Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 08:00 AM EST

PDB ID	:	3CC4
Title	:	Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit
Authors	:	Blaha, G.; Gurel, G.
Deposited on	:	2008-02-24
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

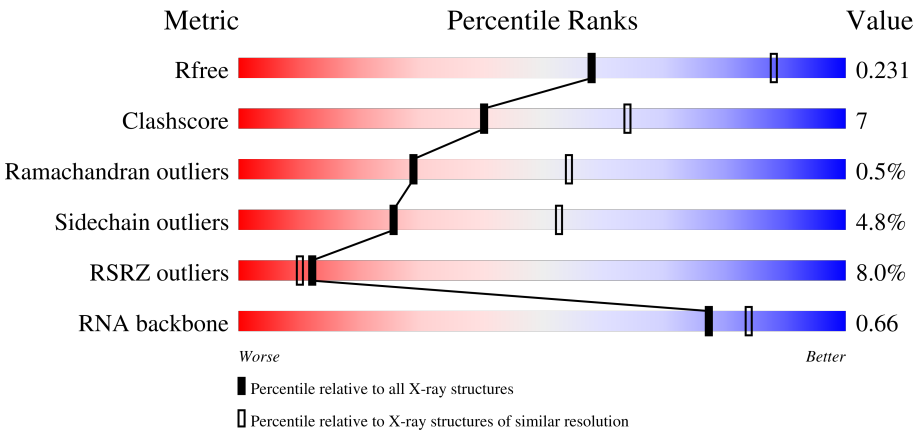
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	9%, 84%, 14%, ··
2	B	338	3%, 87%, 12%, ·
3	C	246	.%, 83%, 14%, ·
4	D	177	40%, 66%, 14%, 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	178	8% 87% 10%
6	F	120	26% 86% 13%
7	G	348	3% 8% 92%
8	H	177	23% 76% 14% 10%
9	I	162	40% 40% 57%
10	J	145	% 86% 10%
11	K	132	2% 86% 13%
12	L	165	16% 76% 12% 12%
13	M	196	% 86% 12%
14	N	187	20% 87% 12%
15	O	116	2% 95%
16	P	149	3% 85% 11%
17	Q	96	% 89% 10%
18	R	155	89% 6%
19	S	85	9% 82% 13% 5%
20	T	120	6% 86% 12%
21	U	67	6% 69% 9% 21%
22	V	71	39% 79% 13% 8%
23	W	154	3% 81% 18%
24	X	92	13% 71% 16% 11%
25	Y	241	2% 54% 5% 41%
26	Z	116	38% 55% 8% 37%
27	1	57	81% 16%
28	2	50	22% 76% 16% 8%
29	3	92	7% 85% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	0	2923	2% 59% 29% 5% 6%
31	9	122	3% 48% 40% 11%

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
32	MG	0	8069	-	-	-	X
32	MG	A	8051	-	-	-	X
34	SR	0	8933	-	-	-	X
34	SR	0	8947	-	-	-	X
34	SR	0	8957	-	-	-	X
34	SR	0	8976	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	8996	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8549	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8554	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	S	8510	-	-	-	X

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 99135 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 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1753	1072	352	324	5	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	337	2625	1616	493	511	5	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	1860	1130	345	384	1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	140	1094	685	195	210	4	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	172	1357	840	224	289	4	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	119	890	551	141	197	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	29	240	149	39	51	1	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	160	1282	798	240	238	6	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	70	519	323	81	114	1	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	142	1120	696	199	222	3	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	132	994	609	189	192	4	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	L	145	1118	670	222	226	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	194	1558	943	333	281	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	186	1445	895	262	286	2	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	O	115	865	529	161	175	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	P	143	1136	683	229	224	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	Q	95	735	450	141	144	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	R	150	1149	713	209	223	4	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	81	641	389	111	138	3	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	T	119	950	568	180	202	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	U	53	410	244	75	86	5	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	V	65	499	304	94	100	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	W	154	1196	737	209	244	6	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	X	82	654	402	129	122	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
25	Y	142	1130	686	228	216	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Z	73	573	343	113	112	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	1	56	431	258	86	83	4	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	2	46	396	239	89	67	1	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	3	92	755	458	153	137	7	0	0	0

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
30	0	2754	59021	26349	10873	19054	2745	0	0	0

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
31	9	122	2599	1160	471	847	121	0	0	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
32	A	1	1	1	0	0
32	B	1	1	1	0	0
32	K	1	1	1	0	0
32	T	1	1	1	0	0
32	Y	1	1	1	0	0
32	0	87	87	87	0	0
32	9	1	1	1	0	0

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
33	A	1	1	1	0	0
33	B	1	1	1	0	0
33	J	3	3	3	0	0
33	L	1	1	1	0	0
33	M	1	1	1	0	0
33	N	1	1	1	0	0
33	O	1	1	1	0	0
33	R	1	1	1	0	0
33	Y	1	1	1	0	0
33	3	1	1	1	0	0
33	0	10	10	10	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
34	A	3	3	3	0	0
34	B	2	2	2	0	0
34	F	1	1	1	0	0
34	H	1	1	1	0	0
34	R	1	1	1	0	0
34	S	1	1	1	0	0
34	1	2	2	2	0	0
34	3	2	2	2	0	0
34	0	92	92	92	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
34	9	3	3	3	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
35	B	1	1	1	0	0
			Total	Na		
35	C	1	1	1	0	0
			Total	Na		
35	J	1	1	1	0	0
			Total	Na		
35	M	1	1	1	0	0
			Total	Na		
35	Q	1	1	1	0	0
			Total	Na		
35	R	1	1	1	0	0
			Total	Na		
35	S	1	1	1	0	0
			Total	Na		
35	0	66	66	66	0	0
			Total	Na		
35	9	2	2	2	0	0

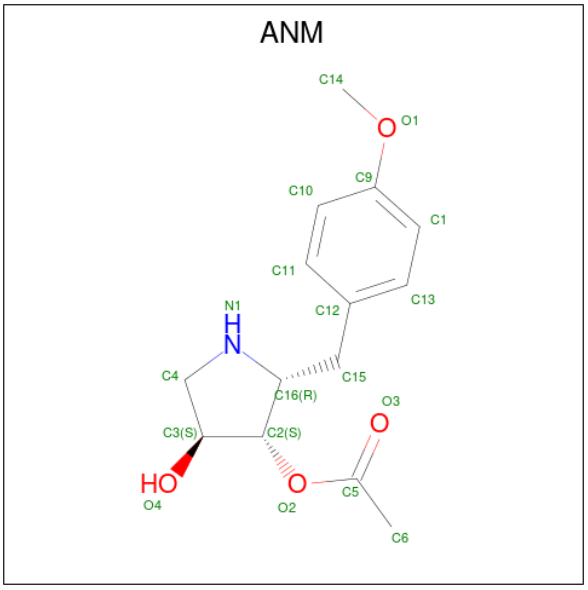
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
36	O	1	1	1	0	0
			Total	Cd		
36	U	1	1	1	0	0
			Total	Cd		
36	Z	1	1	1	0	0
			Total	Cd		
36	1	1	1	1	0	0
			Total	Cd		
36	3	1	1	1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
37	0	2	2	2	0	0

- Molecule 38 is ANISOMYCIN (three-letter code: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
38	0	1	19	14	1	4	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
39	A	110	110	110	0	0
39	B	140	140	140	0	0
39	C	163	163	163	0	0
39	D	46	46	46	0	0
39	E	44	44	44	0	0
39	F	26	26	26	0	0
39	G	17	17	17	0	0
39	H	67	67	67	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	I	6	Total O 6 6	0	0
39	J	49	Total O 49 49	0	0
39	K	56	Total O 56 56	0	0
39	L	85	Total O 85 85	0	0
39	M	121	Total O 121 121	0	0
39	N	61	Total O 61 61	0	0
39	O	44	Total O 44 44	0	0
39	P	62	Total O 62 62	0	0
39	Q	48	Total O 48 48	0	0
39	R	78	Total O 78 78	0	0
39	S	32	Total O 32 32	0	0
39	T	39	Total O 39 39	0	0
39	U	27	Total O 27 27	0	0
39	V	13	Total O 13 13	0	0
39	W	65	Total O 65 65	0	0
39	X	23	Total O 23 23	0	0
39	Y	92	Total O 92 92	0	0
39	Z	31	Total O 31 31	0	0
39	1	48	Total O 48 48	0	0
39	2	38	Total O 38 38	0	0
39	3	66	Total O 66 66	0	0

Continued on next page...

Continued from previous page...

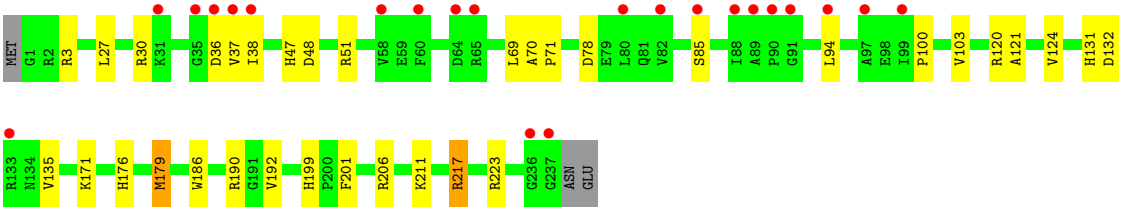
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
39	0	5972	5972	5972	0	0
			Total	O		
39	9	147	147	147	0	0

3 Residue-property plots (i)

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

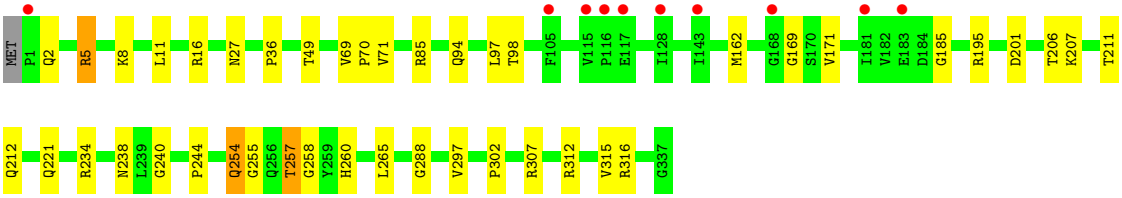
• Molecule 1: 50S ribosomal protein L2P

Chain A:



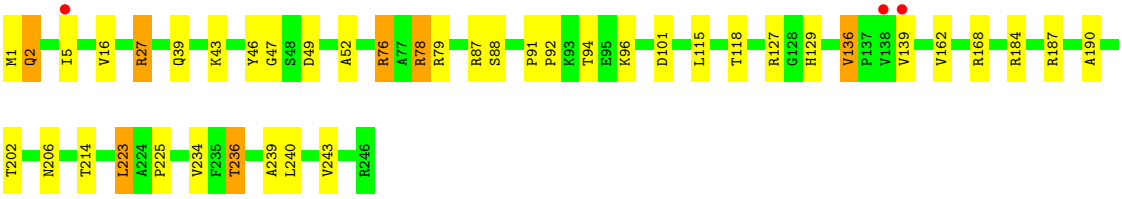
• Molecule 2: 50S ribosomal protein L3P

Chain B:



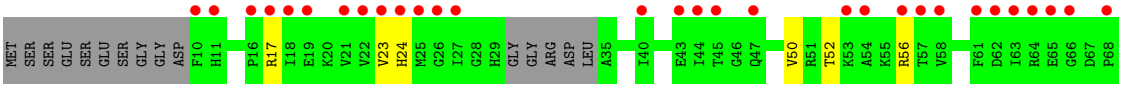
• Molecule 3: 50S ribosomal protein L4P

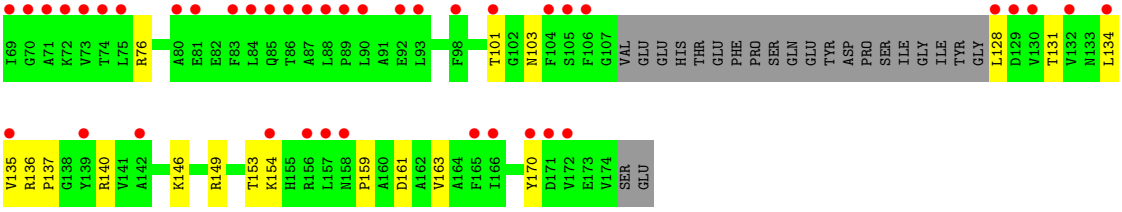
Chain C:



• Molecule 4: 50S ribosomal protein L5P

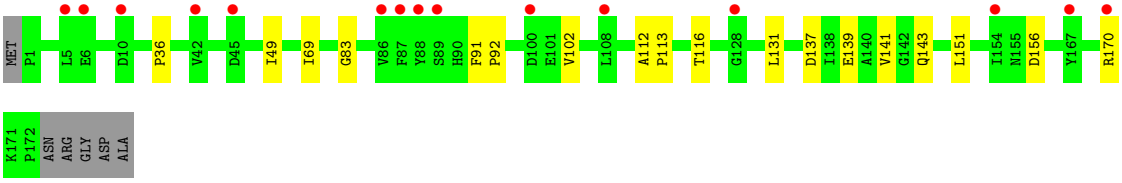
Chain D:





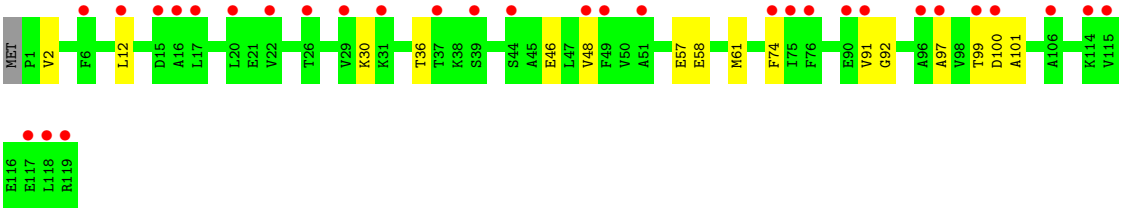
• Molecule 5: 50S ribosomal protein L6P

Chain E:



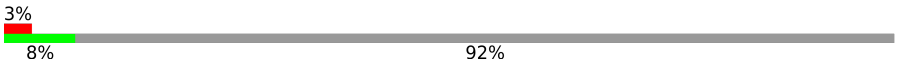
• Molecule 6: 50S ribosomal protein L7Ae

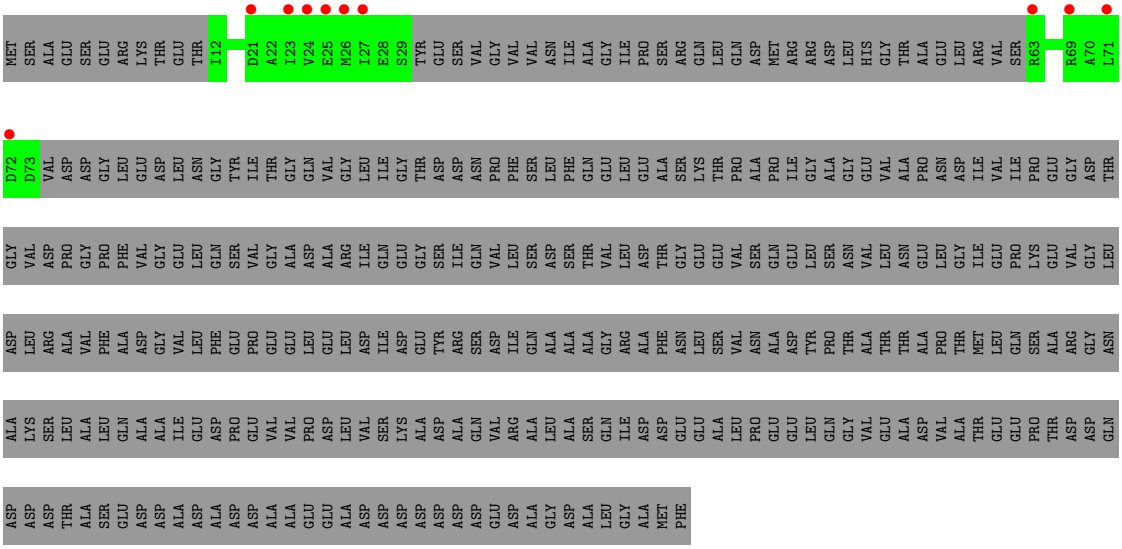
Chain F:



• Molecule 7: 50S ribosomal protein L10E

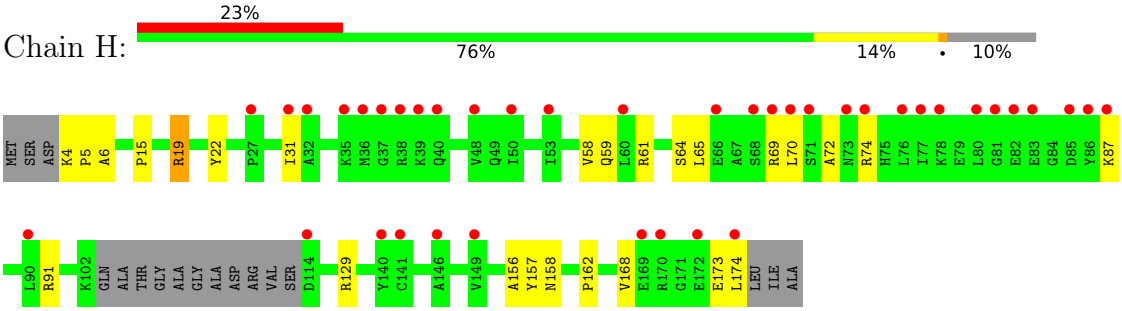
Chain G:





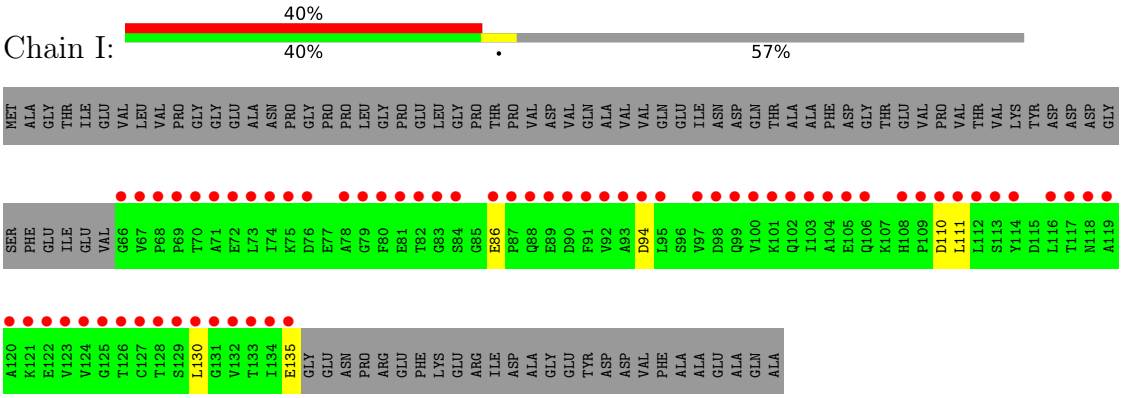
• Molecule 8: 50S ribosomal protein L10e

Chain H:



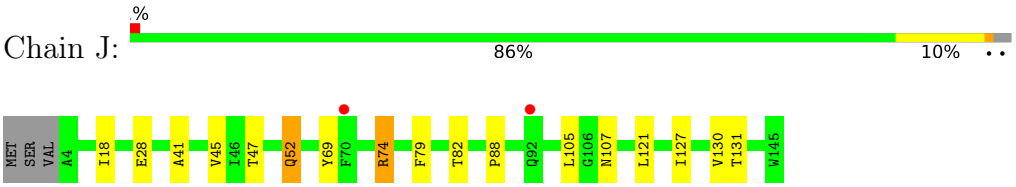
- Molecule 9: 50S ribosomal protein L11P

Chain I:



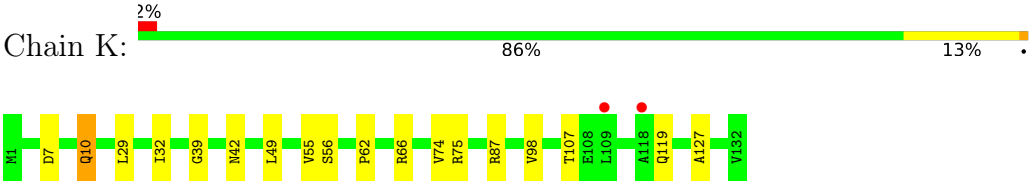
- Molecule 10: 50S ribosomal protein L13P

Chain J:



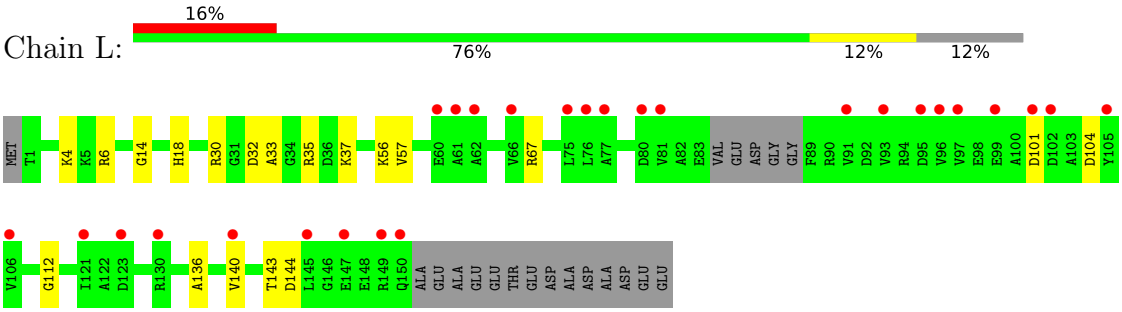
- Molecule 11: 50S ribosomal protein L14P

Chain K:



