:VAL:CG2	2:B:1092:ILE:HD11	2.33	0.58
2:A:210:TYR:HA	2:A:233:ASP:O	2.04	0.58
2:A:339:ASN:O	2:A:342:LYS:HB2	2.04	0.58
2:B:1402:VAL:O	2:B:1406:MET:HB2	2.04	0.58
2:A:130:ARG:HD2	2:B:1203:MET:O	2.03	0.58
2:A:391:MET:HG3	2:A:392:ILE:N	2.18	0.58
2:A:436:PHE:HE1	2:A:462:LEU:HD21	1.69	0.58
2:B:1467:GLU:CD	2:B:1467:GLU:H	2.12	0.58
2:B:1538:LEU:O	2:B:1542:LEU:HD22	2.03	0.58
1:C:976:A:OP1	2:A:171:GLU:O	2.21	0.58
2:B:1010:ARG:NH2	2:B:1088:ALA:HB1	2.19	0.58
2:B:1238:PHE:CE2	2:B:1527:PRO:HD2	2.39	0.58
1:C:916:H2U:H2'	1:C:960:U:O2	2.04	0.57
2:A:41:ARG:NH2	2:B:1208:ARG:H	2.03	0.57
2:B:1050:ASP:HB2	2:B:1051:PRO:CD	2.33	0.57
1:C:972:A:H2'	1:C:973:G:O4'	2.04	0.57
2:B:1009:LEU:O	2:B:1089:THR:HG22	2.04	0.57
2:B:1428:LEU:HD21	2:B:1477:VAL:HB	1.85	0.57
1:D:1941:G:H2'	1:D:1942:C:C6	2.40	0.57
2:B:1485:GLY:O	2:B:1531:LEU:HD22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:126:TYR:CE1	2:A:127:LEU:HD22	2.40	0.57
2:B:1150:ARG:NH2	5:B:2386:HOH:O	2.37	0.57
2:A:356:GLU:O	2:A:363:GLY:HA3	2.06	0.56
1:C:976:A:O2'	2:A:482:GLU:OE1	2.22	0.56
1:D:1924:A:H2'	1:D:1925:U:C6	2.40	0.56
2:B:1013:HIS:O	2:B:1075:VAL:HB	2.05	0.56
1:C:974:C:H2'	1:C:975:C:O4'	2.05	0.56
2:B:1211:GLN:CD	2:B:1213:VAL:CG1	2.79	0.56
2:B:1196:LEU:HD23	2:B:1516:PHE:HZ	1.70	0.56
1:C:933:U:H1'	2:A:33:LEU:CD1	2.36	0.56
2:A:491:HIS:CD2	2:A:527:PRO:HA	2.35	0.56
1:C:976:A:O2'	2:A:482:GLU:CD	2.49	0.56
2:B:1356:GLU:CB	2:B:1359:LYS:HD3	2.35	0.56
2:B:1126:TYR:CD1	2:B:1127:LEU:HD13	2.41	0.55
1:D:1917:G:N2	1:D:1957:A:H2'	2.21	0.55
2:B:1210:TYR:HA	2:B:1233:ASP:O	2.06	0.55
2:B:1549:ARG:HH22	2:B:1558:THR:HG23	1.71	0.55
2:B:1092:ILE:CG2	2:B:1093:GLU:N	2.69	0.55
1:C:909:A:H5''	5:C:2341:HOH:O	2.05	0.55
1:C:976:A:N3	1:C:976:A:C2'	2.70	0.55
2:A:84:ASN:CG	2:A:87:MET:HG3	2.32	0.55
2:A:278:ARG:HD2	2:A:291:GLU:OE2	2.06	0.55
2:A:410:ARG:HD3	5:A:2012:HOH:O	2.06	0.55
2:B:1545:THR:HG21	2:B:1550:ASP:HB2	1.88	0.55
2:A:170:PRO:HG2	2:A:514:PHE:HZ	1.70	0.55
2:A:434:PRO:HD2	2:A:447:MET:HE3	1.88	0.55
2:B:1183:HIS:HB3	2:B:1186:LYS:HD2	1.88	0.55
1:D:1940:U:H2'	1:D:1941:G:H8	1.73	0.54
1:C:976:A:N6	2:A:447:MET:SD	2.81	0.54
2:A:531:LEU:HD23	2:A:532:ALA:N	2.22	0.54
2:B:1428:LEU:CD2	2:B:1477:VAL:HB	2.38	0.54
2:A:545:THR:CG2	2:A:546:ASP:H	2.18	0.54
1:D:1921:A:H61	1:D:1946:A:H2'	1.70	0.54
2:A:466:PRO:HG2	2:A:467:GLU:H	1.73	0.54
1:C:944:A:O2'	1:C:945:G:H5'	2.07	0.54
2:B:1209:TYR:CG	2:B:1210:TYR:N	2.75	0.54
2:B:1048:PHE:CE1	2:B:1050:ASP:HB3	2.37	0.54
2:B:1356:GLU:HA	2:B:1388:ASP:OD2	2.07	0.54
2:B:1026:ARG:NH2	2:B:1027:ARG:HG3	2.23	0.54
2:B:1356:GLU:OE2	2:B:1388:ASP:OD2	2.25	0.54
2:B:1430:VAL:O	2:B:1433:PHE:HE1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1933:U:C2'	1:D:1934:G:OP2	2.56	0.53
2:A:211:GLN:HG2	2:A:213:VAL:HG13	1.88	0.53
2:A:488:VAL:HA	2:A:529:ALA:CB	2.38	0.53
2:B:1151:PHE:CD2	2:B:1251:LEU:HD13	2.43	0.53
2:B:1508:GLU:CD	2:B:1508:GLU:H	2.16	0.53
2:A:304:PHE:CE2	2:A:306:VAL:HB	2.44	0.53
2:A:491:HIS:HD1	2:A:491:HIS:C	2.16	0.53
2:A:211:GLN:CG	2:A:213:VAL:HG13	2.38	0.53
2:B:1537:ARG:O	2:B:1541:LEU:HD13	2.09	0.53
2:A:297:ASP:OD2	2:A:383:ARG:NH2	2.42	0.53
2:A:188:TYR:CZ	2:B:1568:PRO:HG3	2.43	0.53
2:A:253:ARG:HG3	2:A:253:ARG:HH11	1.73	0.53
1:C:912:U:H3'	5:C:2108:HOH:O	2.09	0.53
1:D:1906:G:H2'	1:D:1907:A:C8	2.44	0.53
1:D:1944:A:O2'	1:D:1945:G:H5'	2.09	0.53
2:A:198:LYS:HD2	2:A:235:GLU:HB2	1.90	0.53
2:B:1033:LEU:HD22	2:B:1048:PHE:HZ	1.74	0.53
2:B:1304:PHE:CZ	2:B:1306:VAL:HG22	2.44	0.53
1:D:1911:U:O2'	2:B:1114:HIS:HE1	1.92	0.52
2:A:129:LEU:HB2	2:B:1204:SER:HB3	1.90	0.52
2:B:1033:LEU:HD22	2:B:1048:PHE:CZ	2.43	0.52
2:A:77:ALA:HA	2:A:92:ILE:HD12	1.91	0.52
2:B:1064:ARG:HB2	2:B:1067:PHE:CE2	2.44	0.52
2:B:1161:GLU:HA	2:B:1211:GLN:OE1	2.09	0.52
2:B:1372:LEU:HD23	2:B:1376:ILE:CG2	2.39	0.52
2:B:1286:LEU:HB2	2:B:1426:ALA:HB1	1.90	0.52
