



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 AM UTC

PDB ID : 2XB2 / pdb_00002xb2
Title : Crystal structure of the core Mago-Y14-eIF4AIII-Barentsz-UPF3b assembly shows how the EJC is bridged to the NMD machinery
Authors : Buchwald, G.; Ebert, J.; Basquin, C.; Sauliere, J.; Jayachandran, U.; Bono, F.; Le Hir, H.; Conti, E.
Deposited on : 2010-04-03
Resolution : 3.40 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

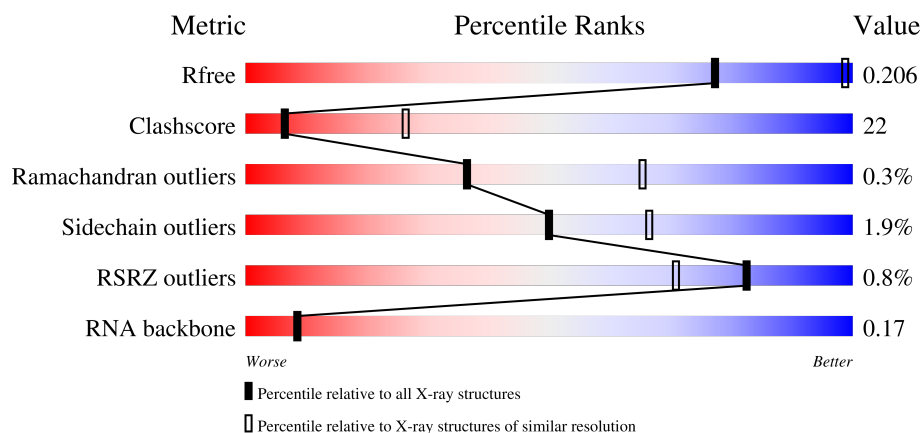
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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	411	55% 37% 5%
1	X	411	59% 31% 5%
2	C	146	59% 37% ..

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Mol	Chain	Length	Quality of chain
2	Y	146	60%38%
3	D	90	58%40%
3	Z	90	52%47%
4	E	15	27%27%47%
4	R	15	27%20%53%
5	F	3	67%33%
6	G	60	2%12%12%75%
6	U	60	3%18%8%72%
7	S	150	%22%15%62%
7	T	150	%19%18%61%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11710 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 EUKARYOTIC INITIATION FACTOR 4A-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3131	1976	546	590	19			
1	X	390	Total	C	N	O	S	0	0	0
			3131	1976	546	590	19			

- Molecule 2 is a protein called PROTEIN MAGO NASHI HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	143	Total	C	N	O	S	0	0	0
			1190	769	199	219	3			
2	Y	143	Total	C	N	O	S	0	0	0
			1190	769	199	219	3			

- Molecule 3 is a protein called RNA-BINDING PROTEIN 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	89	Total	C	N	O	S	0	0	0
			719	456	120	140	3			
3	Z	89	Total	C	N	O	S	0	0	0
			719	456	120	140	3			

- Molecule 4 is a RNA chain called RNA POLY-U-RIBONUCLEOTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	8	Total	C	N	O	P	0	0	0
			157	72	16	62	7			
4	R	7	Total	C	N	O	P	0	0	0
			137	63	14	54	6			

- Molecule 5 is a protein called PUTATIVE REGULATOR OF NONSENSE TRANSCRIPTS 3B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			25	14	6	5			

- Molecule 6 is a protein called REGULATOR OF NONSENSE TRANSCRIPTS 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	15	Total	C	N	O	S	0	0	0
			124	77	25	21	1			
6	U	17	Total	C	N	O	S	0	0	1
			120	74	23	22	1			

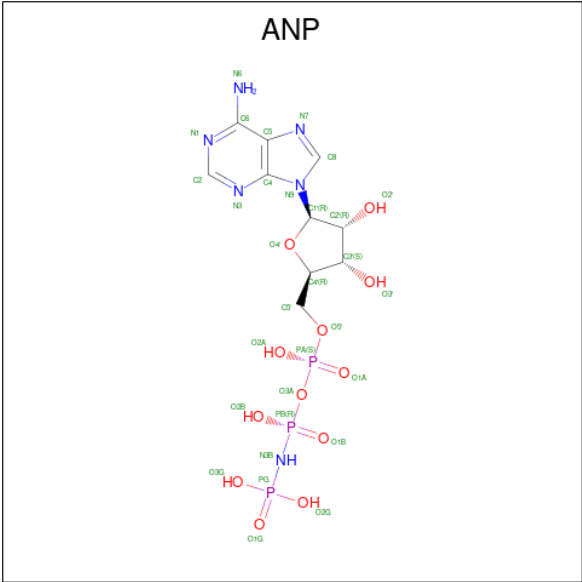
- Molecule 7 is a protein called PROTEIN CASC3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	S	57	Total	C	N	O	0	0	0
			494	309	92	93			
7	T	59	Total	C	N	O	0	0	0
			509	318	96	95			

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	X	1	Total	Mg	0	0
			1	1		

- Molecule 9 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

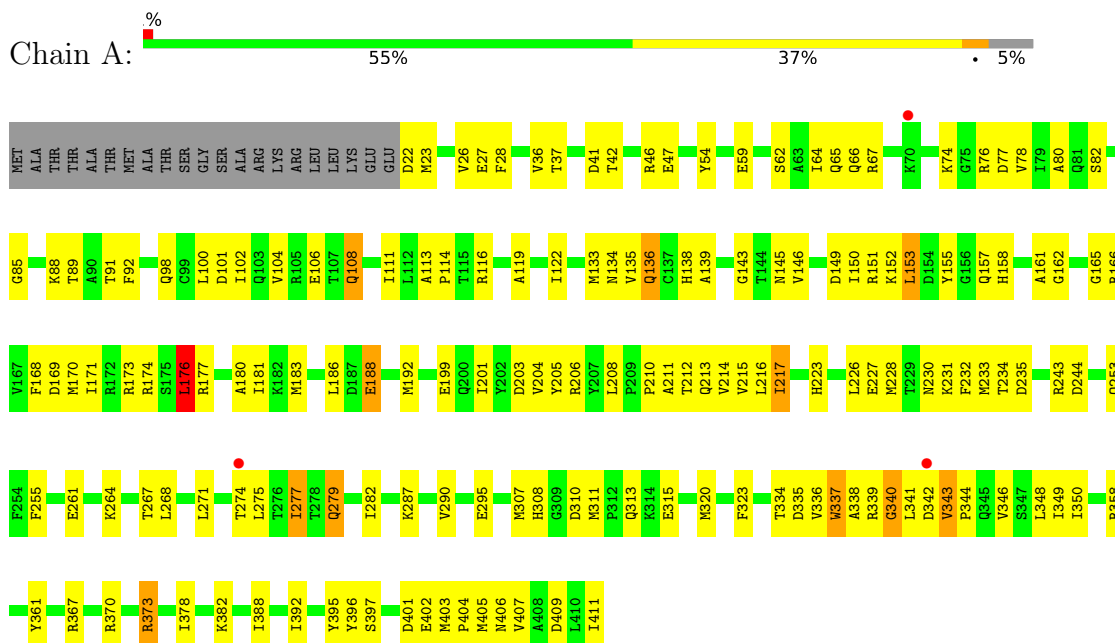


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
9	X	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

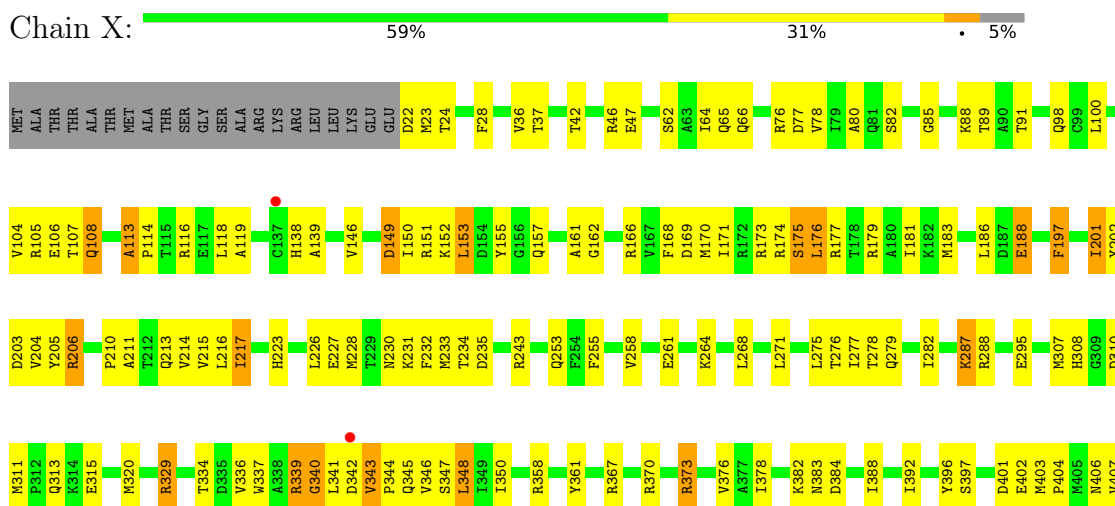
3 Residue-property plots

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: EUKARYOTIC INITIATION FACTOR 4A-III



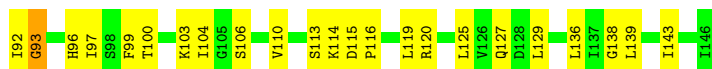
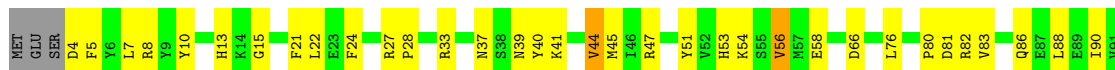
• Molecule 1: EUKARYOTIC INITIATION FACTOR 4A-III





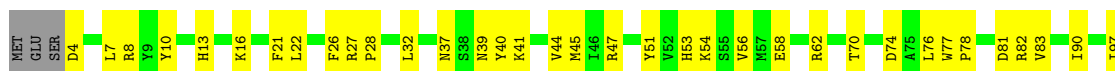
• Molecule 2: PROTEIN MAGO NASHI HOMOLOG

Chain C: 59% 37% ..



• Molecule 2: PROTEIN MAGO NASHI HOMOLOG

Chain Y: 60% 38% .



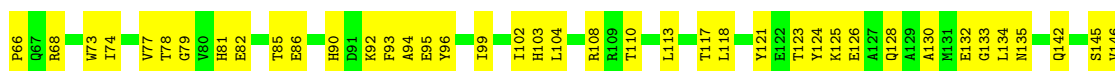
• Molecule 3: RNA-BINDING PROTEIN 8A

Chain D: 58% 40% ..



• Molecule 3: RNA-BINDING PROTEIN 8A

Chain Z: 52% 47% .

