



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:51 pm BST

PDB ID : 2I91
Title : 60kDa Ro autoantigen in complex with a fragment of misfolded RNA
Authors : Reinisch, K.M.; Stein, A.J.
Deposited on : 2006-09-04
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

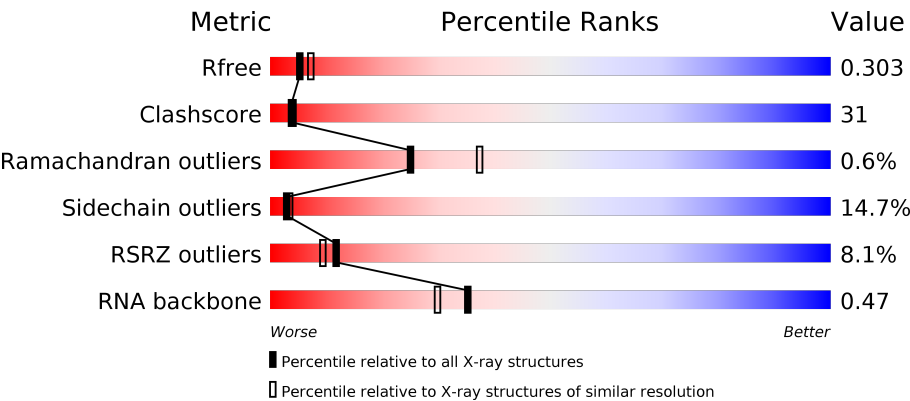
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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

Mol	Chain	Length	Quality of chain
1	C	8	<div><div>13%</div><div>100%</div></div>
1	E	8	<div><div>13%</div><div>13%</div><div>75%</div><div>13%</div></div>
2	D	15	<div><div>27%</div><div>20%</div><div>27%</div><div>40%</div><div>7%</div><div>7%</div></div>
2	F	15	<div><div>27%</div><div>13%</div><div>40%</div><div>33%</div><div>13%</div></div>

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Mol	Chain	Length	Quality of chain
3	A	538	
3	B	538	

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
4	ACT	A	601	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9774 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 5'-R(*GP*CP*CP*UP*AP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	8	Total	C	N	O	P	0	0	0
			162	74	27	54	7			
1	E	8	Total	C	N	O	P	0	0	0
			162	74	27	54	7			

- Molecule 2 is a RNA chain called 5'-R(*C*GP*GP*UP*AP*GP*GP*CP*UP*UP*UP*UP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	P	0	0	0
			295	133	51	98	13			
2	F	15	Total	C	N	O	P	0	0	0
			315	142	54	105	14			

- Molecule 3 is a protein called 60 kDa SS-A/Ro ribonucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	520	Total	C	N	O	S	0	0	0
			4108	2605	708	764	31			
3	B	526	Total	C	N	O	S	0	0	0
			4161	2639	717	774	31			

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	12	Total	O	0	0
			12	12		
6	D	25	Total	O	0	0
			25	25		
6	E	12	Total	O	0	0
			12	12		
6	F	20	Total	O	0	0
			20	20		
6	A	283	Total	O	0	0
			283	283		

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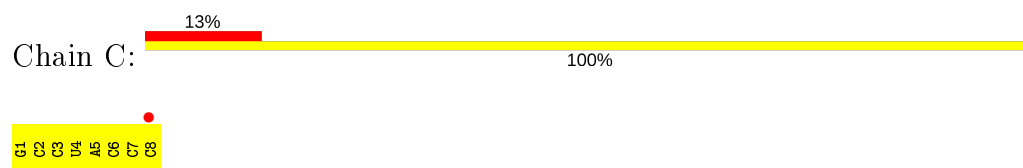
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	209	Total 209	O 209	0	0

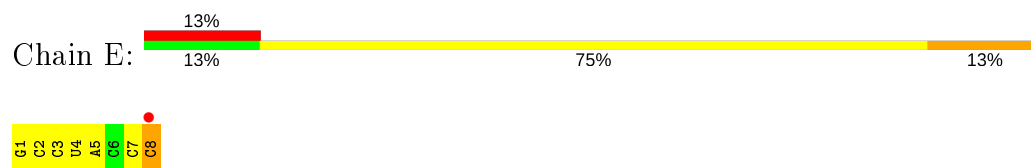
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

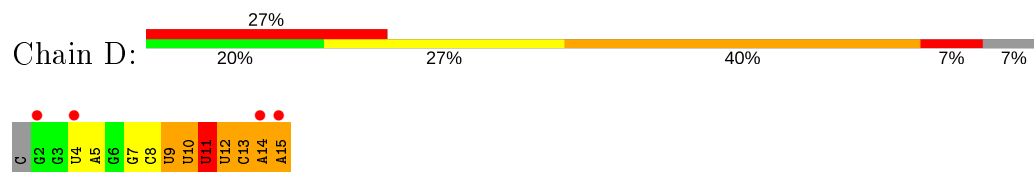
- Molecule 1: 5'-R(*GP*CP*CP*UP*AP*CP*CP*C)-3'



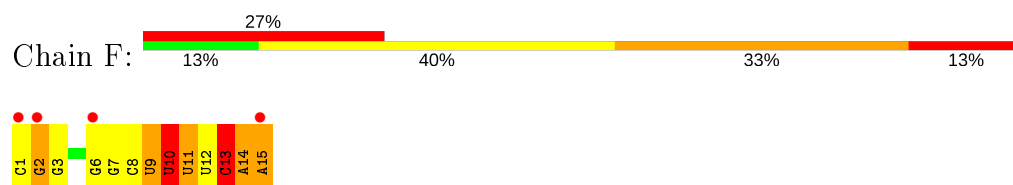
- Molecule 1: 5'-R(*GP*CP*CP*UP*AP*CP*CP*C)-3'



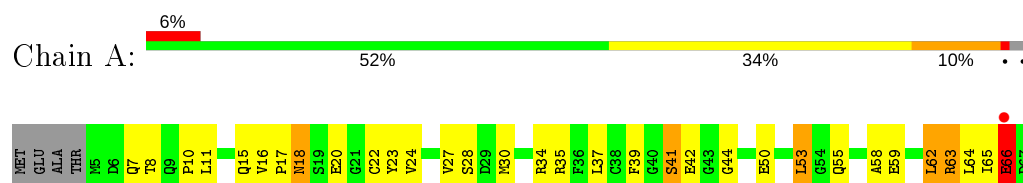
- Molecule 2: 5'-R(*C*GP*GP*UP*AP*GP*GP*CP*UP*UP*UP*UP*CP*AP*A)-3'

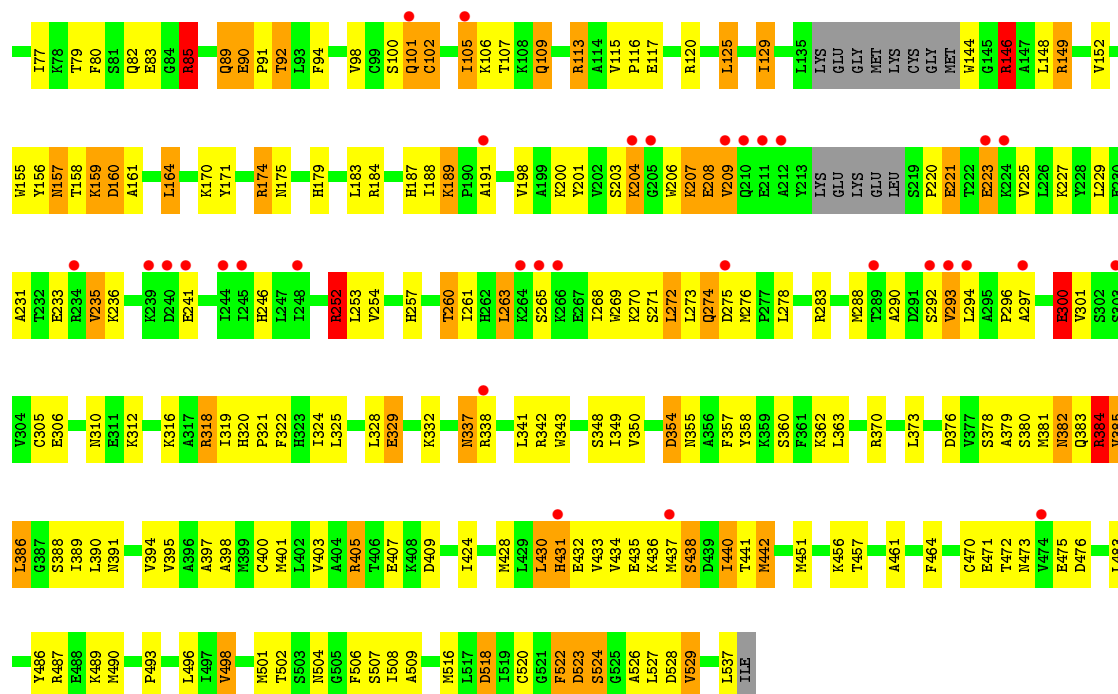


- Molecule 2: 5'-R(*C*GP*GP*UP*AP*GP*GP*CP*UP*UP*UP*UP*CP*AP*A)-3'