2:A:545:THR:CG2	2:A:546:ASP:N	2.73	0.52
1:D:1922:G:O6	1:D:1946:A:N1	2.43	0.52
2:A:323:VAL:HG22	2:A:326:GLY:HA3	1.91	0.52
2:A:11:LEU:HA	2:A:92:ILE:HD13	1.92	0.52
2:A:241:ALA:HB3	2:A:242:PRO:HD3	1.92	0.52
2:A:248:MET:HA	2:A:248:MET:CE	2.31	0.52
1:C:962:C:H2'	1:C:963:C:H6	1.75	0.51
1:D:1914:A:O2'	1:D:1915:A:H5'	2.11	0.51
2:A:11:LEU:O	2:A:14:VAL:HG23	2.10	0.51
2:B:1167:LYS:HD3	2:B:1516:PHE:HE2	1.73	0.51
2:B:1194:PRO:HG2	2:B:1213:VAL:HG21	1.91	0.51
2:A:92:ILE:HG23	2:A:93:GLU:N	2.25	0.51
2:A:488:VAL:HA	2:A:529:ALA:HB2	1.91	0.51
2:B:1567:ALA:CB	2:B:1568:PRO:HD3	2.37	0.51
2:A:50:ASP:OD2	2:A:50:ASP:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:563:LEU:H	2:A:563:LEU:HD22	1.75	0.51
2:B:1010:ARG:H	2:B:1013:HIS:CD2	2.28	0.51
2:A:182:VAL:HG23	2:A:183:HIS:CD2	2.46	0.51
2:A:270:MET:O	2:A:430:VAL:HA	2.11	0.51
1:C:906:G:O2'	1:C:907:A:H5'	2.11	0.51
1:C:952:G:O2'	1:C:953:G:H5'	2.11	0.51
2:A:315:LYS:O	2:A:399:LYS:HG3	2.11	0.51
2:B:1033:LEU:O	2:B:1033:LEU:HD12	2.11	0.51
2:A:196:LEU:HD13	2:A:516:PHE:HZ	1.75	0.51
2:A:260:LYS:CB	2:A:262:VAL:HG12	2.33	0.51
2:A:357:ARG:HH11	2:A:357:ARG:HG2	1.75	0.51
2:B:1256:TRP:CD1	2:B:1264:LEU:HD21	2.46	0.51
2:B:1323:VAL:HG22	2:B:1323:VAL:O	2.09	0.51
2:B:1584:VAL:HG23	2:B:1584:VAL:O	2.11	0.51
1:D:1966:U:H2'	1:D:1967:C:C6	2.46	0.51
2:B:1192:GLN:HA	2:B:1216:PHE:O	2.11	0.51
2:A:221:LEU:HD12	2:A:221:LEU:H	1.77	0.50
2:A:270:MET:HE3	2:A:275:ALA:CB	2.40	0.50
1:C:962:C:H2'	1:C:963:C:C6	2.47	0.50
2:A:173:ALA:CB	2:A:217:ARG:HB3	2.42	0.50
2:B:1020:LEU:HB2	2:B:1038:MET:HE1	1.94	0.50
2:B:1330:THR:OG1	2:B:1333:GLN:HG3	2.11	0.50
2:A:252:VAL:HG21	2:A:476:MET:SD	2.52	0.50
2:B:1079:ASP:O	2:B:1080:GLU:C	2.53	0.50
2:B:1148:VAL:O	2:B:1152:MET:HG2	2.11	0.50
2:B:1111:ASP:HB3	2:B:1114:HIS:CE1	2.47	0.50
2:A:26:ARG:NH1	2:A:113:ASN:HD21	2.10	0.50
2:A:521:LEU:HA	2:A:525:THR:CG2	2.40	0.50
2:B:1537:ARG:NH2	4:B:1831:AMO:H2'2	2.26	0.50
2:A:574:THR:O	2:A:577:ALA:HB3	2.12	0.50
1:C:939:G:O2'	1:C:940:U:H5'	2.12	0.49
2:B:1078:ARG:HD2	2:B:1090:GLY:O	2.12	0.49
1:D:1941:G:H2'	1:D:1942:C:H6	1.76	0.49
2:B:1326:GLY:HA2	2:B:1329:LEU:HD13	1.94	0.49
2:A:141:ARG:HG2	2:A:539:THR:HG21	1.94	0.49
2:A:157:PHE:CD2	2:A:208:ARG:HB3	2.47	0.49
2:B:1236:THR:O	2:B:1528:HIS:HB2	2.12	0.49
2:A:13:HIS:O	2:A:16:GLN:HB2	2.13	0.49
2:A:40:ASP:O	2:A:42:GLU:N	2.45	0.49
2:B:1202:MET:HE2	2:B:1237:SER:HB3	1.93	0.49
2:A:333:GLN:O	2:A:336:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:123:LYS:HD2	2:A:124:TYR:CE1	2.48	0.49
2:A:323:VAL:CG2	2:A:323:VAL:O	2.60	0.49
2:A:545:THR:HG21	2:A:550:ASP:CB	2.42	0.49
2:B:1149:ARG:CZ	2:B:1212:ILE:HD12	2.42	0.49
1:D:1916:H2U:H2'	1:D:1960:U:O2	2.13	0.49
2:A:516:PHE:CD2	2:B:1565:THR:HG22	2.48	0.49
2:B:1164:MET:HE3	2:B:1216:PHE:CZ	2.47	0.49
2:A:238:PHE:CE2	2:B:1021:CYS:HB3	2.47	0.49
2:A:253:ARG:HG3	2:A:253:ARG:NH1	2.28	0.49
2:A:468:ASN:N	2:A:468:ASN:ND2	2.61	0.49
2:A:326:GLY:C	2:A:391:MET:HB2	2.38	0.49
2:B:1372:LEU:HD23	2:B:1376:ILE:HG21	1.93	0.49
2:B:1372:LEU:N	2:B:1372:LEU:HD12	2.28	0.49
1:C:917:G:H4'	1:C:960:U:C2	2.48	0.48
1:C:962:C:O2'	1:C:963:C:H5'	2.12	0.48
2:A:211:GLN:CD	2:A:213:VAL:CG1	2.82	0.48
2:A:445:THR:HG22	2:A:446:ALA:N	2.29	0.48
2:B:1109:PRO:HD2	2:B:1127:LEU:HD23	1.94	0.48
2:A:130:ARG:HG2	5:A:2066:HOH:O	2.12	0.48
2:B:1066:GLU:HG2	2:B:1108:LEU:HD11	1.95	0.48
2:B:1111:ASP:N	2:B:1116:ASN:HD21	2.03	0.48
2:B:1476:MET:HE2	2:B:1483:VAL:HG23	1.95	0.48
2:A:47:VAL:CG2	2:A:49:PHE:CE1	2.97	0.48
1:C:942:C:O2'	1:C:943:C:H5'	2.14	0.48
1:C:976:A:H5'	2:A:217:ARG:HH12	1.78	0.48
2:A:164:MET:HG3	2:B:1216:PHE:HZ	1.79	0.48
2:B:1179:PRO:HB2	2:B:1579:LEU:HD13	1.95	0.48
2:B:1238:PHE:HE2	2:B:1527:PRO:HD2	1.78	0.48
2:B:1488:VAL:HA	2:B:1529:ALA:HB2	1.96	0.48
1:C:912:U:C5'	2:A:116:ASN:HA	2.44	0.48
1:C:941:G:H2'	1:C:942:C:C6	2.49	0.48