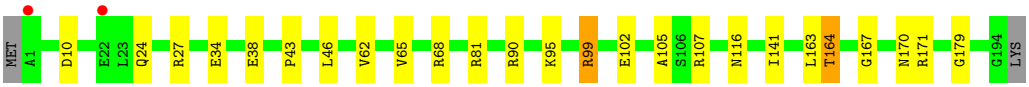
- Molecule 12: 50S ribosomal protein L15P

Chain L:



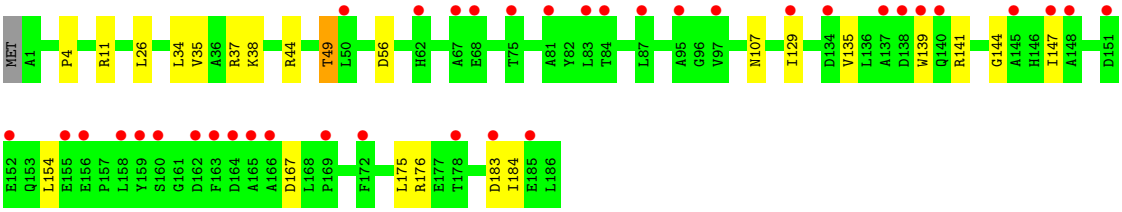
- Molecule 13: 50S ribosomal protein L15e

Chain M:

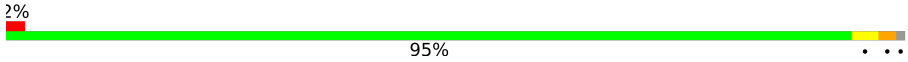


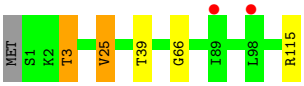
- Molecule 14: 50S ribosomal protein L18P

Chain N:



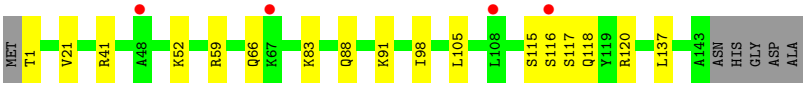
- Molecule 15: 50S ribosomal protein L18e

Chain O: 



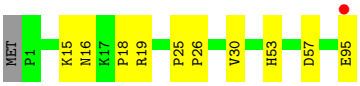
- Molecule 16: 50S ribosomal protein L19e

Chain P:



- Molecule 17: 50S ribosomal protein L21e

Chain Q:



- Molecule 18: 50S ribosomal protein L22P

Chain R:

- Molecule 19: 50S ribosomal protein L23P

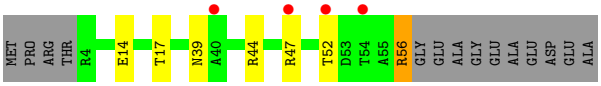
Chain S:

• Molecule 20: 50S ribosomal protein L24P

Chain T:

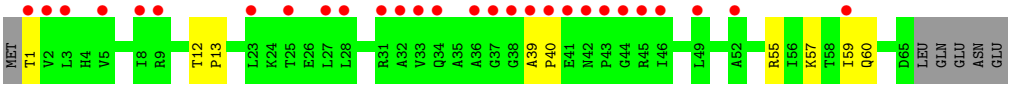
• Molecule 21: 50S ribosomal protein L24e

Chain U:



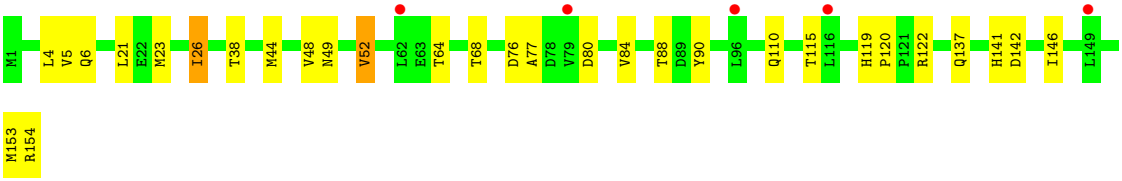
• Molecule 22: 50S ribosomal protein L29P

Chain V:



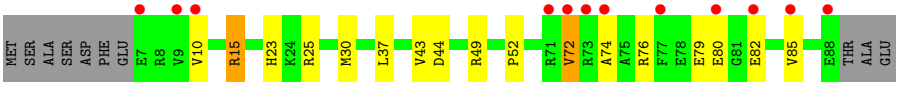
• Molecule 23: 50S ribosomal protein L30P

Chain W:



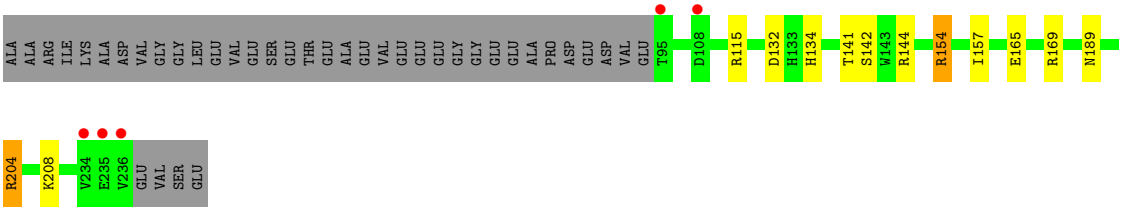
• Molecule 24: 50S ribosomal protein L31e

Chain X:



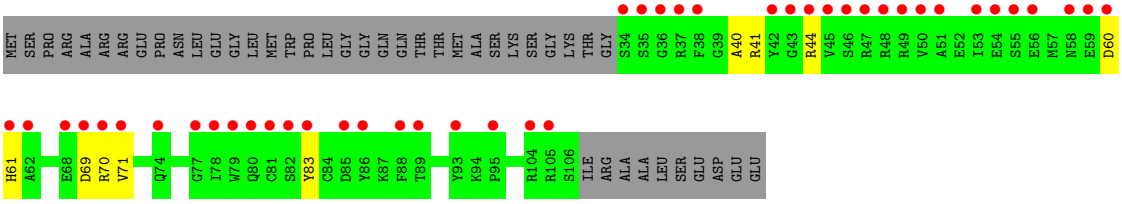
• Molecule 25: 50S ribosomal protein L32e

Chain Y:



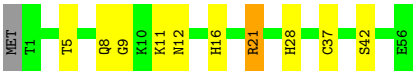
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



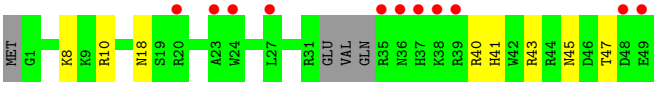
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



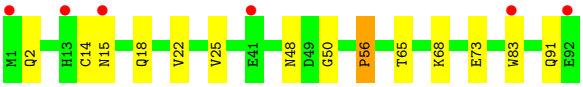
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



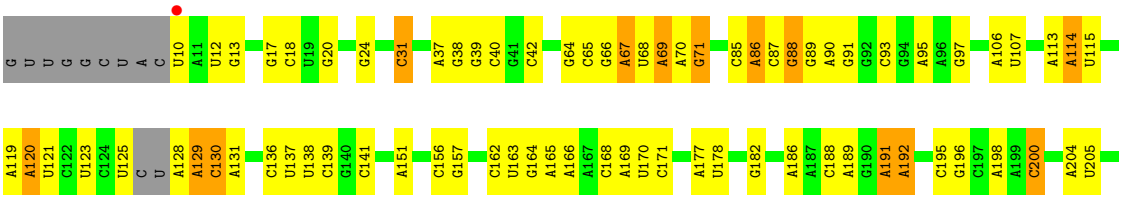
- Molecule 29: 50S ribosomal protein L44E

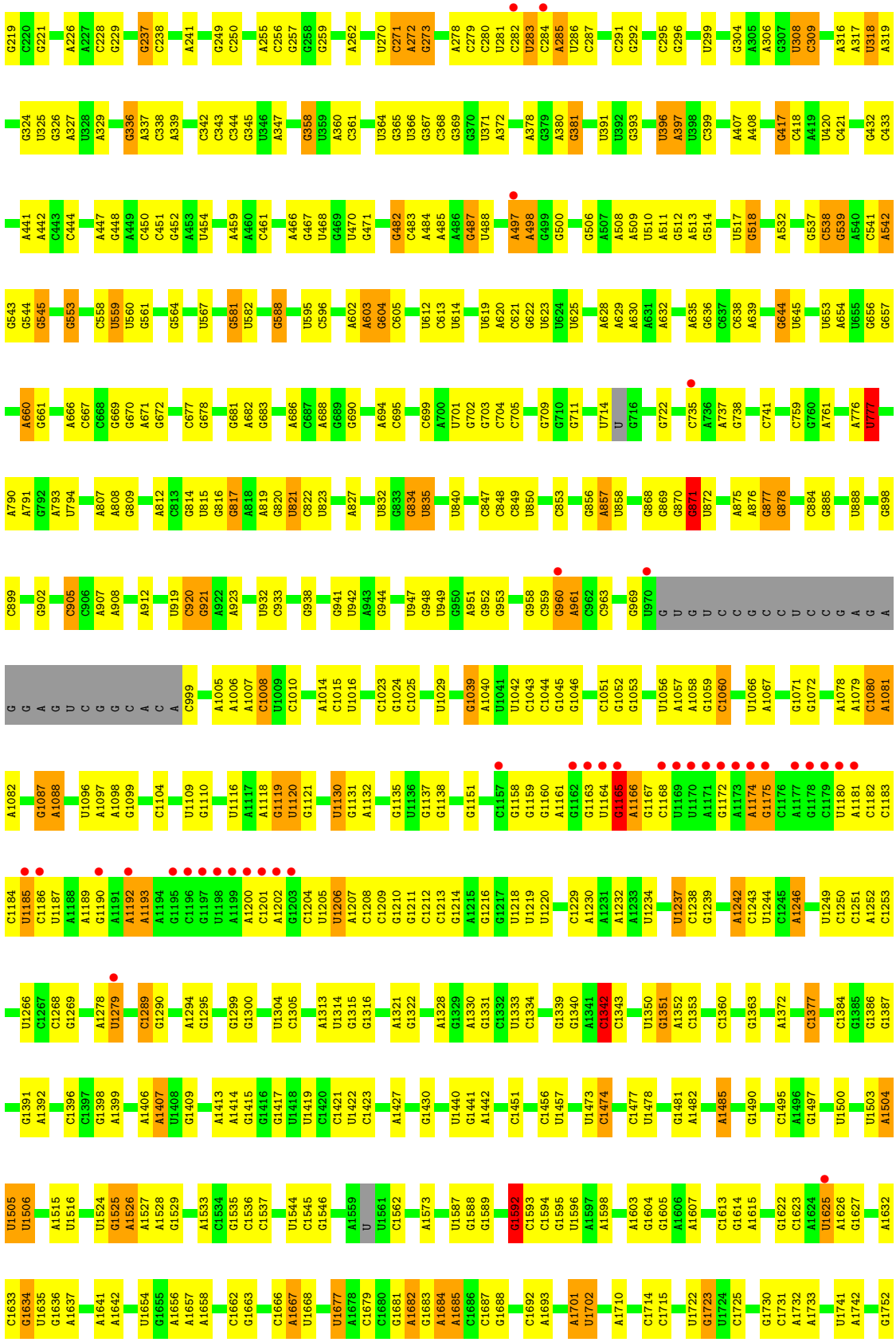
Chain 3:

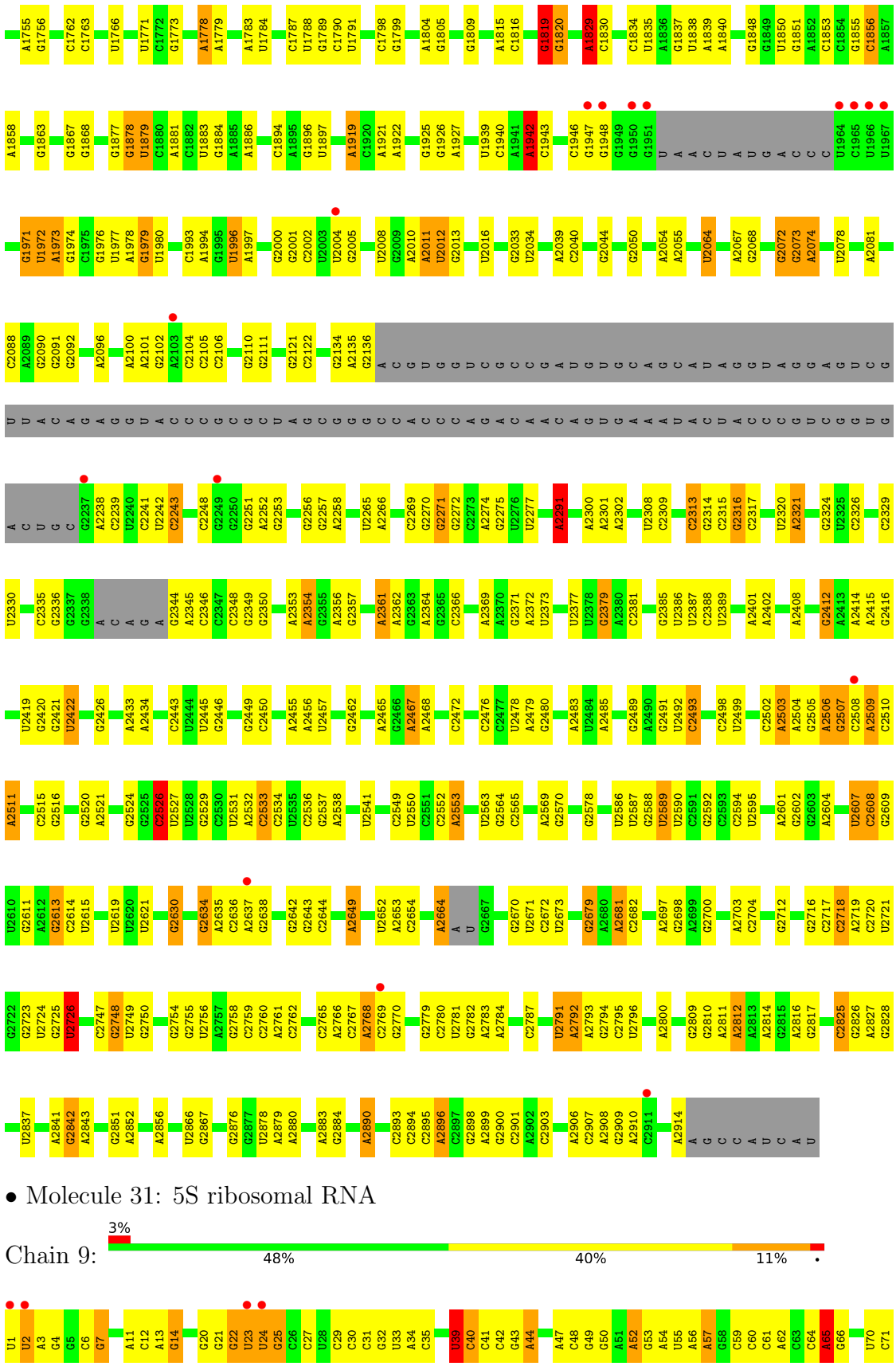


- Molecule 30: 23S ribosomal RNA

Chain 0:

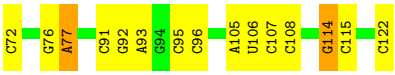



G219 C220 G221 A226 A227 C228 G229 G237 C238 A241 G249 C250 A255 C256 G257 G258 G259 A262 U270 C271 A272 G273 A278 C279 C280 U281 C282 U283 C284 A285 U286 C287 C291 G292 C295 G296 U299 G304 A305 A306 G307 U308 C309 A316 A317 U318 A319
G324 U325 G326 A327 U328 A329 G336 A337 C338 A339 C342 C343 C344 G345 U346 A347 G358 U359 A360 C361 U364 G365 U366 G367 C368 G369 G370 U371 A372 A378 G379 A380 G381 U391 U392 G393 U396 A397 U398 C399 A407 A408 G417 C418 A419 U420 C421 G432 C433
A441 A442 C443 C444 A447 G448 A449 C450 C451 G452 A453 U454 A459 A460 C461 A466 G467 U468 G469 U470 G471 G492 C483 A484 A485 A486 G487 U488 A497 A498 G499 G500 G506 A507 A508 A509 U510 A511 G512 A513 G514 U517 G518 A532 G537 C538 G539 A540 C541 A542
G543 G544 G545 G553 C558 U559 U560 G561 G564 U567 G581 U582 G588 U595 C596 A602 A603 G604 C605 U612 C613 U614 U619 A620 C621 G622 U623 U624 U625 A628 A629 A630 A631 A632 A635 G636 C637 C638 A639 G644 U645 U653 A654 U655 G656 G657
A660 G661 A666 C667 C668 G669 G670 A671 G672 C677 G678 G681 A682 G683 A686 C687 A688 G689 G690 A694 C695 C699 A700 U701 G702 G703 C704 C705 G709 G710 G711 U714 U G716 G722 C735 A736 A737 G738 C741 C759 G760 A761 A776 U777
A790 A791 G792 A793 U794 A807 A808 C809 A812 C813 G814 U815 G816 G817 A818 A819 G820 U821 C822 U823 A827 U832 G833 G834 U835 U840 C847 C848 C849 U850 C853 G856 A857 U858 G868 G869 G870 G871 U872 A875 A876 G877 G878 C884 G885 U888 G898
C899 G902 G905 C906 A907 A908 A912 U919 C920 G921 A922 A923 U932 C933 G938 G941 U942 A943 G944 U947 G948 U949 G950 A951 G952 G953 G958 C959 G960 A961 C962 C963 G969 U970 G U G U C C G C A A G A
G G A G U C G G C A C A C999 A1005 A1006 A1007 C1008 U1009 C1010 A1014 C1015 U1016 C1023 G1024 C1025 U1029 G1039 A1040 U1041 U1042 C1043 C1044 G1045 G1046 C1051 G1052 G1053 U1056 A1057 A1058 G1059 C1060 U1066 A1067 G1071 G1072 A1078 A1079 C1080 A1081
A1082 G1087 A1088 U1096 A1097 A1098 G1099 C1104 U1109 G1110 U1116 A1117 A1118 G1119 U1120 G1121 U1130 G1131 A1132 G1135 U1136 G1137 G1138 G1151 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 C1179 U1180 A1181 C1182 C1183
C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 U1220 C1229 A1230 A1231 A1232 A1233 U1234 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253
U1266 C1267 C1268 G1269 A1278 U1279 C1289 G1290 A1294 G1295 G1299 G1300 U1304 C1305 A1313 U1314 G1315 G1316 A1321 G1322 A1328 G1329 A1330 G1331 C1332 U1333 C1334 G1339 G1340 A1341 C1342 C1343 U1350 G1351 A1352 C1353 C1360 G1363 A1372 C1377 C1384 G1385 G1386 G1387
G1391 A1392 C1396 C1397 G1398 A1399 A1406 A1407 U1408 G1409 A1413 A1414 G1415 G1416 G1417 U1418 U1419 C1420 C1421 U1422 C1423 A1427 G1430 U1440 G1441 A1442 C1451 C1456 U1457 U1473 C1474 C1477 U1478 G1481 A1482 A1485 G1490 C1495 A1496 G1497 U1500 U1503 A1504
U1505 U1506 A1515 U1516 U1524 G1525 A1526 A1527 A1528 G1529 A1533 C1534 G1535 C1536 C1537 U1544 C1545 G1546 A1559 U U1561 C1562 A1573 U1587 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 A1606 A1607 C1613 G1614 A1615 G1622 C1623 A1624 U1625 A1626 G1627 A1632
C1633 G1634 U1635 G1636 A1637 A1641 A1642 U1654 G1655 A1656 A1657 A1658 C1662 G1663 C1666 A1667 U1668 U1677 A1678 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 G1688 C1692 A1693 A1701 U1702 A1710 C1714 C1715 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 U1741 A1742 G1752



• Molecule 31: 5S ribosomal RNA

Chain 9:


C72
G76
A77
C91
G92
A93
G94
C95
C96
A105
U106
C107
C108
G114
C115
C122

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.78Å 299.08Å 573.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.70 85.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.70) 96.9 (85.45-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.244 0.191 , 0.231	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	99135	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UR3, OMG, PSU, NA, ANM, SR, 1MA, CL, OMU, CD, K

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	0.51	0/1786	0.78	0/2408
2	B	0.53	0/2690	0.78	0/3652
3	C	0.54	0/1885	0.77	0/2552
4	D	0.65	0/1111	0.71	1/1498 (0.1%)
5	E	0.60	0/1382	0.68	0/1880
6	F	0.54	0/901	0.71	0/1224
7	G	0.51	0/241	0.67	0/324
8	H	0.60	0/1302	0.79	0/1743
9	I	0.59	0/526	0.62	0/716
10	J	0.61	0/1136	0.72	0/1530
11	K	0.51	0/1004	0.80	0/1351
12	L	0.49	0/1130	0.76	0/1509
13	M	0.51	0/1582	0.77	0/2116
14	N	0.55	0/1474	0.77	0/1999
15	O	0.47	0/874	0.73	1/1181 (0.1%)
16	P	0.52	0/1147	0.67	0/1528
17	Q	0.49	0/749	0.77	0/1005
18	R	0.54	0/1172	0.74	0/1578
19	S	0.54	0/648	0.67	0/875
20	T	0.46	0/958	0.76	1/1289 (0.1%)
21	U	0.57	0/417	0.71	0/562
22	V	0.44	0/502	0.67	0/675
23	W	0.52	0/1219	0.78	1/1655 (0.1%)
24	X	0.52	0/664	0.72	0/895
25	Y	0.52	0/1146	0.74	0/1536
26	Z	0.69	0/584	0.74	0/781
27	1	0.55	0/438	0.75	0/578
28	2	0.45	0/401	0.70	0/529
29	3	0.59	0/771	0.70	0/1024
30	0	0.37	0/65958	0.68	15/102869 (0.0%)
31	9	0.32	0/2904	0.69	1/4526 (0.0%)
All	All	0.43	0/98702	0.70	20/147588 (0.0%)