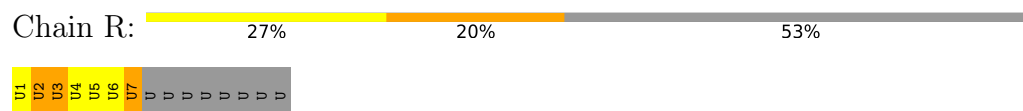


• Molecule 4: RNA POLY-U-RIBONUCLEOTIDE

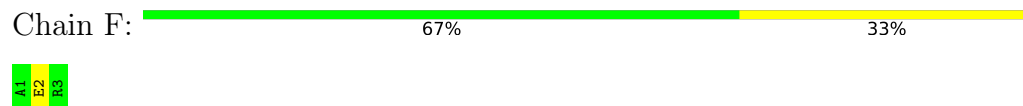
Chain E: 27% 27% 47%



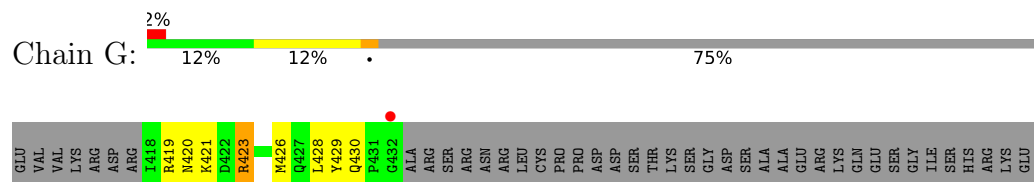
• Molecule 4: RNA POLY-U-RIBONUCLEOTIDE



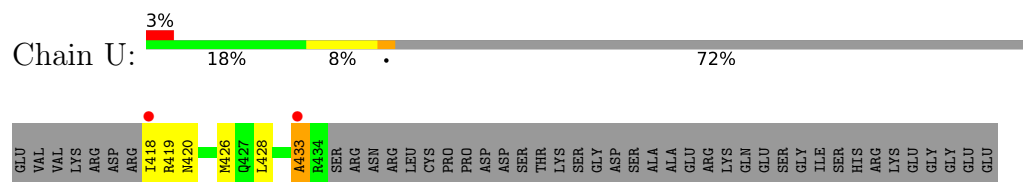
● Molecule 5: PUTATIVE REGULATOR OF NONSENSE TRANSCRIPTS 3B



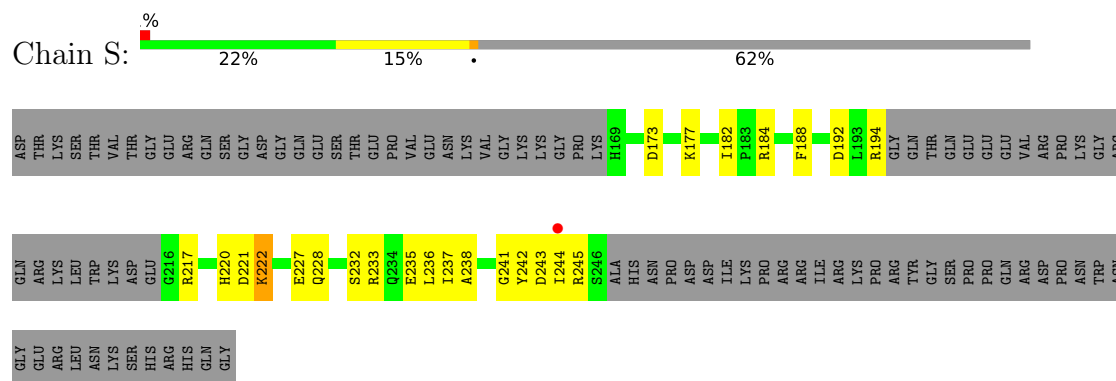
- Molecule 6: REGULATOR OF NONSENSE TRANSCRIPTS 3B



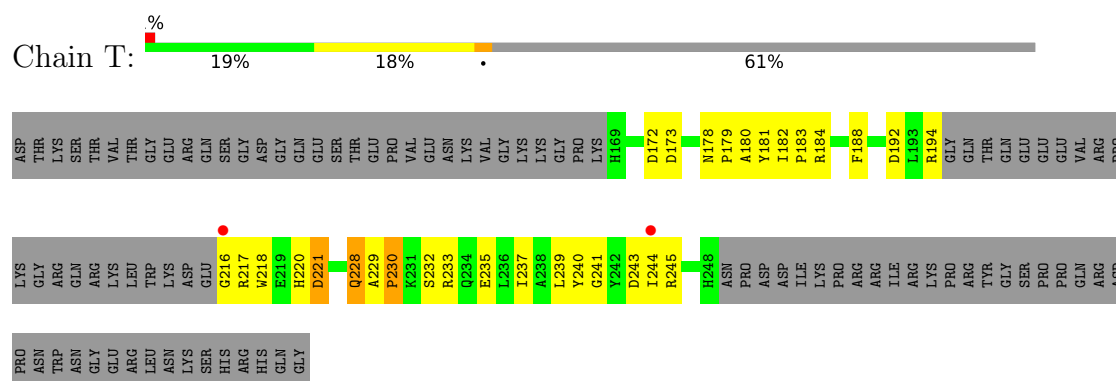
- Molecule 6: REGULATOR OF NONSENSE TRANSCRIPTS 3B



- Molecule 7: PROTEIN CASC3



- Molecule 7: PROTEIN CASC3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.80Å 134.80Å 227.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.40 60.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.00-3.40) 100.0 (60.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.260 0.212 , 0.206	Depositor DCC
R_{free} test set	1634 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11710	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: ANP, MG

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	0.74	4/3180 (0.1%)	1.03	9/4291 (0.2%)
1	X	0.66	3/3180 (0.1%)	1.01	15/4291 (0.3%)
2	C	0.63	1/1219 (0.1%)	0.89	4/1640 (0.2%)
2	Y	0.66	1/1219 (0.1%)	0.87	4/1640 (0.2%)
3	D	0.51	0/736	0.84	0/995
3	Z	0.59	0/736	0.86	0/995
4	E	0.33	0/172	0.67	0/264
4	R	0.32	0/150	0.70	0/230
5	F	0.63	0/24	0.78	0/30
6	G	0.46	0/126	1.09	1/168 (0.6%)
6	U	0.81	1/122 (0.8%)	0.88	0/166
7	S	0.67	0/506	0.81	0/677
7	T	0.69	0/522	0.99	2/699 (0.3%)
All	All	0.66	10/11892 (0.1%)	0.95	35/16086 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	VAL	CB-CG1	-9.89	1.19	1.52
1	A	26	VAL	CB-CG2	-9.41	1.21	1.52
2	Y	39	ASN	CG-ND2	-6.81	1.19	1.33
2	C	39	ASN	CG-ND2	-6.70	1.19	1.33
1	A	176	LEU	CG-CD2	-5.75	1.33	1.52
1	A	176	LEU	CG-CD1	-5.70	1.33	1.52
1	X	176	LEU	CG-CD1	-5.69	1.33	1.52
6	U	433	ALA	C-N	-5.62	1.25	1.33
1	X	176	LEU	CG-CD2	-5.25	1.35	1.52
1	X	276	THR	CB-CG2	-5.15	1.35	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	VAL	O-C-N	7.68	129.86	121.10
1	X	340	GLY	N-CA-C	7.50	130.97	113.18
1	A	340	GLY	N-CA-C	7.31	130.50	113.18
1	A	136	GLN	N-CA-C	7.17	120.59	108.90
1	A	26	VAL	CG1-CB-CG2	-7.04	95.32	110.80
1	X	149	ASP	N-CA-C	-6.91	103.75	111.28
1	X	383	ASN	CB-CA-C	-6.83	108.68	116.54
6	G	423	ARG	N-CA-C	6.74	118.20	109.64
1	A	149	ASP	N-CA-C	-6.44	104.26	111.28
2	C	93	GLY	N-CA-C	-5.93	100.55	111.34
1	A	188	GLU	N-CA-C	-5.83	103.36	111.52
2	Y	144	LYS	CA-C-N	5.82	125.95	119.32
2	Y	144	LYS	C-N-CA	5.82	125.95	119.32
1	X	188	GLU	N-CA-C	-5.78	103.94	111.74
2	C	44	VAL	N-CA-C	5.74	117.11	108.96
1	X	228	MET	N-CA-C	5.74	120.15	113.20
1	A	228	MET	N-CA-C	5.69	120.09	113.20
2	Y	44	VAL	N-CA-C	5.68	117.02	108.96
1	X	339	ARG	N-CA-C	5.49	118.42	109.59
1	X	36	VAL	N-CA-C	5.47	115.82	108.17
1	A	78	VAL	N-CA-C	5.46	116.34	108.48
1	X	78	VAL	N-CA-C	5.37	116.21	108.48
7	T	221	ASP	N-CA-C	5.32	116.76	111.07
1	A	36	VAL	N-CA-C	5.29	115.57	108.17
1	X	175	SER	N-CA-C	-5.27	105.62	111.36
2	Y	56	VAL	N-CA-C	-5.24	105.74	110.82
2	C	90	ILE	CB-CA-C	-5.24	103.33	110.77
1	X	206	ARG	CG-CD-NE	5.23	123.51	112.00
7	T	221	ASP	O-C-N	5.21	127.43	122.07
1	X	113	ALA	CA-C-N	5.18	124.69	119.19
1	X	113	ALA	C-N-CA	5.18	124.69	119.19
1	X	343	VAL	N-CA-C	-5.14	97.77	108.88
1	X	287	LYS	N-CA-C	-5.13	105.81	111.71
2	C	56	VAL	N-CA-C	-5.13	105.84	110.82
1	X	329	ARG	N-CA-C	5.09	117.95	111.69

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	3131	0	3173	165	0
1	X	3131	0	3172	144	0
2	C	1190	0	1177	49	0
2	Y	1190	0	1177	40	0
3	D	719	0	680	30	0
3	Z	719	0	680	35	0
4	E	157	0	82	15	0
4	R	137	0	72	16	0
5	F	25	0	26	1	0
6	G	124	0	126	15	0
6	U	120	0	109	4	0
7	S	494	0	459	37	0
7	T	509	0	471	33	0
8	A	1	0	0	0	0
8	X	1	0	0	0	0
9	A	31	0	13	6	0
9	X	31	0	13	6	0
All	All	11710	0	11430	506	0