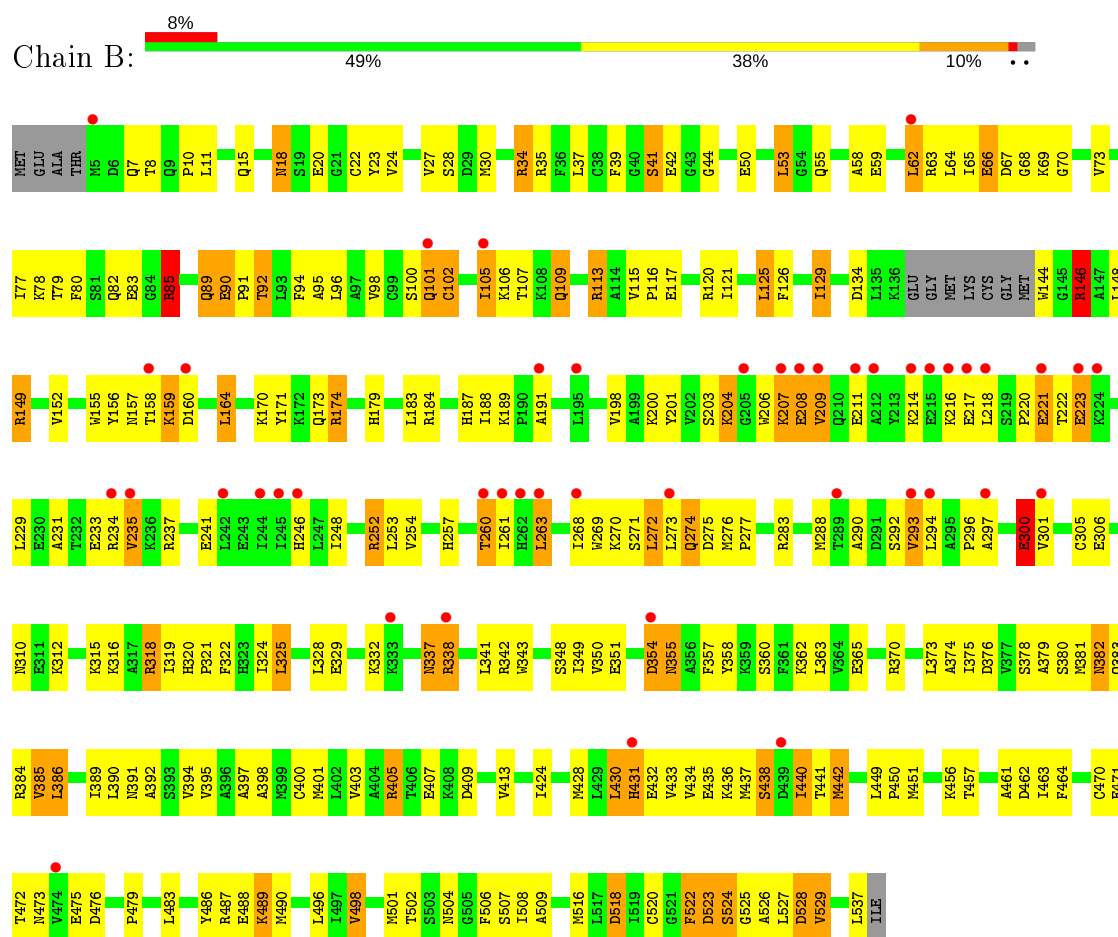


- Molecule 3: 60 kDa SS-A/Ro ribonucleoprotein





• Molecule 3: 60 kDa SS-A/Ro ribonucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.68Å 119.98Å 73.54Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 37.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.65) 94.9 (37.25-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.285 0.264 , 0.303	Depositor DCC
R_{free} test set	4252 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9774	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8704e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.44	0/179	0.80	0/276
1	E	0.36	0/179	0.66	0/276
2	D	0.63	0/329	1.17	2/511 (0.4%)
2	F	0.51	0/351	1.07	3/545 (0.6%)
3	A	0.53	4/4181 (0.1%)	1.24	47/5643 (0.8%)
3	B	0.55	5/4235 (0.1%)	1.22	47/5714 (0.8%)
All	All	0.54	9/9454 (0.1%)	1.20	99/12965 (0.8%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	42	GLU	CD-OE1	-13.70	1.10	1.25
3	A	42	GLU	CD-OE1	-13.28	1.11	1.25
3	A	42	GLU	CD-OE2	-9.74	1.15	1.25
3	B	42	GLU	CD-OE2	-9.43	1.15	1.25
3	B	208	GLU	CD-OE1	-6.72	1.18	1.25
3	B	208	GLU	CG-CD	-6.55	1.42	1.51
3	B	208	GLU	CD-OE2	-5.83	1.19	1.25
3	A	208	GLU	CD-OE1	-5.35	1.19	1.25
3	A	208	GLU	CD-OE2	-5.04	1.20	1.25

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	146	ARG	NE-CZ-NH1	20.63	130.62	120.30
3	B	318	ARG	NE-CZ-NH1	-19.11	110.75	120.30
3	B	146	ARG	NE-CZ-NH1	-18.92	110.84	120.30
3	A	146	ARG	NE-CZ-NH2	-18.36	111.12	120.30
3	B	318	ARG	NE-CZ-NH2	17.80	129.20	120.30
3	A	34	ARG	NE-CZ-NH2	-16.45	112.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	42	GLU	OE1-CD-OE2	-16.13	103.94	123.30
3	A	42	GLU	OE1-CD-OE2	-16.08	104.01	123.30
3	A	174	ARG	NE-CZ-NH2	-15.91	112.34	120.30
3	B	34	ARG	NE-CZ-NH2	14.77	127.68	120.30
3	B	34	ARG	NE-CZ-NH1	-14.73	112.94	120.30
3	A	174	ARG	NE-CZ-NH1	14.69	127.64	120.30
3	B	146	ARG	NE-CZ-NH2	14.25	127.42	120.30
3	A	384	ARG	NE-CZ-NH1	-14.21	113.20	120.30
3	B	342	ARG	NE-CZ-NH1	-14.13	113.23	120.30
3	A	252	ARG	NE-CZ-NH1	14.07	127.34	120.30
3	A	384	ARG	NE-CZ-NH2	13.97	127.28	120.30
3	B	384	ARG	NE-CZ-NH1	13.83	127.21	120.30
3	A	85	ARG	NE-CZ-NH2	13.79	127.19	120.30
3	B	384	ARG	NE-CZ-NH2	-13.70	113.45	120.30
3	A	34	ARG	NE-CZ-NH1	13.70	127.15	120.30
3	A	342	ARG	NE-CZ-NH1	13.69	127.14	120.30
3	A	342	ARG	NE-CZ-NH2	-13.68	113.46	120.30
3	B	174	ARG	NE-CZ-NH1	-13.64	113.48	120.30
3	A	252	ARG	NE-CZ-NH2	-13.50	113.55	120.30
3	B	342	ARG	NE-CZ-NH2	13.50	127.05	120.30
3	A	487	ARG	NE-CZ-NH2	-13.33	113.64	120.30
3	A	318	ARG	NE-CZ-NH1	13.10	126.85	120.30
3	A	85	ARG	NE-CZ-NH1	-13.05	113.78	120.30
3	B	85	ARG	NE-CZ-NH1	13.00	126.80	120.30
3	A	338	ARG	NE-CZ-NH1	12.93	126.76	120.30
3	B	338	ARG	NE-CZ-NH1	-12.86	113.87	120.30
3	B	63	ARG	NE-CZ-NH2	-12.79	113.91	120.30
3	B	174	ARG	NE-CZ-NH2	12.77	126.69	120.30
3	A	63	ARG	NE-CZ-NH1	-12.63	113.98	120.30
3	A	113	ARG	NE-CZ-NH1	-12.63	113.98	120.30
3	B	113	ARG	NE-CZ-NH2	-12.62	113.99	120.30
3	A	338	ARG	NE-CZ-NH2	-12.62	113.99	120.30
3	A	318	ARG	NE-CZ-NH2	-12.52	114.04	120.30
3	B	113	ARG	NE-CZ-NH1	12.31	126.46	120.30
3	A	63	ARG	NE-CZ-NH2	12.10	126.35	120.30
3	B	338	ARG	NE-CZ-NH2	11.98	126.29	120.30
3	B	63	ARG	NE-CZ-NH1	11.97	126.29	120.30
3	B	487	ARG	NE-CZ-NH1	-11.97	114.31	120.30
3	B	85	ARG	NE-CZ-NH2	-11.94	114.33	120.30
3	A	487	ARG	NE-CZ-NH1	11.74	126.17	120.30
3	A	113	ARG	NE-CZ-NH2	11.41	126.01	120.30
3	B	149	ARG	NE-CZ-NH2	-11.35	114.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	149	ARG	NE-CZ-NH1	-11.21	114.69	120.30
3	B	318	ARG	CD-NE-CZ	10.71	138.59	123.60
3	B	149	ARG	NE-CZ-NH1	10.09	125.34	120.30
3	B	146	ARG	CG-CD-NE	-9.72	91.39	111.80
3	A	149	ARG	NE-CZ-NH2	9.71	125.16	120.30
3	B	252	ARG	NE-CZ-NH1	-9.59	115.51	120.30
3	B	487	ARG	NE-CZ-NH2	9.55	125.07	120.30
3	A	34	ARG	CD-NE-CZ	9.33	136.66	123.60
3	A	146	ARG	CD-NE-CZ	9.05	136.27	123.60
2	D	11	U	N1-C1'-C2'	8.95	125.64	114.00
3	B	252	ARG	NE-CZ-NH2	8.69	124.65	120.30
3	B	318	ARG	CG-CD-NE	-8.62	93.71	111.80
3	B	146	ARG	CD-NE-CZ	8.56	135.58	123.60
3	B	34	ARG	CD-NE-CZ	8.38	135.33	123.60
3	A	318	ARG	CD-NE-CZ	8.28	135.19	123.60
3	A	174	ARG	CD-NE-CZ	7.65	134.31	123.60
3	A	342	ARG	CD-NE-CZ	7.40	133.96	123.60
3	A	34	ARG	CG-CD-NE	-7.36	96.35	111.80
3	B	342	ARG	CD-NE-CZ	7.21	133.69	123.60
3	A	384	ARG	CD-NE-CZ	6.99	133.39	123.60
2	F	11	U	N1-C1'-C2'	6.87	122.93	114.00
3	B	174	ARG	CD-NE-CZ	6.74	133.04	123.60
3	B	85	ARG	CD-NE-CZ	6.69	132.97	123.60
3	A	487	ARG	CD-NE-CZ	6.69	132.96	123.60
3	B	384	ARG	CD-NE-CZ	6.65	132.90	123.60
3	B	338	ARG	CD-NE-CZ	6.59	132.82	123.60
3	A	42	GLU	CG-CD-OE2	6.51	131.32	118.30
3	B	42	GLU	CG-CD-OE2	6.49	131.29	118.30
3	B	63	ARG	CD-NE-CZ	6.44	132.61	123.60
3	B	487	ARG	CD-NE-CZ	6.41	132.57	123.60
3	A	85	ARG	CD-NE-CZ	6.40	132.56	123.60
3	B	149	ARG	CD-NE-CZ	6.35	132.50	123.60
2	F	10	U	N1-C1'-C2'	6.34	122.24	114.00
3	A	113	ARG	CD-NE-CZ	6.31	132.43	123.60
3	A	300	GLU	CA-CB-CG	6.26	127.18	113.40
3	B	208	GLU	CA-CB-CG	-6.25	99.66	113.40
3	B	18	ASN	CB-CA-C	-6.23	97.95	110.40
3	B	113	ARG	CD-NE-CZ	6.22	132.31	123.60
3	B	300	GLU	CA-CB-CG	6.14	126.92	113.40
3	A	338	ARG	CD-NE-CZ	6.09	132.12	123.60
3	A	63	ARG	CD-NE-CZ	6.08	132.11	123.60
3	A	252	ARG	CD-NE-CZ	5.98	131.97	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	66	GLU	CA-CB-CG	5.94	126.47	113.40
3	A	149	ARG	CD-NE-CZ	5.85	131.79	123.60
3	B	66	GLU	CA-CB-CG	5.83	126.22	113.40
3	A	523	ASP	N-CA-C	-5.64	95.77	111.00
2	F	13	C	N1-C1'-C2'	5.58	121.26	114.00
3	A	208	GLU	CA-CB-CG	-5.54	101.21	113.40
3	A	18	ASN	CB-CA-C	-5.50	99.39	110.40
3	B	523	ASP	N-CA-C	-5.48	96.20	111.00
2	D	12	U	N1-C1'-C2'	5.20	120.76	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	162	0	89	9	0
1	E	162	0	89	6	0
2	D	295	0	151	24	0
2	F	315	0	162	22	0
3	A	4108	0	4171	263	0
3	B	4161	0	4234	275	0
4	A	4	0	3	2	0
4	B	4	0	3	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	283	0	0	13	0
6	B	209	0	0	18	0
6	C	12	0	0	0	0
6	D	25	0	0	0	0
6	E	12	0	0	0	0
6	F	20	0	0	0	0
All	All	9774	0	8902	559	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 31.