2:B:1215:CYS:SG	2:B:1231:GLN:HG3	2.53	0.48
1:C:976:A:H1'	2:A:482:GLU:OE2	2.13	0.48
2:A:9:LEU:O	2:A:10:ARG:HD3	2.14	0.48
2:A:102:ILE:HD12	2:A:102:ILE:H	1.78	0.48
2:A:377:ILE:O	2:A:381:LEU:HG	2.14	0.48
2:A:567:ALA:HA	2:A:568:PRO:C	2.38	0.48
2:B:1270:MET:HG3	2:B:1274:GLU:HB3	1.96	0.48
2:B:1283:LYS:HG3	2:B:1283:LYS:O	2.14	0.48
2:B:1222:ARG:HD2	2:B:1224:ASP:OD2	2.13	0.48
2:A:161:GLU:HA	2:A:211:GLN:HE21	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:C:H42	1:C:941:G:H1	1.61	0.47
2:A:297:ASP:CG	2:A:383:ARG:HH22	2.22	0.47
2:A:330:THR:HG22	2:A:331:ARG:N	2.29	0.47
2:B:1304:PHE:CE1	2:B:1306:VAL:HG13	2.49	0.47
1:C:975:C:H1'	2:A:225:ARG:NH2	2.29	0.47
1:D:1928:G:O2'	1:D:1929:C:H5'	2.14	0.47
2:A:545:THR:CG2	2:A:547:ASN:H	2.10	0.47
2:B:1111:ASP:H	2:B:1116:ASN:ND2	2.02	0.47
2:B:1245:ARG:NH2	5:B:2107:HOH:O	2.47	0.47
1:D:1931:C:O2'	1:D:1932:PSU:H5''	2.14	0.47
2:A:253:ARG:NH1	2:A:265:GLY:O	2.48	0.47
1:D:1918:G:O2'	1:D:1919:H2U:P	2.73	0.47
2:B:1576:LEU:HB3	2:B:1581:ILE:O	2.14	0.47
1:C:935:U:O2'	2:A:28:ARG:HD2	2.14	0.47
2:B:1318:VAL:HG22	2:B:1396:ALA:HB1	1.97	0.47
2:B:1324:PRO:HA	2:B:1390:ASP:OD1	2.14	0.47
1:C:928:G:O2'	1:C:929:C:H5'	2.15	0.47
2:B:1092:ILE:HG23	2:B:1093:GLU:N	2.29	0.47
2:B:1472:ASN:HA	5:B:2081:HOH:O	2.13	0.47
1:C:944:A:C2'	1:C:945:G:H5'	2.45	0.47
2:A:58:LYS:HD3	2:A:58:LYS:C	2.40	0.47
2:A:226:GLN:HB3	5:A:2064:HOH:O	2.14	0.47
2:B:1412:LYS:O	2:B:1413:VAL:C	2.58	0.47
2:B:1235:GLU:OE2	2:B:1530:GLY:HA3	2.15	0.47
2:A:283:LYS:N	2:A:284:PRO:CD	2.77	0.46
2:B:1146:SER:O	2:B:1150:ARG:HG3	2.15	0.46
2:B:1435:MET:CE	2:B:1454:PRO:HG3	2.46	0.46
2:A:304:PHE:CZ	2:A:306:VAL:HB	2.51	0.46
2:B:1026:ARG:HE	2:B:1026:ARG:HA	1.80	0.46
2:B:1211:GLN:HG3	2:B:1213:VAL:HG13	1.98	0.46
1:C:923:A:H2'	1:C:924:A:C8	2.50	0.46
2:A:168:ALA:HB3	5:A:2370:HOH:O	2.14	0.46
2:A:236:THR:CG2	2:A:239:MET:HE3	2.45	0.46
2:B:1167:LYS:HB2	2:B:1167:LYS:HE3	1.72	0.46
2:A:76:ARG:O	2:A:92:ILE:HG13	2.15	0.46
2:A:126:TYR:CE1	2:A:127:LEU:CD2	2.98	0.46
2:A:234:VAL:HG13	2:A:531:LEU:O	2.15	0.46
2:A:299:LEU:HD12	2:A:318:VAL:HG11	1.97	0.46
2:B:1567:ALA:HB3	2:B:1568:PRO:CD	2.38	0.46
2:A:565:THR:HB	2:B:1167:LYS:CD	2.46	0.46
2:B:1300:LYS:HG2	5:B:2305:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1330:THR:O	2:B:1334:ILE:HD13	2.16	0.46
2:B:1492:ASN:HB2	5:B:2273:HOH:O	2.14	0.46
2:B:1030:LEU:N	2:B:1030:LEU:HD12	2.30	0.46
2:B:1166:THR:HG21	2:B:1197:PHE:CE2	2.51	0.46
2:B:1196:LEU:HD11	2:B:1451:PHE:CE1	2.50	0.46
2:B:1567:ALA:O	2:B:1568:PRO:C	2.53	0.46
2:A:162:THR:HB	2:A:163:PRO:HD2	1.98	0.46
2:A:313:ASP:OD1	2:A:315:LYS:N	2.47	0.46
2:A:498:THR:O	2:A:502:ILE:HG13	2.16	0.46
2:B:1038:MET:O	2:B:1044:ILE:HA	2.15	0.46
1:C:933:U:C1'	2:A:33:LEU:HD13	2.45	0.46
2:A:206:PHE:O	5:A:2336:HOH:O	2.20	0.46
2:A:324:PRO:HD2	2:A:419:LEU:HD13	1.97	0.46
2:B:1329:LEU:HA	2:B:1333:GLN:OE1	2.15	0.46
1:C:971:G:O2'	1:C:972:A:H5'	2.16	0.46
2:A:196:LEU:HD13	2:A:516:PHE:CZ	2.50	0.46
2:B:1066:GLU:O	2:B:1105:ALA:HB2	2.16	0.45
2:A:306:VAL:HG12	2:A:307:PHE:CD2	2.51	0.45
2:A:579:LEU:HB3	2:A:581:ILE:HG12	1.97	0.45
2:B:1327:ALA:CB	2:B:1389:GLY:O	2.65	0.45
1:D:1910:G:C2	1:D:1926:G:H1'	2.51	0.45
2:B:1202:MET:HE2	2:B:1237:SER:CB	2.46	0.45
2:B:1262:VAL:CG1	2:B:1263:ASP:N	2.80	0.45
2:B:1336:GLU:O	2:B:1339:ASN:N	2.49	0.45
2:A:111:ASP:HB3	2:A:114:HIS:HE2	1.82	0.45
2:B:1009:LEU:O	2:B:1010:ARG:HD2	2.16	0.45
2:B:1248:MET:HA	2:B:1248:MET:CE	2.43	0.45
2:A:278:ARG:HB2	2:A:279:TYR:CE1	2.51	0.45
2:B:1208:ARG:NH2	2:B:1239:MET:SD	2.88	0.45
2:B:1241:ALA:HB3	2:B:1242:PRO:CD	2.40	0.45
2:B:1506:ASN:O	2:B:1510:GLN:HG3	2.17	0.45
2:B:1505:ILE:HG23	2:B:1509:GLU:CG	2.47	0.45
1:D:1923:A:H2'	1:D:1924:A:C8	2.52	0.45
2:A:41:ARG:HG3	2:A:42:GLU:N	2.32	0.45
2:B:1196:LEU:HD11	2:B:1451:PHE:CZ	2.52	0.45
2:B:1297:ASP:OD2	2:B:1383:ARG:NH2	2.49	0.45