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
23	W	0	1
30	0	0	42
31	9	0	2
All	All	0	45

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	4	LEU	CA-CB-CG	7.59	132.77	115.30
30	0	1942	A	C5'-C4'-C3'	6.82	126.92	116.00
30	0	871	G	C5'-C4'-O4'	-6.64	101.13	109.10
30	0	1504	A	N9-C1'-C2'	5.91	121.68	114.00
30	0	2726	U	N1-C1'-C2'	5.85	121.60	114.00
31	9	39	U	N1-C1'-C2'	5.84	121.59	114.00
30	0	1504	A	C1'-O4'-C4'	-5.62	105.40	109.90
15	O	66	GLY	N-CA-C	5.61	127.11	113.10
30	0	1592	G	N9-C1'-C2'	5.49	121.14	114.00
30	0	1819	G	C5'-C4'-C3'	5.49	124.78	116.00
30	0	2467	A	C1'-O4'-C4'	-5.47	105.52	109.90
20	T	52	ARG	N-CA-C	5.42	125.64	111.00
30	0	1829	A	N9-C1'-C2'	-5.39	106.08	112.00
30	0	2313	C	C5'-C4'-O4'	5.32	115.48	109.10
30	0	1120	U	C5'-C4'-C3'	-5.21	107.66	116.00
4	D	170	TYR	N-CA-C	5.14	124.87	111.00
30	0	1165	G	C1'-O4'-C4'	-5.12	105.80	109.90
30	0	777	U	O4'-C1'-N1	5.12	112.29	108.20
30	0	2316	G	C5'-C4'-C3'	-5.09	107.86	116.00
30	0	2291	A	N9-C1'-C2'	5.05	120.56	114.00

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	0	1342	C	Sidechain
30	0	1351	G	Sidechain
30	0	1417	G	Sidechain
30	0	1430	G	Sidechain
30	0	1677	U	Sidechain
30	0	1702	U	Sidechain
30	0	1809	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	1993	C	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2526	C	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	2679	G	Sidechain
30	0	270	U	Sidechain
30	0	2726	U	Sidechain
30	0	2842	G	Sidechain
30	0	391	U	Sidechain
30	0	396	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	817	G	Sidechain
30	0	888	U	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	21	0
2	B	2625	0	2533	29	0
3	C	1860	0	1813	22	0
4	D	1094	0	1085	11	0
5	E	1357	0	1266	10	0
6	F	890	0	843	8	0
7	G	240	0	231	0	0
8	H	1282	0	1292	18	0
9	I	519	0	500	4	0
10	J	1120	0	1098	14	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	12	0
13	M	1558	0	1573	19	0
14	N	1445	0	1401	16	0
15	O	865	0	873	4	0
16	P	1136	0	1123	11	0
17	Q	735	0	729	6	0
18	R	1149	0	1122	11	0
19	S	641	0	605	5	0
20	T	950	0	924	8	0
21	U	410	0	364	3	0
22	V	499	0	511	4	0
23	W	1196	0	1137	22	0
24	X	654	0	653	11	0
25	Y	1130	0	1133	13	0
26	Z	573	0	532	6	0
27	1	431	0	426	10	0
28	2	396	0	413	5	0
29	3	755	0	729	7	0
30	0	59021	0	29812	846	0
31	9	2599	0	1325	64	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	0	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	1	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	19	0	19	5	0
39	0	5972	0	0	121	0
39	1	48	0	0	0	0
39	2	38	0	0	0	0
39	3	66	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	9	147	0	0	5	0
39	A	110	0	0	4	0
39	B	140	0	0	5	0
39	C	163	0	0	2	0
39	D	46	0	0	0	0
39	E	44	0	0	0	0
39	F	26	0	0	0	0
39	G	17	0	0	0	0
39	H	67	0	0	3	0
39	I	6	0	0	1	0
39	J	49	0	0	1	0
39	K	56	0	0	0	0
39	L	85	0	0	2	0
39	M	121	0	0	1	0
39	N	61	0	0	1	0
39	O	44	0	0	0	0
39	P	62	0	0	0	0
39	Q	48	0	0	0	0
39	R	78	0	0	0	0
39	S	32	0	0	0	0
39	T	39	0	0	0	0
39	U	27	0	0	0	0
39	V	13	0	0	0	0
39	W	65	0	0	2	0
39	X	23	0	0	1	0
39	Y	92	0	0	3	0
39	Z	31	0	0	1	0
All	All	99135	0	59934	1085	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 7.