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

All (506) 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:X:348:LEU:HD23	1:X:411:ILE:HD12	1.20	1.16
1:X:307:MET:HE1	1:X:320:MET:HG2	1.44	0.97
1:A:307:MET:HE1	1:A:320:MET:HG2	1.48	0.96
6:G:423:ARG:HH11	6:G:423:ARG:HG2	1.39	0.87
1:A:104:VAL:HG22	1:A:106:GLU:HG3	1.57	0.86
7:S:244:ILE:HD12	1:X:151:ARG:NH2	1.96	0.81
1:X:307:MET:HA	1:X:311:MET:SD	2.21	0.80
1:A:136:GLN:HE22	1:A:155:TYR:HE2	1.27	0.80
1:X:348:LEU:CD2	1:X:376:VAL:HB	2.12	0.80
3:D:152:ARG:HD3	1:X:47:GLU:OE2	1.81	0.80
1:A:108:GLN:HA	1:A:181:ILE:HA	1.64	0.79
7:S:245:ARG:O	1:X:105:ARG:NH1	2.16	0.78
1:A:150:ILE:HD13	1:A:170:MET:HE1	1.67	0.77
1:A:279:GLN:HB3	1:A:346:VAL:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:MET:HE1	6:G:430:GLN:HE22	1.51	0.75
1:A:146:VAL:O	1:A:150:ILE:HG12	1.87	0.75
1:A:307:MET:HA	1:A:311:MET:SD	2.26	0.75
1:X:146:VAL:O	1:X:150:ILE:HG12	1.86	0.74
7:S:182:ILE:O	7:S:184:ARG:HG3	1.87	0.74
6:G:423:ARG:HG2	6:G:423:ARG:NH1	2.00	0.74
4:R:6:U:H1'	1:X:169:ASP:HB2	1.70	0.74
2:C:15:GLY:HA3	7:T:192:ASP:OD1	1.88	0.73
1:X:150:ILE:HD13	1:X:170:MET:HE1	1.71	0.72
1:X:88:LYS:HB2	9:X:1413:ANP:O2B	1.89	0.71
1:X:279:GLN:HB2	1:X:346:VAL:HA	1.72	0.71
2:Y:116:PRO:O	2:Y:120:ARG:HG3	1.90	0.71
1:A:342:ASP:OD1	9:A:1413:ANP:H3'	1.90	0.71
3:D:104:LEU:HD11	3:D:113:LEU:HD13	1.70	0.71
1:A:348:LEU:C	1:A:348:LEU:HD13	2.16	0.71
1:X:348:LEU:HD23	1:X:411:ILE:CD1	2.10	0.71
2:C:116:PRO:O	2:C:120:ARG:HG3	1.91	0.71
3:D:135:ASN:ND2	3:D:146:VAL:H	1.88	0.70
7:S:228:GLN:O	1:X:179:ARG:HB2	1.90	0.70
1:X:153:LEU:HD21	1:X:176:LEU:HD22	1.73	0.70
7:S:177:LYS:O	1:X:288:ARG:NH2	2.25	0.69
7:S:237:ILE:HG12	7:S:242:TYR:HA	1.73	0.69
7:S:237:ILE:HA	7:S:242:TYR:N	2.05	0.69
1:A:104:VAL:CG2	1:A:106:GLU:HG3	2.23	0.69
7:S:194:ARG:HB3	2:Y:82:ARG:HG3	1.74	0.69
1:X:174:ARG:HE	1:X:177:ARG:HH12	1.41	0.69
2:Y:127:GLN:HB3	3:Z:108:ARG:HG3	1.74	0.69
2:C:13:HIS:HD2	2:C:103:LYS:NZ	1.91	0.68
1:A:402:GLU:OE2	2:C:106:SER:HB2	1.94	0.67
7:S:243:ASP:HB2	7:S:245:ARG:HG2	1.75	0.67
1:X:37:THR:O	1:X:66:GLN:HG2	1.94	0.67
1:X:108:GLN:HA	1:X:181:ILE:HA	1.75	0.67
3:D:81:HIS:CE1	3:D:83:GLU:HB2	2.29	0.67
7:T:244:ILE:H	7:T:244:ILE:HD12	1.60	0.67
2:C:82:ARG:HG3	7:T:194:ARG:HB3	1.76	0.66
1:X:347:SER:HB2	1:X:411:ILE:HD11	1.76	0.66
7:S:237:ILE:O	7:S:241:GLY:HA2	1.95	0.66
1:X:348:LEU:HD21	1:X:376:VAL:HB	1.78	0.66
1:A:271:LEU:O	1:A:275:LEU:HD13	1.95	0.66
1:X:348:LEU:HD22	1:X:376:VAL:HB	1.78	0.66
3:Z:104:LEU:HD11	3:Z:113:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:341:LEU:N	1:X:341:LEU:HD12	2.11	0.65
1:A:382:LYS:HE2	7:T:173:ASP:OD1	1.95	0.65
5:F:2:GLU:OE1	1:X:329:ARG:NE	2.29	0.65
1:A:169:ASP:HB2	4:E:6:U:H1'	1.79	0.65
7:T:240:TYR:CG	7:T:244:ILE:HD11	2.32	0.65
7:T:181:TYR:HE2	7:T:183:PRO:HG3	1.62	0.64
1:A:116:ARG:HD3	1:A:313:GLN:OE1	1.97	0.64
2:C:113:SER:O	2:C:116:PRO:HD3	1.96	0.64
1:X:116:ARG:HD3	1:X:313:GLN:OE1	1.98	0.64
3:Z:104:LEU:HD13	3:Z:117:THR:HB	1.79	0.64
3:D:104:LEU:HG	3:D:113:LEU:HD22	1.80	0.64
1:X:169:ASP:O	1:X:173:ARG:HG3	1.98	0.64
1:A:88:LYS:HB2	9:A:1413:ANP:O2B	1.99	0.63
7:S:220:HIS:ND1	1:X:210:PRO:HA	2.13	0.63
1:A:152:LYS:HG3	1:A:157:GLN:OE1	1.98	0.63
3:D:123:THR:OG1	3:D:126:GLU:HG3	1.99	0.63
1:A:388:ILE:HD11	7:T:184:ARG:HH22	1.64	0.63
4:E:2:U:C3'	4:E:3:U:H5'	2.29	0.63
1:A:230:ASN:OD1	1:A:231:LYS:N	2.32	0.62
1:A:307:MET:HE1	1:A:320:MET:CG	2.26	0.62
6:G:420:ASN:HA	6:G:423:ARG:HD2	1.81	0.62
1:A:341:LEU:HD12	1:A:341:LEU:N	2.12	0.62
7:S:233:ARG:O	7:S:237:ILE:HG13	1.99	0.62
1:A:47:GLU:OE2	3:Z:152:ARG:HD3	2.00	0.62
7:S:184:ARG:HH22	1:X:388:ILE:HD11	1.65	0.61
1:X:138:HIS:HB2	1:X:157:GLN:OE1	2.01	0.61
2:Y:54:LYS:O	2:Y:58:GLU:HG2	2.00	0.61
2:C:54:LYS:O	2:C:58:GLU:HG2	2.00	0.61
4:R:2:U:H2'	4:R:2:U:O2	2.01	0.60
1:X:104:VAL:HG22	1:X:106:GLU:HG3	1.83	0.60
7:S:232:SER:HB3	7:S:235:GLU:HG3	1.83	0.60
1:A:151:ARG:NH1	7:T:240:TYR:CD1	2.70	0.60
2:C:45:MET:HE3	2:C:47:ARG:NH2	2.17	0.60
7:S:244:ILE:O	1:X:155:TYR:CE1	2.54	0.60
1:A:169:ASP:O	1:A:173:ARG:HG3	2.02	0.60
7:T:178:ASN:OD1	7:T:179:PRO:HD2	2.01	0.60
3:Z:123:THR:OG1	3:Z:126:GLU:HG3	2.02	0.59
1:A:119:ALA:HB1	1:A:162:GLY:HA2	1.83	0.59
1:X:85:GLY:HA2	9:X:1413:ANP:HNB1	1.67	0.59
3:Z:104:LEU:HG	3:Z:113:LEU:HD22	1.84	0.59
2:Y:13:HIS:HD2	2:Y:103:LYS:NZ	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:ASN:HB2	2:C:45:MET:SD	2.42	0.59
3:D:135:ASN:HD22	3:D:146:VAL:H	1.49	0.59
3:Z:135:ASN:ND2	3:Z:146:VAL:H	2.01	0.59
1:A:27:GLU:HG2	2:C:44:VAL:HG21	1.85	0.59
1:X:367:ARG:HA	1:X:367:ARG:NE	2.18	0.59
7:T:181:TYR:CE2	7:T:183:PRO:HG3	2.36	0.58
1:X:307:MET:HE1	1:X:320:MET:CG	2.26	0.58
1:A:62:SER:OG	1:A:65:GLN:HG3	2.03	0.58
1:A:177:ARG:HB3	7:T:228:GLN:O	2.03	0.58
1:A:199:GLU:HA	1:A:199:GLU:OE1	2.04	0.58
7:S:244:ILE:HG12	1:X:155:TYR:HD1	1.68	0.58
1:A:344:PRO:HB3	1:A:373:ARG:CZ	2.34	0.58
1:X:350:ILE:HD13	1:X:378:ILE:HB	1.84	0.58
7:S:173:ASP:OD1	1:X:382:LYS:HE2	2.03	0.57
1:X:77:ASP:HB3	1:X:233:MET:HE2	1.85	0.57
4:R:2:U:C3'	4:R:3:U:H5'	2.34	0.57
4:R:2:U:H3'	4:R:3:U:H5'	1.86	0.57
2:Y:51:TYR:CE1	3:Z:154:PRO:HD3	2.39	0.57
1:X:223:HIS:O	1:X:227:GLU:HG3	2.04	0.57
1:X:46:ARG:HG3	1:X:98:GLN:OE1	2.04	0.57
1:X:342:ASP:OD1	9:X:1413:ANP:H3'	2.04	0.57
1:X:341:LEU:N	1:X:341:LEU:CD1	2.67	0.57
2:Y:70:THR:HA	2:Y:97:ILE:HD13	1.86	0.56
1:A:150:ILE:HD13	1:A:170:MET:CE	2.35	0.56
7:S:192:ASP:OD1	2:Y:16:LYS:HG2	2.05	0.56
1:A:231:LYS:HD2	7:T:217:ARG:HA	1.86	0.56
1:X:119:ALA:HB1	1:X:162:GLY:HA2	1.86	0.56
2:Y:37:ASN:HB2	2:Y:45:MET:SD	2.45	0.56
1:X:347:SER:HB2	1:X:411:ILE:CD1	2.36	0.56
1:A:342:ASP:OD2	1:A:344:PRO:HD3	2.04	0.56
4:E:2:U:H2'	4:E:3:U:H5'	1.86	0.56
2:Y:13:HIS:HD2	2:Y:103:LYS:HZ1	1.54	0.56
3:D:68:ARG:HB2	3:D:73:TRP:CZ2	2.40	0.56
3:D:99:ILE:HG21	3:D:102:ILE:HD11	1.88	0.56
3:Z:92:LYS:O	3:Z:134:LEU:HD11	2.06	0.56
2:Y:45:MET:HE3	2:Y:47:ARG:NH2	2.21	0.55