2:B:1355:ASN:HB2	2:B:1363:GLY:O	2.17	0.45
2:A:450:PRO:HB3	2:A:503:LEU:CD1	2.47	0.45
2:B:1108:LEU:HA	2:B:1109:PRO:HD3	1.67	0.45
2:A:323:VAL:HG22	2:A:323:VAL:O	2.16	0.45
2:A:366:SER:HA	2:A:367:PRO:HD3	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1226:GLN:HG2	2:B:1548:ILE:HD13	1.99	0.45
2:A:207:ASP:HA	5:A:2336:HOH:O	2.16	0.44
2:A:240:THR:HB	2:A:242:PRO:HD2	1.99	0.44
2:A:251:LEU:O	2:A:254:HIS:HB3	2.18	0.44
2:A:490:ILE:HD13	2:A:495:MET:HG3	1.98	0.44
2:B:1325:GLY:O	2:B:1389:GLY:O	2.34	0.44
2:A:333:GLN:HA	2:A:336:GLU:HG2	2.00	0.44
2:B:1026:ARG:HA	2:B:1065:ASN:HD21	1.82	0.44
2:B:1439:ASP:OD2	2:B:1440:GLY:N	2.50	0.44
2:A:102:ILE:HD12	2:A:102:ILE:N	2.33	0.44
2:B:1391:MET:HG3	2:B:1392:ILE:N	2.33	0.44
2:A:79:ASP:O	2:A:80:GLU:C	2.61	0.44
2:A:247:VAL:HG13	2:A:248:MET:HE3	1.99	0.44
2:B:1304:PHE:CE2	2:B:1306:VAL:HG22	2.51	0.44
2:B:1359:LYS:HB2	2:B:1363:GLY:HA3	2.00	0.44
2:A:298:LEU:HD21	2:A:379:ASP:CB	2.43	0.44
2:B:1004:GLU:HG2	2:B:1009:LEU:HD21	1.98	0.44
2:B:1366:SER:HB3	2:B:1369:ALA:HB2	2.00	0.44
1:C:950:G:O2'	1:C:951:G:H5'	2.17	0.44
1:D:1933:U:O2'	1:D:1934:G:OP2	2.35	0.44
2:A:215:CYS:SG	2:A:231:GLN:HG3	2.58	0.44
2:A:424:LYS:HD2	2:A:424:LYS:HA	1.73	0.44
2:B:1040:ASP:OD2	2:B:1040:ASP:C	2.61	0.44
2:B:1488:VAL:HA	2:B:1529:ALA:CB	2.47	0.44
1:C:975:C:H4'	2:A:219:GLU:HG3	2.00	0.44
2:A:49:PHE:HB3	2:A:57:LEU:HD22	2.00	0.44
2:A:169:THR:HG21	2:A:195:GLN:HB3	2.00	0.44
2:A:187:PHE:N	2:A:187:PHE:CD1	2.85	0.44
2:A:199:GLN:HG2	2:A:528:HIS:CD2	2.53	0.44
2:A:454:PRO:HG2	2:A:462:LEU:HD12	2.00	0.44
2:B:1270:MET:O	2:B:1430:VAL:HA	2.18	0.44
2:B:1370:LYS:HG3	2:B:1371:PHE:N	2.32	0.44
1:C:955:PSU:H2'	1:C:957:A:OP2	2.17	0.44
2:B:1198:LYS:HD2	2:B:1235:GLU:HB2	1.99	0.44
2:B:1322:ARG:O	2:B:1322:ARG:HD3	2.18	0.44
2:A:286:LEU:HB2	2:A:426:ALA:HB1	1.99	0.44
2:A:491:HIS:C	2:A:491:HIS:ND1	2.75	0.44
2:B:1039:ARG:NH2	2:B:1066:GLU:OE1	2.51	0.44
2:B:1132:PRO:HD2	2:B:1133:GLU:OE1	2.17	0.44
2:B:1356:GLU:CD	2:B:1388:ASP:OD2	2.61	0.44
2:B:1327:ALA:HB3	2:B:1389:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1435:MET:CE	2:B:1452:THR:O	2.66	0.43
2:A:188:TYR:CE1	2:B:1568:PRO:HG3	2.54	0.43
2:B:1087:MET:HE1	5:B:2099:HOH:O	2.18	0.43
2:B:1521:LEU:HA	2:B:1525:THR:OG1	2.18	0.43
2:A:49:PHE:CZ	2:A:99:LEU:HD22	2.53	0.43
2:B:1039:ARG:HB2	2:B:1044:ILE:HG12	2.01	0.43
2:B:1283:LYS:HA	2:B:1477:VAL:HG21	2.00	0.43
1:C:976:A:O2'	2:A:482:GLU:OE2	2.36	0.43
2:A:111:ASP:HB3	2:A:114:HIS:CD2	2.53	0.43
2:A:174:ARG:NE	2:B:1578:GLU:OE2	2.49	0.43
2:A:557:THR:C	2:A:559:ALA:H	2.26	0.43
2:B:1127:LEU:HD12	2:B:1127:LEU:HA	1.85	0.43
1:D:1936:C:O3'	1:D:1937:1MG:H3'	2.19	0.43
1:C:921:A:O2'	1:C:922:G:C8	2.69	0.43
2:A:5:TYR:HB3	2:A:42:GLU:HB2	1.99	0.43
2:A:26:ARG:HH12	2:A:113:ASN:HD21	1.67	0.43
2:B:1302:VAL:HG12	2:B:1304:PHE:N	2.29	0.43
2:B:1579:LEU:O	2:B:1580:SER:C	2.61	0.43
2:B:1026:ARG:HH21	2:B:1027:ARG:HG3	1.83	0.43
1:D:1934:G:O2'	2:B:1081:LYS:HE3	2.19	0.43
2:A:357:ARG:HG2	2:A:357:ARG:NH1	2.34	0.43
2:A:496:GLN:NE2	2:A:500:PHE:CE2	2.86	0.43
2:B:1196:LEU:HD23	2:B:1516:PHE:CZ	2.52	0.43
2:B:1262:VAL:HG12	2:B:1263:ASP:N	2.34	0.43
1:C:920:C:C2'	1:C:921:A:H5''	2.47	0.43
2:A:176:TYR:OH	2:A:227:PRO:HB2	2.18	0.43
1:C:951:G:H2'	1:C:952:G:O4'	2.19	0.42
2:A:59:LEU:C	2:A:59:LEU:HD13	2.44	0.42
2:B:1505:ILE:HG23	2:B:1509:GLU:HG2	2.00	0.42
2:A:205:GLY:O	2:A:206:PHE:C	2.57	0.42
2:B:1165:LEU:HD23	2:B:1165:LEU:HA	1.89	0.42
2:B:1227:PRO:HG3	2:B:1556:LYS:HG3	1.99	0.42
2:A:426:ALA:N	2:A:479:ASN:HD21	2.14	0.42
2:A:568:PRO:HD3	2:B:1188:TYR:CZ	2.54	0.42
2:B:1157:PHE:CD2	2:B:1208:ARG:HB3	2.54	0.42
2:A:409:LEU:CD2	2:A:413:VAL:CG2	2.98	0.42
2:A:424:LYS:HG3	2:A:425:TRP:H	1.84	0.42
2:A:434:PRO:HG3	5:A:2236:HOH:O	2.18	0.42
2:B:1548:ILE:O	2:B:1551:VAL:HG22	2.18	0.42
2:A:169:THR:HG23	2:A:196:LEU:HG	2.01	0.42