All (559) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:A:H3'	2:D:15:A:C5'	1.60	1.29
3:B:337:ASN:OD1	3:B:389:ILE:HD11	1.47	1.13
3:B:146:ARG:HE	3:B:146:ARG:HA	1.11	1.11
2:D:14:A:H3'	2:D:15:A:H5'	1.18	1.09
3:B:157:ASN:ND2	3:B:188:ILE:HD11	1.70	1.07
3:A:337:ASN:OD1	3:A:389:ILE:HD11	1.52	1.05
3:A:157:ASN:ND2	3:A:188:ILE:HD11	1.73	1.03
3:B:78:LYS:HE3	6:B:710:HOH:O	1.62	0.98
2:F:1:C:HO5'	2:F:1:C:H6	1.09	0.97
2:D:15:A:O2'	3:A:316:LYS:HG2	1.67	0.95
3:A:254:VAL:H	3:A:257:HIS:HD2	1.11	0.94
3:A:83:GLU:HB3	3:A:362:LYS:NZ	1.83	0.93
3:B:146:ARG:CA	3:B:146:ARG:HE	1.78	0.91
3:B:254:VAL:H	3:B:257:HIS:HD2	1.13	0.91
2:D:14:A:H3'	2:D:15:A:H5"	1.50	0.90
3:A:120:ARG:CD	3:A:318:ARG:HH21	1.84	0.90
3:A:85:ARG:HA	3:A:524:SER:OG	1.71	0.89
3:A:207:LYS:HD3	6:A:887:HOH:O	1.72	0.88
2:D:14:A:C3'	2:D:15:A:C5'	2.50	0.88
3:A:428:MET:HE1	3:A:436:LYS:HE2	1.53	0.87
2:D:15:A:O2'	3:A:316:LYS:HE2	1.73	0.87
3:B:44:GLY:HA2	3:B:53:LEU:HD12	1.57	0.87
3:B:401:MET:O	3:B:405:ARG:HG3	1.75	0.86
3:A:44:GLY:HA2	3:A:53:LEU:HD12	1.57	0.86
3:B:157:ASN:HD21	3:B:188:ILE:HD11	1.34	0.85
3:B:428:MET:HE1	3:B:436:LYS:HE2	1.56	0.85
3:B:83:GLU:HB3	3:B:362:LYS:NZ	1.92	0.85
3:A:157:ASN:HD21	3:A:188:ILE:HD11	1.40	0.84
3:A:105:ILE:HD12	6:A:703:HOH:O	1.77	0.83
3:B:428:MET:CE	3:B:436:LYS:HE2	2.08	0.83
3:B:85:ARG:HA	3:B:524:SER:OG	1.78	0.83
3:A:337:ASN:C	3:A:337:ASN:HD22	1.77	0.82
3:A:395:VAL:HG13	3:A:522:PHE:CD2	2.14	0.82
3:B:337:ASN:C	3:B:337:ASN:HD22	1.79	0.82
3:B:395:VAL:HG13	3:B:522:PHE:CD2	2.13	0.82
3:A:27:VAL:HG22	3:A:518:ASP:OD1	1.79	0.82
3:B:18:ASN:HB2	3:B:20:GLU:H	1.42	0.81
3:A:82:GLN:NE2	3:A:117:GLU:HB3	1.94	0.81
3:A:379:ALA:HB3	4:A:601:ACT:H1	1.62	0.80
3:B:82:GLN:NE2	3:B:117:GLU:HB3	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:A:O2'	3:A:316:LYS:CG	2.29	0.80
3:A:428:MET:CE	3:A:436:LYS:HE2	2.11	0.80
3:B:105:ILE:HD12	6:B:714:HOH:O	1.80	0.80
3:B:389:ILE:HG22	3:B:389:ILE:O	1.81	0.79
2:F:9:U:H4'	2:F:10:U:OP1	1.81	0.79
3:B:120:ARG:NE	3:B:318:ARG:HH21	1.81	0.79
2:D:14:A:C3'	2:D:15:A:H5'	2.09	0.79
3:A:146:ARG:HH11	3:A:146:ARG:HA	1.49	0.78
3:B:149:ARG:HH21	3:B:187:HIS:CD2	2.01	0.78
3:A:27:VAL:HG21	3:A:35:ARG:CZ	2.13	0.78
3:B:85:ARG:HD3	3:B:362:LYS:NZ	1.99	0.77
2:D:14:A:C4	3:A:252:ARG:NH2	2.52	0.77
1:E:4:U:H2'	1:E:5:A:C8	2.19	0.77
3:A:83:GLU:HB3	3:A:362:LYS:HZ3	1.49	0.77
3:B:27:VAL:HG22	3:B:518:ASP:OD1	1.84	0.77
3:B:11:LEU:HB2	3:B:15:GLN:OE1	1.85	0.76
3:B:83:GLU:HB3	3:B:362:LYS:HZ1	1.51	0.76
3:A:332:LYS:NZ	3:A:431:HIS:HB2	2.00	0.76
3:B:37:LEU:HD22	3:B:92:THR:HG23	1.66	0.76
3:B:370:ARG:HG2	3:B:409:ASP:OD1	1.86	0.75
3:A:89:GLN:HE21	3:A:89:GLN:HA	1.50	0.75
3:B:146:ARG:NE	3:B:146:ARG:HA	1.95	0.75
3:B:39:PHE:HA	3:B:386:LEU:HD21	1.68	0.75
3:A:389:ILE:HG22	3:A:389:ILE:O	1.84	0.75
3:A:11:LEU:HB2	3:A:15:GLN:OE1	1.87	0.74
3:B:27:VAL:HG21	3:B:35:ARG:CZ	2.17	0.74
3:B:332:LYS:NZ	3:B:431:HIS:HB2	2.03	0.74
3:A:204:LYS:HD2	3:A:208:GLU:OE2	1.88	0.73
3:A:436:LYS:O	3:A:440:ILE:HG22	1.89	0.73
3:B:184:ARG:HG3	6:B:836:HOH:O	1.87	0.73
3:A:120:ARG:CD	3:A:318:ARG:NH2	2.52	0.73
3:A:370:ARG:HG2	3:A:409:ASP:OD1	1.88	0.73
1:E:4:U:H2'	1:E:5:A:H8	1.53	0.73
3:A:227:LYS:HG3	6:A:928:HOH:O	1.89	0.72
3:B:395:VAL:HG13	3:B:522:PHE:HD2	1.52	0.72
3:B:435:GLU:O	3:B:438:SER:HB2	1.89	0.72
3:A:146:ARG:CA	3:A:146:ARG:HH11	2.02	0.72
3:A:401:MET:O	3:A:405:ARG:HG3	1.90	0.72
3:A:120:ARG:HD3	3:A:318:ARG:HH21	1.53	0.72
3:B:461:ALA:HB3	3:B:464:PHE:HE1	1.55	0.72
2:D:9:U:H4'	2:D:10:U:OP1	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:435:GLU:O	3:A:438:SER:HB2	1.89	0.72
3:A:433:VAL:O	3:A:437:MET:HG2	1.89	0.72
3:B:120:ARG:CD	3:B:318:ARG:NH2	2.53	0.72
3:B:89:GLN:HA	3:B:89:GLN:HE21	1.54	0.72
3:B:204:LYS:HD2	3:B:208:GLU:OE2	1.91	0.71
3:A:37:LEU:HD22	3:A:92:THR:HG23	1.72	0.71
3:B:436:LYS:O	3:B:440:ILE:HG22	1.91	0.71
3:A:39:PHE:HA	3:A:386:LEU:HD21	1.73	0.71
3:B:433:VAL:O	3:B:437:MET:HG2	1.90	0.71
3:B:325:LEU:HD13	3:B:390:LEU:HD13	1.72	0.71
3:A:379:ALA:O	3:A:382:ASN:HB2	1.91	0.70
2:F:15:A:N3	2:F:15:A:H3'	2.07	0.70
3:B:27:VAL:HG23	3:B:507:SER:HB2	1.73	0.70
3:B:149:ARG:NH2	3:B:187:HIS:CD2	2.59	0.70
3:A:332:LYS:CE	3:A:431:HIS:HB2	2.21	0.70
3:A:27:VAL:HG23	3:A:507:SER:HB2	1.74	0.70
3:B:85:ARG:HD3	3:B:362:LYS:HZ2	1.55	0.70
3:B:365:GLU:HG3	6:B:858:HOH:O	1.92	0.69
3:B:362:LYS:HG2	6:B:815:HOH:O	1.91	0.69
3:A:120:ARG:HD3	3:A:318:ARG:NH2	2.07	0.69
3:A:18:ASN:HB2	3:A:20:GLU:H	1.57	0.69
3:A:149:ARG:NH2	3:A:187:HIS:CD2	2.61	0.69
3:B:379:ALA:O	3:B:382:ASN:HB2	1.92	0.68
3:B:207:LYS:HD2	3:B:207:LYS:N	2.08	0.68
3:B:157:ASN:HD21	3:B:188:ILE:CD1	2.06	0.68
3:B:379:ALA:HB3	4:B:602:ACT:H1	1.75	0.68
3:A:395:VAL:HG13	3:A:522:PHE:HD2	1.56	0.68
3:B:475:GLU:HB3	6:B:861:HOH:O	1.93	0.68
3:A:120:ARG:NE	3:A:318:ARG:HH21	1.91	0.68
3:A:381:MET:HE1	3:A:501:MET:HG3	1.76	0.68
3:A:275:ASP:OD2	3:B:221:GLU:HB2	1.93	0.68
3:A:204:LYS:CD	3:A:208:GLU:OE2	2.43	0.67
3:A:204:LYS:HB3	3:A:208:GLU:OE2	1.95	0.67
3:B:479:PRO:HG2	6:B:821:HOH:O	1.95	0.67
3:A:221:GLU:HB2	3:B:275:ASP:OD2	1.94	0.67
3:A:58:ALA:O	3:A:62:LEU:HD12	1.95	0.67
1:C:4:U:H2'	1:C:5:A:C8	2.30	0.67
3:A:325:LEU:HD13	3:A:390:LEU:HD13	1.77	0.67
3:B:498:VAL:HG21	3:B:509:ALA:HB2	1.77	0.67
3:A:504:ASN:ND2	3:A:506:PHE:H	1.93	0.66
3:B:496:LEU:HB3	3:B:516:MET:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:204:LYS:CD	3:B:208:GLU:OE2	2.44	0.66
1:E:1:G:O2'	1:E:2:C:H5'	1.95	0.66
3:B:332:LYS:CE	3:B:431:HIS:HB2	2.25	0.66
3:A:83:GLU:HB3	3:A:362:LYS:HZ1	1.57	0.66
3:A:461:ALA:HB3	3:A:464:PHE:HE1	1.59	0.66
3:B:337:ASN:C	3:B:337:ASN:ND2	2.48	0.66
3:A:337:ASN:C	3:A:337:ASN:ND2	2.47	0.66
3:A:207:LYS:HD2	3:A:207:LYS:N	2.10	0.65
1:C:7:C:O2'	1:C:8:C:H5'	1.95	0.65
3:B:504:ASN:ND2	3:B:506:PHE:CD2	2.62	0.65
2:F:13:C:H5''	2:F:14:A:OP2	1.96	0.65
3:B:58:ALA:O	3:B:62:LEU:HD12	1.95	0.65
3:A:175:ASN:ND2	6:A:965:HOH:O	2.29	0.65
3:A:498:VAL:HG21	3:A:509:ALA:HB2	1.78	0.65
3:A:27:VAL:HG21	3:A:35:ARG:NH2	2.12	0.65
2:F:15:A:H4'	3:B:316:LYS:HE2	1.79	0.64
3:A:496:LEU:HB3	3:A:516:MET:HG2	1.79	0.64
3:B:432:GLU:O	3:B:436:LYS:HG3	1.96	0.64
3:A:332:LYS:HD3	3:A:431:HIS:ND1	2.11	0.64
3:B:125:LEU:HD22	3:B:129:ILE:HD12	1.80	0.64
2:D:8:C:O3'	2:D:9:U:H3'	1.97	0.64
3:B:79:THR:HG23	3:B:83:GLU:OE1	1.97	0.64
3:A:337:ASN:OD1	3:A:389:ILE:CD1	2.38	0.64
3:A:125:LEU:HD22	3:A:129:ILE:HD12	1.79	0.63
3:B:204:LYS:HB3	3:B:208:GLU:OE2	1.98	0.63
3:B:231:ALA:O	3:B:235:VAL:HG12	1.97	0.63
3:B:381:MET:HE1	3:B:501:MET:HG3	1.81	0.63
3:A:432:GLU:O	3:A:436:LYS:HG3	1.97	0.63
3:B:206:TRP:CG	3:B:233:GLU:HG3	2.34	0.63
3:A:146:ARG:NH1	3:A:146:ARG:HA	2.14	0.62
3:B:41:SER:O	3:B:50:GLU:HG3	1.99	0.62
3:B:389:ILE:CG2	3:B:389:ILE:O	2.47	0.62
3:A:89:GLN:NE2	3:A:89:GLN:HA	2.15	0.62
3:A:206:TRP:CG	3:A:233:GLU:HG3	2.35	0.62
3:A:70:GLY:HA3	3:A:107:THR:OG1	2.00	0.61
3:B:79:THR:CG2	3:B:83:GLU:OE1	2.48	0.61
3:A:231:ALA:O	3:A:235:VAL:HG12	1.99	0.61
2:D:10:U:O2'	2:D:11:U:OP2	2.18	0.61
3:A:146:ARG:HH11	3:A:146:ARG:C	2.04	0.61
1:C:2:C:O2'	1:C:3:C:H5'	2.01	0.61
3:A:149:ARG:NH1	6:A:745:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:70:GLY:HA3	3:B:107:THR:OG1	2.00	0.61
3:A:254:VAL:N	3:A:257:HIS:HD2	1.93	0.61
2:F:8:C:O3'	2:F:9:U:H3'	2.01	0.61
3:A:79:THR:HG23	3:A:83:GLU:OE1	2.01	0.61
3:B:431:HIS:C	3:B:431:HIS:CD2	2.75	0.60
3:B:332:LYS:HD3	3:B:431:HIS:ND1	2.16	0.60
2:D:15:A:HO3'	3:A:316:LYS:C	2.05	0.60
3:A:319:ILE:HG21	3:A:324:ILE:HD11	1.83	0.60
3:A:85:ARG:HD2	3:A:362:LYS:NZ	2.16	0.60
3:A:79:THR:CG2	3:A:83:GLU:OE1	2.49	0.60
3:A:206:TRP:CD1	3:A:233:GLU:HG3	2.37	0.60
3:B:395:VAL:HG12	3:B:501:MET:HE1	1.84	0.60
3:A:320:HIS:HD2	3:A:322:PHE:HB3	1.65	0.60
3:A:41:SER:O	3:A:50:GLU:HG3	2.02	0.59
3:B:89:GLN:HA	3:B:89:GLN:NE2	2.16	0.59
1:C:6:C:OP1	3:A:236:LYS:NZ	2.35	0.59
3:B:113:ARG:HB3	6:B:704:HOH:O	2.03	0.59
3:B:320:HIS:HD2	3:B:322:PHE:HB3	1.67	0.59
3:B:206:TRP:CD1	3:B:233:GLU:HG3	2.38	0.59
3:A:431:HIS:C	3:A:431:HIS:CD2	2.75	0.59
3:B:288:MET:O	3:B:293:VAL:HG13	2.02	0.59
3:B:27:VAL:HG21	3:B:35:ARG:NH2	2.17	0.59
3:A:90:GLU:N	3:A:90:GLU:OE2	2.36	0.59
3:B:380:SER:O	3:B:383:GLN:NE2	2.35	0.58
3:A:332:LYS:HZ3	3:A:431:HIS:HB2	1.68	0.58
3:A:65:ILE:HG21	3:A:102:CYS:HB2	1.85	0.58
3:B:65:ILE:HG21	3:B:102:CYS:HB2	1.84	0.58