All (1085) 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)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.22	1.16
31:9:76:G:H3'	31:9:77:A:H5"	1.34	1.02
15:O:3:THR:HG22	30:0:656:G:H5'	1.43	1.00
30:0:871:G:H5'	30:0:871:G:H8	1.27	0.98
30:0:871:G:H5'	30:0:871:G:C8	1.98	0.97
30:0:2717:C:H2'	30:0:2718:C:H5"	1.46	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:171:ARG:HD3	30:0:156:C:H5"	1.44	0.96
10:J:82:THR:HG23	30:0:1242:A:H5'	1.47	0.96
30:0:2717:C:C2'	30:0:2718:C:H5"	1.97	0.94
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.15	0.93
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.13	0.93
14:N:37:ARG:NH1	31:9:6:C:H5"	1.83	0.93
31:9:56:A:H2'	31:9:57:A:H5"	1.48	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.91
30:0:870:G:H2'	30:0:871:G:H5"	1.53	0.90
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.54	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.20	0.89
30:0:1474:C:H5'	30:0:1474:C:H6	1.37	0.89
30:0:1116:U:HO2'	30:0:1118:A:H2	0.87	0.87
30:0:1160:G:H5'	30:0:1161:A:C5'	2.04	0.87
30:0:1160:G:C5'	30:0:1161:A:H5'	2.03	0.86
30:0:2506:A:HO2'	30:0:2507:G:H8	0.89	0.86
30:0:2812:A:H2	30:0:2814:A:H62	1.24	0.85
30:0:1667:A:H5'	30:0:1667:A:H8	1.42	0.85
30:0:1603:A:H5'	30:0:1605:G:O4'	1.75	0.85
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
30:0:1701:A:H4'	30:0:1702:U:H5"	1.56	0.84
11:K:10:GLN:H	11:K:10:GLN:HE21	1.25	0.83
30:0:2586:U:H3	30:0:2592:G:H22	1.21	0.83
39:N:8843:HOH:O	31:9:49:G:H5"	1.77	0.83
30:0:381:G:H5"	39:0:4352:HOH:O	1.77	0.83
30:0:1835:U:H5	30:0:1840:A:N7	1.76	0.83
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.61	0.82
30:0:541:C:H2'	30:0:542:A:H5"	1.61	0.82
30:0:559:U:H6	30:0:559:U:H5'	1.45	0.81
30:0:545:G:H5'	30:0:545:G:H8	1.44	0.81
30:0:2533:C:H6	30:0:2533:C:H5'	1.46	0.81
30:0:1979:G:H2'	39:0:3320:HOH:O	1.82	0.79
30:0:2291:A:C8	30:0:2309:C:H5'	2.18	0.78
30:0:871:G:H8	30:0:871:G:C5'	1.96	0.78
30:0:2908:A:H2'	30:0:2909:G:O4'	1.83	0.78
30:0:506:G:H22	30:0:509:A:C5'	1.97	0.78
38:0:2924:ANM:H151	38:0:2924:ANM:H63	1.63	0.78
30:0:1300:G:H1'	39:0:4716:HOH:O	1.82	0.77
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.85	0.77
30:0:1205:U:H2'	30:0:1206:U:H5"	1.66	0.77
30:0:506:G:H22	30:0:509:A:H5"	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:853:C:H3'	39:0:4586:HOH:O	1.83	0.77
30:0:541:C:C2'	30:0:542:A:H5"	2.15	0.76
30:0:1666:C:O2'	30:0:1667:A:H5"	1.86	0.75
28:2:41:HIS:H	28:2:45:ASN:HD22	1.34	0.75
31:9:29:C:H2'	31:9:30:C:H5'	1.68	0.75
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.75
3:C:27:ARG:NH2	30:0:657:G:OP1	2.20	0.75
30:0:1118:A:H3'	30:0:1118:A:C8	2.22	0.75
30:0:1118:A:H3'	30:0:1118:A:H8	1.51	0.75
30:0:2506:A:O2'	30:0:2507:G:H8	1.69	0.75
30:0:182:G:H5'	39:0:5189:HOH:O	1.86	0.74
31:9:14:G:H5'	31:9:14:G:H8	1.51	0.74
30:0:1474:C:H5'	30:0:1474:C:C6	2.22	0.74
13:M:163:LEU:HD21	30:0:188:C:H5"	1.71	0.73
30:0:1120:U:H5'	30:0:1121:G:OP2	1.89	0.73
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
18:R:98:ASN:HD21	30:0:500:G:H21	1.34	0.73
22:V:1:THR:HB	30:0:93:C:H5"	1.70	0.73
30:0:877:G:H5'	30:0:878:G:OP1	1.90	0.72
30:0:1166:A:H61	30:0:1180:U:H3	1.35	0.72
30:0:544:G:H2'	30:0:545:G:H5"	1.72	0.72
30:0:1973:A:H5'	30:0:1973:A:H8	1.55	0.72
31:9:56:A:C2'	31:9:57:A:H5"	2.20	0.72
30:0:282:C:H1'	30:0:368:C:N4	2.04	0.72
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.37	0.71
30:0:1189:A:H1'	30:0:1209:C:O4'	1.90	0.71
30:0:1206:U:H6	30:0:1206:U:H5'	1.53	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.05	0.71
30:0:1878:G:H1'	39:0:6168:HOH:O	1.91	0.71
30:0:2491:G:H1'	39:0:6923:HOH:O	1.91	0.70
30:0:2534:C:H1'	39:0:3522:HOH:O	1.91	0.70
3:C:184:ARG:NH2	30:0:450:C:OP1	2.24	0.70
30:0:1741:U:H5'	30:0:1742:A:OP1	1.91	0.70
30:0:1183:C:H2'	39:0:6292:HOH:O	1.91	0.70
2:B:5:ARG:HH11	2:B:8:LYS:HE2	1.56	0.70
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.70
1:A:211:LYS:HB2	39:A:9075:HOH:O	1.91	0.69
30:0:1701:A:H5'	39:0:6332:HOH:O	1.92	0.69
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.69
30:0:823:U:H3'	39:0:4481:HOH:O	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:116:SER:O	30:0:1593:C:H5'	1.92	0.69
2:B:206:THR:HG21	30:0:2716:G:H5"	1.72	0.69
30:0:2851:G:O2'	30:0:2852:A:H5'	1.92	0.69
30:0:541:C:H2'	30:0:542:A:C5'	2.23	0.69
30:0:1159:G:H21	30:0:1189:A:H8	1.39	0.69
31:9:39:U:H1'	31:9:44:A:H61	1.57	0.68
30:0:870:G:C2'	30:0:871:G:H5"	2.21	0.68
30:0:1527:A:H1'	30:0:1528:A:C8	2.29	0.68
30:0:2533:C:H5'	30:0:2533:C:C6	2.27	0.68
30:0:12:U:H2'	30:0:13:G:H5'	1.75	0.68
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.58	0.68
3:C:139:VAL:HG13	39:C:8643:HOH:O	1.92	0.68
30:0:1119:G:N2	30:0:1246:A:C2	2.58	0.68
30:0:2769:C:C2'	30:0:2770:G:H5'	2.23	0.68
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.75	0.67
30:0:603:A:H5"	30:0:604:G:OP1	1.94	0.67
30:0:681:G:N3	30:0:681:G:H5'	2.09	0.67
30:0:2783:A:H3'	39:0:5264:HOH:O	1.93	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.76	0.67
30:0:1205:U:H2'	30:0:1206:U:C5'	2.24	0.67
30:0:1666:C:C2'	30:0:1667:A:H5"	2.25	0.67
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.78	0.66
30:0:2538:A:H8	38:0:2924:ANM:H61	1.61	0.65
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.93	0.65
30:0:558:C:C2'	30:0:559:U:H5"	2.26	0.65
30:0:1701:A:H4'	30:0:1702:U:C5'	2.23	0.65
30:0:1377:C:H6	30:0:1377:C:H5'	1.61	0.65
30:0:1667:A:H5'	30:0:1667:A:C8	2.29	0.65
30:0:2613:G:O2'	30:0:2614:C:H5'	1.96	0.65
11:K:39:GLY:HA2	39:0:5253:HOH:O	1.97	0.65
10:J:52:GLN:HE22	30:0:1119:G:H8	1.43	0.65
12:L:136:ALA:HB3	39:L:8874:HOH:O	1.96	0.65
30:0:2073:G:H5"	39:0:3853:HOH:O	1.95	0.65
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.65
18:R:128:ARG:NH2	30:0:2054:A:N3	2.44	0.65
31:9:23:U:O2'	31:9:24:U:H4'	1.96	0.65
30:0:119:A:H2'	30:0:120:A:H5"	1.78	0.65
2:B:238:ASN:HD22	2:B:240:GLY:H	1.44	0.64
30:0:2005:G:OP2	30:0:2005:G:H3'	1.97	0.64
30:0:2766:A:H5'	39:0:9579:HOH:O	1.96	0.64
30:0:1183:C:N4	30:0:1184:C:H41	1.95	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2578:G:H5'	30:0:2578:G:H8	1.62	0.64
30:0:2765:C:H4'	39:0:5557:HOH:O	1.98	0.64
30:0:542:A:H5'	30:0:542:A:C8	2.24	0.64
30:0:545:G:H5'	30:0:545:G:C8	2.29	0.64
2:B:212:GLN:HA	30:0:1733:A:H4'	1.80	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
30:0:1947:G:H2'	30:0:1948:G:H8	1.62	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.62	0.64
30:0:2637:A:H5'	39:0:9282:HOH:O	1.96	0.64
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.64
30:0:1701:A:H5"	30:0:1702:U:H3'	1.79	0.64
30:0:2635:A:O2'	30:0:2636:C:H5'	1.98	0.64
30:0:2756:U:H3	30:0:2896:A:H2	1.45	0.63
30:0:871:G:C8	30:0:871:G:C5'	2.73	0.63
30:0:2878:U:H2'	30:0:2879:A:O4'	1.97	0.63
30:0:1189:A:H3'	39:0:7737:HOH:O	1.97	0.63
30:0:2502:C:C2'	30:0:2503:A:H5'	2.28	0.63
30:0:2717:C:O2'	30:0:2718:C:H5"	1.98	0.63
30:0:1116:U:O2'	30:0:1118:A:H2	1.70	0.63
30:0:544:G:C2'	30:0:545:G:H5"	2.28	0.63
4:D:154:LYS:H	4:D:154:LYS:HD2	1.63	0.62
30:0:2426:G:H1'	39:0:6139:HOH:O	1.97	0.62
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.92	0.62
30:0:1165:G:H4'	30:0:1174:A:O2'	1.99	0.62
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.15	0.62
30:0:90:A:H2'	30:0:91:G:O4'	1.98	0.62
30:0:1166:A:H1'	30:0:1192:A:C2	2.34	0.62
30:0:1205:U:C2'	30:0:1206:U:H5"	2.30	0.62
30:0:2004:U:H4'	39:0:5340:HOH:O	1.99	0.62
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.65	0.62
30:0:1666:C:H2'	30:0:1667:A:C5'	2.29	0.62
30:0:2679:G:H2'	30:0:2681:A:OP2	1.99	0.62
30:0:2896:A:H5"	39:0:6146:HOH:O	1.99	0.62
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.62
30:0:1184:C:H1'	39:0:7526:HOH:O	1.99	0.62
31:9:7:G:H5'	39:9:9098:HOH:O	2.00	0.62
8:H:19:ARG:HH12	30:0:1008:C:H5"	1.65	0.62
30:0:832:U:OP2	39:0:7839:HOH:O	2.16	0.62
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.61
31:9:20:G:O2'	31:9:21:G:H5'	1.99	0.61
23:W:154:ARG:NH1	30:0:588:G:O6	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1441:G:O2'	30:0:1442:A:H5'	1.99	0.61
30:0:123:U:H5'	39:0:6705:HOH:O	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:H	1.64	0.61
20:T:52:ARG:HD2	30:0:317:A:H5"	1.82	0.61
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.48	0.61
30:0:1666:C:H2'	30:0:1667:A:H5'	1.83	0.61
30:0:2768:A:H2'	30:0:2769:C:O4'	2.00	0.61
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.82	0.61
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.81	0.61
30:0:69:A:H5'	30:0:69:A:C8	2.36	0.61
30:0:282:C:O2'	30:0:283:U:H5'	2.00	0.61
30:0:2717:C:H2'	30:0:2718:C:C5'	2.26	0.61
11:K:87:ARG:NH2	30:0:2720:C:O2	2.34	0.60
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.83	0.60
29:3:48:ASN:HD21	30:0:2468:A:H61	1.49	0.60
30:0:848:C:H5'	39:0:7329:HOH:O	2.00	0.60
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.83	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
30:0:558:C:O2'	30:0:559:U:H5"	2.02	0.60
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.60
30:0:1819:G:H2'	30:0:1820:G:H4'	1.81	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
30:0:1278:A:H4'	30:0:1279:U:C4	2.37	0.60
30:0:2502:C:H2'	30:0:2503:A:H5'	1.83	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5"	1.84	0.60
31:9:39:U:H3'	31:9:40:C:H5"	1.84	0.60
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.99	0.60
30:0:905:C:H3'	39:0:5219:HOH:O	2.00	0.60
30:0:2241:C:O2'	30:0:2242:U:H5'	2.01	0.59
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.59
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.50	0.59
14:N:144:GLY:O	14:N:147:ILE:HG22	2.02	0.59
30:0:920:C:H5"	30:0:921:G:O5'	2.02	0.59
30:0:1372:A:H3'	39:0:7247:HOH:O	2.02	0.59
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.59
30:0:447:A:O2'	30:0:448:G:H5'	2.03	0.59
30:0:2507:G:H2'	30:0:2510:C:H42	1.67	0.59
30:0:2638:G:H5'	39:0:4962:HOH:O	2.02	0.59
30:0:2851:G:C2'	30:0:2852:A:H5'	2.32	0.58
30:0:2748:G:H5'	39:0:7599:HOH:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:969:G:H1	30:0:999:C:H42	1.50	0.58
30:0:69:A:H5'	30:0:69:A:H8	1.68	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.69	0.58
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.86	0.58
30:0:1681:G:H5"	30:0:1682:A:H5'	1.84	0.58
31:9:29:C:C2'	31:9:30:C:H5'	2.34	0.58
30:0:292:G:H2'	30:0:358:G:N2	2.19	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.36	0.58
30:0:2769:C:H2'	30:0:2770:G:H5'	1.85	0.57
30:0:2816:A:H5"	30:0:2817:G:H5'	1.86	0.57
31:9:71:C:H2'	31:9:72:C:H6	1.69	0.57
30:0:506:G:H22	30:0:509:A:H5'	1.70	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57
30:0:1201:C:H5"	39:0:6282:HOH:O	2.03	0.57
30:0:1632:A:H2'	30:0:1633:C:H5'	1.86	0.57
31:9:76:G:C3'	31:9:77:A:H5"	2.20	0.57
30:0:558:C:H2'	30:0:559:U:C5'	2.33	0.57
30:0:2372:A:H2'	30:0:2373:U:H6	1.69	0.57
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.85	0.57
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.70	0.57
30:0:1947:G:H2'	30:0:1948:G:C8	2.40	0.57
16:P:115:SER:H	16:P:118:GLN:NE2	1.98	0.57
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.05	0.57
30:0:2529:G:H3'	39:0:7241:HOH:O	2.05	0.57
30:0:2712:G:H5'	39:0:5253:HOH:O	2.05	0.57
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.56
30:0:2795:C:O2'	30:0:2796:U:H5'	2.05	0.56
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.87	0.56
30:0:2769:C:H2'	30:0:2770:G:O4'	2.05	0.56
31:9:64:C:C2'	31:9:65:A:H5'	2.34	0.56
30:0:317:A:H5'	39:0:3798:HOH:O	2.05	0.56
30:0:2301:A:H5"	30:0:2302:A:H5'	1.86	0.56
5:E:143:GLN:NE2	30:0:2779:G:H21	2.03	0.56
30:0:1080:C:H4'	30:0:1081:A:OP1	2.05	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.85	0.56
30:0:1835:U:C5	30:0:1840:A:N7	2.66	0.56
11:K:66:ARG:HH22	30:0:1994:A:P	2.28	0.56
30:0:1116:U:O2'	30:0:1118:A:C2	2.52	0.56
30:0:2505:G:O2'	30:0:2506:A:H5'	2.05	0.56
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.53	0.56
30:0:1175:G:H1'	30:0:1193:A:H2'	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1790:C:H2'	30:0:1791:U:H6	1.71	0.56
30:0:625:U:H5"	30:0:1044:C:N4	2.21	0.56
28:2:10:ARG:NH2	30:0:121:U:OP2	2.36	0.56
30:0:441:A:H1'	30:0:442:A:N7	2.21	0.56
30:0:711:G:H1'	39:0:7152:HOH:O	2.06	0.56
30:0:1406:A:H4'	30:0:1407:A:H5"	1.87	0.56
30:0:2700:G:H3'	39:0:3609:HOH:O	2.06	0.56
31:9:39:U:H1'	31:9:44:A:N6	2.20	0.56
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.21	0.55
30:0:1377:C:H5'	30:0:1377:C:C6	2.41	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
30:0:2748:G:H1'	39:0:7956:HOH:O	2.06	0.55
30:0:644:G:N3	30:0:644:G:H5'	2.20	0.55
30:0:1187:U:O2'	30:0:1189:A:H2	1.89	0.55
30:0:2472:C:O2'	30:0:2634:G:H4'	2.07	0.55
30:0:2670:G:O2'	30:0:2671:U:H5'	2.06	0.55
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.88	0.55
30:0:907:A:H4'	30:0:1328:A:C2	2.41	0.55
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.87	0.55
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.22	0.55
30:0:2768:A:H5"	39:0:4460:HOH:O	2.06	0.55
30:0:138:U:H5"	30:0:139:C:OP2	2.07	0.55
30:0:669:G:O2'	30:0:670:G:H5'	2.06	0.55
30:0:2769:C:O2'	30:0:2770:G:H5'	2.07	0.55
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.88	0.55
29:3:2:GLN:HE21	29:3:91:GLN:HE21	1.54	0.55
30:0:602:A:O2'	30:0:605:C:H4'	2.07	0.54
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.22	0.54
30:0:2718:C:H5'	30:0:2718:C:H6	1.72	0.54
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.05	0.54
30:0:272:A:H3'	39:0:7588:HOH:O	2.07	0.54
30:0:595:U:H2'	30:0:596:C:H6	1.72	0.54
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.05	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.07	0.54
30:0:1625:U:H4'	39:0:4699:HOH:O	2.06	0.54
30:0:1666:C:C2'	30:0:1667:A:C5'	2.85	0.54
30:0:1682:A:H5"	39:0:9470:HOH:O	2.06	0.54
30:0:1174:A:C5	30:0:1201:C:H4'	2.43	0.54
30:0:1741:U:O2'	30:0:2723:G:H4'	2.07	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1130:U:H2'	30:0:1131:G:O4'	2.07	0.54
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.23	0.54
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.22	0.53
30:0:1528:A:H2'	30:0:1529:G:O4'	2.08	0.53
30:0:1634:G:H3'	39:0:3923:HOH:O	2.06	0.53
30:0:2419:U:H5"	30:0:2420:G:H5'	1.90	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.38	0.53
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.89	0.53
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.89	0.53
23:W:84:VAL:HG12	39:W:6679:HOH:O	2.07	0.53
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.53
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.53
30:0:1477:C:H5'	30:0:1868:G:C5'	2.38	0.53
30:0:2420:G:O2'	30:0:2421:G:H5'	2.08	0.53
31:9:54:A:O2'	31:9:55:U:H5'	2.08	0.53
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.43	0.53
14:N:37:ARG:NH1	31:9:6:C:C5'	2.67	0.53
29:3:48:ASN:ND2	29:3:50:GLY:H	2.06	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.74	0.53
30:0:1058:A:H2'	30:0:1060:C:H5"	1.89	0.53
30:0:380:A:H2'	39:0:7284:HOH:O	2.09	0.53
30:0:2265:U:H2'	30:0:2266:A:C8	2.44	0.53
30:0:2768:A:O2'	30:0:2769:C:H5'	2.08	0.53
30:0:272:A:H5'	30:0:273:G:OP2	2.09	0.53
30:0:671:A:O2'	30:0:672:G:H2'	2.09	0.53
30:0:899:C:H5'	39:0:3228:HOH:O	2.08	0.53
17:Q:95:GLU:HA	30:0:949:U:H4'	1.90	0.53
30:0:31:C:H2'	39:0:7745:HOH:O	2.08	0.53
30:0:1641:A:C2'	30:0:1642:A:H5'	2.39	0.53
31:9:64:C:H2'	31:9:65:A:H5'	1.90	0.53
30:0:2346:C:H6	30:0:2346:C:O5'	1.92	0.53
29:3:65:THR:HB	29:3:83:TRP:H	1.73	0.53
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.71	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:1456:C:H2'	30:0:1457:U:C6	2.44	0.53
30:0:2526:C:H5'	30:0:2526:C:C6	2.44	0.53
30:0:558:C:H2'	30:0:559:U:H5"	1.90	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.24	0.52
30:0:1279:U:H2'	30:0:1279:U:O2	2.08	0.52
30:0:2251:G:H2'	30:0:2252:A:C8	2.44	0.52
30:0:17:G:H2'	30:0:18:C:C6	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:2:U:OP2	31:9:3:A:H5'	2.09	0.52
39:Z:8706:HOH:O	30:0:1886:A:H4'	2.10	0.52
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.52
30:0:849:C:H1'	39:0:6667:HOH:O	2.10	0.52
30:0:2787:C:H5	39:0:4665:HOH:O	1.92	0.52
39:I:1549:HOH:O	30:0:1180:U:H1'	2.08	0.52
30:0:482:G:H4'	30:0:508:A:N1	2.24	0.52
30:0:814:G:H4'	39:0:3158:HOH:O	2.09	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.09	0.52
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.92	0.52
30:0:304:G:H1'	30:0:347:A:N6	2.24	0.52
30:0:343:C:O2'	30:0:344:C:H5'	2.08	0.52
30:0:1766:U:O2	30:0:1778:A:H5'	2.10	0.52
1:A:48:ASP:HB3	39:A:9064:HOH:O	2.08	0.52
3:C:76:ARG:HH22	30:0:1363:G:P	2.32	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.92	0.52
30:0:468:U:H3'	39:0:7628:HOH:O	2.10	0.52
30:0:1118:A:H8	30:0:1119:G:H5"	1.73	0.52
3:C:236:THR:HG22	3:C:239:ALA:H	1.75	0.52
12:L:6:ARG:HD3	30:0:1299:G:O6	2.09	0.52
15:O:3:THR:CG2	30:0:656:G:H5'	2.30	0.52
20:T:52:ARG:O	30:0:317:A:OP1	2.27	0.52
4:D:146:LYS:HZ1	14:N:38:LYS:HE2	1.75	0.52
30:0:88:G:H2'	30:0:89:G:C8	2.44	0.52
30:0:1314:U:H2'	39:0:5916:HOH:O	2.08	0.52
30:0:2010:A:H2'	39:0:6002:HOH:O	2.09	0.52
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.75	0.52
30:0:1714:C:O2'	30:0:1715:C:H5'	2.10	0.52
30:0:2320:U:H4'	30:0:2321:A:O4'	2.10	0.52
30:0:2538:A:C8	38:0:2924:ANM:H61	2.44	0.52
30:0:1250:C:O2'	30:0:1251:C:H5'	2.10	0.51
30:0:1506:U:H6	30:0:1506:U:H5'	1.74	0.51
30:0:280:C:H2'	30:0:281:U:O4'	2.10	0.51
30:0:1972:U:H2'	30:0:1973:A:H5"	1.92	0.51
30:0:2748:G:H2'	39:0:7599:HOH:O	2.10	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.10	0.51
30:0:2111:G:H1'	39:0:9050:HOH:O	2.10	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.94	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.98	0.51
30:0:2783:A:H2'	30:0:2784:A:C8	2.46	0.51
4:D:103:ASN:HD22	4:D:134:LEU:H	1.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.75	0.51
23:W:80:ASP:O	23:W:84:VAL:HG23	2.11	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51
1:A:199:HIS:HD2	1:A:201:PHE:H	1.58	0.51
4:D:76:ARG:NE	31:9:44:A:O4'	2.42	0.51
30:0:1014:A:H2'	30:0:1015:C:H5'	1.92	0.51
30:0:1132:A:N6	30:0:1229:C:H2'	2.25	0.51
30:0:1189:A:O2'	30:0:1208:C:H2'	2.10	0.51
30:0:1268:C:O2'	30:0:1269:G:H5'	2.11	0.51
30:0:2604:A:H5'	39:0:5833:HOH:O	2.10	0.51
12:L:18:HIS:HD2	30:0:902:G:N7	2.09	0.51
12:L:143:THR:HG22	12:L:144:ASP:H	1.76	0.51
30:0:136:C:H2'	30:0:137:U:O4'	2.11	0.51
30:0:794:U:H3	30:0:819:A:H61	1.57	0.51
30:0:820:G:O2'	30:0:856:G:H4'	2.11	0.51
30:0:1249:U:H2'	30:0:1250:C:C6	2.45	0.51
30:0:2243:C:H5"	39:0:3776:HOH:O	2.11	0.51
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.91	0.51
30:0:2344:G:N3	30:0:2344:G:H2'	2.25	0.51
31:9:54:A:H2	39:9:9064:HOH:O	1.93	0.51
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.43	0.51
30:0:1755:A:H2'	30:0:1756:G:O4'	2.10	0.51
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.57	0.50
18:R:117:HIS:HD2	30:0:20:G:H21	1.59	0.50
30:0:67:A:H5"	30:0:69:A:C8	2.46	0.50
30:0:182:G:H5"	39:0:3749:HOH:O	2.11	0.50
30:0:1211:G:O2'	30:0:1212:C:H5'	2.11	0.50
30:0:2385:G:H2'	30:0:2386:U:C6	2.46	0.50
14:N:141:ARG:NH2	31:9:48:C:H4'	2.26	0.50
24:X:30:MET:HG2	30:0:1384:C:H5'	1.93	0.50
30:0:396:U:O2'	30:0:418:C:H4'	2.12	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.46	0.50
30:0:71:G:H5"	39:0:3940:HOH:O	2.10	0.50
30:0:1015:C:H2'	30:0:1016:U:C6	2.46	0.50
30:0:1200:A:H3'	39:0:5796:HOH:O	2.10	0.50
30:0:407:A:H5'	39:0:6070:HOH:O	2.10	0.50
30:0:1940:C:H4'	39:0:7406:HOH:O	2.10	0.50
8:H:168:VAL:HG13	39:H:9008:HOH:O	2.11	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.92	0.50
14:N:11:ARG:HD3	31:9:114:G:O6	2.11	0.50
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1172:G:H5"	39:0:7316:HOH:O	2.11	0.50
30:0:1596:U:H2'	30:0:1598:A:OP2	2.11	0.50
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.92	0.50
30:0:271:C:H41	30:0:378:A:H2	1.58	0.50
30:0:396:U:H1'	39:0:7686:HOH:O	2.09	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.93	0.50
30:0:125:U:H2'	39:0:3792:HOH:O	2.10	0.50
30:0:1185:U:H2'	30:0:1186:C:C6	2.46	0.50
30:0:1925:G:O2'	30:0:1926:G:H5'	2.12	0.50
30:0:2252:A:C5	30:0:2253:G:H1'	2.46	0.50
27:1:12:ASN:O	30:0:1415:G:H5'	2.11	0.50
30:0:485:A:N3	30:0:487:G:H5"	2.27	0.50
30:0:1819:G:H2'	30:0:1820:G:C5'	2.42	0.50
30:0:1972:U:C2'	30:0:1973:A:H5"	2.42	0.50
30:0:2415:A:H2'	30:0:2416:G:H5'	1.94	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
30:0:255:A:H2'	30:0:256:C:C6	2.46	0.50
30:0:559:U:H5'	30:0:559:U:C6	2.36	0.50
30:0:2104:C:O2	30:0:2485:A:N1	2.45	0.50
1:A:121:ALA:O	1:A:124:VAL:HG22	2.12	0.49
30:0:1562:C:H2'	30:0:1562:C:O2	2.12	0.49
1:A:192:VAL:HG12	39:A:9054:HOH:O	2.11	0.49
30:0:564:G:H1'	39:0:6359:HOH:O	2.12	0.49
30:0:2498:C:O2'	30:0:2499:U:H5'	2.12	0.49
12:L:14:GLY:O	30:0:1295:G:H5"	2.12	0.49
31:9:52:A:H2'	31:9:53:G:O4'	2.12	0.49
31:9:92:G:H2'	31:9:93:A:H8	1.76	0.49
8:H:31:ILE:HG23	39:H:9028:HOH:O	2.13	0.49
30:0:1350:U:H4'	39:0:5156:HOH:O	2.12	0.49
30:0:2256:G:O2'	30:0:2257:G:H5'	2.12	0.49
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.38	0.49
30:0:660:A:H4'	30:0:661:G:O5'	2.13	0.49
30:0:1181:A:N1	30:0:1192:A:O2'	2.44	0.49
30:0:249:G:O2'	30:0:250:C:H5'	2.13	0.49
30:0:958:G:H2'	30:0:959:C:C6	2.47	0.49
30:0:1419:U:H2'	30:0:1685:A:C2	2.47	0.49
39:B:9096:HOH:O	30:0:2672:C:H1'	2.12	0.49
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.95	0.49
6:F:91:VAL:HG11	30:0:262:A:OP2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:120:A:N3	30:0:120:A:H2'	2.28	0.49
30:0:1894:C:N4	30:0:1939:U:H2'	2.27	0.49
30:0:2508:C:H2'	39:0:6808:HOH:O	2.12	0.49
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.49
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.49
31:9:34:A:H2'	31:9:35:C:O4'	2.12	0.49
31:9:35:C:H5"	39:9:9077:HOH:O	2.12	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	1.94	0.49
30:0:1135:G:H5'	39:0:5971:HOH:O	2.13	0.49
30:0:1838:U:O2'	30:0:2644:C:H5'	2.13	0.49
30:0:2758:G:H2'	30:0:2759:C:C6	2.48	0.49
31:9:61:C:H2'	31:9:62:A:H8	1.77	0.49
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.95	0.49
30:0:459:A:H5"	39:0:9053:HOH:O	2.13	0.49
30:0:1046:G:N3	30:0:1082:A:H2	2.11	0.49
30:0:1632:A:C2'	30:0:1633:C:H5'	2.43	0.49
30:0:1919:A:H4'	39:0:4884:HOH:O	2.12	0.49
30:0:2248:C:H3'	39:0:5478:HOH:O	2.13	0.49
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.95	0.49
4:D:159:PRO:O	4:D:163:VAL:HG23	2.13	0.49
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.94	0.49
30:0:64:G:H2'	30:0:65:C:O4'	2.13	0.49
30:0:567:U:OP1	39:0:5320:HOH:O	2.19	0.49
30:0:1603:A:H5"	30:0:1605:G:H5'	1.95	0.49
5:E:137:ASP:O	5:E:141:VAL:HG23	2.12	0.48
8:H:70:LEU:O	8:H:74:ARG:HB2	2.13	0.48
30:0:1189:A:H1'	30:0:1209:C:H1'	1.94	0.48
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.48
2:B:16:ARG:NH1	39:B:9082:HOH:O	2.45	0.48
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.95	0.48
39:Y:8908:HOH:O	30:0:1330:A:H5"	2.12	0.48
30:0:1044:C:H5	39:0:6654:HOH:O	1.94	0.48
30:0:1946:C:H2'	30:0:1971:G:C8	2.48	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.48	0.48
13:M:164:THR:HG22	13:M:167:GLY:H	1.78	0.48
30:0:1441:G:H1'	39:0:7823:HOH:O	2.11	0.48
31:9:114:G:H2'	31:9:115:C:C6	2.49	0.48
14:N:44:ARG:NH1	31:9:4:G:H21	2.11	0.48
30:0:324:G:O2'	30:0:325:U:H5'	2.13	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:432:G:O2'	30:0:433:C:H5'	2.14	0.48
30:0:558:C:H2'	30:0:559:U:H5'	1.95	0.48
30:0:947:U:O2'	30:0:948:G:H5'	2.13	0.48
20:T:38:ARG:HH21	30:0:306:A:P	2.37	0.48
6:F:91:VAL:HG12	6:F:92:GLY:N	2.29	0.48
18:R:40:ALA:O	18:R:44:VAL:HG23	2.13	0.48
30:0:42:C:H1'	39:0:4709:HOH:O	2.13	0.48
30:0:318:U:H5'	30:0:339:A:C2	2.49	0.48
30:0:932:U:H2'	30:0:933:C:C6	2.49	0.48
30:0:1819:G:H2'	30:0:1820:G:C4'	2.44	0.48
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.14	0.48
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.28	0.48
30:0:2011:A:H4'	30:0:2012:U:O5'	2.14	0.48
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.48
30:0:2608:C:H2'	39:0:7867:HOH:O	2.14	0.48
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.29	0.48
30:0:1066:U:H2'	30:0:1067:A:C8	2.49	0.48
30:0:1183:C:H42	30:0:1184:C:H41	1.61	0.48
30:0:2000:G:O2'	30:0:2001:G:H5'	2.14	0.48
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.78	0.47
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.14	0.47
16:P:41:ARG:HH22	30:0:1500:U:P	2.37	0.47
27:1:28:HIS:HE1	30:0:776:A:OP1	1.97	0.47
30:0:622:G:O2'	30:0:623:U:H5'	2.14	0.47
30:0:1087:G:H4'	30:0:1088:A:OP1	2.14	0.47
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.47
30:0:1613:C:H2'	30:0:1614:G:O4'	2.14	0.47
30:0:1855:G:H4'	30:0:1856:C:O5'	2.13	0.47
30:0:2135:A:O2'	30:0:2136:G:H5'	2.14	0.47
30:0:790:A:H1'	30:0:1710:A:H2'	1.96	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
1:A:51:ARG:NH1	1:A:120:ARG:O	2.47	0.47
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.27	0.47
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.95	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.29	0.47
30:0:635:A:H2'	30:0:636:G:H5"	1.95	0.47
30:0:2329:C:O2'	30:0:2330:U:H5'	2.13	0.47
30:0:2526:C:O2'	30:0:2527:U:H5'	2.14	0.47
30:0:2755:G:H1'	39:0:4715:HOH:O	2.14	0.47
2:B:244:PRO:HB3	30:0:1234:U:N3	2.28	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:14:GLU:O	21:U:17:THR:HB	2.15	0.47
30:0:961:A:H4'	39:0:6826:HOH:O	2.14	0.47
30:0:1166:A:OP1	30:0:1174:A:H4'	2.14	0.47
30:0:1926:G:H2'	30:0:1927:A:C8	2.50	0.47
30:0:2842:G:H2'	30:0:2843:A:H5'	1.95	0.47
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.47
30:0:1181:A:C2'	30:0:1182:C:H5'	2.45	0.47
30:0:1342:C:C2'	30:0:1343:C:H5'	2.45	0.47
30:0:1603:A:H5'	30:0:1605:G:C4'	2.44	0.47
31:9:107:C:O2'	31:9:108:C:H5'	2.14	0.47
13:M:95:LYS:HE2	30:0:157:G:H4'	1.97	0.47
16:P:83:LYS:HG2	30:0:793:A:H5"	1.97	0.47
20:T:38:ARG:NH1	39:0:6736:HOH:O	2.47	0.47
23:W:23:MET:O	30:0:1025:C:H5'	2.15	0.47
29:3:15:ASN:O	30:0:2408:A:H4'	2.15	0.47
30:0:368:C:H2'	30:0:369:G:H5'	1.97	0.47
30:0:1535:G:H2'	30:0:1536:C:C6	2.50	0.47
30:0:1622:G:H2'	30:0:1623:C:H5'	1.97	0.47
30:0:1829:A:H2'	30:0:1830:C:H5'	1.97	0.47
30:0:2064:U:H5'	30:0:2652:U:O3'	2.15	0.47
30:0:2105:C:H2'	30:0:2106:C:C6	2.49	0.47
31:9:39:U:HO2'	31:9:42:C:H5	1.57	0.47
27:1:16:HIS:HD2	30:0:470:U:O2'	1.97	0.47
30:0:560:U:H2'	30:0:561:G:H8	1.79	0.47
30:0:714:U:H3'	39:0:6997:HOH:O	2.15	0.47
30:0:2414:A:H2'	30:0:2415:A:C8	2.50	0.47
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.47
30:0:653:U:H2'	30:0:654:A:C8	2.49	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
30:0:1016:U:H1'	39:0:3685:HOH:O	2.13	0.47
30:0:1588:G:C6	30:0:1589:G:N1	2.83	0.47
30:0:1662:C:H2'	30:0:1663:G:O4'	2.15	0.47
3:C:118:THR:O	3:C:136:VAL:HG13	2.15	0.47
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.49	0.47
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.97	0.47
17:Q:15:LYS:HD3	30:0:2364:A:H5"	1.97	0.47
30:0:255:A:H2'	30:0:256:C:H6	1.80	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
30:0:1595:G:O2'	30:0:1596:U:H5'	2.15	0.47
30:0:1815:A:H2'	30:0:1816:C:O4'	2.15	0.47
2:B:211:THR:HG21	39:0:7515:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:141:ARG:HH21	31:9:48:C:H4'	1.79	0.46
26:Z:40:ALA:HA	30:0:1773:G:C8	2.51	0.46
30:0:299:U:H5'	39:0:7395:HOH:O	2.16	0.46
30:0:2064:U:H4'	30:0:2653:A:OP1	2.14	0.46
17:Q:19:ARG:HH21	31:9:11:A:P	2.37	0.46
30:0:256:C:H2'	30:0:257:G:O4'	2.15	0.46
30:0:559:U:H2'	30:0:560:U:O4'	2.15	0.46
30:0:704:C:H2'	30:0:705:C:H6	1.80	0.46
30:0:951:A:O2'	30:0:952:G:H5'	2.15	0.46
30:0:960:G:C2'	30:0:960:G:N3	2.78	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.97	0.46
30:0:595:U:H2'	30:0:596:C:C6	2.49	0.46
30:0:834:G:H3'	30:0:835:U:H4'	1.98	0.46
30:0:1592:G:H2'	30:0:1593:C:C6	2.51	0.46
30:0:1603:A:C5'	30:0:1605:G:H5'	2.45	0.46
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.45	0.46
30:0:192:A:H5'	39:0:7700:HOH:O	2.16	0.46
30:0:1057:A:H1'	30:0:2492:U:O2'	2.15	0.46
30:0:2072:G:C6	30:0:2533:C:H1'	2.51	0.46
30:0:2909:G:H2'	30:0:2910:A:H8	1.80	0.46
19:S:33:SER:O	19:S:37:VAL:HG23	2.15	0.46
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.44	0.46
30:0:694:A:H2'	30:0:695:C:H5'	1.97	0.46
30:0:1137:G:H1'	39:0:3907:HOH:O	2.15	0.46
30:0:2781:U:C2'	30:0:2782:G:H5'	2.45	0.46
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.98	0.46
30:0:12:U:C2'	30:0:13:G:H5'	2.46	0.46
30:0:821:U:H3'	39:0:3796:HOH:O	2.15	0.46
30:0:1118:A:C8	30:0:1119:G:H5"	2.51	0.46
30:0:1973:A:H5'	30:0:1973:A:C8	2.42	0.46
30:0:645:U:O2	30:0:761:A:H2	1.98	0.46
30:0:702:G:O2'	30:0:703:G:H5'	2.16	0.46
30:0:1158:G:O2'	30:0:1159:G:H5'	2.16	0.46
30:0:1218:U:H2'	30:0:1219:U:C6	2.51	0.46
30:0:1804:A:H2'	30:0:1805:G:C8	2.50	0.46
30:0:2361:A:H5'	30:0:2361:A:H8	1.81	0.46
30:0:2531:U:O2'	30:0:2532:A:H5'	2.15	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.55	0.46
30:0:407:A:H2'	30:0:408:A:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1060:C:H6	30:0:1060:C:H5'	1.81	0.46
30:0:1614:G:H2'	39:0:4660:HOH:O	2.16	0.46
30:0:1771:U:O2'	30:0:1773:G:N7	2.48	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.50	0.46
30:0:2879:A:H2'	30:0:2880:A:O4'	2.16	0.46
30:0:2894:C:O2'	30:0:2895:C:H5'	2.15	0.46
30:0:2900:G:H2'	30:0:2901:C:O4'	2.16	0.46
2:B:238:ASN:HD22	2:B:240:GLY:N	2.11	0.46
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.19	0.46
30:0:113:A:OP2	30:0:114:A:H2'	2.15	0.46
30:0:807:A:O2'	30:0:808:A:H5'	2.16	0.46
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.97	0.46
39:C:8656:HOH:O	30:0:2100:A:H5'	2.15	0.46
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.64	0.46
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.97	0.46
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.97	0.46
30:0:538:C:H5"	30:0:539:G:C8	2.50	0.46
30:0:612:U:H2'	30:0:613:C:C6	2.51	0.46
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.97	0.45
30:0:876:A:H2'	30:0:876:A:N3	2.31	0.45
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.45
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.45
30:0:1972:U:H2'	30:0:1973:A:H5'	1.98	0.45
30:0:2421:G:H3'	30:0:2422:U:C5'	2.46	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	1.97	0.45
30:0:2852:A:H5"	39:0:5266:HOH:O	2.17	0.45
8:H:64:SER:OG	30:0:2520:G:H5'	2.16	0.45
30:0:95:A:H5"	30:0:97:G:O4'	2.16	0.45
30:0:319:A:H4'	30:0:338:C:C4	2.52	0.45
30:0:960:G:N3	30:0:960:G:H3'	2.31	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.16	0.45
30:0:1413:A:H2'	30:0:1414:A:O4'	2.16	0.45
30:0:2326:C:H4'	30:0:2412:G:C4'	2.47	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
11:K:55:VAL:HG12	11:K:56:SER:N	2.32	0.45
14:N:35:VAL:HG11	31:9:6:C:H4'	1.97	0.45
15:O:25:VAL:HG13	30:0:709:G:O2'	2.16	0.45
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.82	0.45
30:0:629:A:H2'	30:0:630:A:O4'	2.16	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.99	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:HB2	39:A:9064:HOH:O	2.17	0.45
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.53	0.45
18:R:39:THR:HG23	18:R:107:GLU:O	2.17	0.45
30:0:281:U:O2'	30:0:282:C:H5'	2.16	0.45
30:0:1485:A:H8	39:0:9975:HOH:O	1.99	0.45
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.45
30:0:1787:C:H4'	30:0:2883:A:O4'	2.17	0.45
30:0:1973:A:H2'	30:0:1974:G:O4'	2.16	0.45
30:0:2766:A:O2'	30:0:2767:C:H5'	2.16	0.45
38:0:2924:ANM:H62	38:0:2924:ANM:H2	1.87	0.45
31:9:13:A:O2'	31:9:14:G:H5"	2.17	0.45
31:9:24:U:H3'	31:9:25:G:H5'	1.97	0.45
8:H:69:ARG:HD3	39:H:9028:HOH:O	2.16	0.45
30:0:17:G:H2'	30:0:18:C:H6	1.81	0.45
30:0:812:A:H1'	39:0:3988:HOH:O	2.16	0.45
30:0:1304:U:H2'	30:0:1305:C:C6	2.52	0.45
30:0:1497:G:H4'	30:0:1627:G:O2'	2.16	0.45
30:0:2781:U:H2'	30:0:2782:G:H5'	1.98	0.45
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.99	0.45
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.65	0.45
30:0:777:U:H4'	30:0:777:U:OP2	2.16	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:2589:U:H2'	30:0:2590:U:C6	2.52	0.45
30:0:2758:G:H2'	30:0:2759:C:H6	1.82	0.45
31:9:49:G:H2'	31:9:50:G:O4'	2.17	0.45
3:C:88:SER:HB3	3:C:91:PRO:HB3	1.99	0.45
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.45
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.45
30:0:1160:G:HO2'	30:0:1190:G:H8	1.64	0.45
30:0:1181:A:H2'	30:0:1182:C:H5'	1.98	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:1398:G:H2'	30:0:1399:A:C8	2.51	0.45
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.45
30:0:2387:U:H2'	30:0:2388:C:C6	2.51	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.97	0.45
30:0:308:U:H5'	30:0:309:C:OP1	2.16	0.45
30:0:1015:C:H2'	30:0:1016:U:H6	1.80	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.52	0.45
2:B:94:GLN:O	30:0:2673:U:H4'	2.17	0.45
4:D:140:ARG:HB3	31:9:29:C:H5"	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:107:ARG:NH1	39:M:8871:HOH:O	2.49	0.45
30:0:168:C:H6	30:0:168:C:O5'	2.00	0.45
30:0:847:C:H4'	39:0:3779:HOH:O	2.16	0.45
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.45
30:0:2401:A:H2'	30:0:2402:A:C8	2.52	0.45
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.82	0.45
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.97	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.32	0.45
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.45
30:0:397:A:O2'	30:0:417:G:N3	2.37	0.45
30:0:2509:A:H2'	30:0:2510:C:O4'	2.17	0.45
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.45
1:A:36:ASP:O	1:A:38:ILE:N	2.44	0.44
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.44
2:B:254:GLN:HG2	2:B:255:GLY:N	2.32	0.44
19:S:11:THR:H	19:S:14:ALA:HB3	1.80	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.53	0.44
30:0:907:A:H2'	30:0:908:A:H8	1.80	0.44
30:0:2371:G:H5'	39:0:5043:HOH:O	2.17	0.44
30:0:2510:C:H5'	30:0:2511:A:OP2	2.18	0.44
30:0:2607:U:H4'	39:0:9455:HOH:O	2.16	0.44
31:9:22:G:H5'	31:9:23:U:OP1	2.17	0.44
23:W:44:MET:CE	30:0:944:G:H21	2.31	0.44
30:0:1204:C:H2'	30:0:1205:U:O4'	2.17	0.44
30:0:2866:U:H4'	30:0:2867:G:H5'	1.99	0.44
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.99	0.44
1:A:206:ARG:NH2	30:0:2630:G:O6	2.50	0.44
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.32	0.44
30:0:737:A:H2'	30:0:738:G:O4'	2.17	0.44
30:0:821:U:H2'	30:0:822:C:C6	2.53	0.44
30:0:1167:G:H2'	30:0:1168:C:C6	2.51	0.44
30:0:1878:G:O2'	30:0:1879:U:C6	2.68	0.44
30:0:1942:A:H3'	39:0:7406:HOH:O	2.17	0.44
30:0:2524:G:H21	30:0:2526:C:N4	2.16	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
30:0:168:C:H5'	30:0:2277:U:OP1	2.17	0.44
30:0:690:G:H4'	30:0:741:C:O2	2.17	0.44
30:0:960:G:N3	30:0:960:G:H2'	2.31	0.44
30:0:1594:C:O2'	30:0:1607:A:H4'	2.17	0.44
30:0:1878:G:O2'	30:0:1879:U:P	2.74	0.44
12:L:30:ARG:NH2	39:L:8818:HOH:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:5:THR:HG23	30:0:1688:G:O2'	2.18	0.44
30:0:1996:U:O2'	30:0:1997:A:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
3:C:115:LEU:O	3:C:118:THR:HB	2.18	0.44
12:L:33:ALA:HB2	30:0:165:A:H5"	2.00	0.44
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
25:Y:165:GLU:HB3	39:Y:8889:HOH:O	2.17	0.44
29:3:73:GLU:HB3	39:3:9051:HOH:O	2.17	0.44
30:0:454:U:H5"	39:0:7834:HOH:O	2.17	0.44
30:0:2421:G:H3'	30:0:2422:U:H5"	2.00	0.44
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.44
1:A:132:ASP:HB3	1:A:135:VAL:H	1.82	0.44
30:0:128:A:O2'	30:0:129:A:H5'	2.17	0.44
30:0:162:C:H2'	30:0:163:U:H5'	1.99	0.44
30:0:666:A:H2'	30:0:667:C:O4'	2.18	0.44
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.44
30:0:1252:A:H2'	30:0:1253:C:O4'	2.18	0.44
30:0:1477:C:H5'	30:0:1868:G:H5"	2.00	0.44
30:0:1683:G:C2	30:0:1693:A:O4'	2.71	0.44
30:0:2092:G:H2'	30:0:2613:G:OP1	2.18	0.44
30:0:2256:G:C2'	30:0:2257:G:H5'	2.48	0.44
30:0:2899:A:O2'	30:0:2900:G:H5'	2.18	0.44
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
30:0:71:G:H8	39:0:3940:HOH:O	2.00	0.44
30:0:137:U:OP1	30:0:259:G:O2'	2.36	0.44
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.44
30:0:1165:G:H1'	30:0:1174:A:H1'	1.98	0.44
30:0:1172:G:H1'	39:0:5007:HOH:O	2.17	0.44
30:0:1422:U:H2'	30:0:1423:C:C6	2.52	0.44
30:0:2379:G:N7	30:0:2408:A:N1	2.65	0.44
30:0:2809:G:H2'	30:0:2810:G:O4'	2.18	0.44
30:0:138:U:OP2	30:0:139:C:H5	2.00	0.44
30:0:920:C:H5'	30:0:921:G:C4	2.53	0.44
30:0:1130:U:H5'	39:0:7729:HOH:O	2.17	0.44
30:0:1592:G:H2'	30:0:1593:C:H6	1.83	0.44
30:0:2039:A:H2'	30:0:2040:C:C6	2.52	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.90	0.43
2:B:315:VAL:HG23	2:B:316:ARG:HG2	2.00	0.43
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.33	0.43
30:0:466:A:H2'	30:0:467:G:O4'	2.18	0.43
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
30:0:1421:C:O2'	30:0:1422:U:H5'	2.17	0.43
30:0:1790:C:H2'	30:0:1791:U:C6	2.52	0.43
30:0:2326:C:H4'	30:0:2412:G:H4'	2.00	0.43
30:0:2703:A:H2'	30:0:2704:C:H6	1.83	0.43
31:9:91:C:H2'	31:9:92:G:O4'	2.18	0.43
3:C:47:GLY:HA2	3:C:92:PRO:HB2	2.00	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.83	0.43
30:0:558:C:C2'	30:0:559:U:C5'	2.92	0.43
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.33	0.43
30:0:2533:C:H6	30:0:2533:C:C5'	2.24	0.43
30:0:2578:G:H5'	30:0:2578:G:C8	2.49	0.43
16:P:1:THR:O	30:0:1396:C:H1'	2.18	0.43
19:S:17:ASP:HB3	19:S:23:LYS:HB2	2.00	0.43
30:0:371:U:H2'	30:0:372:A:H8	1.83	0.43
30:0:2765:C:H2'	30:0:2766:A:C8	2.54	0.43
13:M:171:ARG:CD	30:0:156:C:H5"	2.31	0.43
16:P:88:GLN:HE22	30:0:1799:G:H21	1.65	0.43
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.19	0.43
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.33	0.43
23:W:119:HIS:HE1	39:0:9570:HOH:O	2.01	0.43
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.16	0.43
30:0:603:A:H1'	30:0:605:C:C2	2.53	0.43
30:0:1377:C:H1'	39:0:9041:HOH:O	2.18	0.43
30:0:1504:A:H5'	39:0:4450:HOH:O	2.19	0.43
30:0:1544:U:H2'	30:0:1545:C:C6	2.54	0.43
30:0:1837:G:H3'	39:0:7851:HOH:O	2.18	0.43
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.43
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.88	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
30:0:417:G:P	39:0:7478:HOH:O	2.75	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.43
30:0:1039:G:H2'	30:0:1040:A:O4'	2.19	0.43
30:0:1042:U:O2'	30:0:1043:C:H5'	2.18	0.43
30:0:1138:G:H4'	39:0:5749:HOH:O	2.18	0.43
30:0:1213:C:O2'	30:0:1214:G:H5'	2.18	0.43
30:0:1788:U:O2'	30:0:1789:G:H5'	2.19	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2274:A:O2'	30:0:2275:G:H5'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
30:0:2791:U:H1'	30:0:2792:A:H5"	2.00	0.43
31:9:33:U:H2'	39:9:9068:HOH:O	2.19	0.43
12:L:37:LYS:NZ	30:0:919:U:O3'	2.50	0.43
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.52	0.43
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.99	0.43
30:0:271:C:H4'	30:0:272:A:OP1	2.18	0.43
30:0:364:U:H2'	30:0:365:G:O4'	2.19	0.43
30:0:407:A:H8	39:0:4495:HOH:O	2.00	0.43
30:0:497:A:H2'	30:0:498:A:C5'	2.49	0.43
30:0:1096:U:O2'	30:0:1097:A:H5'	2.18	0.43
2:B:297:VAL:HG23	39:B:9071:HOH:O	2.17	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.53	0.43
30:0:195:C:H2'	30:0:196:G:H5'	2.00	0.43
30:0:603:A:H4'	30:0:604:G:O5'	2.18	0.43
30:0:722:G:H22	30:0:938:G:P	2.41	0.43
30:0:1477:C:O2'	30:0:1478:U:H5'	2.18	0.43
30:0:1921:A:O2'	30:0:1922:A:H5'	2.19	0.43
30:0:2653:A:H2'	30:0:2654:C:C6	2.54	0.43
18:R:98:ASN:ND2	30:0:500:G:H21	2.10	0.43
24:X:43:VAL:HG12	24:X:44:ASP:H	1.83	0.43
30:0:488:U:H2'	39:0:4037:HOH:O	2.18	0.43
30:0:517:U:H1'	39:0:7636:HOH:O	2.19	0.43
30:0:815:U:O2'	30:0:1598:A:H4'	2.18	0.43
30:0:1926:G:H2'	30:0:1927:A:H8	1.84	0.43
30:0:2039:A:H4'	30:0:2760:C:O2'	2.19	0.43
31:9:47:A:C2	31:9:48:C:C2	3.07	0.43
2:B:36:PRO:HG3	2:B:169:GLY:H	1.83	0.43
10:J:52:GLN:NE2	30:0:1119:G:H8	2.13	0.43
30:0:1278:A:H4'	30:0:1279:U:N3	2.34	0.43
30:0:1481:G:H2'	30:0:1482:A:O4'	2.19	0.43
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.43
30:0:2001:G:O2'	30:0:2002:C:H5'	2.18	0.43
30:0:2256:G:H2'	30:0:2257:G:C5'	2.49	0.43
5:E:83:GLY:HA3	5:E:170:ARG:HE	1.83	0.43
22:V:39:ALA:N	22:V:40:PRO:HD2	2.34	0.43
25:Y:141:THR:HG23	39:Y:8884:HOH:O	2.18	0.43
30:0:65:C:O2'	30:0:66:G:H5'	2.19	0.43
30:0:238:C:H4'	30:0:287:C:OP1	2.19	0.43
30:0:285:A:H2'	30:0:286:U:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1342:C:O2'	30:0:1343:C:H5'	2.19	0.43
30:0:1451:C:H5'	30:0:1505:U:C5	2.54	0.43
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.52	0.42
27:1:42:SER:HB3	30:0:1473:U:O4'	2.18	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.54	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.18	0.42
3:C:46:TYR:CE1	30:0:450:C:H4'	2.53	0.42
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.51	0.42
23:W:5:VAL:HG11	23:W:153:MET:HE3	2.00	0.42
30:0:1490:G:H4'	30:0:1533:A:OP1	2.18	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:1834:C:H2'	30:0:1840:A:N6	2.34	0.42
30:0:2515:C:H2'	30:0:2516:G:O4'	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:C6	2.53	0.42
30:0:85:C:H5"	30:0:86:A:OP2	2.19	0.42
30:0:164:G:H3'	39:0:3671:HOH:O	2.18	0.42
30:0:204:A:C2'	30:0:205:U:H5'	2.49	0.42
30:0:255:A:H2'	30:0:256:C:O4'	2.19	0.42
30:0:1187:U:H2'	39:0:6950:HOH:O	2.18	0.42
30:0:2526:C:H5'	30:0:2526:C:H6	1.84	0.42
30:0:2793:A:H2'	30:0:2794:G:H5'	2.01	0.42
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.42
23:W:115:THR:HG23	39:W:5420:HOH:O	2.18	0.42
30:0:952:G:H4'	39:0:4063:HOH:O	2.18	0.42
30:0:1159:G:H1	30:0:1208:C:H42	1.68	0.42
30:0:2324:G:N2	30:0:2377:U:H1'	2.34	0.42
30:0:2433:A:H2'	30:0:2434:A:C8	2.54	0.42
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.42
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
25:Y:134:HIS:CD2	25:Y:134:HIS:H	2.37	0.42
30:0:661:G:C5	30:0:686:A:C2	3.08	0.42
30:0:1339:G:C6	30:0:1340:G:N1	2.87	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1850:U:H2'	30:0:1851:G:H8	1.84	0.42
30:0:1942:A:O2'	30:0:1943:C:H5'	2.20	0.42
30:0:2614:C:O2'	30:0:2615:U:H5'	2.20	0.42
23:W:44:MET:HE2	30:0:944:G:H21	1.84	0.42
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.55	0.42
30:0:1079:A:H4'	30:0:2078:U:H5'	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1622:G:C2'	30:0:1623:C:H5'	2.49	0.42
30:0:1839:A:H5'	30:0:2643:G:H4'	2.01	0.42
31:9:56:A:C3'	31:9:57:A:H5"	2.49	0.42
30:0:129:A:O2'	30:0:131:A:OP1	2.37	0.42
30:0:204:A:H2'	30:0:205:U:H5'	2.01	0.42
30:0:278:A:H2'	30:0:279:C:O4'	2.20	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
30:0:1386:G:O2'	30:0:1387:G:H5'	2.19	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.20	0.42
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.39	0.42
10:J:41:ALA:HB3	39:J:5907:HOH:O	2.20	0.42
12:L:30:ARG:HD3	30:0:164:G:H4'	2.01	0.42
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.88	0.42
30:0:1525:G:H5'	30:0:1526:A:OP2	2.19	0.42
30:0:1682:A:H2'	39:0:9817:HOH:O	2.20	0.42
30:0:2269:C:C2'	30:0:2270:G:H5'	2.50	0.42
31:9:27:C:H1'	39:9:9053:HOH:O	2.17	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.38	0.42
30:0:816:G:C6	30:0:817:G:N1	2.88	0.42
30:0:1052:G:N3	30:0:1052:G:H2'	2.35	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.50	0.42
30:0:1186:C:H42	30:0:1190:G:H22	1.68	0.42
30:0:1243:C:H3'	39:0:4869:HOH:O	2.20	0.42
30:0:1537:C:H1'	39:0:6638:HOH:O	2.19	0.42
30:0:2672:C:H2'	30:0:2673:U:H6	1.85	0.42
3:C:79:ARG:O	3:C:87:ARG:HG2	2.20	0.42
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.28	0.42
10:J:74:ARG:NH1	10:J:105:LEU:HD11	2.35	0.42
10:J:82:THR:CG2	30:0:1242:A:H5'	2.34	0.42
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.02	0.42
30:0:39:G:N2	30:0:444:C:C2	2.88	0.42
30:0:200:C:H2'	39:0:3470:HOH:O	2.19	0.42
30:0:304:G:H1'	30:0:347:A:H61	1.84	0.42
30:0:567:U:H6	30:0:567:U:O5'	2.02	0.42
30:0:1023:C:O2'	30:0:1024:G:H5'	2.20	0.42
30:0:1406:A:H5'	30:0:1407:A:C8	2.55	0.42
30:0:1477:C:C5'	30:0:1868:G:H5"	2.49	0.42
30:0:1544:U:H2'	30:0:1545:C:H6	1.85	0.42
30:0:1883:U:H5'	30:0:2012:U:OP2	2.19	0.42
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:2724:U:H2'	30:0:2725:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:80:TYR:O	30:0:2050:G:H5"	2.20	0.41
30:0:360:A:H2'	30:0:361:C:O4'	2.19	0.41
30:0:821:U:H5"	39:0:3074:HOH:O	2.20	0.41
30:0:1098:A:H2'	30:0:1099:G:O4'	2.20	0.41
30:0:1587:U:H2'	30:0:1588:G:O4'	2.20	0.41
30:0:1679:C:H5'	39:0:9335:HOH:O	2.20	0.41
30:0:1856:C:H5'	30:0:1858:A:O4'	2.20	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.41
30:0:2134:G:N2	30:0:2242:U:C2	2.88	0.41
30:0:2335:C:H2'	30:0:2336:G:C8	2.55	0.41
30:0:2842:G:C2'	30:0:2843:A:H5'	2.50	0.41
31:9:60:C:O2'	31:9:61:C:H5'	2.19	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.20	0.41
4:D:103:ASN:ND2	4:D:134:LEU:H	2.17	0.41
4:D:146:LYS:HZ1	14:N:107:ASN:HD21	1.68	0.41
24:X:10:VAL:HG23	24:X:72:VAL:HG12	2.03	0.41
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.02	0.41
30:0:68:U:O2'	30:0:69:A:H5"	2.20	0.41
30:0:177:A:H2'	30:0:178:U:O4'	2.20	0.41
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.38	0.41
30:0:2664:A:H8	30:0:2664:A:OP1	2.02	0.41
2:B:5:ARG:HE	2:B:5:ARG:HB3	1.69	0.41
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.96	0.41
24:X:25:ARG:HD2	39:X:5356:HOH:O	2.19	0.41
30:0:1615:A:H4'	39:0:5927:HOH:O	2.20	0.41
31:9:1:U:H5"	31:9:3:A:OP1	2.20	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.93	0.41
2:B:238:ASN:HD21	30:0:2609:G:N2	2.18	0.41
2:B:302:PRO:HA	30:0:2717:C:H5'	2.02	0.41
20:T:9:LYS:HD3	39:0:3781:HOH:O	2.20	0.41
23:W:122:ARG:HH12	23:W:154:ARG:N	2.19	0.41
30:0:308:U:C4	30:0:342:C:H1'	2.55	0.41
30:0:1315:G:H4'	30:0:1316:G:OP2	2.20	0.41
30:0:2073:G:C6	30:0:2489:G:H4'	2.55	0.41
30:0:2366:C:H6	30:0:2366:C:O5'	2.03	0.41
38:0:2924:ANM:H63	38:0:2924:ANM:C15	2.43	0.41
31:9:31:C:H2'	31:9:32:G:O4'	2.21	0.41
30:0:241:A:C2	30:0:378:A:H4'	2.55	0.41
30:0:932:U:H2'	30:0:933:C:H6	1.86	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:105:A:H2'	31:9:106:U:O4'	2.21	0.41
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.03	0.41
30:0:1205:U:C2'	30:0:1206:U:C5'	2.95	0.41
30:0:2379:G:H5'	30:0:2381:C:O4'	2.21	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:2672:C:O2'	30:0:2673:U:H5'	2.20	0.41
30:0:2781:U:H2'	30:0:2782:G:C5'	2.50	0.41
31:9:29:C:H2'	31:9:30:C:C5'	2.45	0.41
19:S:37:VAL:O	19:S:41:VAL:HG23	2.21	0.41
30:0:326:G:O2'	30:0:327:A:H5'	2.20	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.85	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.41
30:0:1603:A:H5"	30:0:1604:G:H3'	2.03	0.41
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.41
30:0:2349:G:O2'	30:0:2350:G:H5'	2.20	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
31:9:23:U:C2'	31:9:24:U:H4'	2.51	0.41
15:O:39:THR:O	15:O:115:ARG:NH2	2.54	0.41
26:Z:41:ARG:HH12	30:0:821:U:H4'	1.86	0.41
30:0:629:A:C2	30:0:2074:A:C2	3.09	0.41
30:0:1495:C:H1'	30:0:1573:A:H1'	2.03	0.41
30:0:2238:A:O2'	30:0:2239:C:H5'	2.21	0.41
31:9:24:U:H3'	31:9:25:G:C5'	2.51	0.41
31:9:39:U:H3'	31:9:40:C:C5'	2.50	0.41
1:A:171:LYS:HB2	30:0:820:G:C5	2.56	0.41
2:B:85:ARG:NH1	39:B:9096:HOH:O	2.53	0.41
2:B:254:GLN:NE2	39:B:9055:HOH:O	2.54	0.41
3:C:49:ASP:HB3	3:C:52:ALA:HB2	2.02	0.41
13:M:163:LEU:CD2	30:0:188:C:H5"	2.45	0.41
20:T:2:LYS:HG2	30:0:447:A:OP1	2.21	0.41
27:1:9:GLY:HA2	30:0:1687:C:O2	2.21	0.41
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.41
30:0:1321:A:H2'	30:0:1322:G:C8	2.56	0.41
30:0:1829:A:C2'	30:0:1830:C:H5'	2.50	0.41
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.41
30:0:2067:A:H2'	30:0:2068:G:O4'	2.21	0.41
30:0:2271:G:H2'	30:0:2271:G:N3	2.36	0.41
30:0:2837:U:H2'	39:0:6892:HOH:O	2.21	0.41
30:0:2896:A:N3	30:0:2896:A:H2'	2.36	0.41
1:A:176:HIS:CD2	30:0:857:A:H4'	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:ASN:HB2	30:0:329:A:OP2	2.21	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.88	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.20	0.41
30:0:1398:G:O2'	30:0:1399:A:H5'	2.21	0.41
30:0:1783:A:O2'	30:0:1784:U:H5'	2.21	0.41
30:0:2016:U:H6	30:0:2016:U:O5'	2.03	0.41
30:0:2553:A:N3	30:0:2553:A:H2'	2.35	0.41
13:M:179:GLY:O	30:0:399:C:H5'	2.22	0.40
16:P:117:SER:HB3	30:0:1593:C:OP1	2.21	0.40
30:0:130:C:H2'	39:0:3186:HOH:O	2.21	0.40
30:0:226:A:H1'	30:0:393:G:C5	2.56	0.40
30:0:827:A:H1'	39:0:6263:HOH:O	2.20	0.40
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.86	0.40
30:0:2385:G:H2'	30:0:2386:U:H6	1.83	0.40
30:0:2493:C:H2'	30:0:2493:C:O2	2.21	0.40
30:0:2549:C:H2'	30:0:2550:U:O4'	2.22	0.40
30:0:2642:G:H2'	30:0:2643:G:O4'	2.21	0.40
9:I:110:ASP:O	30:0:1163:G:H5'	2.21	0.40
12:L:67:ARG:HB2	12:L:112:GLY:HA3	2.04	0.40
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.04	0.40
30:0:228:C:H2'	30:0:229:G:H5'	2.03	0.40
30:0:613:C:H2'	30:0:614:U:H6	1.87	0.40
30:0:912:A:C4	30:0:1294:A:C2	3.09	0.40
30:0:1185:U:H5'	39:0:7526:HOH:O	2.21	0.40
30:0:1268:C:H2'	30:0:1269:G:H8	1.86	0.40
30:0:1972:U:C2'	30:0:1973:A:C5'	2.99	0.40
30:0:2449:G:H2'	30:0:2450:C:O4'	2.21	0.40
30:0:2812:A:C2	30:0:2814:A:N6	2.75	0.40
6:F:30:LYS:HE2	6:F:99:THR:HG21	2.04	0.40
14:N:147:ILE:HD11	31:9:50:G:OP1	2.22	0.40
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.37	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.22	0.40
30:0:849:C:O2'	30:0:850:U:H5'	2.21	0.40
30:0:876:A:N3	30:0:876:A:C2'	2.85	0.40
30:0:2419:U:H5"	30:0:2420:G:C5'	2.51	0.40
3:C:1:MET:HG2	3:C:2:GLN:H	1.87	0.40
23:W:21:LEU:HD23	23:W:21:LEU:HA	1.86	0.40
27:1:16:HIS:CD2	30:0:470:U:O2'	2.73	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.22	0.40
30:0:441:A:O5'	30:0:441:A:H8	2.04	0.40
30:0:1080:C:H6	30:0:1080:C:O5'	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1299:G:N2	39:0:4716:HOH:O	2.54	0.40
30:0:1545:C:H2'	30:0:1546:G:O4'	2.22	0.40
30:0:1762:C:O2'	30:0:1763:C:H5'	2.21	0.40
30:0:2291:A:N9	30:0:2309:C:H5'	2.35	0.40
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.36	0.40
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.55	0.40
30:0:396:U:HO2'	30:0:397:A:P	2.45	0.40
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
30:0:877:G:C5'	30:0:878:G:OP1	2.65	0.40
30:0:1051:C:H2'	30:0:1052:G:O4'	2.21	0.40
30:0:1119:G:C5	30:0:1243:C:C4	3.10	0.40
30:0:2478:U:O2'	30:0:2479:A:H5'	2.21	0.40
30:0:2893:C:O2'	30:0:2894:C:H5'	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	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	17 40
2	B	335/338 (99%)	314 (94%)	19 (6%)	2 (1%)	25 50
3	C	244/246 (99%)	229 (94%)	15 (6%)	0	100 100
4	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	10 26
5	E	170/178 (96%)	159 (94%)	11 (6%)	0	100 100
6	F	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	5 13
7	G	25/348 (7%)	25 (100%)	0	0	100 100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	25 50
9	I	68/162 (42%)	60 (88%)	8 (12%)	0	100 100
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	19	43
12	L	141/165 (86%)	134 (95%)	7 (5%)	0	100	100
13	M	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
14	N	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	5	12
15	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
22	V	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
23	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	12	30
24	X	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	64 (90%)	6 (8%)	1 (1%)	11	28
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	14	34
All	All	3705/4472 (83%)	3524 (95%)	161 (4%)	20 (0%)	29	54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
14	N	154	LEU
14	N	184	ILE
14	N	183	ASP
1	A	27	LEU
4	D	56	ARG
8	H	19	ARG
14	N	139	TRP
14	N	167	ASP
23	W	77	ALA
2	B	2	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	100	ASP
6	F	101	ALA
11	K	127	ALA
2	B	185	GLY
4	D	137	PRO
23	W	49	ASN
26	Z	44	ARG
6	F	61	MET
29	3	56	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	179/182 (98%)	170 (95%)	9 (5%)	24	51
2	B	282/283 (100%)	269 (95%)	13 (5%)	27	54
3	C	193/193 (100%)	177 (92%)	16 (8%)	11	25
4	D	117/148 (79%)	107 (92%)	10 (8%)	10	24
5	E	152/156 (97%)	148 (97%)	4 (3%)	46	75
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	79
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	127 (95%)	7 (5%)	23	49
9	I	58/130 (45%)	56 (97%)	2 (3%)	37	66
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	36
11	K	106/106 (100%)	99 (93%)	7 (7%)	16	38
12	L	113/127 (89%)	107 (95%)	6 (5%)	22	48
13	M	158/160 (99%)	150 (95%)	8 (5%)	24	50
14	N	149/150 (99%)	144 (97%)	5 (3%)	37	66
15	O	93/94 (99%)	91 (98%)	2 (2%)	52	79
16	P	113/117 (97%)	109 (96%)	4 (4%)	36	65
17	Q	79/80 (99%)	76 (96%)	3 (4%)	33	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	117/122 (96%)	114 (97%)	3 (3%)	46	75
19	S	71/74 (96%)	69 (97%)	2 (3%)	43	73
20	T	105/106 (99%)	96 (91%)	9 (9%)	10	24
21	U	44/53 (83%)	41 (93%)	3 (7%)	16	36
22	V	51/57 (90%)	49 (96%)	2 (4%)	32	61
23	W	130/130 (100%)	123 (95%)	7 (5%)	22	47
24	X	66/74 (89%)	59 (89%)	7 (11%)	6	15
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38	67
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	45 (98%)	1 (2%)	52	79
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	77
29	3	79/79 (100%)	75 (95%)	4 (5%)	24	50
All	All	3095/3646 (85%)	2946 (95%)	149 (5%)	25	53