2:B:1198:LYS:HB3	2:B:1209:TYR:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1941:G:O2'	1:D:1942:C:H5'	2.20	0.42
2:A:32:SER:O	2:A:33:LEU:HD12	2.19	0.42
2:B:1211:GLN:CG	2:B:1213:VAL:HG13	2.50	0.42
2:B:1267:PHE:CD2	2:B:1267:PHE:N	2.87	0.42
2:B:1345:GLY:O	2:B:1401:ILE:HD13	2.19	0.42
1:D:1904:G:H2'	1:D:1905:U:O4'	2.20	0.42
1:D:1970:G:C2'	1:D:1971:G:H5'	2.49	0.42
2:A:127:LEU:HA	2:A:130:ARG:HD3	2.01	0.42
2:A:330:THR:CG2	2:A:331:ARG:N	2.83	0.42
1:C:927:G:O2'	1:C:928:G:H5'	2.20	0.42
2:A:202:MET:HE2	2:A:202:MET:CA	2.47	0.42
2:A:239:MET:HE2	5:A:2061:HOH:O	2.20	0.42
2:A:428:LEU:HG	2:A:477:VAL:HG22	2.01	0.42
2:B:1030:LEU:N	2:B:1030:LEU:CD1	2.82	0.42
2:B:1315:LYS:HE2	2:B:1315:LYS:HB3	1.78	0.42
2:A:552:ILE:O	2:A:555:PRO:HG3	2.19	0.42
2:B:1279:TYR:CD1	2:B:1284:PRO:HB3	2.55	0.42
2:B:1364:ILE:C	2:B:1364:ILE:CD1	2.93	0.42
2:B:1293:THR:HG21	2:B:1383:ARG:HG2	2.02	0.41
2:B:1298:LEU:HD13	2:B:1383:ARG:HH22	1.82	0.41
1:C:976:A:H4'	3:C:701:SO4:O3	2.20	0.41
2:B:1014:VAL:HG22	2:B:1092:ILE:HD11	2.02	0.41
2:B:1330:THR:HG23	2:B:1333:GLN:OE1	2.20	0.41
2:B:1549:ARG:NH2	2:B:1558:THR:HG23	2.36	0.41
1:D:1965:G:H2'	1:D:1966:U:C6	2.55	0.41
2:A:146:SER:O	2:A:150:ARG:HG3	2.20	0.41
2:A:178:VAL:HB	2:A:188:TYR:HB2	2.01	0.41
2:A:435:MET:HA	2:A:471:ALA:HB2	2.03	0.41
2:A:557:THR:C	2:A:559:ALA:N	2.76	0.41
2:A:564:MET:SD	2:B:1200:LEU:HD13	2.60	0.41
2:B:1298:LEU:HD21	2:B:1379:ASP:HB3	2.03	0.41
2:B:1567:ALA:CB	2:B:1568:PRO:CD	2.98	0.41
2:B:1196:LEU:O	2:B:1200:LEU:HG	2.21	0.41
2:B:1221:LEU:HD11	2:B:1227:PRO:HD3	2.02	0.41
1:D:1933:U:O2'	1:D:1934:G:P	2.79	0.41
2:A:4:GLU:HG3	5:A:2304:HOH:O	2.20	0.41
2:A:38:MET:O	2:A:44:ILE:HA	2.20	0.41
2:A:58:LYS:O	2:A:61:SER:HB2	2.20	0.41
2:A:138:LEU:HD12	2:B:1206:PHE:CZ	2.55	0.41
2:A:181:ARG:HG3	2:A:578:GLU:HB2	2.02	0.41
3:C:701:SO4:O1	2:A:537:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:ARG:HG2	2:A:40:ASP:N	2.34	0.41
2:A:353:LYS:HE2	2:A:391:MET:HE1	2.03	0.41
2:A:46:GLN:HE22	2:A:78:ARG:HH11	1.69	0.41
2:A:140:THR:O	2:A:144:ILE:HG13	2.21	0.41
2:A:364:ILE:HD12	2:A:365:ASN:N	2.36	0.41
2:B:1066:GLU:CG	2:B:1108:LEU:HD11	2.50	0.41
2:B:1360:GLY:O	2:B:1363:GLY:N	2.51	0.41
2:B:1536:ASP:HB2	5:B:2015:HOH:O	2.21	0.41
1:D:1926:G:O2'	1:D:1927:G:H5'	2.20	0.41
2:A:50:ASP:C	2:A:57:LEU:HD23	2.45	0.41
2:A:108:LEU:HA	2:A:109:PRO:HD3	1.69	0.41
2:A:200:LEU:HD13	2:B:1564:MET:SD	2.61	0.41
2:A:344:TYR:CD1	2:A:344:TYR:N	2.88	0.41
2:B:1003:THR:HG23	2:B:1019:THR:HB	2.02	0.41
2:B:1173:ALA:O	2:B:1192:GLN:NE2	2.53	0.41
2:B:1332:LYS:HD2	2:B:1335:ASP:HB2	2.02	0.41
1:C:924:A:H2'	1:C:925:U:C6	2.56	0.41
2:A:138:LEU:HD23	2:A:138:LEU:HA	1.82	0.40
1:C:939:G:H2'	1:C:940:U:O4'	2.21	0.40
2:A:536:ASP:HB2	5:A:2328:HOH:O	2.21	0.40
2:A:63:LEU:HD11	2:A:99:LEU:HD21	2.02	0.40
2:B:1020:LEU:HB2	2:B:1038:MET:CE	2.51	0.40
2:B:1026:ARG:HA	2:B:1065:ASN:ND2	2.35	0.40
2:B:1126:TYR:CE1	2:B:1127:LEU:HD13	2.56	0.40
2:B:1430:VAL:O	2:B:1433:PHE:CE1	2.72	0.40
2:B:1456:ASP:C	2:B:1457:MET:HG3	2.46	0.40
2:B:1565:THR:O	2:B:1566:GLU:HB2	2.21	0.40
1:C:949:5MC:H2'	1:C:950:G:C8	2.56	0.40
1:C:949:5MC:H2'	1:C:950:G:H8	1.87	0.40
2:A:584:VAL:HG22	2:B:1580:SER:CA	2.51	0.40
2:B:1306:VAL:O	2:B:1310:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	583/590 (99%)	539 (92%)	40 (7%)	4 (1%)	18	38
2	B	583/590 (99%)	520 (89%)	55 (9%)	8 (1%)	9	19
All	All	1166/1180 (99%)	1059 (91%)	95 (8%)	12 (1%)	12	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	41	ARG
2	A	115	VAL
2	B	1305	ALA
2	B	1326	GLY
2	B	1567	ALA
2	A	54	ALA
2	A	195	GLN
2	B	1371	PHE
2	B	1031	GLY
2	B	1450	PRO
2	B	1306	VAL
2	B	1544	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	
2	A	486/490 (99%)	452 (93%)	34 (7%)	14	31
2	B	486/490 (99%)	461 (95%)	25 (5%)	21	45
All	All	972/980 (99%)	913 (94%)	59 (6%)	17	37