1:A:232:PHE:CD1	1:A:233:MET:HG3	2.42	0.55
1:A:77:ASP:HB3	1:A:233:MET:HE2	1.89	0.55
7:S:236:LEU:HD11	7:S:245:ARG:NH2	2.21	0.55
7:T:244:ILE:HD12	7:T:244:ILE:N	2.21	0.55
1:X:105:ARG:NH1	1:X:155:TYR:CZ	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:7:LEU:HD13	2:Y:90:ILE:HG12	1.89	0.55
4:R:1:U:H3'	4:R:1:U:H6	1.71	0.55
1:A:350:ILE:HD13	1:A:378:ILE:HB	1.89	0.55
2:C:115:ASP:C	2:C:115:ASP:OD1	2.50	0.55
7:S:244:ILE:HG12	1:X:155:TYR:CD1	2.42	0.55
1:A:104:VAL:HG13	1:A:108:GLN:HE22	1.72	0.54
1:A:234:THR:O	1:A:235:ASP:C	2.49	0.54
1:A:279:GLN:NE2	1:A:323:PHE:O	2.41	0.54
2:Y:4:ASP:OD2	2:Y:4:ASP:N	2.40	0.54
1:A:206:ARG:HE	7:T:221:ASP:HB2	1.71	0.54
6:U:426:MET:HB2	3:Z:110:THR:O	2.07	0.54
2:C:127:GLN:HB3	3:D:108:ARG:HG3	1.89	0.54
2:Y:76:LEU:O	2:Y:114:LYS:HB2	2.08	0.54
1:A:232:PHE:HB3	7:T:218:TRP:CE3	2.42	0.54
1:A:46:ARG:HG3	1:A:98:GLN:OE1	2.08	0.54
1:A:153:LEU:HD21	1:A:176:LEU:HD22	1.89	0.54
2:C:92:ILE:O	2:C:93:GLY:C	2.49	0.54
2:Y:113:SER:O	2:Y:116:PRO:HD3	2.08	0.54
7:S:217:ARG:HA	1:X:231:LYS:HD2	1.90	0.54
7:T:240:TYR:CD2	7:T:244:ILE:HD11	2.43	0.54
1:X:232:PHE:CD1	1:X:233:MET:HG3	2.43	0.54
2:C:81:ASP:OD1	2:C:83:VAL:HB	2.08	0.53
3:D:78:THR:HG22	3:D:79:GLY:N	2.23	0.53
2:C:13:HIS:HD2	2:C:103:LYS:HZ1	1.55	0.53
1:A:85:GLY:HA2	9:A:1413:ANP:HNB1	1.72	0.53
1:A:367:ARG:HA	1:A:367:ARG:NE	2.23	0.53
1:A:186:LEU:HD12	1:A:216:LEU:CD2	2.38	0.53
1:A:367:ARG:O	1:A:370:ARG:HD3	2.09	0.53
1:X:261:GLU:OE2	1:X:264:LYS:HD2	2.07	0.53
1:X:308:HIS:CD2	1:X:310:ASP:HB2	2.44	0.53
3:Z:68:ARG:HB2	3:Z:73:TRP:CZ2	2.44	0.53
2:C:110:VAL:O	2:C:116:PRO:HB3	2.08	0.53
1:X:343:VAL:HB	1:X:346:VAL:HG23	1.91	0.53
1:X:153:LEU:HD23	1:X:176:LEU:HB2	1.91	0.53
1:X:308:HIS:HD2	1:X:310:ASP:HB2	1.73	0.53
2:C:76:LEU:O	2:C:114:LYS:HB2	2.08	0.53
2:Y:70:THR:HG22	2:Y:97:ILE:HD13	1.90	0.53
1:X:277:ILE:HG22	1:X:278:THR:HG23	1.91	0.52
3:Z:78:THR:HG22	3:Z:79:GLY:N	2.24	0.52
1:X:210:PRO:O	1:X:211:ALA:HB3	2.10	0.52
3:Z:85:THR:HG22	3:Z:86:GLU:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:92:LYS:O	3:D:134:LEU:HD11	2.10	0.52
1:A:54:TYR:CD1	3:Z:125:LYS:HB2	2.44	0.52
3:Z:85:THR:HG22	3:Z:86:GLU:N	2.23	0.52
1:A:214:VAL:HG12	1:A:233:MET:HE3	1.92	0.52
3:D:104:LEU:HD13	3:D:117:THR:HB	1.91	0.52
7:T:182:ILE:O	7:T:184:ARG:HG3	2.10	0.52
1:X:153:LEU:CD2	1:X:176:LEU:HB2	2.40	0.52
1:X:340:GLY:CA	1:X:367:ARG:HH12	2.22	0.52
1:A:308:HIS:HD2	1:A:310:ASP:HB2	1.74	0.52
7:S:245:ARG:O	1:X:105:ARG:CZ	2.58	0.52
1:X:62:SER:OG	1:X:65:GLN:HG3	2.10	0.52
1:X:215:VAL:HG12	1:X:217:ILE:CD1	2.39	0.52
1:X:403:MET:CG	1:X:407:VAL:HG21	2.40	0.52
1:A:37:THR:O	1:A:66:GLN:HG2	2.10	0.52
1:X:64:ILE:HD11	1:X:80:ALA:HB1	1.91	0.52
3:Z:99:ILE:HG21	3:Z:102:ILE:HD11	1.92	0.52
1:A:153:LEU:HD22	1:A:170:MET:HE3	1.92	0.52
1:A:210:PRO:O	1:A:211:ALA:HB3	2.10	0.52
1:X:153:LEU:HD22	1:X:170:MET:HE3	1.92	0.52
1:A:308:HIS:CD2	1:A:310:ASP:HB2	2.45	0.52
1:A:268:LEU:HD11	1:A:282:ILE:CD1	2.40	0.51
2:C:143:ILE:HG23	3:D:71:GLU:OE1	2.10	0.51
1:A:403:MET:CG	1:A:407:VAL:HG21	2.39	0.51
4:E:1:U:O4	7:T:181:TYR:OH	2.24	0.51
2:Y:115:ASP:C	2:Y:115:ASP:OD1	2.50	0.51
1:A:348:LEU:C	1:A:348:LEU:CD1	2.83	0.51
3:D:95:GLU:HG2	3:D:95:GLU:O	2.09	0.51
1:X:278:THR:OG1	1:X:347:SER:HB2	2.11	0.51
1:X:234:THR:O	1:X:235:ASP:C	2.54	0.51
1:X:150:ILE:HD13	1:X:170:MET:CE	2.38	0.51
2:Y:110:VAL:O	2:Y:116:PRO:HB3	2.11	0.51
1:A:145:ASN:HA	4:E:8:U:H1'	1.93	0.51
1:X:268:LEU:HD11	1:X:282:ILE:CD1	2.41	0.51
7:S:217:ARG:HG3	1:X:231:LYS:O	2.10	0.51
2:Y:104:ILE:HD11	2:Y:119:LEU:HD22	1.92	0.51
3:Z:77:VAL:HG22	3:Z:146:VAL:HG22	1.93	0.51
1:A:101:ASP:OD2	1:A:104:VAL:HG12	2.11	0.50
4:E:2:U:C2'	4:E:3:U:H5'	2.39	0.50
2:C:104:ILE:HD11	2:C:119:LEU:HD22	1.92	0.50
3:D:85:THR:HG22	3:D:86:GLU:H	1.75	0.50
3:D:85:THR:HG22	3:D:86:GLU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:343:VAL:CG1	1:X:346:VAL:HG23	2.41	0.50
1:A:152:LYS:CD	1:A:157:GLN:OE1	2.59	0.50
1:A:171:ILE:CD1	1:A:204:VAL:HG13	2.40	0.50
7:S:227:GLU:O	1:X:177:ARG:NH1	2.43	0.50
4:E:2:U:H3'	4:E:3:U:H5'	1.94	0.50
7:S:228:GLN:O	1:X:179:ARG:CB	2.57	0.50
1:X:334:THR:C	1:X:336:VAL:H	2.20	0.50
1:A:188:GLU:OE1	1:A:339:ARG:HB3	2.12	0.50
1:A:287:LYS:HE2	4:E:3:U:P	2.52	0.50
1:X:342:ASP:OD2	1:X:370:ARG:NE	2.21	0.50
1:A:223:HIS:O	1:A:227:GLU:HG3	2.11	0.50
1:A:274:THR:O	1:A:277:ILE:HG13	2.11	0.50
1:X:168:PHE:CE1	1:X:203:ASP:HB3	2.47	0.50
4:E:1:U:O2'	4:E:2:U:C5'	2.59	0.50
1:X:104:VAL:HG13	1:X:108:GLN:HE22	1.77	0.50
1:A:261:GLU:OE2	1:A:264:LYS:HD2	2.12	0.49
1:A:340:GLY:CA	1:A:367:ARG:HH12	2.24	0.49
1:A:404:PRO:HB3	6:G:426:MET:HE3	1.94	0.49
6:U:426:MET:HE3	6:U:428:LEU:CD1	2.42	0.49
1:X:100:LEU:CD2	1:X:108:GLN:HG3	2.41	0.49
1:A:22:ASP:O	1:A:23:MET:HB2	2.10	0.49
4:R:2:U:C4	7:S:188:PHE:HB3	2.47	0.49
1:X:214:VAL:HG12	1:X:233:MET:HE3	1.93	0.49
1:X:28:PHE:CE2	1:X:226:LEU:HB3	2.48	0.49
6:G:430:GLN:O	6:G:430:GLN:HG2	2.13	0.49
1:A:406:ASN:HB2	1:A:409:ASP:OD2	2.13	0.49
2:C:115:ASP:CG	2:C:115:ASP:O	2.54	0.49
2:Y:40:TYR:CE2	2:Y:41:LYS:HG3	2.48	0.49
1:A:139:ALA:HA	1:A:161:ALA:O	2.12	0.49
1:X:116:ARG:CD	1:X:313:GLN:OE1	2.59	0.49
1:X:406:ASN:HB2	1:X:409:ASP:OD2	2.13	0.49
2:Y:81:ASP:OD1	2:Y:83:VAL:HB	2.13	0.49
2:Y:115:ASP:CG	2:Y:115:ASP:O	2.54	0.48
1:A:168:PHE:CE1	1:A:203:ASP:HB3	2.48	0.48
1:X:104:VAL:HG13	1:X:108:GLN:NE2	2.28	0.48
1:X:88:LYS:HD2	1:X:217:ILE:HG23	1.96	0.48
1:X:255:PHE:CE2	1:X:401:ASP:HA	2.49	0.48
1:A:88:LYS:HD2	1:A:217:ILE:HG23	1.96	0.48
2:C:10:TYR:C	2:C:10:TYR:CD2	2.91	0.48
1:A:28:PHE:CE2	1:A:226:LEU:HB3	2.48	0.48
1:A:67:ARG:NH2	2:C:143:ILE:HD13	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:CD2	1:A:108:GLN:HG3	2.43	0.48
1:A:116:ARG:CD	1:A:313:GLN:OE1	2.62	0.48
1:A:343:VAL:O	1:A:346:VAL:HG23	2.14	0.48
1:A:343:VAL:CG1	1:A:346:VAL:HG23	2.44	0.48
2:C:66:ASP:HA	6:G:421:LYS:CE	2.43	0.48
1:X:268:LEU:HD11	1:X:282:ILE:HD11	1.95	0.48
1:X:402:GLU:OE2	2:Y:106:SER:HB2	2.13	0.48