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	69	LEU
1	A	78	ASP
1	A	85	SER
1	A	94	LEU
1	A	131	HIS
1	A	179	MET
1	A	217	ARG
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	162	MET
2	B	171	VAL
2	B	195	ARG
2	B	254	GLN
2	B	257	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	265	LEU
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU
3	C	243	VAL
4	D	17	ARG
4	D	23	VAL
4	D	24	HIS
4	D	50	VAL
4	D	52	THR
4	D	101	THR
4	D	128	LEU
4	D	149	ARG
4	D	153	THR
4	D	161	ASP
5	E	36	PRO
5	E	102	VAL
5	E	131	LEU
5	E	156	ASP
6	F	12	LEU
6	F	46	GLU
8	H	58	VAL
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	162	PRO
8	H	173	GLU
9	I	94	ASP
9	I	135	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	28	GLU
10	J	47	THR
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	49	LEU
11	K	62	PRO
11	K	98	VAL
11	K	107	THR
11	K	119	GLN
12	L	4	LYS
12	L	32	ASP
12	L	35	ARG
12	L	101	ASP
12	L	104	ASP
12	L	140	VAL
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	99	ARG
13	M	116	ASN
13	M	141	ILE
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	135	VAL
14	N	175	LEU
14	N	176	ARG
15	O	3	THR
15	O	25	VAL
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	16	ASN
17	Q	18	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	132	ARG
19	S	10	VAL
19	S	81	ILE
20	T	39	ASN
20	T	48	VAL
20	T	61	GLU
20	T	71	VAL
20	T	82	THR
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	47	ARG
21	U	52	THR
21	U	56	ARG
22	V	12	THR
22	V	13	PRO
23	W	26	ILE
23	W	38	THR
23	W	52	VAL
23	W	76	ASP
23	W	120	PRO
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	154	ARG
25	Y	157	ILE
25	Y	189	ASN
25	Y	204	ARG
27	1	21	ARG
28	2	18	ASN
29	3	14	CYS
29	3	18	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	3	22	VAL
29	3	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	260	HIS
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	42	ASN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	42	ASN
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	107	ASN
14	N	140	GLN
16	P	50	GLN
16	P	66	GLN
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	22	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	94	ASN
18	R	98	ASN
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	9	HIS
19	S	44	GLN
19	S	51	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	12	ASN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	249 (8%)	29 (1%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	285	A
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	735	C
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1485	A
30	0	1505	U
30	0	1506	U
30	0	1524	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1525	G
30	0	1526	A
30	0	1592	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	G
30	0	2613	G
30	0	2634	G
30	0	2649	A
30	0	2664	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	129	A
30	0	169	A
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1684	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2791	U
31	9	65	A