3:B:157:ASN:HD22	3:B:188:ILE:HD11	1.61	0.58
3:A:269:TRP:HA	3:A:272:LEU:HB2	1.85	0.58
3:B:269:TRP:HA	3:B:272:LEU:HB2	1.85	0.58
3:B:120:ARG:HD3	3:B:318:ARG:NH2	2.18	0.58
3:B:373:LEU:HD11	3:B:403:VAL:HG12	1.85	0.58
3:A:275:ASP:OD2	3:B:221:GLU:CB	2.50	0.58
3:A:386:LEU:N	3:A:386:LEU:HD23	2.19	0.58
3:B:254:VAL:N	3:B:257:HIS:HD2	1.94	0.58
3:B:376:ASP:O	3:B:381:MET:HG3	2.03	0.58
3:B:184:ARG:NH2	6:B:713:HOH:O	2.32	0.58
3:B:7:GLN:NE2	3:B:472:THR:OG1	2.37	0.58
1:C:1:G:O2'	1:C:2:C:H5'	2.04	0.57
3:A:504:ASN:ND2	3:A:506:PHE:CD2	2.72	0.57
3:B:85:ARG:CD	3:B:362:LYS:HZ2	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:389:ILE:CG2	3:A:389:ILE:O	2.52	0.57
3:B:337:ASN:OD1	3:B:389:ILE:CD1	2.38	0.57
3:A:395:VAL:HG13	3:A:522:PHE:CE2	2.39	0.57
3:B:386:LEU:N	3:B:386:LEU:HD23	2.19	0.57
2:D:7:G:OP1	3:A:341:LEU:HD21	2.05	0.57
2:D:14:A:C3'	2:D:15:A:H5''	2.28	0.57
3:A:502:THR:OG1	3:A:504:ASN:OD1	2.23	0.57
3:B:82:GLN:HE21	3:B:117:GLU:HB3	1.70	0.57
3:B:83:GLU:HB3	3:B:362:LYS:HZ3	1.70	0.57
3:A:288:MET:O	3:A:293:VAL:HG13	2.04	0.57
3:A:376:ASP:O	3:A:381:MET:HG3	2.05	0.57
2:F:13:C:H5''	3:B:171:TYR:OH	2.04	0.57
3:B:332:LYS:HZ3	3:B:431:HIS:HB2	1.68	0.57
3:A:82:GLN:HE21	3:A:117:GLU:HB3	1.66	0.56
3:A:77:ILE:HG23	3:A:92:THR:HG22	1.87	0.56
3:A:155:TRP:O	3:A:159:LYS:HD2	2.05	0.56
3:A:373:LEU:HD11	3:A:403:VAL:HG12	1.87	0.56
3:A:146:ARG:NH1	3:A:146:ARG:O	2.39	0.56
3:A:328:LEU:HD21	3:A:431:HIS:HB3	1.87	0.56
3:B:39:PHE:HA	3:B:386:LEU:CD2	2.35	0.56
3:B:451:MET:HG3	3:B:464:PHE:CE2	2.41	0.56
3:B:155:TRP:O	3:B:159:LYS:HD2	2.06	0.56
3:A:80:PHE:HA	3:A:85:ARG:HG3	1.88	0.56
3:A:90:GLU:HB2	3:A:91:PRO:HD3	1.88	0.56
3:B:65:ILE:HD13	3:B:102:CYS:HB3	1.87	0.56
3:A:221:GLU:CB	3:B:275:ASP:OD2	2.53	0.56
3:B:207:LYS:CD	3:B:207:LYS:H	2.19	0.56
3:B:77:ILE:HG23	3:B:92:THR:HG22	1.88	0.56
1:C:1:G:O2'	1:C:2:C:C5'	2.54	0.56
3:A:171:TYR:O	3:A:179:HIS:HE1	1.89	0.55
3:A:322:PHE:N	3:A:522:PHE:HE1	2.04	0.55
3:B:237:ARG:NH1	6:B:742:HOH:O	2.39	0.55
3:A:386:LEU:H	3:A:386:LEU:HD23	1.71	0.55
3:A:451:MET:HG3	3:A:464:PHE:CE2	2.42	0.55
3:A:7:GLN:NE2	3:A:472:THR:OG1	2.40	0.55
3:B:386:LEU:H	3:B:386:LEU:HD23	1.70	0.55
3:A:254:VAL:H	3:A:257:HIS:CD2	2.04	0.55
3:A:65:ILE:HD13	3:A:102:CYS:HB3	1.88	0.55
3:B:207:LYS:H	3:B:207:LYS:HD2	1.72	0.55
3:B:319:ILE:HG21	3:B:324:ILE:HD11	1.88	0.55
3:B:328:LEU:HD21	3:B:431:HIS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301:VAL:HG13	3:A:349:ILE:HD11	1.89	0.54
3:B:498:VAL:CG2	3:B:509:ALA:HB2	2.38	0.54
2:D:10:U:O4'	2:D:10:U:O2	2.26	0.54
3:B:301:VAL:HG13	3:B:349:ILE:HD11	1.89	0.54
3:A:157:ASN:HD21	3:A:188:ILE:CD1	2.18	0.54
3:A:385:VAL:HG23	3:A:390:LEU:O	2.07	0.54
2:D:13:C:H4'	2:D:14:A:OP2	2.07	0.54
3:A:310:ASN:ND2	3:B:191:ALA:O	2.41	0.54
3:A:436:LYS:O	3:A:440:ILE:CG2	2.55	0.54
3:B:120:ARG:CD	3:B:318:ARG:HH21	2.18	0.54
3:B:320:HIS:CD2	3:B:322:PHE:H	2.26	0.54
3:B:395:VAL:HG13	3:B:522:PHE:CE2	2.42	0.54
3:B:90:GLU:HB2	3:B:91:PRO:HD3	1.88	0.54
3:B:120:ARG:HD3	3:B:318:ARG:HH22	1.72	0.54
3:A:207:LYS:H	3:A:207:LYS:CD	2.21	0.53
3:B:322:PHE:N	3:B:522:PHE:HE1	2.06	0.53
3:A:91:PRO:HB2	6:A:773:HOH:O	2.08	0.53
3:A:319:ILE:CG2	3:A:324:ILE:HD11	2.39	0.53
3:A:430:LEU:O	3:A:434:VAL:HG23	2.08	0.53
3:B:171:TYR:O	3:B:179:HIS:HE1	1.91	0.53
3:A:395:VAL:HG12	3:A:501:MET:HE1	1.90	0.53
3:A:328:LEU:O	3:A:332:LYS:HG2	2.09	0.53
3:B:218:LEU:HD23	3:B:222:THR:CG2	2.39	0.53
3:A:498:VAL:CG2	3:A:509:ALA:HB2	2.39	0.53
3:A:39:PHE:HA	3:A:386:LEU:CD2	2.38	0.53
3:B:385:VAL:HG23	3:B:390:LEU:O	2.08	0.53
3:B:90:GLU:OE2	3:B:90:GLU:N	2.42	0.53
2:F:14:A:N3	2:F:14:A:H2'	2.24	0.53
3:B:296:PRO:O	3:B:297:ALA:HB3	2.09	0.53
3:B:273:LEU:HA	3:B:276:MET:HE3	1.90	0.52
3:A:207:LYS:CD	3:A:207:LYS:N	2.72	0.52
3:B:430:LEU:O	3:B:434:VAL:HG23	2.09	0.52
3:A:55:GLN:O	3:A:59:GLU:HG3	2.09	0.52
3:B:315:LYS:CE	6:B:815:HOH:O	2.57	0.52
3:B:504:ASN:HD22	3:B:506:PHE:HD2	1.52	0.52
3:B:207:LYS:CD	3:B:207:LYS:N	2.72	0.52
3:B:85:ARG:HH11	3:B:525:GLY:HA3	1.74	0.52
3:A:105:ILE:HD13	3:B:537:LEU:HD13	1.91	0.52
3:B:436:LYS:O	3:B:440:ILE:CG2	2.56	0.51
3:B:486:TYR:CE1	3:B:490:MET:HG3	2.45	0.51
3:A:358:TYR:O	3:A:363:LEU:HD21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:89:GLN:CA	3:A:89:GLN:HE21	2.20	0.51
3:B:8:THR:CG2	3:B:475:GLU:HG2	2.41	0.51
3:A:235:VAL:HG11	3:A:253:LEU:HD13	1.92	0.51
3:B:488:GLU:HG3	6:B:891:HOH:O	2.10	0.51
1:E:7:C:O3'	1:E:8:C:H3'	2.11	0.51
3:A:526:ALA:O	3:A:529:VAL:HG23	2.10	0.51
3:B:254:VAL:H	3:B:257:HIS:CD2	2.06	0.51
3:B:397:ALA:O	3:B:400:CYS:HB3	2.11	0.51
3:B:24:VAL:HG21	3:B:506:PHE:HB3	1.91	0.51
3:B:67:ASP:HB3	6:B:830:HOH:O	2.10	0.51
3:A:201:TYR:CD2	3:A:229:LEU:HD22	2.44	0.51
3:A:329:GLU:OE2	3:A:332:LYS:HE3	2.10	0.51
3:A:296:PRO:O	3:A:297:ALA:HB3	2.10	0.51
3:A:320:HIS:CD2	3:A:322:PHE:H	2.29	0.51
3:A:63:ARG:O	3:A:66:GLU:HB2	2.11	0.51
3:A:260:THR:HA	3:A:263:LEU:HD22	1.93	0.51
3:A:401:MET:O	3:A:405:ARG:CG	2.58	0.51
3:B:329:GLU:OE2	3:B:332:LYS:HE3	2.11	0.51
3:B:502:THR:OG1	3:B:504:ASN:OD1	2.29	0.51
3:A:157:ASN:HD22	3:A:157:ASN:N	2.09	0.51
3:A:504:ASN:HD21	3:A:506:PHE:HB2	1.76	0.51
3:B:358:TYR:O	3:B:363:LEU:HD21	2.10	0.50
3:A:397:ALA:O	3:A:400:CYS:HB3	2.10	0.50
3:A:273:LEU:HA	3:A:276:MET:HE3	1.93	0.50
3:B:395:VAL:CG1	3:B:522:PHE:HD2	2.20	0.50
3:B:65:ILE:HD13	3:B:102:CYS:CB	2.42	0.50
3:B:157:ASN:ND2	3:B:188:ILE:CD1	2.57	0.50
3:A:312:LYS:HA	3:A:312:LYS:HE3	1.94	0.50
3:B:260:THR:HA	3:B:263:LEU:HD22	1.92	0.50
1:E:7:C:OP1	1:E:8:C:H2'	2.12	0.50
3:A:461:ALA:HB3	3:A:464:PHE:CE1	2.45	0.50
3:B:80:PHE:HA	3:B:85:ARG:HG3	1.92	0.50
3:B:319:ILE:CG2	3:B:324:ILE:HD11	2.42	0.50
3:B:328:LEU:O	3:B:332:LYS:HG2	2.12	0.50
3:B:357:PHE:CD2	3:B:430:LEU:HD11	2.47	0.50
3:B:7:GLN:HG3	3:B:476:ASP:O	2.12	0.50
2:D:14:A:H2'	2:D:14:A:N3	2.26	0.50
3:A:274:GLN:HG2	3:B:220:PRO:HD2	1.94	0.49
3:A:380:SER:O	3:A:383:GLN:NE2	2.34	0.49
3:B:305:CYS:SG	3:B:349:ILE:HD13	2.52	0.49
3:B:483:LEU:HD22	3:B:496:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:320:HIS:CG	3:B:321:PRO:HD2	2.47	0.49
3:B:55:GLN:O	3:B:59:GLU:HG3	2.12	0.49
3:A:305:CYS:SG	3:A:349:ILE:HD13	2.53	0.49
3:A:357:PHE:CD2	3:A:430:LEU:HD11	2.47	0.49
3:A:470:CYS:SG	3:A:507:SER:HA	2.52	0.49
3:B:276:MET:SD	3:B:288:MET:HE1	2.52	0.49
3:B:470:CYS:SG	3:B:507:SER:HA	2.52	0.49
3:B:428:MET:HE1	3:B:432:GLU:HG2	1.94	0.49
3:B:486:TYR:CZ	3:B:490:MET:HG3	2.47	0.49
1:C:4:U:H2'	1:C:5:A:H8	1.76	0.49
3:A:486:TYR:CE1	3:A:490:MET:HG3	2.47	0.49
3:B:18:ASN:ND2	3:B:472:THR:O	2.45	0.49
3:B:526:ALA:O	3:B:529:VAL:HG23	2.13	0.49
3:A:113:ARG:HB3	6:A:707:HOH:O	2.12	0.49
2:F:1:C:H2'	2:F:2:G:C8	2.47	0.49
3:A:170:LYS:HD3	3:A:171:TYR:CE1	2.48	0.49
3:A:241:GLU:HG2	3:A:268:ILE:HD11	1.95	0.49
3:B:378:SER:HA	3:B:442:MET:O	2.13	0.49
3:A:65:ILE:HD13	3:A:102:CYS:CB	2.43	0.49
3:A:157:ASN:HD22	3:A:188:ILE:HD11	1.71	0.48
3:A:24:VAL:HG21	3:A:506:PHE:HB3	1.94	0.48
3:A:275:ASP:OD2	3:B:221:GLU:CG	2.61	0.48
3:B:146:ARG:HH11	3:B:146:ARG:HA	1.78	0.48
2:F:14:A:H3'	2:F:15:A:O4'	2.13	0.48
3:B:504:ASN:HD21	3:B:506:PHE:HB2	1.77	0.48
3:A:7:GLN:HG3	3:A:476:ASP:O	2.12	0.48
3:A:378:SER:HA	3:A:442:MET:O	2.13	0.48
3:B:241:GLU:HG2	3:B:268:ILE:HD11	1.95	0.48
3:B:407:GLU:HB3	6:B:740:HOH:O	2.12	0.48
3:A:320:HIS:CG	3:A:321:PRO:HD2	2.49	0.48
3:B:149:ARG:NH2	3:B:187:HIS:NE2	2.60	0.48
3:B:270:LYS:HE2	3:B:300:GLU:OE2	2.14	0.48
3:A:207:LYS:H	3:A:207:LYS:HD2	1.76	0.48
3:A:380:SER:C	3:A:382:ASN:H	2.17	0.48
2:F:1:C:H2'	2:F:2:G:H8	1.79	0.48
3:A:20:GLU:HA	3:A:20:GLU:OE2	2.14	0.48
3:A:486:TYR:CZ	3:A:490:MET:HG3	2.49	0.48
3:B:188:ILE:HG12	3:B:189:LYS:N	2.29	0.48
3:B:204:LYS:CE	3:B:208:GLU:OE2	2.62	0.47
3:A:221:GLU:CG	3:B:275:ASP:OD2	2.62	0.47
3:B:216:LYS:O	3:B:218:LEU:HD12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:483:LEU:HD22	3:A:496:LEU:HB2	1.94	0.47
3:A:322:PHE:HB2	3:A:522:PHE:CE1	2.49	0.47
3:B:18:ASN:HB3	3:B:471:GLU:OE2	2.13	0.47
3:B:204:LYS:HE2	3:B:208:GLU:OE2	2.15	0.47
3:B:391:ASN:OD1	3:B:394:VAL:HG23	2.14	0.47
3:B:89:GLN:CA	3:B:89:GLN:HE21	2.22	0.47
3:A:332:LYS:HE2	3:A:431:HIS:HB2	1.95	0.47
3:A:537:LEU:HD13	3:B:105:ILE:HD13	1.96	0.47
3:B:312:LYS:HA	3:B:312:LYS:HE3	1.95	0.47
3:A:379:ALA:HB3	4:A:601:ACT:CH3	2.41	0.47
3:B:201:TYR:CD2	3:B:229:LEU:HD22	2.50	0.47
3:B:235:VAL:HG11	3:B:253:LEU:HD13	1.95	0.47