1:X:344:PRO:HB3	1:X:373:ARG:CZ	2.44	0.48
1:X:367:ARG:NE	1:X:367:ARG:CA	2.76	0.48
4:E:1:U:H5''	7:T:188:PHE:HE1	1.79	0.48
1:X:104:VAL:CG2	1:X:106:GLU:HG3	2.43	0.48
4:R:7:U:H6	4:R:7:U:H3'	1.77	0.47
2:Y:76:LEU:HB3	2:Y:114:LYS:CB	2.44	0.47
1:A:404:PRO:O	1:A:407:VAL:HG23	2.14	0.47
3:D:118:LEU:N	3:D:118:LEU:HD12	2.30	0.47
1:X:149:ASP:OD2	1:X:170:MET:HE2	2.15	0.47
2:C:40:TYR:CE2	2:C:41:LYS:HG3	2.50	0.47
1:X:287:LYS:HB3	1:X:308:HIS:CD2	2.50	0.47
2:Y:10:TYR:C	2:Y:10:TYR:CD2	2.92	0.47
1:A:47:GLU:OE1	3:Z:66:PRO:N	2.47	0.47
1:A:173:ARG:O	1:A:174:ARG:HB2	2.13	0.47
1:A:255:PHE:CE2	1:A:401:ASP:HA	2.49	0.47
3:D:77:VAL:HG22	3:D:146:VAL:HG22	1.96	0.47
7:T:237:ILE:O	7:T:241:GLY:HA2	2.15	0.47
6:U:420:ASN:ND2	3:Z:82:GLU:HG2	2.29	0.47
1:X:215:VAL:HG12	1:X:217:ILE:HD12	1.96	0.47
1:X:350:ILE:CD1	1:X:378:ILE:HB	2.44	0.47
2:Y:62:ARG:NH2	3:Z:78:THR:HG21	2.29	0.47
1:A:243:ARG:HG2	1:A:243:ARG:HH11	1.80	0.47
1:A:343:VAL:HB	1:A:346:VAL:HG23	1.96	0.47
2:C:13:HIS:HD2	2:C:103:LYS:HZ2	1.62	0.47
2:C:53:HIS:CE1	2:C:54:LYS:HG2	2.50	0.47
1:X:85:GLY:CA	9:X:1413:ANP:HNB1	2.28	0.47
1:A:268:LEU:HD11	1:A:282:ILE:HD11	1.95	0.46
1:X:82:SER:HB3	1:X:88:LYS:HG3	1.97	0.46
1:A:215:VAL:HG12	1:A:217:ILE:CD1	2.46	0.46
2:C:51:TYR:CE1	3:D:154:PRO:HD3	2.50	0.46
2:C:96:HIS:C	2:C:96:HIS:CD2	2.92	0.46
4:R:6:U:H3'	4:R:6:U:H6	1.80	0.46
1:X:42:THR:O	1:X:42:THR:HG22	2.14	0.46
1:X:188:GLU:OE1	1:X:339:ARG:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:95:GLU:HG2	3:Z:95:GLU:O	2.15	0.46
1:A:165:GLY:HA3	4:E:6:U:O5'	2.16	0.46
1:A:267:THR:HG23	6:G:429:TYR:CE2	2.50	0.46
7:T:233:ARG:O	7:T:237:ILE:HG13	2.14	0.46
2:Y:53:HIS:CE1	2:Y:54:LYS:HG2	2.50	0.46
1:A:153:LEU:CD2	1:A:176:LEU:HB2	2.46	0.46
7:S:235:GLU:O	7:S:238:ALA:HB3	2.15	0.46
1:X:171:ILE:CD1	1:X:204:VAL:HG13	2.46	0.46
1:A:253:GLN:NE2	1:A:361:TYR:OH	2.44	0.46
3:Z:128:GLN:HG2	3:Z:132:GLU:OE2	2.15	0.46
1:X:183:MET:HE2	1:X:213:GLN:OE1	2.16	0.46
7:T:235:GLU:O	7:T:239:LEU:HG	2.15	0.46
1:A:64:ILE:HD11	1:A:80:ALA:HB1	1.97	0.45
7:S:243:ASP:HB2	7:S:245:ARG:CG	2.46	0.45
1:A:287:LYS:HB3	1:A:308:HIS:CD2	2.51	0.45
1:A:295:GLU:OE2	1:A:295:GLU:HA	2.16	0.45
6:G:430:GLN:CD	6:G:430:GLN:H	2.24	0.45
1:A:253:GLN:NE2	1:A:361:TYR:CE2	2.85	0.45
1:A:335:ASP:O	1:A:338:ALA:HB3	2.17	0.45
7:S:221:ASP:OD2	7:S:222:LYS:HG2	2.16	0.45
7:T:229:ALA:HB1	7:T:230:PRO:HD2	1.98	0.45
1:X:22:ASP:O	1:X:23:MET:HB3	2.17	0.45
1:X:295:GLU:OE2	1:X:295:GLU:HA	2.16	0.45
1:X:343:VAL:HB	1:X:346:VAL:CG2	2.46	0.45
1:A:100:LEU:HD23	1:A:108:GLN:HG3	1.99	0.45
1:A:138:HIS:ND1	1:A:152:LYS:HG2	2.32	0.45
1:A:340:GLY:HA2	9:A:1413:ANP:O2G	2.16	0.45
2:C:125:LEU:O	2:C:129:LEU:HG	2.17	0.45
1:X:100:LEU:HD23	1:X:108:GLN:HG3	1.97	0.45
1:A:336:VAL:HG13	1:A:337:TRP:N	2.31	0.45
1:A:403:MET:HG3	1:A:407:VAL:CG2	2.47	0.45
4:R:5:U:OP1	1:X:116:ARG:HG3	2.16	0.45
1:X:186:LEU:HD12	1:X:216:LEU:CD2	2.46	0.45
1:X:65:GLN:HG2	1:X:91:THR:OG1	2.17	0.45
1:X:404:PRO:O	1:X:407:VAL:HG23	2.15	0.45
3:Z:124:TYR:HE2	3:Z:128:GLN:NE2	2.15	0.45
4:E:4:U:C4	4:E:5:U:N3	2.85	0.45
1:X:226:LEU:HD23	1:X:226:LEU:HA	1.73	0.45
1:X:271:LEU:O	1:X:275:LEU:HG	2.17	0.45
1:A:344:PRO:HB3	1:A:373:ARG:NH2	2.31	0.45
1:A:350:ILE:CD1	1:A:378:ILE:HB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:89:THR:HB	9:X:1413:ANP:O2A	2.17	0.45
1:X:139:ALA:HA	1:X:161:ALA:O	2.16	0.45
1:X:255:PHE:HE2	1:X:401:ASP:HA	1.82	0.45
1:A:42:THR:HG22	1:A:42:THR:O	2.16	0.45
6:G:419:ARG:HG3	6:G:420:ASN:N	2.32	0.45
3:Z:96:TYR:CD2	3:Z:130:ALA:HA	2.52	0.45
2:Y:139:LEU:HB3	3:Z:74:ILE:CD1	2.48	0.44
1:A:274:THR:O	1:A:277:ILE:CG1	2.65	0.44
1:A:208:LEU:O	7:T:220:HIS:ND1	2.51	0.44
3:D:112:TYR:CZ	6:G:423:ARG:NH1	2.85	0.44
7:T:243:ASP:HB2	7:T:245:ARG:HG2	2.00	0.44
1:A:104:VAL:HG13	1:A:104:VAL:O	2.17	0.44
1:A:143:GLY:N	4:E:7:U:OP1	2.49	0.44
3:D:90:HIS:CE1	3:D:94:ALA:HB2	2.52	0.44
7:S:184:ARG:HH22	1:X:388:ILE:CD1	2.28	0.44
7:T:172:ASP:HB3	7:T:180:ALA:HB3	1.99	0.44
1:A:343:VAL:HB	1:A:346:VAL:CG2	2.47	0.44
4:R:3:U:C2'	4:R:4:U:O5'	2.66	0.44
1:X:403:MET:HG3	1:X:407:VAL:CG2	2.48	0.44
1:A:59:GLU:HG2	3:Z:125:LYS:HE2	1.99	0.44
1:A:102:ILE:HD11	1:A:133:MET:HE2	2.00	0.44
2:C:5:PHE:O	2:C:28:PRO:HB3	2.16	0.44
1:A:88:LYS:O	1:A:91:THR:HB	2.17	0.44
1:A:405:MET:HE1	6:G:430:GLN:NE2	2.25	0.44
3:Z:118:LEU:N	3:Z:118:LEU:HD12	2.33	0.44
1:A:388:ILE:CD1	7:T:184:ARG:HH22	2.29	0.44
3:D:81:HIS:HA	3:D:142:GLN:OE1	2.18	0.44
4:R:2:U:C5	7:S:188:PHE:HB3	2.53	0.44
2:Y:27:ARG:HB3	2:Y:28:PRO:HD2	2.00	0.44
1:A:100:LEU:HD13	1:A:135:VAL:HG21	2.00	0.43
2:C:86:GLN:O	2:C:100:THR:HA	2.18	0.43
1:X:202:TYR:O	1:X:206:ARG:HG3	2.18	0.43
1:X:258:VAL:O	1:X:382:LYS:HA	2.18	0.43
2:Y:125:LEU:O	2:Y:129:LEU:HG	2.18	0.43
3:Z:135:ASN:ND2	3:Z:145:SER:HA	2.33	0.43
1:A:152:LYS:CG	1:A:157:GLN:OE1	2.65	0.43
6:G:419:ARG:HG3	6:G:420:ASN:H	1.84	0.43
1:X:152:LYS:HG3	1:X:157:GLN:CD	2.43	0.43
1:X:334:THR:C	1:X:336:VAL:N	2.76	0.43
1:A:113:ALA:HB1	1:A:114:PRO:HD2	2.01	0.43
1:A:367:ARG:NE	1:A:367:ARG:CA	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:LEU:HB3	2:C:114:LYS:HB2	2.01	0.43
1:A:138:HIS:CG	1:A:152:LYS:HG2	2.54	0.43
1:A:403:MET:HG3	1:A:407:VAL:HG21	2.00	0.43
2:C:76:LEU:HB3	2:C:114:LYS:CB	2.48	0.43
4:R:1:U:C3'	4:R:1:U:C6	3.02	0.43
1:X:107:THR:HA	1:X:157:GLN:O	2.17	0.43
1:A:82:SER:HB3	1:A:88:LYS:HG3	2.00	0.43
1:X:243:ARG:HH11	1:X:243:ARG:HG2	1.84	0.43
3:Z:93:PHE:HB3	3:Z:121:TYR:OH	2.19	0.43
1:X:403:MET:HG3	1:X:407:VAL:HG21	2.01	0.43
3:Z:81:HIS:HA	3:Z:142:GLN:OE1	2.18	0.43
1:A:231:LYS:HD2	7:T:216:GLY:O	2.19	0.43
1:A:76:ARG:NH1	1:A:76:ARG:HG3	2.34	0.43
1:A:342:ASP:CG	1:A:344:PRO:HD3	2.43	0.43
4:R:2:U:C3'	4:R:3:U:C5'	2.97	0.43
7:S:232:SER:O	7:S:233:ARG:C	2.62	0.43
7:S:244:ILE:HD12	1:X:151:ARG:CZ	2.49	0.43
1:X:104:VAL:HG13	1:X:104:VAL:O	2.19	0.43
2:Y:135:SER:OG	3:Z:103:HIS:HD2	2.01	0.43
1:A:108:GLN:CA	1:A:181:ILE:HA	2.42	0.42
1:A:341:LEU:N	1:A:341:LEU:CD1	2.82	0.42