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	ARG

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Mol	Chain	Res	Type
2	A	4	GLU
2	A	16	GLN
2	A	47	VAL
2	A	52	ASP
2	A	57	LEU
2	A	62	GLU
2	A	71	VAL
2	A	72	THR
2	A	92	ILE
2	A	94	VAL
2	A	114	HIS
2	A	125	ARG
2	A	127	LEU
2	A	141	ARG
2	A	158	LEU
2	A	213	VAL
2	A	222	ARG
2	A	234	VAL
2	A	253	ARG
2	A	262	VAL
2	A	302	VAL
2	A	323	VAL
2	A	335	ASP
2	A	383	ARG
2	A	409	LEU
2	A	428	LEU
2	A	439	ASP
2	A	462	LEU
2	A	477	VAL
2	A	525	THR
2	A	531	LEU
2	A	538	LEU
2	A	563	LEU
2	B	1011	LEU
2	B	1026	ARG
2	B	1057	LEU
2	B	1074	THR
2	B	1094	VAL
2	B	1095	LEU
2	B	1122	LEU
2	B	1125	ARG
2	B	1127	LEU

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Mol	Chain	Res	Type
2	B	1196	LEU
2	B	1209	TYR
2	B	1213	VAL
2	B	1222	ARG
2	B	1234	VAL
2	B	1274	GLU
2	B	1286	LEU
2	B	1303	GLU
2	B	1306	VAL
2	B	1323	VAL
2	B	1383	ARG
2	B	1503	LEU
2	B	1542	LEU
2	B	1545	THR
2	B	1563	LEU
2	B	1581	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	13	HIS
2	A	70	GLN
2	A	113	ASN
2	A	136	GLN
2	A	195	GLN
2	A	199	GLN
2	A	211	GLN
2	A	226	GLN
2	A	339	ASN
2	A	365	ASN
2	A	468	ASN
2	A	479	ASN
2	A	491	HIS
2	A	528	HIS
2	B	1008	GLN
2	B	1013	HIS
2	B	1065	ASN
2	B	1113	ASN
2	B	1114	HIS
2	B	1116	ASN
2	B	1195	GLN
2	B	1231	GLN

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Mol	Chain	Res	Type
2	B	1497	GLN
2	B	1510	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	6 (8%)	0
1	D	69/75 (92%)	6 (8%)	1 (1%)
All	All	143/150 (95%)	12 (8%)	1 (0%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	917	G
1	C	919	H2U
1	C	933	U
1	C	934	G
1	C	937	1MG
1	C	948	U
1	D	1917	G
1	D	1919	H2U
1	D	1920	C
1	D	1934	G
1	D	1937	1MG
1	D	1948	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	1933	U

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

16 non-standard protein/DNA/RNA residues 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
1	H2U	C	916	1	18,21,22	0.89	1 (5%)	19,30,33	0.68	0
1	5MU	D	1954	1	19,22,23	0.33	0	27,32,35	0.54	0
1	H2U	D	1916	1	18,21,22	0.71	1 (5%)	19,30,33	0.62	0
1	1MG	D	1937	1	23,26,27	0.51	0	33,39,42	1.22	3 (9%)
1	5MC	D	1949	1	19,22,23	0.39	0	26,32,35	0.85	2 (7%)
1	PSU	D	1955	1	18,21,22	1.86	1 (5%)	21,30,33	0.68	1 (4%)
1	1MG	C	937	1	23,26,27	0.53	0	33,39,42	1.16	3 (9%)
1	PSU	C	932	1	18,21,22	1.83	1 (5%)	21,30,33	0.81	1 (4%)
1	H2U	D	1919	1	18,21,22	0.71	1 (5%)	19,30,33	0.72	0
1	PSU	C	913	1	18,21,22	1.81	1 (5%)	21,30,33	0.86	2 (9%)
1	5MU	C	954	1	19,22,23	0.27	0	27,32,35	0.37	0
1	5MC	C	949	1	19,22,23	0.53	0	26,32,35	0.87	2 (7%)
1	PSU	C	955	1	18,21,22	1.79	1 (5%)	21,30,33	0.75	1 (4%)
1	PSU	D	1932	1	18,21,22	1.82	1 (5%)	21,30,33	0.81	1 (4%)
1	H2U	C	919	1	18,21,22	0.62	1 (5%)	19,30,33	0.78	0
1	PSU	D	1913	1	18,21,22	1.86	1 (5%)	21,30,33	0.87	2 (9%)

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
1	H2U	C	916	1	-	0/7/38/39	0/2/2/2
1	5MU	D	1954	1	-	0/7/25/26	0/2/2/2
1	H2U	D	1916	1	-	0/7/38/39	0/2/2/2
1	1MG	D	1937	1	-	1/7/25/26	0/3/3/3
1	5MC	D	1949	1	-	0/7/25/26	0/2/2/2
1	PSU	D	1955	1	-	0/7/25/26	0/2/2/2
1	1MG	C	937	1	-	0/7/25/26	0/3/3/3
1	PSU	C	932	1	-	1/7/25/26	0/2/2/2
1	H2U	D	1919	1	-	4/7/38/39	0/2/2/2
1	PSU	C	913	1	-	2/7/25/26	0/2/2/2
1	5MU	C	954	1	-	0/7/25/26	0/2/2/2
1	5MC	C	949	1	-	2/7/25/26	0/2/2/2
1	PSU	C	955	1	-	1/7/25/26	0/2/2/2
1	PSU	D	1932	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	H2U	C	919	1	-	0/7/38/39	0/2/2/2
1	PSU	D	1913	1	-	3/7/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1913	PSU	C6-N1	-7.36	1.24	1.36
1	D	1932	PSU	C6-N1	-7.35	1.24	1.36
1	D	1955	PSU	C6-N1	-7.25	1.24	1.36
1	C	913	PSU	C6-N1	-7.25	1.24	1.36
1	C	955	PSU	C6-N1	-7.21	1.24	1.36
1	C	932	PSU	C6-N1	-7.15	1.24	1.36
1	C	916	H2U	C2-N1	3.08	1.39	1.35
1	D	1919	H2U	C2-N1	2.51	1.39	1.35
1	D	1916	H2U	C2-N1	2.32	1.38	1.35
1	C	919	H2U	C2-N1	2.02	1.38	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1937	1MG	C2-N1-C6	4.39	124.65	120.99
1	C	937	1MG	C2-N1-C6	4.27	124.55	120.99
1	D	1937	1MG	N2-C2-N1	-3.36	116.08	118.79
1	C	937	1MG	N2-C2-N1	-3.22	116.19	118.79
1	D	1949	5MC	C5-C6-N1	-3.08	119.97	123.31
1	D	1937	1MG	CM1-N1-C2	-2.96	117.64	120.70
1	C	949	5MC	C5-C6-N1	-2.77	120.30	123.31
1	C	937	1MG	CM1-N1-C2	-2.69	117.92	120.70
1	D	1932	PSU	C5-C6-N1	2.55	125.69	122.14
1	C	932	PSU	C5-C6-N1	2.37	125.43	122.14
1	C	949	5MC	CM5-C5-C6	-2.28	119.77	122.85
1	C	955	PSU	C5-C6-N1	2.16	125.14	122.14
1	D	1913	PSU	O4'-C1'-C2'	2.09	108.05	105.15
1	D	1913	PSU	C5-C6-N1	2.05	124.99	122.14
1	C	913	PSU	C5-C6-N1	2.05	124.98	122.14
1	D	1949	5MC	CM5-C5-C6	-2.02	120.12	122.85
1	C	913	PSU	O4'-C1'-C2'	2.02	107.94	105.15
1	D	1955	PSU	C5-C6-N1	2.01	124.93	122.14