3:A:451:MET:HG3	3:A:464:PHE:HE2	1.80	0.47
3:A:18:ASN:HB3	3:A:471:GLU:OE2	2.15	0.47
3:B:170:LYS:HD3	3:B:171:TYR:CE1	2.49	0.47
3:A:171:TYR:HA	3:A:174:ARG:NH2	2.30	0.47
3:A:493:PRO:HG3	6:A:846:HOH:O	2.14	0.47
1:C:3:C:H4'	2:D:11:U:C5	2.50	0.47
3:A:204:LYS:HE2	3:A:208:GLU:OE2	2.15	0.46
3:B:134:ASP:HA	6:B:744:HOH:O	2.15	0.46
3:B:200:LYS:HB3	3:B:209:VAL:HG23	1.97	0.46
3:A:191:ALA:O	3:B:310:ASN:ND2	2.47	0.46
3:A:156:TYR:HD2	3:A:164:LEU:HD11	1.80	0.46
3:A:188:ILE:HG12	3:A:189:LYS:N	2.31	0.46
3:B:424:ILE:HA	3:B:428:MET:SD	2.55	0.46
3:B:451:MET:HG3	3:B:464:PHE:HE2	1.79	0.46
3:A:341:LEU:HD12	3:A:341:LEU:N	2.30	0.46
3:A:325:LEU:HD22	3:A:390:LEU:CD1	2.46	0.46
3:A:8:THR:CG2	3:A:475:GLU:HG2	2.45	0.46
3:B:10:PRO:HB3	3:B:23:TYR:CD2	2.51	0.46
3:A:276:MET:SD	3:A:288:MET:HE1	2.55	0.46
3:B:235:VAL:CG2	3:B:235:VAL:O	2.63	0.46
3:A:189:LYS:HG3	6:A:795:HOH:O	2.15	0.46
3:A:105:ILE:CD1	3:B:537:LEU:HD22	2.46	0.46
3:A:10:PRO:HB3	3:A:23:TYR:CD2	2.51	0.46
3:B:20:GLU:OE2	3:B:20:GLU:HA	2.15	0.46
3:B:211:GLU:O	3:B:214:LYS:HG3	2.15	0.46
3:A:204:LYS:CE	3:A:208:GLU:OE2	2.64	0.46
3:A:85:ARG:HD2	3:A:362:LYS:HZ2	1.80	0.46
3:B:431:HIS:C	3:B:431:HIS:HD2	2.19	0.46
3:B:395:VAL:CG1	3:B:522:PHE:CD2	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:337:ASN:CG	3:A:389:ILE:HD11	2.31	0.45
3:A:85:ARG:NH1	3:A:523:ASP:OD1	2.49	0.45
3:B:218:LEU:HD23	3:B:222:THR:HG21	1.99	0.45
3:B:337:ASN:CG	3:B:389:ILE:HD11	2.27	0.45
3:A:430:LEU:HA	3:A:433:VAL:HG13	1.98	0.45
3:B:341:LEU:N	3:B:341:LEU:HD12	2.30	0.45
3:A:504:ASN:ND2	3:A:506:PHE:HB2	2.31	0.45
3:B:430:LEU:HA	3:B:433:VAL:HG13	1.97	0.45
3:A:235:VAL:O	3:A:235:VAL:CG2	2.64	0.45
3:B:325:LEU:HD22	3:B:390:LEU:CD1	2.47	0.45
2:F:14:A:C8	3:B:252:ARG:NH2	2.85	0.45
3:A:35:ARG:HA	3:A:520:CYS:SG	2.57	0.45
3:B:156:TYR:HD2	3:B:164:LEU:HD11	1.81	0.45
3:B:35:ARG:HA	3:B:520:CYS:SG	2.57	0.45
3:B:395:VAL:HG12	3:B:501:MET:CE	2.47	0.45
3:B:504:ASN:ND2	3:B:506:PHE:HB2	2.32	0.45
3:A:483:LEU:O	3:A:486:TYR:HB3	2.17	0.45
3:B:234:ARG:CZ	6:B:811:HOH:O	2.65	0.45
3:B:350:VAL:O	3:B:354:ASP:HB3	2.17	0.45
3:A:27:VAL:HG12	3:A:28:SER:O	2.17	0.45
3:A:407:GLU:HB3	6:A:705:HOH:O	2.17	0.45
3:B:380:SER:C	3:B:382:ASN:H	2.19	0.45
3:B:332:LYS:HE2	3:B:431:HIS:HB2	1.98	0.44
3:A:101:GLN:HE21	3:A:101:GLN:HB3	1.53	0.44
3:A:357:PHE:CZ	3:A:398:ALA:HB1	2.52	0.44
3:A:294:LEU:HD23	3:A:294:LEU:HA	1.90	0.44
3:B:126:PHE:HD1	3:B:174:ARG:HB2	1.82	0.44
3:B:483:LEU:O	3:B:486:TYR:HB3	2.18	0.44
3:A:431:HIS:HE1	6:A:893:HOH:O	2.00	0.44
3:A:395:VAL:CG1	3:A:522:PHE:HD2	2.25	0.44
3:B:22:CYS:SG	3:B:473:ASN:HA	2.57	0.44
3:B:320:HIS:HD2	3:B:322:PHE:H	1.64	0.44
3:B:157:ASN:HD21	3:B:188:ILE:CG1	2.31	0.44
3:B:294:LEU:HD22	3:B:301:VAL:HG22	2.00	0.44
3:B:498:VAL:HG11	3:B:508:ILE:HG12	2.00	0.44
3:A:350:VAL:O	3:A:354:ASP:HB3	2.17	0.44
3:A:384:ARG:HG2	3:A:388:SER:O	2.17	0.44
3:A:431:HIS:C	3:A:431:HIS:HD2	2.20	0.44
3:A:441:THR:O	3:A:442:MET:HB3	2.18	0.44
3:B:155:TRP:O	3:B:159:LYS:CD	2.65	0.43
3:A:184:ARG:O	3:A:187:HIS:ND1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:50:GLU:HG2	6:A:728:HOH:O	2.18	0.43
3:A:312:LYS:CE	3:A:312:LYS:HA	2.48	0.43
3:A:395:VAL:CG1	3:A:522:PHE:CD2	2.93	0.43
3:B:27:VAL:HG12	3:B:28:SER:O	2.19	0.43
3:B:504:ASN:ND2	3:B:506:PHE:HD2	2.10	0.43
2:D:15:A:O2'	3:A:316:LYS:CE	2.54	0.43
3:A:105:ILE:HD13	3:B:537:LEU:CD1	2.48	0.43
3:A:278:LEU:HA	3:A:278:LEU:HD23	1.84	0.43
3:A:155:TRP:O	3:A:159:LYS:CD	2.65	0.43
3:A:149:ARG:HH21	3:A:187:HIS:CD2	2.34	0.43
3:B:312:LYS:CE	3:B:312:LYS:HA	2.48	0.43
3:B:357:PHE:CZ	3:B:398:ALA:HB1	2.53	0.43
3:A:254:VAL:O	3:A:257:HIS:HB2	2.19	0.43
3:A:391:ASN:OD1	3:A:394:VAL:HG23	2.19	0.43
1:E:2:C:O2'	1:E:3:C:H5'	2.19	0.43
3:A:424:ILE:HA	3:A:428:MET:SD	2.58	0.43
3:B:223:GLU:OE2	3:B:223:GLU:HA	2.19	0.43
3:A:428:MET:HE1	3:A:432:GLU:HG2	2.01	0.43
3:B:105:ILE:O	3:B:109:GLN:HB3	2.19	0.43
3:A:294:LEU:HD22	3:A:301:VAL:HG22	2.01	0.42
3:B:109:GLN:HG3	6:B:859:HOH:O	2.19	0.42
3:B:173:GLN:O	3:B:174:ARG:HD3	2.19	0.42
3:B:164:LEU:HD13	3:B:198:VAL:HG11	2.01	0.42
3:B:101:GLN:HE21	3:B:101:GLN:HB3	1.53	0.42
3:B:395:VAL:CG1	3:B:501:MET:HE1	2.49	0.42
3:B:89:GLN:CA	3:B:89:GLN:NE2	2.81	0.42
3:A:290:ALA:HB2	3:A:343:TRP:HB3	2.01	0.42
3:A:537:LEU:HD22	3:B:105:ILE:CD1	2.49	0.42
3:B:322:PHE:HB2	3:B:522:PHE:CE1	2.55	0.42
3:A:272:LEU:HD12	3:A:272:LEU:HA	1.87	0.42
3:B:273:LEU:O	3:B:274:GLN:C	2.58	0.42
2:F:14:A:N3	2:F:14:A:C2'	2.83	0.42
2:F:6:G:H2'	2:F:7:G:O4'	2.20	0.42
3:A:223:GLU:OE2	3:A:223:GLU:HA	2.19	0.42
3:A:161:ALA:HB1	3:A:225:VAL:HG21	2.02	0.42
3:A:293:VAL:O	3:A:300:GLU:HG2	2.19	0.42
2:F:13:C:OP2	3:B:277:PRO:HB2	2.19	0.42
3:B:294:LEU:HD23	3:B:294:LEU:HA	1.89	0.42
3:A:200:LYS:HB3	3:A:209:VAL:HG23	2.02	0.42
3:A:220:PRO:HD2	3:B:274:GLN:HG2	2.02	0.42
3:B:94:PHE:O	3:B:98:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:U:C2	3:A:283:ARG:HA	2.55	0.42
3:A:105:ILE:O	3:A:109:GLN:HB3	2.19	0.42
3:B:144:TRP:HZ3	3:B:152:VAL:HG21	1.84	0.42
3:B:375:ILE:HD13	3:B:397:ALA:HA	2.01	0.42
2:F:7:G:O2'	2:F:8:C:H5'	2.20	0.42
3:A:316:LYS:HE3	3:B:158:THR:O	2.19	0.42
3:B:381:MET:HE1	3:B:392:ALA:HB1	2.01	0.42
3:B:374:ALA:HA	3:B:413:VAL:O	2.20	0.42
3:B:77:ILE:HD11	3:B:95:ALA:HB1	2.00	0.42
3:A:115:VAL:N	3:A:116:PRO:HD2	2.35	0.41
3:A:144:TRP:HZ3	3:A:152:VAL:HG21	1.85	0.41
3:A:149:ARG:NH2	3:A:187:HIS:NE2	2.68	0.41
3:A:395:VAL:HG12	3:A:501:MET:CE	2.50	0.41
3:A:537:LEU:CD1	3:B:105:ILE:HD13	2.50	0.41
3:B:489:LYS:HD3	3:B:489:LYS:HA	1.71	0.41
3:B:8:THR:HG21	3:B:475:GLU:HG2	2.02	0.41
1:C:3:C:O4'	2:D:11:U:C4	2.73	0.41
3:A:320:HIS:HD2	3:A:322:PHE:H	1.68	0.41
3:A:22:CYS:SG	3:A:473:ASN:HA	2.60	0.41
3:B:64:LEU:HD13	3:B:73:VAL:HG22	2.02	0.41
3:B:171:TYR:O	3:B:179:HIS:CE1	2.73	0.41
3:B:221:GLU:OE1	3:B:221:GLU:HA	2.21	0.41
2:F:8:C:H2'	3:B:338:ARG:HB2	2.01	0.41
3:A:221:GLU:OE1	3:A:221:GLU:HA	2.21	0.41
3:A:270:LYS:HE2	3:A:300:GLU:OE2	2.20	0.41
3:A:325:LEU:HD22	3:A:390:LEU:HD11	2.02	0.41
3:A:325:LEU:HD23	3:A:325:LEU:O	2.20	0.41
3:A:431:HIS:HD2	3:A:432:GLU:N	2.19	0.41
3:B:290:ALA:HB2	3:B:343:TRP:HB3	2.03	0.41
3:B:351:GLU:O	3:B:355:ASN:HB2	2.21	0.41
3:A:109:GLN:NE2	3:B:528:ASP:OD1	2.53	0.41
2:F:13:C:H4'	3:B:121:ILE:HG21	2.01	0.41
3:A:498:VAL:HG11	3:A:508:ILE:HG12	2.02	0.41
3:A:64:LEU:HD13	3:A:73:VAL:HG22	2.03	0.41
3:A:68:GLY:C	3:A:70:GLY:H	2.24	0.41
2:D:15:A:H4'	3:A:316:LYS:CE	2.51	0.41
3:A:273:LEU:O	3:A:274:GLN:C	2.59	0.41
3:A:436:LYS:HD3	6:A:898:HOH:O	2.20	0.41
3:B:101:GLN:O	3:B:102:CYS:O	2.39	0.41
3:B:115:VAL:N	3:B:116:PRO:HD2	2.36	0.41
3:B:120:ARG:NE	3:B:318:ARG:NH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:G:OP1	3:B:341:LEU:HD21	2.21	0.41
3:A:158:THR:O	3:B:316:LYS:HE3	2.21	0.41
2:F:2:G:H2'	2:F:3:G:O4'	2.20	0.41
3:A:27:VAL:CG2	3:A:507:SER:HB2	2.48	0.41
3:B:146:ARG:CA	3:B:146:ARG:NE	2.62	0.41
3:B:325:LEU:HD22	3:B:390:LEU:HD11	2.02	0.41
3:B:68:GLY:C	3:B:70:GLY:H	2.23	0.41
3:A:164:LEU:HD13	3:A:198:VAL:HG11	2.02	0.41
3:A:27:VAL:CG2	3:A:35:ARG:NH2	2.82	0.41
3:B:462:ASP:O	3:B:463:ILE:HD13	2.20	0.41
2:D:4:U:O2'	2:D:5:A:H5'	2.20	0.41
3:B:248:ILE:HD13	3:B:272:LEU:HD13	2.02	0.41
3:B:325:LEU:HD22	3:B:390:LEU:CD2	2.51	0.41
2:F:9:U:C2	3:B:283:ARG:HA	2.56	0.41
3:A:16:VAL:HB	3:A:17:PRO:HD2	2.03	0.40
3:A:94:PHE:O	3:A:98:VAL:HG23	2.22	0.40
3:B:518:ASP:HB2	6:B:820:HOH:O	2.21	0.40
3:A:105:ILE:HD11	3:B:537:LEU:HD22	2.04	0.40
3:A:160:ASP:N	3:A:160:ASP:OD1	2.53	0.40
3:A:430:LEU:O	3:A:433:VAL:HG13	2.21	0.40
3:B:441:THR:O	3:B:442:MET:HB3	2.20	0.40
3:B:461:ALA:HB3	3:B:464:PHE:CE1	2.44	0.40
3:B:449:LEU:HB2	3:B:450:PRO:HD3	2.04	0.40
3:B:85:ARG:HB3	3:B:523:ASP:OD2	2.21	0.40
2:F:1:C:H2'	2:F:2:G:O4'	2.22	0.40
3:A:265:SER:OG	3:A:268:ILE:HG12	2.21	0.40
3:B:96:LEU:O	3:B:96:LEU:HD23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	514/538 (96%)	473 (92%)	38 (7%)	3 (1%)	25	37
3	B	522/538 (97%)	480 (92%)	39 (8%)	3 (1%)	25	37
All	All	1036/1076 (96%)	953 (92%)	77 (7%)	6 (1%)	25	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	102	CYS
3	B	102	CYS
3	A	442	MET
3	B	442	MET
3	A	69	LYS
3	B	69	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	452/467 (97%)	384 (85%)	68 (15%)	3	3
3	B	458/467 (98%)	392 (86%)	66 (14%)	3	3
All	All	910/934 (97%)	776 (85%)	134 (15%)	3	3