3:D:77:VAL:HB	3:D:117:THR:HG23	2.01	0.42
4:E:2:U:C3'	4:E:3:U:C5'	2.96	0.42
1:X:76:ARG:NH1	1:X:76:ARG:HG3	2.34	0.42
3:Z:96:TYR:CE2	3:Z:133:GLY:HA3	2.54	0.42
1:A:402:GLU:HG2	6:G:428:LEU:HD23	2.01	0.42
1:X:150:ILE:HG23	1:X:175:SER:OG	2.19	0.42
2:Y:122:PHE:O	2:Y:126:VAL:HG23	2.19	0.42
1:A:89:THR:HA	1:A:92:PHE:CE2	2.54	0.42
2:C:7:LEU:HD12	2:C:8:ARG:H	1.85	0.42
4:R:5:U:H6	4:R:5:U:O5'	2.01	0.42
1:X:253:GLN:NE2	1:X:361:TYR:CE2	2.88	0.42
2:Y:7:LEU:HD12	2:Y:8:ARG:H	1.85	0.42
1:A:111:ILE:HG21	1:A:122:ILE:HG21	2.02	0.42
1:X:88:LYS:HB2	9:X:1413:ANP:PB	2.59	0.42
1:X:253:GLN:NE2	1:X:361:TYR:OH	2.49	0.42
2:Y:21:PHE:CE2	2:Y:37:ASN:HB3	2.55	0.42
1:A:88:LYS:HB2	9:A:1413:ANP:PB	2.59	0.42
1:A:104:VAL:HG13	1:A:108:GLN:NE2	2.32	0.42
1:A:183:MET:HE2	1:A:213:GLN:OE1	2.19	0.42
1:X:46:ARG:HG3	1:X:46:ARG:H	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASP:OD1	9:A:1413:ANP:C3'	2.63	0.42
2:C:21:PHE:CE2	2:C:37:ASN:HB3	2.54	0.42
2:C:66:ASP:O	6:G:421:LYS:HE2	2.20	0.42
7:T:178:ASN:OD1	7:T:179:PRO:CD	2.68	0.42
1:A:136:GLN:O	1:A:158:HIS:N	2.49	0.42
1:A:168:PHE:CZ	1:A:203:ASP:HB3	2.55	0.42
4:R:1:U:H3'	4:R:1:U:C6	2.55	0.42
7:T:232:SER:HB3	7:T:235:GLU:HG3	2.01	0.42
1:X:173:ARG:O	1:X:174:ARG:HB2	2.20	0.42
2:C:40:TYR:OH	2:C:41:LYS:HE3	2.19	0.41
7:S:244:ILE:O	1:X:155:TYR:HE1	2.01	0.41
1:X:367:ARG:O	1:X:370:ARG:HD3	2.19	0.41
1:A:244:ASP:HB2	1:A:397:SER:HB2	2.02	0.41
1:A:255:PHE:HE2	1:A:401:ASP:HA	1.83	0.41
1:A:337:TRP:HH2	1:A:343:VAL:CG2	2.33	0.41
1:A:76:ARG:HG3	1:A:76:ARG:HH11	1.86	0.41
1:A:334:THR:C	1:A:336:VAL:H	2.27	0.41
2:C:56:VAL:HA	3:D:76:PHE:CE2	2.55	0.41
3:D:93:PHE:HB3	3:D:121:TYR:OH	2.20	0.41
1:A:65:GLN:HG2	1:A:91:THR:OG1	2.20	0.41
1:A:74:LYS:O	1:A:74:LYS:HG2	2.20	0.41
1:A:208:LEU:HD13	1:A:212:THR:HG21	2.01	0.41
1:A:343:VAL:HG12	1:A:346:VAL:HG23	2.02	0.41
1:A:348:LEU:HD13	1:A:349:ILE:N	2.36	0.41
2:C:27:ARG:HB3	2:C:28:PRO:HD2	2.02	0.41
3:D:135:ASN:ND2	3:D:145:SER:HA	2.35	0.41
4:R:4:U:O2'	1:X:114:PRO:O	2.33	0.41
7:S:237:ILE:HG23	7:S:241:GLY:C	2.45	0.41
1:X:188:GLU:OE1	1:X:339:ARG:HD3	2.20	0.41
1:A:253:GLN:HE22	1:A:361:TYR:HE2	1.67	0.41
1:A:358:ARG:HG2	1:A:392:ILE:HG12	2.03	0.41
1:X:278:THR:HB	1:X:345:GLN:O	2.20	0.41
2:Y:26:PHE:CE1	2:Y:32:LEU:HD22	2.55	0.41
2:Y:130:LYS:HB3	2:Y:134:PHE:CE2	2.55	0.41
1:A:275:LEU:HG	1:A:348:LEU:HD12	2.02	0.41
4:E:1:U:H5''	7:T:188:PHE:CE1	2.55	0.41
1:X:358:ARG:HG2	1:X:392:ILE:HG12	2.03	0.41
2:Y:76:LEU:HB3	2:Y:114:LYS:HB2	2.01	0.41
1:A:205:TYR:CD2	1:A:205:TYR:C	2.99	0.41
1:A:334:THR:C	1:A:336:VAL:N	2.77	0.41
2:C:13:HIS:CD2	2:C:103:LYS:HZ2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:LEU:HB3	3:D:74:ILE:CD1	2.51	0.41
1:A:348:LEU:HB2	1:A:411:ILE:HD12	2.01	0.41
2:C:96:HIS:CD2	2:C:97:ILE:N	2.89	0.41
1:X:105:ARG:NH1	1:X:155:TYR:CE2	2.89	0.41
1:A:106:GLU:HB2	1:A:180:ALA:CB	2.50	0.41
1:A:311:MET:HE3	1:A:315:GLU:OE2	2.20	0.41
2:C:27:ARG:HG2	2:C:27:ARG:HH11	1.86	0.41
3:D:68:ARG:HB2	3:D:73:TRP:CH2	2.56	0.41
7:S:220:HIS:CD2	1:X:205:TYR:CE2	3.08	0.41
7:S:228:GLN:HA	7:S:228:GLN:OE1	2.20	0.41
1:X:113:ALA:HB1	1:X:118:LEU:HD23	2.03	0.41
1:X:311:MET:HE3	1:X:315:GLU:OE2	2.21	0.41
2:Y:74:ASP:HB3	2:Y:99:PHE:HD1	1.86	0.41
2:Y:77:TRP:HA	2:Y:78:PRO:HD3	1.98	0.41
1:A:155:TYR:HE1	7:T:244:ILE:O	2.04	0.41
1:A:215:VAL:HG12	1:A:217:ILE:HD12	2.02	0.41
1:A:396:TYR:O	1:A:397:SER:C	2.64	0.41
2:C:88:LEU:HB3	2:C:99:PHE:HB2	2.03	0.41
1:X:396:TYR:O	1:X:397:SER:C	2.64	0.41
3:Z:90:HIS:CE1	3:Z:94:ALA:HB2	2.55	0.41
1:A:192:MET:HE3	1:A:201:ILE:HD11	2.02	0.40
2:C:4:ASP:O	2:C:5:PHE:HB2	2.21	0.40
2:C:80:PRO:CG	2:C:100:THR:HG22	2.52	0.40
1:A:133:MET:O	1:A:134:ASN:C	2.62	0.40
1:A:243:ARG:HD3	1:A:395:TYR:CZ	2.56	0.40
2:C:24:PHE:HA	2:C:33:ARG:O	2.21	0.40
2:C:136:LEU:C	2:C:138:GLY:N	2.80	0.40
3:D:128:GLN:HG2	3:D:132:GLU:OE2	2.20	0.40
6:U:418:ILE:HG22	6:U:419:ARG:O	2.21	0.40
1:A:135:VAL:C	1:A:136:GLN:HG3	2.45	0.40
1:X:279:GLN:HB2	1:X:346:VAL:CA	2.47	0.40
2:Y:27:ARG:NH1	2:Y:27:ARG:HG2	2.36	0.40
3:Z:77:VAL:HB	3:Z:117:THR:HG23	2.02	0.40
1:A:41:ASP:HB3	3:Z:68:ARG:NH1	2.36	0.40
1:A:153:LEU:HD23	1:A:176:LEU:HB2	2.03	0.40
2:C:115:ASP:OD1	2:C:115:ASP:O	2.40	0.40
7:T:237:ILE:O	7:T:237:ILE:HG22	2.21	0.40
1:X:113:ALA:HB1	1:X:114:PRO:HD2	2.04	0.40
1:X:230:ASN:OD1	1:X:231:LYS:N	2.54	0.40
1:A:290:VAL:HG21	1:A:334:THR:HG23	2.03	0.40
1:X:197:PHE:O	1:X:201:ILE:HD13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/411 (94%)	365 (94%)	23 (6%)	0	100	100
1	X	388/411 (94%)	366 (94%)	21 (5%)	1 (0%)	36	65
2	C	141/146 (97%)	129 (92%)	12 (8%)	0	100	100
2	Y	141/146 (97%)	128 (91%)	13 (9%)	0	100	100
3	D	87/90 (97%)	81 (93%)	6 (7%)	0	100	100
3	Z	87/90 (97%)	81 (93%)	6 (7%)	0	100	100
5	F	1/3 (33%)	1 (100%)	0	0	100	100
6	G	13/60 (22%)	13 (100%)	0	0	100	100
6	U	15/60 (25%)	13 (87%)	1 (7%)	1 (7%)	1	6
7	S	53/150 (35%)	46 (87%)	6 (11%)	1 (2%)	6	26
7	T	55/150 (37%)	48 (87%)	6 (11%)	1 (2%)	6	26
All	All	1369/1717 (80%)	1271 (93%)	94 (7%)	4 (0%)	36	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	S	222	LYS
6	U	433	ALA
1	X	384	ASP
7	T	230	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/361 (96%)	336 (97%)	9 (3%)	40	61
1	X	345/361 (96%)	335 (97%)	10 (3%)	37	60
2	C	131/134 (98%)	130 (99%)	1 (1%)	73	77
2	Y	131/134 (98%)	130 (99%)	1 (1%)	73	77
3	D	75/76 (99%)	74 (99%)	1 (1%)	61	71
3	Z	75/76 (99%)	75 (100%)	0	100	100
5	F	2/2 (100%)	2 (100%)	0	100	100
6	G	13/51 (26%)	13 (100%)	0	100	100
6	U	11/51 (22%)	11 (100%)	0	100	100
7	S	51/133 (38%)	51 (100%)	0	100	100
7	T	52/133 (39%)	51 (98%)	1 (2%)	50	66
All	All	1231/1512 (81%)	1208 (98%)	23 (2%)	50	66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	153	LEU
1	A	166	ARG
1	A	176	LEU
1	A	217	ILE
1	A	277	ILE
1	A	279	GLN
1	A	337	TRP
1	A	373	ARG
2	C	22	LEU
3	D	83	GLU
7	T	228	GLN
1	X	24	THR
1	X	108	GLN
1	X	153	LEU
1	X	166	ARG
1	X	197	PHE
1	X	201	ILE
1	X	217	ILE
1	X	337	TRP