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	1919	H2U	O4'-C1'-N1-C2
1	D	1919	H2U	O4'-C1'-N1-C6
1	D	1913	PSU	O4'-C4'-C5'-O5'
1	D	1919	H2U	C2'-C1'-N1-C6
1	D	1919	H2U	C2'-C1'-N1-C2
1	C	949	5MC	O4'-C4'-C5'-O5'
1	D	1913	PSU	C3'-C4'-C5'-O5'
1	C	949	5MC	C3'-C4'-C5'-O5'
1	C	913	PSU	O4'-C1'-C5-C4
1	C	955	PSU	O4'-C1'-C5-C4
1	D	1913	PSU	O4'-C1'-C5-C4
1	C	913	PSU	O4'-C4'-C5'-O5'
1	D	1937	1MG	C4'-C5'-O5'-P
1	C	932	PSU	O4'-C1'-C5-C6
1	D	1932	PSU	O4'-C1'-C5-C6

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	916	H2U	3	0
1	D	1916	H2U	1	0
1	D	1937	1MG	1	0
1	D	1919	H2U	1	0
1	C	949	5MC	2	0
1	C	955	PSU	1	0
1	D	1932	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AMO	B	1831	-	32,33,33	0.67	1 (3%)	46,49,49	1.01	1 (2%)
3	SO4	C	701	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	B	1701	-	4,4,4	0.35	0	6,6,6	0.10	0
4	AMO	A	831	-	32,33,33	0.73	1 (3%)	46,49,49	1.21	2 (4%)

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
4	AMO	B	1831	-	-	1/21/39/39	0/3/3/3
4	AMO	A	831	-	-	1/21/39/39	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	831	AMO	P-O3P	2.91	1.65	1.60
4	B	1831	AMO	P-O3P	2.40	1.64	1.60

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	831	AMO	O3P-P-O5'	6.90	123.74	103.00
4	B	1831	AMO	O3P-P-O5'	5.43	119.31	103.00
4	A	831	AMO	O2P-P-O3P	-2.46	96.98	104.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

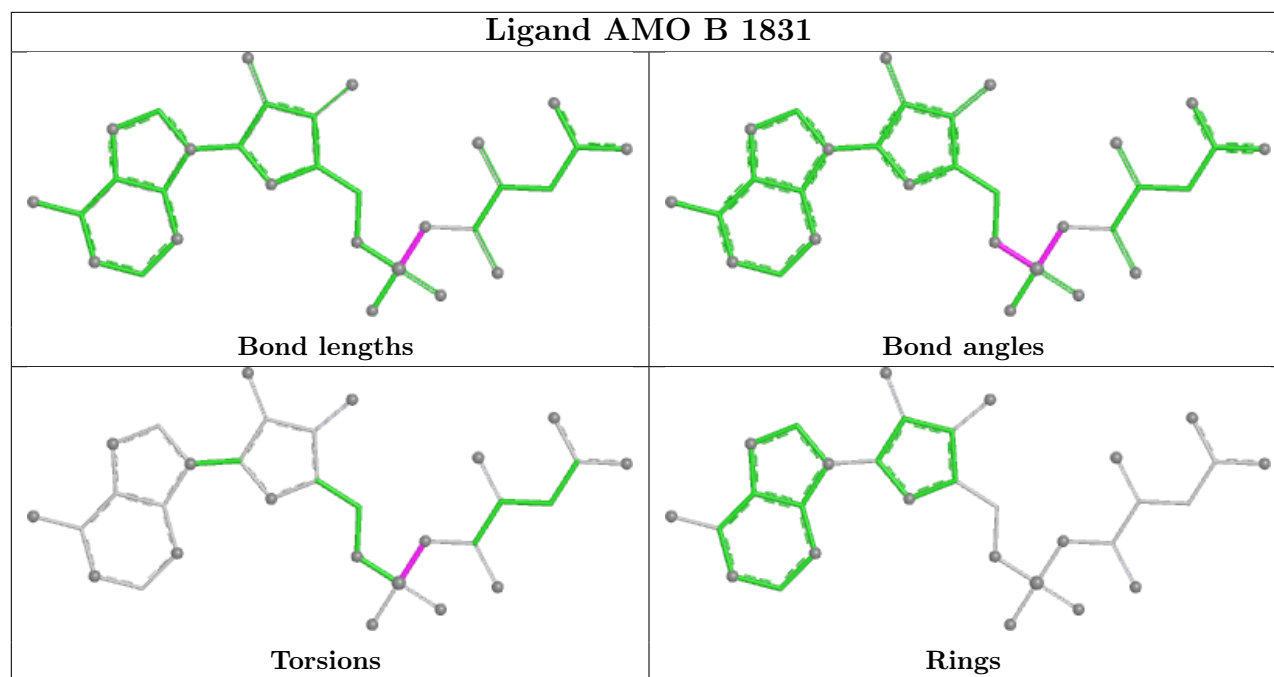
Mol	Chain	Res	Type	Atoms
4	B	1831	AMO	C-O3P-P-O5'
4	A	831	AMO	C-O3P-P-O5'