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	30	MET
3	A	41	SER
3	A	53	LEU
3	A	62	LEU
3	A	66	GLU
3	A	85	ARG
3	A	89	GLN
3	A	90	GLU
3	A	92	THR
3	A	100	SER

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Mol	Chain	Res	Type
3	A	101	GLN
3	A	105	ILE
3	A	106	LYS
3	A	109	GLN
3	A	125	LEU
3	A	129	ILE
3	A	146	ARG
3	A	148	LEU
3	A	157	ASN
3	A	159	LYS
3	A	160	ASP
3	A	164	LEU
3	A	183	LEU
3	A	189	LYS
3	A	203	SER
3	A	204	LYS
3	A	207	LYS
3	A	209	VAL
3	A	221	GLU
3	A	223	GLU
3	A	235	VAL
3	A	246	HIS
3	A	252	ARG
3	A	260	THR
3	A	261	ILE
3	A	263	LEU
3	A	271	SER
3	A	272	LEU
3	A	274	GLN
3	A	292	SER
3	A	293	VAL
3	A	300	GLU
3	A	306	GLU
3	A	329	GLU
3	A	337	ASN
3	A	348	SER
3	A	354	ASP
3	A	355	ASN
3	A	360	SER
3	A	382	ASN
3	A	384	ARG
3	A	385	VAL