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

5 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	$\#\|Z\| > 2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	OMU	0	2587	30	19,22,23	0.27	0	26,31,34	0.44	0
30	PSU	0	2621	30	18,21,22	1.36	2 (11%)	22,30,33	1.20	3 (13%)
30	OMG	0	2588	30	18,26,27	1.03	2 (11%)	19,38,41	0.73	1 (5%)
30	1MA	0	628	30,35	16,25,26	1.36	3 (18%)	18,37,40	1.17	2 (11%)
30	UR3	0	2619	30	19,22,23	0.39	0	26,32,35	0.65	1 (3%)

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
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.32	1.42	1.36
30	0	628	1MA	C2-N3	3.41	1.33	1.29
30	0	2621	PSU	C6-C5	2.73	1.38	1.35
30	0	628	1MA	C6-N6	2.67	1.34	1.27
30	0	2588	OMG	C8-N7	-2.53	1.30	1.35
30	0	2588	OMG	C5-C6	-2.49	1.42	1.47
30	0	628	1MA	C8-N7	-2.09	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	C6-C5-C4	2.97	120.28	118.20
30	0	628	1MA	N1-C2-N3	2.87	129.37	126.02
30	0	2621	PSU	O2-C2-N1	2.68	125.75	122.79
30	0	2621	PSU	C6-N1-C2	-2.62	120.00	122.68
30	0	628	1MA	C5-C6-N1	2.50	117.62	113.90
30	0	2619	UR3	C4-N3-C2	2.35	126.78	124.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2588	OMG	O6-C6-C5	2.21	128.68	124.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
38	ANM	0	2924	37	20,20,20	0.47	0	22,27,27	1.97	6 (27%)

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
38	ANM	0	2924	37	-	4/10/23/23	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	0	2924	ANM	O2-C5-C6	5.23	120.72	111.09
38	0	2924	ANM	C4-C3-C2	-3.85	98.31	103.29
38	0	2924	ANM	C2-O2-C5	-3.75	111.92	117.72
38	0	2924	ANM	C3-C2-C16	-3.01	99.95	104.29
38	0	2924	ANM	C14-O1-C9	-2.79	111.46	117.51
38	0	2924	ANM	O2-C5-O3	-2.07	118.84	122.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	0	2924	ANM	C6-C5-O2-C2
38	0	2924	ANM	O3-C5-O2-C2
38	0	2924	ANM	C10-C9-O1-C14
38	0	2924	ANM	C1-C9-O1-C14

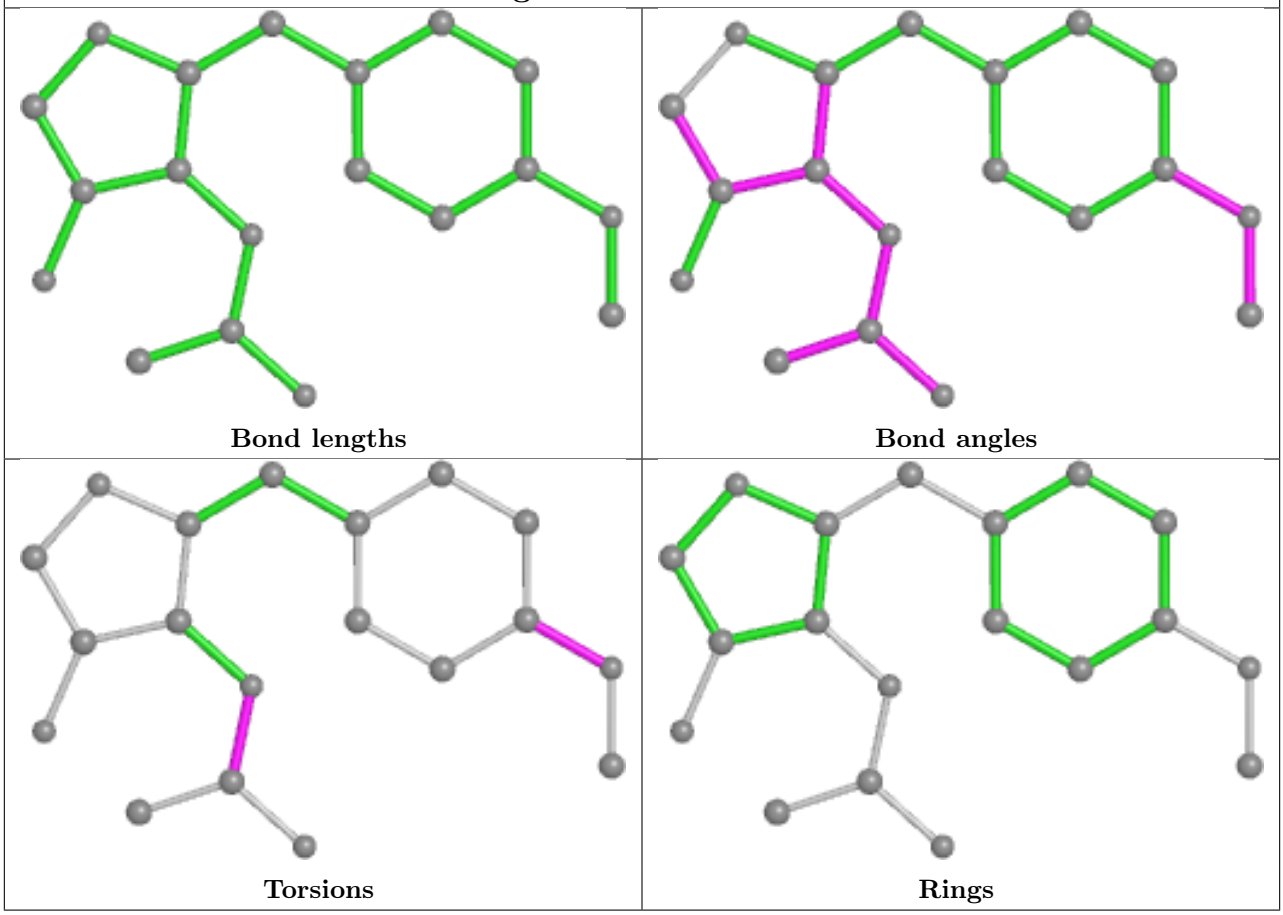
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	ANM	5	0

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

Ligand ANM 0 2924



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	A	237/240 (98%)	0.63	22 (9%)	8	6	24, 49, 88, 107	0
2	B	337/338 (99%)	0.37	10 (2%)	50	51	27, 53, 82, 95	0
3	C	246/246 (100%)	0.29	3 (1%)	79	80	21, 42, 65, 78	0
4	D	140/177 (79%)	2.48	71 (50%)	0	0	61, 99, 124, 134	0
5	E	172/178 (96%)	0.70	15 (8%)	10	8	44, 69, 88, 94	0
6	F	119/120 (99%)	1.32	31 (26%)	0	0	43, 69, 99, 114	0
7	G	29/348 (8%)	1.76	10 (34%)	0	0	77, 95, 103, 106	0
8	H	160/177 (90%)	1.29	40 (25%)	0	0	44, 61, 96, 101	0
9	I	70/162 (43%)	5.14	65 (92%)	0	0	131, 146, 163, 164	0
10	J	142/145 (97%)	0.31	2 (1%)	75	77	35, 50, 71, 91	0
11	K	132/132 (100%)	0.15	2 (1%)	73	76	32, 49, 72, 77	0
12	L	145/165 (87%)	0.94	27 (18%)	1	1	25, 63, 109, 125	0
13	M	194/196 (98%)	0.12	2 (1%)	82	83	28, 40, 56, 62	0
14	N	186/187 (99%)	1.13	37 (19%)	1	0	42, 64, 112, 121	0
15	O	115/116 (99%)	0.50	2 (1%)	70	72	33, 53, 69, 80	0
16	P	143/149 (95%)	0.42	4 (2%)	53	54	38, 53, 67, 74	0
17	Q	95/96 (98%)	0.28	1 (1%)	80	82	34, 45, 62, 73	0
18	R	150/155 (96%)	0.14	0	100	100	30, 43, 63, 71	0
19	S	81/85 (95%)	0.91	8 (9%)	7	5	42, 56, 79, 90	0
20	T	119/120 (99%)	0.65	7 (5%)	22	21	35, 54, 84, 109	0
21	U	53/67 (79%)	0.62	4 (7%)	14	12	40, 56, 78, 84	0
22	V	65/71 (91%)	2.56	28 (43%)	0	0	52, 73, 117, 123	0
23	W	154/154 (100%)	0.54	5 (3%)	47	48	33, 49, 65, 75	0
24	X	82/92 (89%)	0.86	12 (14%)	2	1	43, 60, 85, 101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	142/241 (58%)	0.18	5 (3%) 44 44	22, 41, 64, 89	0
26	Z	73/116 (62%)	2.49	44 (60%) 0 0	58, 76, 89, 100	0
27	1	56/57 (98%)	0.04	0 100 100	24, 30, 36, 43	0
28	2	46/50 (92%)	1.02	11 (23%) 0 0	34, 60, 91, 101	0
29	3	92/92 (100%)	0.70	6 (6%) 18 17	36, 59, 72, 86	0
30	0	2749/2923 (94%)	-0.32	56 (2%) 65 67	18, 43, 87, 165	0
31	9	122/122 (100%)	-0.29	4 (3%) 46 46	34, 65, 86, 145	0
All	All	6646/7517 (88%)	0.31	534 (8%) 12 10	18, 50, 99, 165	0