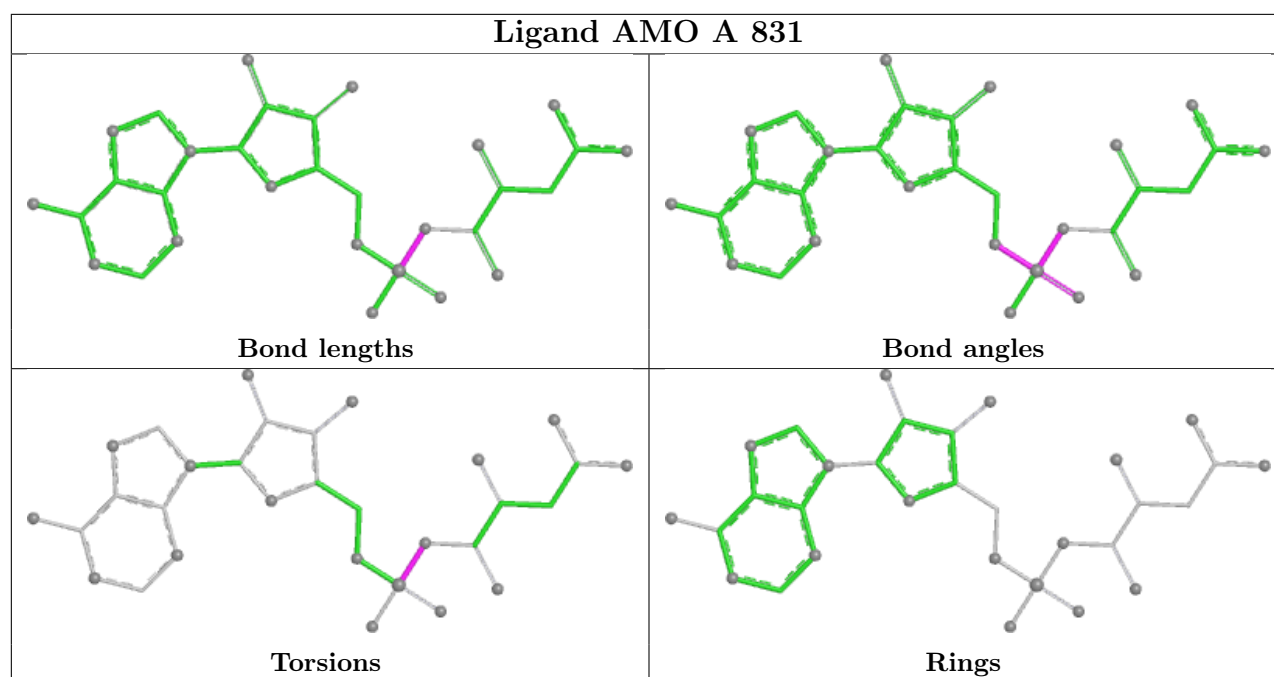
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1831	AMO	1	0
3	C	701	SO4	2	0
4	A	831	AMO	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	C	67/75 (89%)	0.19	2 (2%) 52 47	36, 59, 80, 99	0
1	D	62/75 (82%)	0.11	5 (8%) 18 14	39, 54, 94, 101	0
2	A	585/590 (99%)	-0.47	2 (0%) 90 88	18, 37, 66, 86	0
2	B	585/590 (99%)	-0.41	4 (0%) 84 82	20, 40, 67, 92	0
All	All	1299/1330 (97%)	-0.38	13 (1%) 79 76	18, 41, 70, 101	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1567	ALA	5.0
1	D	1920	C	4.6
1	C	976	A	3.6
1	D	1972	A	3.2
1	D	1902	C	3.0
1	C	920	C	2.8
2	A	169	THR	2.7
2	A	360	GLY	2.6
1	D	1903	C	2.4
2	B	1358	ALA	2.3
2	B	1332	LYS	2.2
1	D	1971	G	2.0
2	B	1568	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	H2U	D	1919	20/21	0.68	0.22	92,101,101,101	0
1	H2U	C	919	20/21	0.71	0.17	99,101,101,101	0
1	5MU	C	954	21/22	0.81	0.13	38,70,83,85	0
1	PSU	C	955	20/21	0.83	0.14	64,76,87,89	0
1	5MC	C	949	21/22	0.83	0.14	50,68,87,89	0
1	PSU	C	932	20/21	0.87	0.11	50,70,76,81	0
1	PSU	D	1932	20/21	0.90	0.12	55,63,66,70	0
1	1MG	D	1937	24/25	0.90	0.11	58,72,100,101	0
1	H2U	D	1916	20/21	0.91	0.09	59,65,69,71	0
1	1MG	C	937	24/25	0.91	0.10	57,66,91,91	0
1	H2U	C	916	20/21	0.92	0.09	63,67,72,73	0
1	PSU	D	1955	20/21	0.93	0.10	37,49,56,57	0
1	PSU	D	1913	20/21	0.94	0.10	43,56,63,64	0
1	5MC	D	1949	21/22	0.94	0.09	46,51,54,57	0
1	PSU	C	913	20/21	0.94	0.09	44,52,60,60	0
1	5MU	D	1954	21/22	0.97	0.07	29,45,51,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

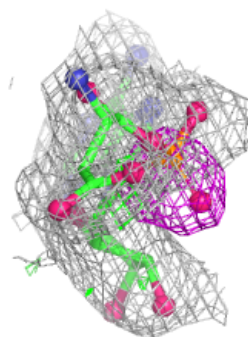
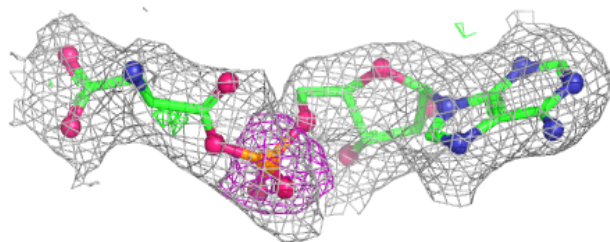
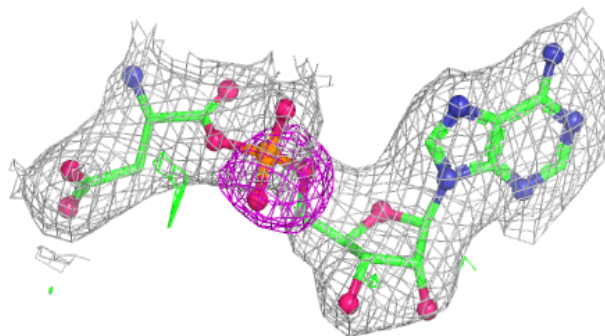
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	701	5/5	0.85	0.20	97,97,100,101	0
4	AMO	B	1831	31/31	0.90	0.11	23,36,65,75	0
4	AMO	A	831	31/31	0.91	0.10	16,33,64,72	0
3	SO4	B	1701	5/5	0.93	0.08	64,68,72,72	0

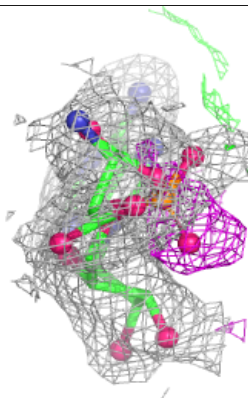
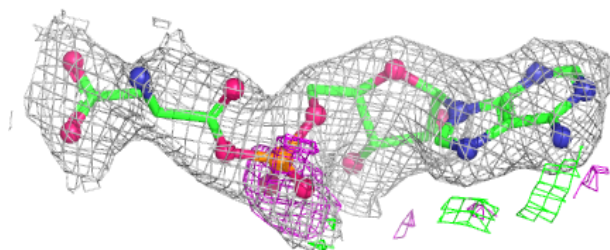
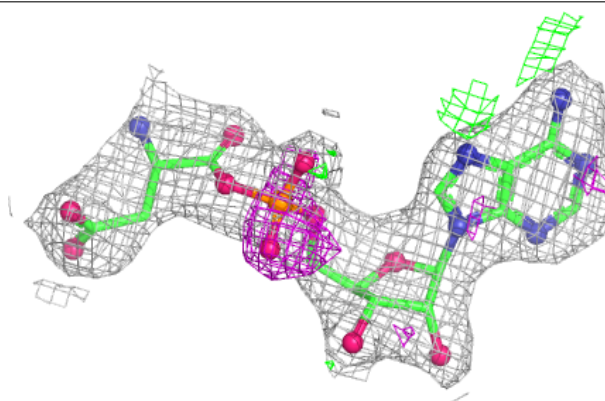
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMO B 1831:

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

**Electron density around AMO A 831:**

$2mF_o-DF_c$ (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.