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Mol	Chain	Res	Type
3	A	386	LEU
3	A	405	ARG
3	A	430	LEU
3	A	431	HIS
3	A	438	SER
3	A	440	ILE
3	A	456	LYS
3	A	457	THR
3	A	489	LYS
3	A	498	VAL
3	A	518	ASP
3	A	522	PHE
3	A	524	SER
3	A	527	LEU
3	A	528	ASP
3	A	529	VAL
3	B	30	MET
3	B	34	ARG
3	B	41	SER
3	B	53	LEU
3	B	62	LEU
3	B	66	GLU
3	B	85	ARG
3	B	89	GLN
3	B	90	GLU
3	B	92	THR
3	B	100	SER
3	B	101	GLN
3	B	105	ILE
3	B	106	LYS
3	B	109	GLN
3	B	125	LEU
3	B	129	ILE
3	B	146	ARG
3	B	148	LEU
3	B	159	LYS
3	B	160	ASP
3	B	164	LEU
3	B	183	LEU
3	B	203	SER
3	B	204	LYS
3	B	207	LYS

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Mol	Chain	Res	Type
3	B	209	VAL
3	B	217	GLU
3	B	221	GLU
3	B	223	GLU
3	B	235	VAL
3	B	246	HIS
3	B	260	THR
3	B	261	ILE
3	B	263	LEU
3	B	271	SER
3	B	272	LEU
3	B	274	GLN
3	B	292	SER
3	B	293	VAL
3	B	300	GLU
3	B	306	GLU
3	B	325	LEU
3	B	337	ASN
3	B	348	SER
3	B	354	ASP
3	B	355	ASN
3	B	360	SER
3	B	382	ASN
3	B	385	VAL
3	B	386	LEU
3	B	405	ARG
3	B	430	LEU
3	B	431	HIS
3	B	438	SER
3	B	440	ILE
3	B	456	LYS
3	B	457	THR
3	B	489	LYS
3	B	498	VAL
3	B	518	ASP
3	B	522	PHE
3	B	524	SER
3	B	527	LEU
3	B	528	ASP
3	B	529	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	7	GLN
3	A	9	GLN
3	A	26	GLN
3	A	57	ASN
3	A	75	GLN
3	A	89	GLN
3	A	157	ASN
3	A	179	HIS
3	A	210	GLN
3	A	257	HIS
3	A	320	HIS
3	A	382	ASN
3	A	431	HIS
3	A	485	GLN
3	A	504	ASN
3	B	7	GLN
3	B	9	GLN
3	B	26	GLN
3	B	57	ASN
3	B	89	GLN
3	B	109	GLN
3	B	157	ASN
3	B	179	HIS
3	B	210	GLN
3	B	257	HIS
3	B	320	HIS
3	B	355	ASN
3	B	431	HIS
3	B	485	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	7/8 (87%)	0	0
1	E	7/8 (87%)	1 (14%)	0
2	D	13/15 (86%)	7 (53%)	5 (38%)
2	F	14/15 (93%)	8 (57%)	5 (35%)
All	All	41/46 (89%)	16 (39%)	10 (24%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	9	U
2	D	10	U
2	D	11	U
2	D	12	U
2	D	13	C
2	D	14	A
2	D	15	A
1	E	8	C
2	F	2	G
2	F	9	U
2	F	10	U
2	F	11	U
2	F	12	U
2	F	13	C
2	F	14	A
2	F	15	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	9	U
2	D	10	U
2	D	11	U
2	D	12	U
2	D	13	C
2	F	9	U
2	F	10	U
2	F	11	U
2	F	12	U
2	F	13	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACT	B	602	5	1,3,3	3.61	1 (100%)	0,3,3	0.00	-
4	ACT	A	601	5	1,3,3	4.37	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	ACT	CH3-C	4.37	1.54	1.48
4	B	602	ACT	CH3-C	3.61	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	ACT	1	0
4	A	601	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	8/8 (100%)	0.87	1 (12%) 3 2	32, 37, 57, 62	0
1	E	8/8 (100%)	1.22	1 (12%) 3 2	31, 39, 54, 67	0
2	D	14/15 (93%)	1.23	4 (28%) 0 0	26, 38, 55, 69	0
2	F	15/15 (100%)	1.62	4 (26%) 0 0	27, 38, 63, 63	0
3	A	520/538 (96%)	0.57	33 (6%) 20 17	11, 30, 47, 59	0
3	B	526/538 (97%)	0.59	45 (8%) 10 8	14, 31, 49, 62	0
All	All	1091/1122 (97%)	0.61	88 (8%) 12 9	11, 31, 50, 69	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	431	HIS	6.7
2	D	15	A	5.1
3	B	215	GLU	4.8
3	A	338	ARG	4.8
2	F	15	A	4.0
3	A	431	HIS	4.0
2	F	1	C	3.9
3	B	105	ILE	3.9
3	B	101	GLN	3.7
3	A	205	GLY	3.7
3	B	338	ARG	3.6
3	A	294	LEU	3.6
3	A	245	ILE	3.6
3	B	205	GLY	3.5
3	B	216	LYS	3.5
3	A	211	GLU	3.5
3	A	240	ASP	3.5
3	B	245	ILE	3.5
1	E	8	C	3.5