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Mol	Chain	Res	Type
1	X	348	LEU
1	X	373	ARG
2	Y	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	253	GLN
1	A	308	HIS
1	A	351	ASN
1	A	356	ASN
2	C	13	HIS
3	D	67	GLN
3	D	103	HIS
3	D	128	GLN
3	D	135	ASN
6	G	430	GLN
6	U	420	ASN
6	U	430	GLN
1	X	194	ASN
1	X	253	GLN
1	X	308	HIS
1	X	351	ASN
1	X	356	ASN
1	X	399	GLN
2	Y	13	HIS
2	Y	86	GLN
2	Y	96	HIS
3	Z	67	GLN
3	Z	103	HIS
3	Z	128	GLN
3	Z	135	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	7/15 (46%)	4 (57%)	0
4	R	6/15 (40%)	3 (50%)	0
All	All	13/30 (43%)	7 (53%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	2	U
4	E	3	U
4	E	7	U
4	E	8	U
4	R	2	U
4	R	3	U
4	R	7	U

There are no RNA pucker outliers to report.

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
9	ANP	A	1413	8	33,33,33	2.59	8 (24%)	45,52,52	2.62	16 (35%)
9	ANP	X	1413	8	33,33,33	2.59	8 (24%)	45,52,52	2.61	16 (35%)

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
9	ANP	A	1413	8	-	7/18/38/38	0/3/3/3
9	ANP	X	1413	8	-	6/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	X	1413	ANP	PG-O1G	8.56	1.59	1.46
9	A	1413	ANP	PG-O1G	8.53	1.59	1.46
9	A	1413	ANP	PB-O1B	7.65	1.57	1.46
9	X	1413	ANP	PB-O1B	7.63	1.57	1.46
9	X	1413	ANP	C8-N9	4.33	1.44	1.37
9	A	1413	ANP	C8-N9	4.33	1.44	1.37
9	A	1413	ANP	PB-O2B	-3.08	1.48	1.56
9	X	1413	ANP	PB-O2B	-3.05	1.48	1.56
9	X	1413	ANP	PG-O3G	-3.04	1.48	1.56
9	A	1413	ANP	PG-O3G	-2.99	1.48	1.56
9	A	1413	ANP	C5-C4	2.76	1.44	1.39
9	X	1413	ANP	C5-C4	2.70	1.43	1.39
9	A	1413	ANP	O3'-C3'	-2.40	1.37	1.43
9	X	1413	ANP	O3'-C3'	-2.38	1.37	1.43
9	X	1413	ANP	C2'-C3'	2.21	1.59	1.53
9	A	1413	ANP	C2'-C3'	2.19	1.59	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1413	ANP	C2'-C1'-N9	6.89	130.42	113.30
9	X	1413	ANP	C2'-C1'-N9	6.87	130.37	113.30
9	X	1413	ANP	O2G-PG-O1G	-6.75	96.52	113.45
9	A	1413	ANP	O2G-PG-O1G	-6.74	96.55	113.45
9	X	1413	ANP	C3'-C2'-C1'	-5.57	90.93	101.46
9	A	1413	ANP	C3'-C2'-C1'	-5.56	90.94	101.46
9	A	1413	ANP	C1'-N9-C8	-5.36	115.21	127.09
9	X	1413	ANP	C1'-N9-C8	-5.34	115.25	127.09
9	A	1413	ANP	C4-N9-C1'	5.24	138.90	126.63
9	X	1413	ANP	C4-N9-C1'	5.24	138.89	126.63
9	A	1413	ANP	O3'-C3'-C4'	4.30	123.42	111.08
9	X	1413	ANP	O3'-C3'-C4'	4.29	123.41	111.08
9	A	1413	ANP	O2B-PB-O1B	4.22	118.92	109.87
9	X	1413	ANP	O2B-PB-O1B	4.18	118.83	109.87
9	X	1413	ANP	O3A-PB-N3B	3.01	114.93	106.59
9	A	1413	ANP	O3A-PB-N3B	2.99	114.89	106.59
9	A	1413	ANP	N3-C4-N9	2.94	132.17	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1413	ANP	O3A-PA-O1A	-2.94	101.87	110.70
9	X	1413	ANP	O4'-C1'-C2'	-2.93	100.34	106.62
9	X	1413	ANP	O3A-PA-O1A	-2.92	101.91	110.70
9	A	1413	ANP	O4'-C1'-C2'	-2.92	100.36	106.62
9	X	1413	ANP	O5'-PA-O1A	-2.92	97.35	108.94
9	A	1413	ANP	O5'-PA-O1A	-2.92	97.36	108.94
9	X	1413	ANP	N3-C4-N9	2.92	132.13	127.17
9	A	1413	ANP	O2G-PG-O3G	2.90	115.38	107.59
9	X	1413	ANP	O2G-PG-O3G	2.90	115.38	107.59
9	A	1413	ANP	C5-C4-N3	-2.75	122.92	126.72
9	X	1413	ANP	C5-C4-N3	-2.74	122.94	126.72
9	A	1413	ANP	O3'-C3'-C2'	2.22	118.93	111.82
9	X	1413	ANP	O3'-C3'-C2'	2.19	118.84	111.82
9	A	1413	ANP	O1G-PG-N3B	-2.07	108.72	111.77
9	X	1413	ANP	O1G-PG-N3B	-2.04	108.77	111.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

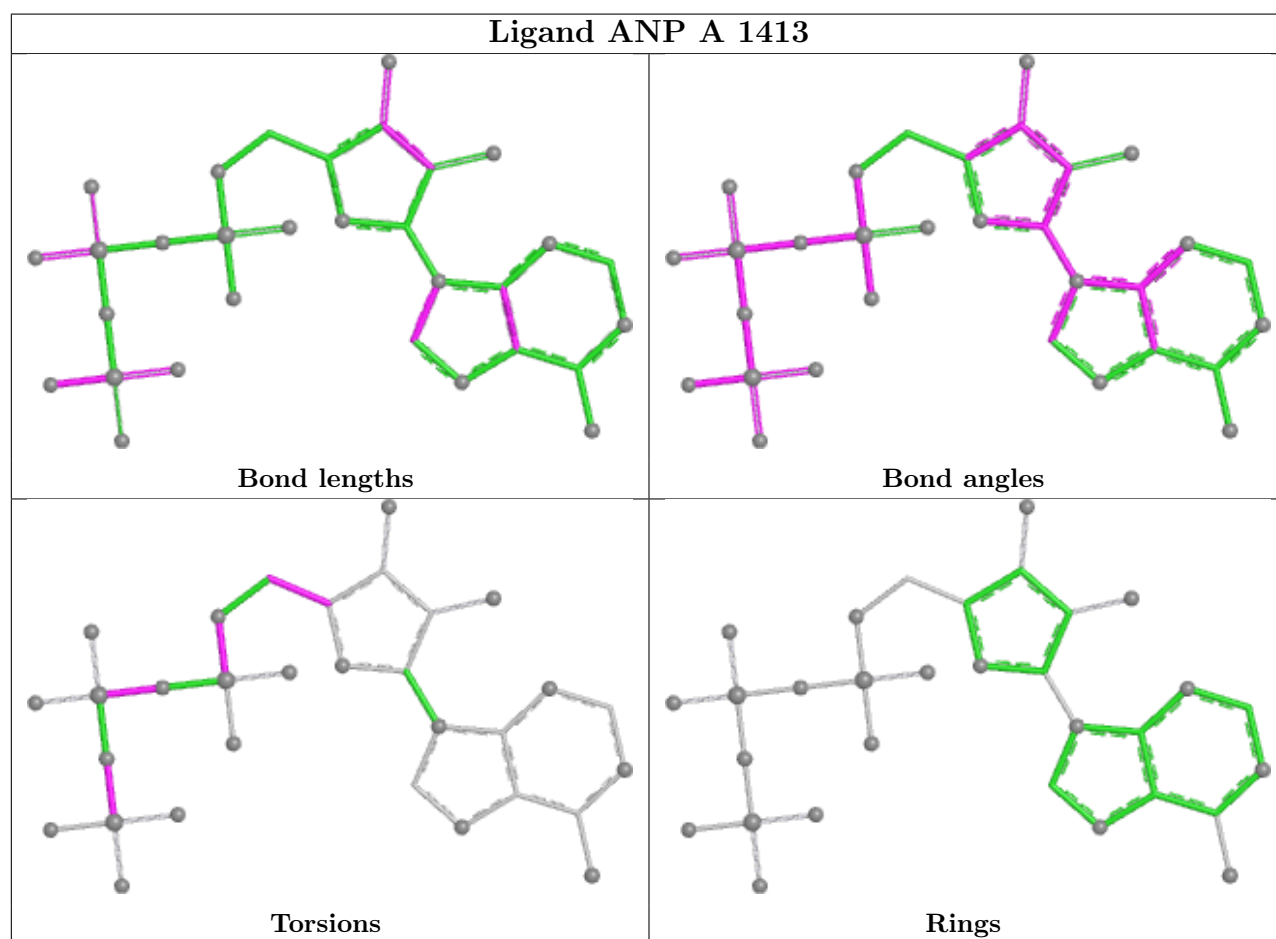
Mol	Chain	Res	Type	Atoms
9	A	1413	ANP	PB-N3B-PG-O1G
9	A	1413	ANP	C5'-O5'-PA-O1A
9	A	1413	ANP	O4'-C4'-C5'-O5'
9	X	1413	ANP	C5'-O5'-PA-O1A
9	X	1413	ANP	O4'-C4'-C5'-O5'
9	A	1413	ANP	C3'-C4'-C5'-O5'
9	X	1413	ANP	C3'-C4'-C5'-O5'
9	A	1413	ANP	C5'-O5'-PA-O2A
9	A	1413	ANP	C5'-O5'-PA-O3A
9	X	1413	ANP	C5'-O5'-PA-O2A
9	X	1413	ANP	C5'-O5'-PA-O3A
9	A	1413	ANP	PA-O3A-PB-O1B
9	X	1413	ANP	PB-N3B-PG-O1G