All (534) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	14.6
22	V	1	THR	12.8
22	V	40	PRO	12.0
9	I	74	ILE	11.8
14	N	166	ALA	10.8
4	D	63	ILE	10.8
9	I	97	VAL	10.4
9	I	70	THR	9.8
9	I	72	GLU	9.0
9	I	66	GLY	8.9
9	I	132	VAL	8.9
9	I	128	THR	8.9
4	D	57	THR	8.5
9	I	100	VAL	8.5
26	Z	35	SER	8.4
22	V	43	PRO	8.3
31	9	1	U	7.9
9	I	91	PHE	7.9
9	I	108	HIS	7.9
26	Z	58	ASN	7.7
9	I	99	GLN	7.7
9	I	71	ALA	7.6
4	D	90	LEU	7.4
22	V	37	GLY	7.1
9	I	79	GLY	7.1
9	I	117	THR	7.0
9	I	102	GLN	7.0
9	I	104	ALA	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	106	GLN	6.7
9	I	98	ASP	6.6
20	T	119	ALA	6.5
9	I	109	PRO	6.5
4	D	10	PHE	6.5
9	I	80	PHE	6.4
9	I	111	LEU	6.2
30	0	1198	U	6.2
4	D	134	LEU	6.2
4	D	18	ILE	6.2
9	I	112	LEU	6.1
4	D	85	GLN	6.1
19	S	81	ILE	6.1
4	D	64	ARG	6.0
9	I	127	CYS	6.0
9	I	78	ALA	5.9
22	V	38	GLY	5.8
1	A	237	GLY	5.8
26	Z	46	SER	5.8
9	I	88	GLN	5.7
30	0	1172	G	5.7
9	I	73	LEU	5.7
9	I	105	GLU	5.6
4	D	89	PRO	5.6
26	Z	45	VAL	5.6
1	A	37	VAL	5.5
4	D	44	ILE	5.5
22	V	41	GLU	5.4
6	F	49	PHE	5.4
9	I	103	ILE	5.4
9	I	130	LEU	5.4
9	I	113	SER	5.4
9	I	120	ALA	5.3
4	D	40	ILE	5.3
9	I	69	PRO	5.3
4	D	88	LEU	5.1
4	D	128	LEU	5.1
30	0	1199	A	5.1
26	Z	44	ARG	5.1
26	Z	104	ARG	5.1
4	D	75	LEU	5.1
9	I	116	LEU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	Y	235	GLU	4.9
4	D	69	ILE	4.9
9	I	76	ASP	4.8
9	I	86	GLU	4.8
9	I	121	LYS	4.8
4	D	104	PHE	4.8
22	V	36	ALA	4.7
26	Z	34	SER	4.7
9	I	94	ASP	4.6
9	I	82	THR	4.6
4	D	130	VAL	4.6
9	I	83	GLY	4.5
9	I	92	VAL	4.5
30	0	1202	A	4.5
8	H	77	ILE	4.5
9	I	93	ALA	4.5
4	D	61	PHE	4.5
24	X	88	GLU	4.5
12	L	60	GLU	4.4
5	E	45	ASP	4.4
9	I	133	THR	4.4
4	D	56	ARG	4.4
6	F	75	ILE	4.4
26	Z	78	ILE	4.4
30	0	735	C	4.4
26	Z	49	ARG	4.3
9	I	110	ASP	4.3
19	S	76	GLU	4.3
7	G	23	ILE	4.3
14	N	155	GLU	4.3
26	Z	69	ASP	4.3
8	H	76	LEU	4.3
9	I	75	LYS	4.3
9	I	118	ASN	4.3
4	D	157	LEU	4.2
14	N	160	SER	4.2
4	D	27	ILE	4.2
9	I	131	GLY	4.2
26	Z	55	SER	4.2
30	0	1171	A	4.2
12	L	106	VAL	4.2
4	D	84	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	Z	82	SER	4.1
30	0	1169	U	4.1
30	0	1163	G	4.1
24	X	7	GLU	4.1
8	H	40	GLN	4.1
22	V	2	VAL	4.1
9	I	67	VAL	4.1
4	D	106	PHE	4.1
8	H	141	CYS	4.1
4	D	26	GLY	4.0
30	0	970	U	4.0
8	H	86	TYR	4.0
14	N	152	GLU	4.0
24	X	74	ALA	4.0
30	0	1173	A	4.0
26	Z	60	ASP	4.0
26	Z	83	TYR	4.0
4	D	23	VAL	4.0
26	Z	50	VAL	4.0
31	9	24	U	3.9
26	Z	62	ALA	3.9
28	2	20	ARG	3.9
28	2	49	GLU	3.9
9	I	126	THR	3.9
28	2	39	ARG	3.8
4	D	58	VAL	3.8
6	F	17	LEU	3.8
24	X	71	ARG	3.8
24	X	77	PHE	3.8
3	C	139	VAL	3.8
14	N	165	ALA	3.7
22	V	3	LEU	3.7
4	D	22	VAL	3.7
24	X	80	GLU	3.7
9	I	123	VAL	3.7
4	D	70	GLY	3.7
4	D	92	GLU	3.7
4	D	24	HIS	3.7
4	D	170	TYR	3.7
10	J	70	PHE	3.6
30	0	282	C	3.6
22	V	46	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	62	ASP	3.6
8	H	81	GLY	3.6
30	0	1170	U	3.6
12	L	96	VAL	3.5
8	H	37	GLY	3.5
12	L	75	LEU	3.5
5	E	108	LEU	3.5
21	U	47	ARG	3.5
6	F	99	THR	3.5
9	I	119	ALA	3.5
7	G	27	ILE	3.5
26	Z	61	HIS	3.4
9	I	124	VAL	3.4
20	T	118	SER	3.4
22	V	32	ALA	3.4
30	0	1177	A	3.4
30	0	1181	A	3.4
26	Z	54	GLU	3.4
26	Z	53	ILE	3.4
14	N	172	PHE	3.4
6	F	106	ALA	3.4
4	D	154	LYS	3.4
4	D	25	MET	3.4
26	Z	68	GLU	3.3
1	A	94	LEU	3.3
8	H	70	LEU	3.3
4	D	68	PRO	3.3
7	G	26	MET	3.3
22	V	44	GLY	3.3
9	I	68	PRO	3.3
4	D	19	GLU	3.3
6	F	91	VAL	3.3
26	Z	42	TYR	3.3
7	G	71	LEU	3.3
8	H	174	LEU	3.3
4	D	158	ASN	3.3
1	A	99	ILE	3.3
4	D	87	ALA	3.3
8	H	35	LYS	3.3
4	D	86	THR	3.2
5	E	87	PHE	3.2
12	L	105	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	Z	79	TRP	3.2
8	H	140	TYR	3.2
22	V	33	VAL	3.2
12	L	80	ASP	3.2
9	I	84	SER	3.2
1	A	58	VAL	3.2
12	L	81	VAL	3.2
9	I	114	TYR	3.2
4	D	73	VAL	3.2
4	D	101	THR	3.2
28	2	37	HIS	3.2
1	A	90	PRO	3.2
28	2	27	LEU	3.2
25	Y	108	ASP	3.1
2	B	181	ILE	3.1
11	K	118	ALA	3.1
4	D	47	GLN	3.1
9	I	89	GLU	3.1
9	I	90	ASP	3.1
30	0	10	U	3.1
6	F	12	LEU	3.1
8	H	73	ASN	3.1
20	T	116	ASP	3.1
4	D	165	PHE	3.1
8	H	82	GLU	3.1
12	L	145	LEU	3.1
14	N	83	LEU	3.1
29	3	15	ASN	3.1
14	N	62	HIS	3.1
4	D	45	THR	3.1
4	D	43	GLU	3.1
5	E	154	ILE	3.1
29	3	13	HIS	3.1
30	0	1186	C	3.1
4	D	171	ASP	3.1
8	H	85	ASP	3.1
30	0	1951	G	3.1
28	2	23	ALA	3.1
30	0	1200	A	3.1
4	D	129	ASP	3.1
9	I	81	GLU	3.1
1	A	35	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	77	VAL	3.0
26	Z	48	ARG	3.0
14	N	159	TYR	3.0
9	I	122	GLU	3.0
28	2	35	ARG	3.0
22	V	59	ILE	3.0
30	0	2637	A	3.0
8	H	38	ARG	3.0
30	0	1203	G	3.0
12	L	91	VAL	3.0
14	N	138	ASP	3.0
22	V	8	ILE	3.0
4	D	98	PHE	3.0
4	D	93	LEU	3.0
28	2	36	ASN	3.0
24	X	85	VAL	3.0
22	V	52	ALA	3.0
12	L	99	GLU	3.0
26	Z	43	GLY	3.0
8	H	53	ILE	2.9
26	Z	38	PHE	2.9
30	0	497	A	2.9
14	N	145	ALA	2.9
30	0	1947	G	2.9
14	N	158	LEU	2.9
30	0	1178	G	2.9
22	V	45	ARG	2.9
26	Z	47	ARG	2.9
6	F	26	THR	2.9
9	I	95	LEU	2.9
4	D	65	GLU	2.9
1	A	31	LYS	2.9
6	F	20	LEU	2.9
6	F	29	VAL	2.9
7	G	24	VAL	2.9
30	0	1279	U	2.9
20	T	117	ASP	2.9
28	2	48	ASP	2.9
6	F	119	ARG	2.9
9	I	129	SER	2.9
30	0	2769	C	2.9
9	I	101	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	74	THR	2.9
1	A	38	ILE	2.8
24	X	10	VAL	2.8
5	E	100	ASP	2.8
12	L	150	GLN	2.8
30	0	1168	C	2.8
8	H	78	LYS	2.8
19	S	78	ALA	2.8
8	H	69	ARG	2.8
5	E	10	ASP	2.8
3	C	138	VAL	2.8
8	H	169	GLU	2.8
10	J	92	GLN	2.8
19	S	20	PHE	2.8
24	X	72	VAL	2.8
14	N	147	ILE	2.8
14	N	163	PHE	2.8
30	0	1197	G	2.8
30	0	1948	G	2.8
8	H	114	ASP	2.7
14	N	164	ASP	2.7
1	A	91	GLY	2.7
30	0	1165	G	2.7
4	D	11	HIS	2.7
8	H	36	MET	2.7
1	A	65	ARG	2.7
26	Z	89	THR	2.7
6	F	44	SER	2.7
30	0	1190	G	2.7
30	0	1164	U	2.7
22	V	34	GLN	2.7
4	D	135	VAL	2.7
6	F	97	ALA	2.7
4	D	139	TYR	2.7
30	0	1180	U	2.7
4	D	132	VAL	2.7
8	H	66	GLU	2.7
12	L	149	ARG	2.7
26	Z	93	TYR	2.7
5	E	170	ARG	2.7
1	A	64	ASP	2.7
6	F	90	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	Q	95	GLU	2.7
26	Z	70	ARG	2.7
14	N	169	PRO	2.7
14	N	178	THR	2.7
1	A	236	GLY	2.6
6	F	16	ALA	2.6
4	D	156	ARG	2.6
25	Y	95	THR	2.6
14	N	67	ALA	2.6
14	N	95	ALA	2.6
1	A	82	VAL	2.6
1	A	60	PHE	2.6
22	V	31	ARG	2.6
24	X	73	ARG	2.6
7	G	21	ASP	2.6
1	A	85	SER	2.6
4	D	66	GLY	2.6
9	I	125	GLY	2.6
8	H	39	LYS	2.6
12	L	97	VAL	2.6
26	Z	56	GLU	2.6
22	V	49	LEU	2.6
31	9	23	U	2.6
30	0	1965	C	2.6
8	H	172	GLU	2.6
26	Z	59	GLU	2.6
1	A	80	LEU	2.6
31	9	2	U	2.6
29	3	41	GLU	2.6
2	B	116	PRO	2.6
24	X	82	GLU	2.6
4	D	17	ARG	2.6
14	N	139	TRP	2.6
19	S	80	ARG	2.6
22	V	42	ASN	2.6
8	H	48	VAL	2.6
4	D	83	PHE	2.6
30	0	1964	U	2.6
12	L	121	ILE	2.6
4	D	71	ALA	2.6
8	H	83	GLU	2.6
4	D	166	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	1	ALA	2.5
14	N	81	ALA	2.5
23	W	62	LEU	2.5
26	Z	81	CYS	2.5
6	F	51	ALA	2.5
8	H	50	ILE	2.5
14	N	97	VAL	2.5
16	P	67	LYS	2.5
19	S	45	TYR	2.5
22	V	23	LEU	2.5
29	3	92	GLU	2.5
2	B	105	PHE	2.5
8	H	68	SER	2.5
6	F	114	LYS	2.5
8	H	74	ARG	2.5
8	H	27	PRO	2.5
2	B	143	ILE	2.5
6	F	96	ALA	2.5
21	U	54	THR	2.5
8	H	149	VAL	2.5
25	Y	236	VAL	2.5
4	D	105	SER	2.5
29	3	1	MET	2.5
4	D	172	VAL	2.5
6	F	6	PHE	2.5
14	N	68	GLU	2.4
30	0	1966	U	2.4
4	D	16	PRO	2.4
22	V	25	THR	2.4
30	0	1179	C	2.4
22	V	5	VAL	2.4
14	N	183	ASP	2.4
8	H	146	ALA	2.4
6	F	115	VAL	2.4
9	I	135	GLU	2.4
26	Z	36	GLY	2.4
30	0	2237	G	2.4
30	0	1192	A	2.4
26	Z	77	GLY	2.4
4	D	142	ALA	2.4
20	T	112	LEU	2.4
1	A	88	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	72	ASP	2.4
8	H	31	ILE	2.4
6	F	74	PHE	2.4
14	N	140	GLN	2.4
25	Y	234	VAL	2.4
26	Z	80	GLN	2.3
14	N	87	LEU	2.3
12	L	147	GLU	2.3
12	L	62	ALA	2.3
30	0	284	C	2.3
8	H	170	ARG	2.3
26	Z	37	ARG	2.3
12	L	66	VAL	2.3
26	Z	85	ASP	2.3
8	H	71	SER	2.3
14	N	185	GLU	2.3
26	Z	86	TYR	2.3
30	0	1185	U	2.3
3	C	5	ILE	2.3
30	0	1196	C	2.3
30	0	1174	A	2.3
4	D	53	LYS	2.3
6	F	48	VAL	2.3
6	F	117	GLU	2.3
14	N	137	ALA	2.3
30	0	1967	U	2.3
23	W	79	VAL	2.3
30	0	2508	C	2.3
1	A	133	ARG	2.3
14	N	84	THR	2.3
30	0	1625	U	2.3
30	0	1162	G	2.3
5	E	5	LEU	2.3
16	P	108	LEU	2.3
26	Z	51	ALA	2.3
1	A	36	ASP	2.3
12	L	102	ASP	2.3
2	B	168	GLY	2.3
19	S	15	MET	2.3
23	W	96	LEU	2.3
30	0	1950	G	2.3
4	D	54	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	101	ASP	2.3
14	N	162	ASP	2.3
30	0	2004	U	2.2
5	E	88	TYR	2.2
26	Z	105	ARG	2.2
26	Z	74	GLN	2.2
6	F	118	LEU	2.2
23	W	116	LEU	2.2
30	0	960	G	2.2
6	F	39	SER	2.2
8	H	60	LEU	2.2
22	V	27	LEU	2.2
1	A	89	ALA	2.2
6	F	15	ASP	2.2
2	B	183	GLU	2.2
4	D	81	GLU	2.2
6	F	22	VAL	2.2
9	I	134	ILE	2.2
5	E	89	SER	2.2
7	G	69	ARG	2.2
12	L	130	ARG	2.2
8	H	80	LEU	2.2
5	E	6	GLU	2.2
24	X	9	VAL	2.2
5	E	128	GLY	2.2
6	F	100	ASP	2.2
12	L	77	ALA	2.2
6	F	37	THR	2.2
4	D	21	VAL	2.2
20	T	40	VAL	2.2
26	Z	95	PRO	2.2
2	B	115	VAL	2.1
5	E	86	VAL	2.1
15	O	89	ILE	2.1
2	B	117	GLU	2.1
13	M	22	GLU	2.1
14	N	156	GLU	2.1
30	0	1157	C	2.1
16	P	48	ALA	2.1
21	U	52	THR	2.1
30	0	2103	A	2.1
26	Z	71	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	123	ASP	2.1
22	V	9	ARG	2.1
1	A	97	ALA	2.1
14	N	75	THR	2.1
2	B	128	ILE	2.1
5	E	42	VAL	2.1
16	P	116	SER	2.1
26	Z	88	PHE	2.1
14	N	134	ASP	2.1
15	O	98	LEU	2.1
8	H	87	LYS	2.1
7	G	63	ARG	2.1
12	L	95	ASP	2.1
8	H	90	LEU	2.1
12	L	76	LEU	2.1
2	B	1	PRO	2.1
14	N	129	ILE	2.1
4	D	80	ALA	2.1
21	U	40	ALA	2.1
30	0	1175	G	2.1
30	0	1195	G	2.1
12	L	140	VAL	2.1
4	D	72	LYS	2.1
6	F	31	LYS	2.1
12	L	61	ALA	2.1
14	N	148	ALA	2.1
6	F	76	PHE	2.1
30	0	2249	G	2.0
14	N	50	LEU	2.0
23	W	149	LEU	2.0
12	L	93	VAL	2.0
30	0	1201	C	2.0
20	T	115	GLU	2.0
14	N	151	ASP	2.0
28	2	24	TRP	2.0
29	3	83	TRP	2.0
9	I	87	PRO	2.0
30	0	2911	C	2.0
11	K	109	LEU	2.0
7	G	25	GLU	2.0
5	E	167	TYR	2.0
8	H	32	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	2	38	LYS	2.0
22	V	28	LEU	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(Å^2)	Q<0.9
30	1MA	0	628	23/24	0.98	0.18	25,28,29,31	0
30	OMU	0	2587	21/22	0.98	0.15	31,33,35,37	0
30	OMG	0	2588	24/25	0.98	0.15	27,30,33,35	0
30	UR3	0	2619	21/22	0.98	0.17	30,34,36,39	0
30	PSU	0	2621	20/21	0.98	0.16	22,26,34,34	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	9	8978	1/1	0.09	0.14	144,144,144,144	0
34	SR	0	9006	1/1	0.15	1.95	200,200,200,200	0
34	SR	0	8955	1/1	0.16	0.35	200,200,200,200	0
34	SR	0	8957	1/1	0.29	0.75	200,200,200,200	0
35	NA	S	8510	1/1	0.35	0.43	79,79,79,79	0
35	NA	9	8572	1/1	0.38	0.43	76,76,76,76	0
34	SR	0	8976	1/1	0.40	0.45	186,186,186,186	0
32	MG	0	8089	1/1	0.43	0.17	48,48,48,48	0
34	SR	0	8919	1/1	0.47	0.24	178,178,178,178	0
34	SR	0	8922	1/1	0.48	0.37	159,159,159,159	0
34	SR	0	8996	1/1	0.50	0.82	200,200,200,200	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8986	1/1	0.51	1.96	200,200,200,200	0
34	SR	0	8947	1/1	0.54	0.47	200,200,200,200	0
34	SR	0	8959	1/1	0.54	0.26	169,169,169,169	0
34	SR	A	8977	1/1	0.54	0.17	172,172,172,172	0
34	SR	0	8979	1/1	0.56	0.29	194,194,194,194	0
35	NA	0	8546	1/1	0.57	1.03	95,95,95,95	0
34	SR	0	8994	1/1	0.60	0.60	190,190,190,190	0
34	SR	9	9003	1/1	0.61	0.10	162,162,162,162	0
34	SR	0	8983	1/1	0.64	0.23	164,164,164,164	0
34	SR	0	8934	1/1	0.64	0.13	90,90,90,90	0
34	SR	0	8984	1/1	0.65	0.10	128,128,128,128	0
34	SR	0	8924	1/1	0.65	0.13	145,145,145,145	0
34	SR	0	8989	1/1	0.67	0.39	187,187,187,187	0
35	NA	0	8522	1/1	0.67	0.52	78,78,78,78	0
34	SR	S	8961	1/1	0.67	0.10	114,114,114,114	0
35	NA	0	8573	1/1	0.67	0.63	69,69,69,69	0
34	SR	B	8987	1/1	0.67	0.69	200,200,200,200	0
32	MG	0	8069	1/1	0.69	0.57	47,47,47,47	0
35	NA	0	8561	1/1	0.69	0.83	74,74,74,74	0
34	SR	0	8993	1/1	0.70	0.17	168,168,168,168	0
34	SR	0	8944	1/1	0.70	0.26	185,185,185,185	0
34	SR	0	8971	1/1	0.70	0.17	170,170,170,170	0
34	SR	0	8916	1/1	0.71	0.15	118,118,118,118	0
35	NA	0	8557	1/1	0.72	0.15	67,67,67,67	0
35	NA	0	8512	1/1	0.72	0.51	43,43,43,43	0
35	NA	0	8571	1/1	0.72	0.32	83,83,83,83	0
32	MG	0	8092	1/1	0.72	0.15	61,61,61,61	0
34	SR	0	8969	1/1	0.72	0.39	150,150,150,150	0
35	NA	0	8553	1/1	0.73	0.41	79,79,79,79	0
32	MG	0	8050	1/1	0.73	0.18	37,37,37,37	0
35	NA	0	8554	1/1	0.74	0.76	65,65,65,65	0
35	NA	0	8549	1/1	0.74	0.42	81,81,81,81	0
35	NA	M	8539	1/1	0.74	0.25	41,41,41,41	0
32	MG	0	8040	1/1	0.75	0.34	83,83,83,83	0
34	SR	0	8956	1/1	0.75	0.14	142,142,142,142	0
34	SR	0	8960	1/1	0.75	0.11	145,145,145,145	0
34	SR	0	8982	1/1	0.76	0.85	180,180,180,180	0
34	SR	0	8949	1/1	0.76	0.20	110,110,110,110	0
34	SR	0	8933	1/1	0.76	0.52	138,138,138,138	0
35	NA	0	8555	1/1	0.77	0.74	54,54,54,54	0
35	NA	0	8533	1/1	0.77	0.25	63,63,63,63	0
34	SR	0	8963	1/1	0.77	0.12	133,133,133,133	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8990	1/1	0.77	0.22	118,118,118,118	0
34	SR	0	8953	1/1	0.77	0.24	160,160,160,160	0
32	MG	A	8051	1/1	0.77	0.50	81,81,81,81	0
35	NA	0	8531	1/1	0.78	0.16	40,40,40,40	0
34	SR	0	8981	1/1	0.78	0.23	167,167,167,167	0
35	NA	0	8560	1/1	0.78	0.46	69,69,69,69	0
32	MG	0	8062	1/1	0.78	0.23	34,34,34,34	0
35	NA	0	8562	1/1	0.78	0.85	69,69,69,69	0
35	NA	0	8568	1/1	0.78	0.39	47,47,47,47	0
35	NA	0	8511	1/1	0.78	0.33	59,59,59,59	0
34	SR	9	8980	1/1	0.78	0.27	182,182,182,182	0
34	SR	0	9002	1/1	0.78	0.15	184,184,184,184	0
34	SR	0	8914	1/1	0.79	0.34	118,118,118,118	0
34	SR	0	8917	1/1	0.79	0.18	119,119,119,119	0
32	MG	0	8079	1/1	0.80	0.24	47,47,47,47	0
34	SR	0	8988	1/1	0.80	0.08	163,163,163,163	0
34	SR	0	8938	1/1	0.80	0.08	159,159,159,159	0
35	NA	9	8543	1/1	0.80	0.08	70,70,70,70	0
34	SR	0	8974	1/1	0.80	0.29	166,166,166,166	0
32	MG	0	8031	1/1	0.81	0.20	61,61,61,61	0
34	SR	0	8951	1/1	0.81	0.07	146,146,146,146	0
32	MG	0	8063	1/1	0.81	0.28	72,72,72,72	0
34	SR	0	8997	1/1	0.81	0.64	184,184,184,184	0
34	SR	0	8958	1/1	0.81	0.11	108,108,108,108	0
34	SR	0	8939	1/1	0.82	0.18	152,152,152,152	0
35	NA	0	8565	1/1	0.82	0.54	62,62,62,62	0
32	MG	0	8024	1/1	0.82	0.57	85,85,85,85	0
32	MG	0	8088	1/1	0.82	0.16	37,37,37,37	0
34	SR	0	8998	1/1	0.82	0.41	173,173,173,173	0
35	NA	0	8575	1/1	0.82	0.34	94,94,94,94	0
34	SR	0	8991	1/1	0.82	0.23	191,191,191,191	0
34	SR	0	8948	1/1	0.82	0.17	102,102,102,102	0
34	SR	0	9000	1/1	0.83	0.17	159,159,159,159	0
34	SR	0	8966	1/1	0.83	0.08	110,110,110,110	0
35	NA	0	8506	1/1	0.83	0.25	47,47,47,47	0
34	SR	0	8995	1/1	0.83	0.19	136,136,136,136	0
34	SR	0	9007	1/1	0.83	0.39	200,200,200,200	0
34	SR	0	8973	1/1	0.83	0.10	137,137,137,137	0
34	SR	0	8928	1/1	0.83	0.20	138,138,138,138	0
34	SR	0	8975	1/1	0.83	0.11	134,134,134,134	0
37	K	0	8401	1/1	0.83	0.41	81,81,81,81	0
35	NA	0	8505	1/1	0.84	0.57	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	9001	1/1	0.84	0.24	169,169,169,169	0
32	MG	0	8072	1/1	0.84	0.28	52,52,52,52	0
32	MG	0	8080	1/1	0.84	0.28	57,57,57,57	0
35	NA	0	8567	1/1	0.85	0.43	78,78,78,78	0
32	MG	0	8043	1/1	0.85	0.15	49,49,49,49	0
32	MG	0	8030	1/1	0.85	0.37	55,55,55,55	0
35	NA	Q	8540	1/1	0.85	0.22	60,60,60,60	0
34	SR	0	8910	1/1	0.85	0.12	97,97,97,97	0
32	MG	0	8016	1/1	0.85	0.33	49,49,49,49	0
34	SR	0	8941	1/1	0.85	0.19	115,115,115,115	0
32	MG	0	8006	1/1	0.85	0.21	30,30,30,30	0
35	NA	0	8501	1/1	0.86	0.20	39,39,39,39	0
32	MG	0	8038	1/1	0.86	0.12	58,58,58,58	0
32	MG	B	8042	1/1	0.86	0.12	50,50,50,50	0
34	SR	0	8945	1/1	0.86	0.11	99,99,99,99	0
32	MG	0	8055	1/1	0.86	0.27	38,38,38,38	0
35	NA	0	8518	1/1	0.86	0.41	79,79,79,79	0
32	MG	0	8071	1/1	0.86	0.27	55,55,55,55	0
34	SR	0	9004	1/1	0.86	0.42	200,200,200,200	0
34	SR	0	8926	1/1	0.86	0.12	115,115,115,115	0
35	NA	0	8504	1/1	0.87	0.28	26,26,26,26	0
34	SR	0	8942	1/1	0.87	0.15	121,121,121,121	0
35	NA	0	8525	1/1	0.87	0.12	69,69,69,69	0
34	SR	0	8970	1/1	0.87	0.07	131,131,131,131	0
35	NA	0	8556	1/1	0.87	0.50	44,44,44,44	0
35	NA	0	8574	1/1	0.87	0.43	53,53,53,53	0
34	SR	A	8930	1/1	0.87	0.08	116,116,116,116	0
35	NA	0	8542	1/1	0.87	0.41	42,42,42,42	0
35	NA	0	8502	1/1	0.87	0.34	67,67,67,67	0
35	NA	0	8548	1/1	0.87	0.37	57,57,57,57	0
34	SR	B	8950	1/1	0.88	0.19	108,108,108,108	0
35	NA	0	8523	1/1	0.88	0.26	48,48,48,48	0
32	MG	0	8044	1/1	0.88	0.12	33,33,33,33	0
32	MG	0	8081	1/1	0.88	0.24	54,54,54,54	0
34	SR	0	8920	1/1	0.88	0.12	124,124,124,124	0
35	NA	0	8509	1/1	0.88	0.34	64,64,64,64	0
34	SR	0	8964	1/1	0.88	0.08	126,126,126,126	0
32	MG	0	8085	1/1	0.88	0.28	80,80,80,80	0
32	MG	0	8066	1/1	0.88	0.22	52,52,52,52	0
32	MG	0	8075	1/1	0.89	0.08	45,45,45,45	0
35	NA	J	8538	1/1	0.89	0.20	56,56,56,56	0
35	NA	0	8530	1/1	0.89	0.27	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8908	1/1	0.89	0.18	107,107,107,107	0
35	NA	0	8508	1/1	0.89	0.23	37,37,37,37	0
34	SR	0	8909	1/1	0.89	0.14	94,94,94,94	0
35	NA	0	8544	1/1	0.89	0.30	64,64,64,64	0
35	NA	R	8532	1/1	0.89	0.18	53,53,53,53	0
34	SR	0	8967	1/1	0.89	0.11	133,133,133,133	0
34	SR	0	8968	1/1	0.89	0.10	143,143,143,143	0
35	NA	0	8519	1/1	0.89	0.42	39,39,39,39	0
35	NA	0	8520	1/1	0.89	0.18	54,54,54,54	0
35	NA	0	8521	1/1	0.89	0.29	61,61,61,61	0
32	MG	0	8039	1/1	0.89	0.33	69,69,69,69	0
35	NA	0	8514	1/1	0.90	0.28	42,42,42,42	0
32	MG	0	8083	1/1	0.90	0.15	56,56,56,56	0
34	SR	0	8911	1/1	0.90	0.08	78,78,78,78	0
34	SR	0	8992	1/1	0.90	0.24	123,123,123,123	0
34	SR	0	9008	1/1	0.90	0.14	90,90,90,90	0
35	NA	0	8545	1/1	0.90	0.30	37,37,37,37	0
32	MG	T	8057	1/1	0.90	0.15	57,57,57,57	0
32	MG	0	8073	1/1	0.90	0.14	76,76,76,76	0
36	CD	O	8705	1/1	0.90	0.06	124,124,124,124	0
32	MG	0	8037	1/1	0.90	0.22	83,83,83,83	0
35	NA	0	8559	1/1	0.91	0.23	75,75,75,75	0
32	MG	0	8008	1/1	0.91	0.19	25,25,25,25	0
32	MG	0	8059	1/1	0.91	0.09	36,36,36,36	0
34	SR	0	8965	1/1	0.91	0.12	120,120,120,120	0
32	MG	0	8077	1/1	0.91	0.16	32,32,32,32	0
34	SR	H	8972	1/1	0.92	0.20	130,130,130,130	0
32	MG	0	8076	1/1	0.92	0.22	35,35,35,35	0
34	SR	0	8923	1/1	0.92	0.19	101,101,101,101	0
32	MG	0	8020	1/1	0.92	0.20	54,54,54,54	0
33	CL	0	8817	1/1	0.92	0.12	53,53,53,53	0
35	NA	B	8552	1/1	0.92	0.34	56,56,56,56	0
35	NA	C	8503	1/1	0.92	0.28	37,37,37,37	0
35	NA	0	8563	1/1	0.92	0.37	60,60,60,60	0
35	NA	0	8564	1/1	0.92	0.19	65,65,65,65	0
34	SR	A	8929	1/1	0.92	0.27	131,131,131,131	0
35	NA	0	8529	1/1	0.93	0.09	37,37,37,37	0
32	MG	0	8036	1/1	0.93	0.12	49,49,49,49	0
33	CL	0	8805	1/1	0.93	0.15	59,59,59,59	0
32	MG	0	8010	1/1	0.93	0.17	26,26,26,26	0
32	MG	0	8078	1/1	0.93	0.37	51,51,51,51	0
34	SR	0	8936	1/1	0.93	0.13	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8047	1/1	0.93	0.44	49,49,49,49	0
32	MG	0	8068	1/1	0.93	0.09	47,47,47,47	0
32	MG	0	8049	1/1	0.93	0.37	55,55,55,55	0
32	MG	0	8017	1/1	0.93	0.19	56,56,56,56	0
34	SR	0	8943	1/1	0.93	0.08	95,95,95,95	0
34	SR	0	8921	1/1	0.93	0.12	92,92,92,92	0
32	MG	0	8033	1/1	0.93	0.11	45,45,45,45	0
32	MG	0	8056	1/1	0.93	0.20	42,42,42,42	0
34	SR	0	8985	1/1	0.93	0.12	110,110,110,110	0
36	CD	Z	8703	1/1	0.93	0.06	81,81,81,81	0
32	MG	0	8034	1/1	0.93	0.11	32,32,32,32	0
37	K	0	8402	1/1	0.93	0.17	64,64,64,64	0
32	MG	0	8070	1/1	0.94	0.17	45,45,45,45	0
34	SR	0	8918	1/1	0.94	0.14	79,79,79,79	0
32	MG	0	8091	1/1	0.94	0.07	42,42,42,42	0
34	SR	F	9005	1/1	0.94	0.06	136,136,136,136	0
32	MG	0	8053	1/1	0.94	0.16	61,61,61,61	0
35	NA	0	8541	1/1	0.94	0.34	53,53,53,53	0
34	SR	0	8962	1/1	0.94	0.26	167,167,167,167	0
33	CL	A	8809	1/1	0.94	0.15	57,57,57,57	0
34	SR	3	8999	1/1	0.94	0.08	95,95,95,95	0
35	NA	0	8569	1/1	0.94	0.26	53,53,53,53	0
35	NA	0	8570	1/1	0.94	0.17	49,49,49,49	0
35	NA	0	8516	1/1	0.94	0.23	30,30,30,30	0
35	NA	0	8547	1/1	0.94	0.42	54,54,54,54	0
35	NA	0	8517	1/1	0.94	0.32	30,30,30,30	0
33	CL	O	8808	1/1	0.94	0.17	61,61,61,61	0
35	NA	0	8550	1/1	0.94	0.25	54,54,54,54	0
32	MG	0	8029	1/1	0.94	0.18	39,39,39,39	0
32	MG	0	8064	1/1	0.94	0.27	38,38,38,38	0
32	MG	0	8007	1/1	0.94	0.30	26,26,26,26	0
32	MG	0	8012	1/1	0.94	0.23	21,21,21,21	0
32	MG	0	8061	1/1	0.94	0.39	37,37,37,37	0
33	CL	Y	8820	1/1	0.95	0.11	38,38,38,38	0
32	MG	0	8018	1/1	0.95	0.24	38,38,38,38	0
32	MG	0	8084	1/1	0.95	0.18	31,31,31,31	0
33	CL	0	8822	1/1	0.95	0.25	68,68,68,68	0
32	MG	K	8054	1/1	0.95	0.16	39,39,39,39	0
32	MG	0	8067	1/1	0.95	0.28	34,34,34,34	0
32	MG	0	8045	1/1	0.95	0.17	32,32,32,32	0
34	SR	0	8946	1/1	0.95	0.16	108,108,108,108	0
35	NA	0	8528	1/1	0.95	0.20	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8035	1/1	0.95	0.10	44,44,44,44	0
32	MG	0	8048	1/1	0.95	0.28	28,28,28,28	0
32	MG	0	8093	1/1	0.95	0.11	29,29,29,29	0
32	MG	9	8074	1/1	0.95	0.13	67,67,67,67	0
35	NA	0	8535	1/1	0.95	0.25	52,52,52,52	0
35	NA	0	8537	1/1	0.95	0.12	34,34,34,34	0
32	MG	0	8032	1/1	0.95	0.09	40,40,40,40	0
34	SR	0	8954	1/1	0.95	0.08	105,105,105,105	0
35	NA	0	8507	1/1	0.95	0.30	45,45,45,45	0
34	SR	0	8927	1/1	0.95	0.15	167,167,167,167	0
33	CL	J	8801	1/1	0.95	0.13	62,62,62,62	0
34	SR	0	8931	1/1	0.95	0.11	108,108,108,108	0
33	CL	J	8821	1/1	0.95	0.15	56,56,56,56	0
33	CL	L	8810	1/1	0.95	0.09	49,49,49,49	0
35	NA	0	8515	1/1	0.95	0.23	33,33,33,33	0
32	MG	0	8041	1/1	0.95	0.33	24,24,24,24	0
38	ANM	0	2924	19/19	0.95	0.22	31,37,40,40	0
33	CL	0	8815	1/1	0.96	0.11	57,57,57,57	0
33	CL	0	8816	1/1	0.96	0.19	60,60,60,60	0
32	MG	0	8058	1/1	0.96	0.12	23,23,23,23	0
35	NA	0	8524	1/1	0.96	0.26	45,45,45,45	0
35	NA	0	8558	1/1	0.96	0.26	44,44,44,44	0
32	MG	0	8023	1/1	0.96	0.18	22,22,22,22	0
35	NA	0	8526	1/1	0.96	0.09	32,32,32,32	0
35	NA	0	8527	1/1	0.96	0.26	52,52,52,52	0
32	MG	0	8060	1/1	0.96	0.10	42,42,42,42	0
32	MG	0	8001	1/1	0.96	0.20	25,25,25,25	0
32	MG	0	8014	1/1	0.96	0.22	30,30,30,30	0
32	MG	0	8019	1/1	0.96	0.30	24,24,24,24	0
35	NA	0	8566	1/1	0.96	0.29	37,37,37,37	0
32	MG	0	8011	1/1	0.96	0.29	23,23,23,23	0
35	NA	0	8534	1/1	0.96	0.28	32,32,32,32	0
32	MG	0	8087	1/1	0.96	0.20	42,42,42,42	0
35	NA	0	8536	1/1	0.96	0.12	50,50,50,50	0
33	CL	N	8807	1/1	0.96	0.14	61,61,61,61	0
32	MG	0	8022	1/1	0.96	0.21	29,29,29,29	0
34	SR	1	8913	1/1	0.96	0.09	85,85,85,85	0
34	SR	3	8932	1/1	0.96	0.13	73,73,73,73	0
32	MG	0	8046	1/1	0.96	0.16	28,28,28,28	0
34	SR	0	8901	1/1	0.96	0.16	58,58,58,58	0
34	SR	0	8902	1/1	0.96	0.15	69,69,69,69	0
32	MG	0	8090	1/1	0.96	0.13	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8937	1/1	0.96	0.21	100,100,100,100	0
33	CL	0	8811	1/1	0.96	0.11	53,53,53,53	0
33	CL	0	8814	1/1	0.96	0.17	47,47,47,47	0
32	MG	0	8082	1/1	0.97	0.33	48,48,48,48	0
32	MG	0	8065	1/1	0.97	0.13	33,33,33,33	0
32	MG	0	8003	1/1	0.97	0.19	30,30,30,30	0
33	CL	0	8813	1/1	0.97	0.07	48,48,48,48	0
34	SR	0	8935	1/1	0.97	0.11	79,79,79,79	0
34	SR	R	8912	1/1	0.97	0.16	84,84,84,84	0
35	NA	0	8551	1/1	0.97	0.23	46,46,46,46	0
32	MG	0	8004	1/1	0.97	0.24	25,25,25,25	0
35	NA	0	8513	1/1	0.97	0.27	44,44,44,44	0
32	MG	0	8025	1/1	0.97	0.13	24,24,24,24	0
34	SR	1	8952	1/1	0.97	0.12	79,79,79,79	0
34	SR	0	8940	1/1	0.97	0.10	85,85,85,85	0
33	CL	J	8802	1/1	0.97	0.15	60,60,60,60	0
32	MG	0	8027	1/1	0.97	0.14	34,34,34,34	0
32	MG	0	8013	1/1	0.97	0.08	26,26,26,26	0
33	CL	M	8818	1/1	0.97	0.15	37,37,37,37	0
32	MG	0	8009	1/1	0.97	0.26	21,21,21,21	0
32	MG	Y	8086	1/1	0.97	0.11	39,39,39,39	0
32	MG	0	8052	1/1	0.98	0.11	40,40,40,40	0
34	SR	0	8925	1/1	0.98	0.12	90,90,90,90	0
32	MG	0	8002	1/1	0.98	0.17	22,22,22,22	0
33	CL	0	8812	1/1	0.98	0.11	48,48,48,48	0
32	MG	0	8021	1/1	0.98	0.13	32,32,32,32	0
32	MG	0	8026	1/1	0.98	0.14	31,31,31,31	0
32	MG	0	8015	1/1	0.98	0.19	27,27,27,27	0
34	SR	0	8903	1/1	0.98	0.20	53,53,53,53	0
32	MG	0	8005	1/1	0.98	0.30	26,26,26,26	0
33	CL	3	8804	1/1	0.98	0.05	54,54,54,54	0
33	CL	0	8803	1/1	0.98	0.07	46,46,46,46	0
32	MG	0	8028	1/1	0.99	0.26	22,22,22,22	0
33	CL	R	8806	1/1	0.99	0.17	43,43,43,43	0
33	CL	B	8819	1/1	0.99	0.12	46,46,46,46	0
34	SR	0	8904	1/1	0.99	0.20	52,52,52,52	0
36	CD	U	8701	1/1	0.99	0.12	58,58,58,58	0
34	SR	0	8905	1/1	0.99	0.26	57,57,57,57	0
36	CD	1	8702	1/1	0.99	0.08	57,57,57,57	0
36	CD	3	8704	1/1	0.99	0.09	66,66,66,66	0
34	SR	0	8915	1/1	0.99	0.06	117,117,117,117	0
34	SR	0	8906	1/1	0.99	0.21	56,56,56,56	0