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Mol	Chain	Res	Type	RSRZ
3	A	293	VAL	3.4
3	B	297	ALA	3.4
3	A	101	GLN	3.3
3	A	204	LYS	3.2
3	B	217	GLU	3.2
3	B	268	ILE	3.2
3	A	248	ILE	3.1
3	A	234	ARG	3.1
3	A	239	LYS	3.1
3	A	474	VAL	3.0
3	B	212	ALA	3.0
3	A	264	LYS	2.9
3	B	235	VAL	2.9
3	A	209	VAL	2.9
3	A	297	ALA	2.9
3	A	289	THR	2.8
3	B	263	LEU	2.8
3	B	294	LEU	2.8
3	A	212	ALA	2.8
3	B	246	HIS	2.8
3	B	333	LYS	2.7
3	B	293	VAL	2.7
3	B	191	ALA	2.7
3	B	234	ARG	2.7
3	B	262	HIS	2.7
1	C	8	C	2.7
3	A	224	LYS	2.7
3	A	241	GLU	2.7
3	B	261	ILE	2.6
3	A	244	ILE	2.6
3	B	223	GLU	2.6
2	D	2	G	2.5
3	B	474	VAL	2.5
3	A	191	ALA	2.5
2	F	2	G	2.5
3	B	221	GLU	2.4
3	B	62	LEU	2.4
3	B	273	LEU	2.4
3	B	160	ASP	2.4
3	B	224	LYS	2.4
3	A	275	ASP	2.4
2	D	14	A	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	5	MET	2.3
3	B	211	GLU	2.3
3	B	209	VAL	2.3
3	A	266	LYS	2.3
3	B	244	ILE	2.3
3	B	195	LEU	2.3
2	D	4	U	2.3
2	F	6	G	2.3
3	B	260	THR	2.3
3	A	265	SER	2.3
3	B	218	LEU	2.2
3	A	210	GLN	2.2
3	B	289	THR	2.2
3	B	439	ASP	2.2
3	B	214	LYS	2.2
3	B	242	LEU	2.2
3	A	223	GLU	2.2
3	A	105	ILE	2.2
3	B	208	GLU	2.2
3	A	292	SER	2.1
3	A	66	GLU	2.1
3	B	301	VAL	2.1
3	B	158	THR	2.0
3	B	354	ASP	2.0
3	A	303	SER	2.0
3	A	437	MET	2.0
3	B	207	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
4	ACT	A	601	4/4	0.64	0.32	22,23,24,26	0
5	MG	A	701	1/1	0.79	0.07	40,40,40,40	0
5	MG	B	702	1/1	0.83	0.09	29,29,29,29	0
4	ACT	B	602	4/4	0.84	0.27	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.