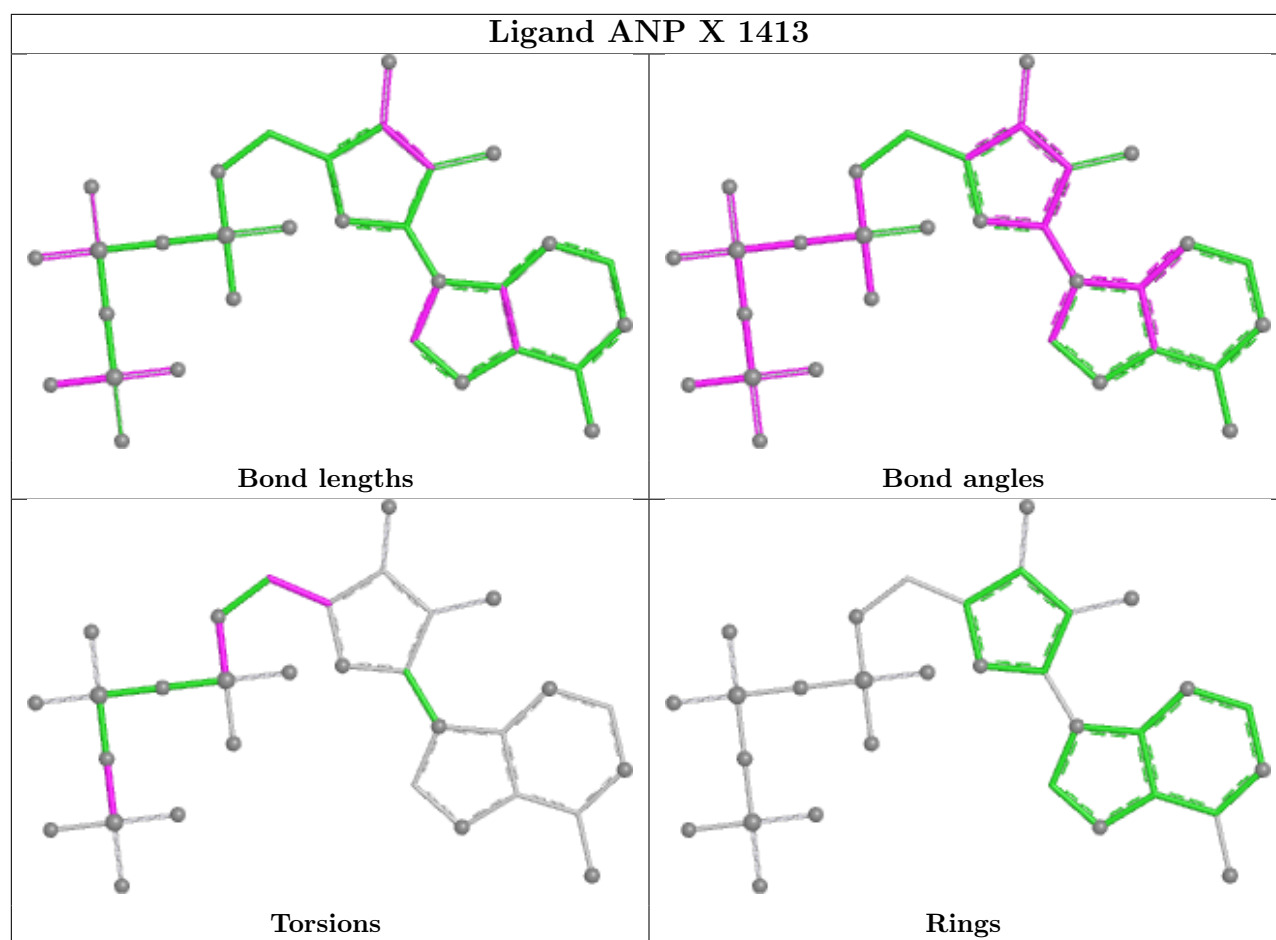
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1413	ANP	6	0
9	X	1413	ANP	6	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

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	390/411 (94%)	-0.03	3 (0%) 82 71	37, 69, 110, 155	0
1	X	390/411 (94%)	-0.00	2 (0%) 87 78	49, 79, 100, 120	0
2	C	143/146 (97%)	-0.12	0 100 100	44, 80, 111, 152	0
2	Y	143/146 (97%)	-0.13	0 100 100	57, 77, 92, 111	0
3	D	89/90 (98%)	0.10	0 100 100	56, 84, 137, 162	0
3	Z	89/90 (98%)	0.10	0 100 100	57, 78, 106, 113	0
4	E	8/15 (53%)	0.13	0 100 100	75, 90, 135, 151	0
4	R	7/15 (46%)	0.24	0 100 100	75, 83, 113, 168	0
5	F	3/3 (100%)	0.93	0 100 100	91, 91, 99, 105	0
6	G	15/60 (25%)	0.46	1 (6%) 24 19	80, 110, 145, 147	0
6	U	17/60 (28%)	0.44	2 (11%) 9 10	66, 88, 133, 140	0
7	S	57/150 (38%)	0.29	1 (1%) 67 53	78, 92, 110, 117	0
7	T	59/150 (39%)	0.29	2 (3%) 48 35	61, 92, 127, 144	0
All	All	1410/1747 (80%)	0.02	11 (0%) 82 71	37, 79, 113, 168	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	S	244	ILE	4.2
1	X	137	CYS	3.6
7	T	216	GLY	2.7
6	U	433	ALA	2.5
6	G	432	GLY	2.4
1	X	342	ASP	2.3
6	U	418	ILE	2.2
1	A	70	LYS	2.2
1	A	274	THR	2.1

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Mol	Chain	Res	Type	RSRZ
7	T	244	ILE	2.1
1	A	342	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

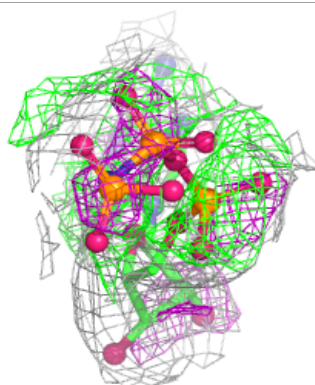
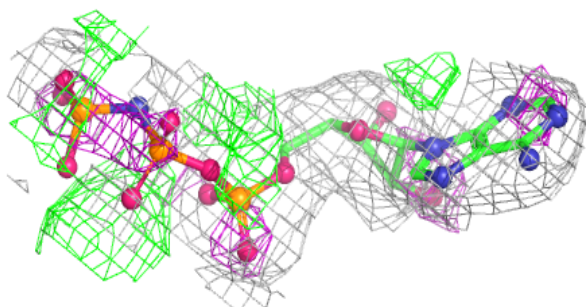
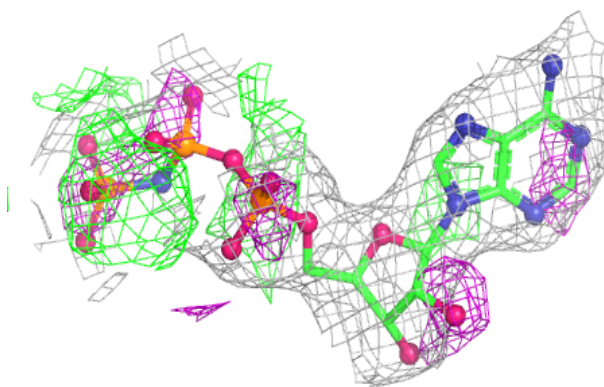
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
8	MG	A	1412	1/1	0.77	0.29	81,81,81,81	0
8	MG	X	1412	1/1	0.78	0.24	81,81,81,81	0
9	ANP	A	1413	31/31	0.91	0.10	30,34,37,39	0
9	ANP	X	1413	31/31	0.92	0.10	30,34,37,39	0

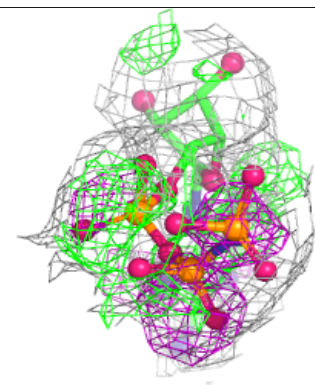
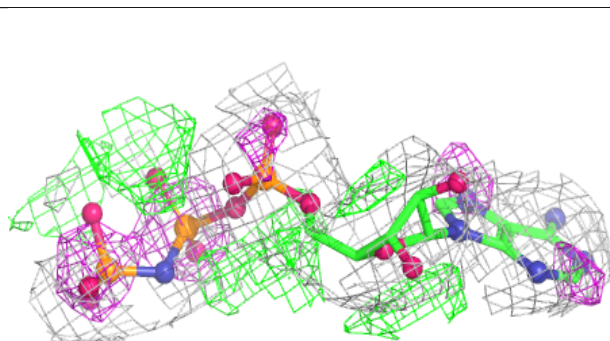
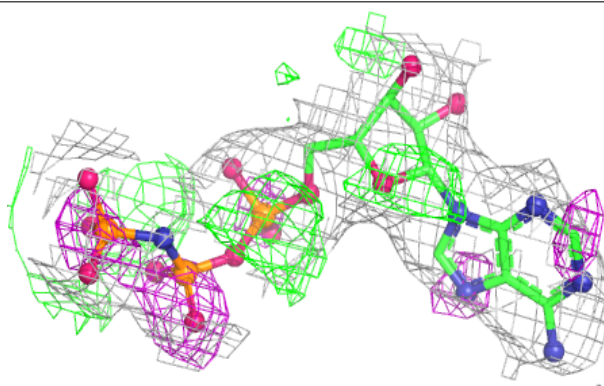
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 1413:

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

**Electron density around ANP X 1413:**

$2mF_o-DF_c$ (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.