Continued on next page...

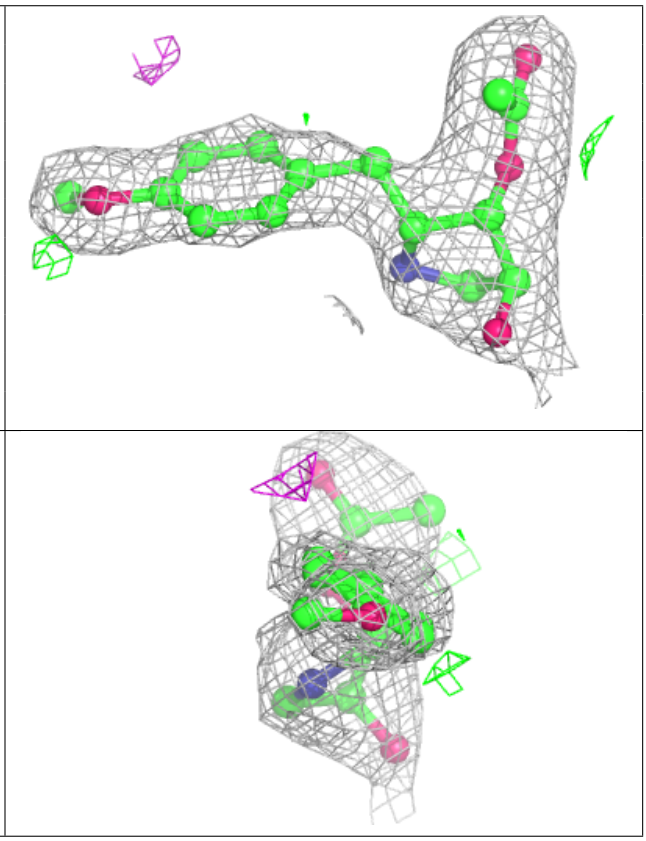
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8907	1/1	0.99	0.32	76,76,76,76	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 ANM 0 2924:

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.