



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 1ZHO / pdb_00001zho
Title : The structure of a ribosomal protein L1 in complex with mRNA
Authors : Nevskaya, N.; Tishchenko, S.; Volchkov, S.; Kljashtorny, V.; Nikonova, E.;
Nikonov, O.; Nikulin, A.; Kohrer, C.; Piendl, W.; Zimmermann, R.; Stockley,
P.; Garber, M.; Nikonov, S.
Deposited on : 2005-04-26
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

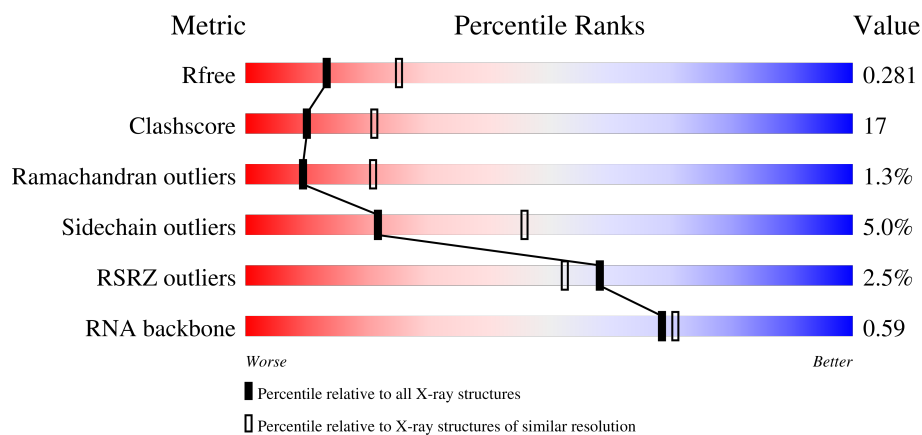
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

Mol	Chain	Length	Quality of chain
1	B	38	61% 32% 8%
1	D	38	68% 24% 8%
1	F	38	5% 47% 39% 5% 8%
1	H	38	5% 42% 42% 13% .

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Mol	Chain	Length	Quality of chain
2	A	228	64%33%
2	C	228	4% 49%45%5%
2	E	228	2% 54%38%7%
2	G	228	3% 65%31%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10515 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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			
1	D	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			
1	F	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			
1	H	38	Total	C	N	O	P	0	0	0
			816	363	150	265	38			

- Molecule 2 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			
2	C	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			
2	E	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			
2	G	228	Total	C	N	O	Se	0	0	0
			1742	1102	318	319	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	MSE	MET	modified residue	UNP P27150
A	120	MSE	MET	modified residue	UNP P27150
A	218	MSE	MET	modified residue	UNP P27150
C	108	MSE	MET	modified residue	UNP P27150
C	120	MSE	MET	modified residue	UNP P27150
C	218	MSE	MET	modified residue	UNP P27150
E	108	MSE	MET	modified residue	UNP P27150
E	120	MSE	MET	modified residue	UNP P27150
E	218	MSE	MET	modified residue	UNP P27150

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Chain	Residue	Modelled	Actual	Comment	Reference
G	108	MSE	MET	modified residue	UNP P27150
G	120	MSE	MET	modified residue	UNP P27150
G	218	MSE	MET	modified residue	UNP P27150

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total K 1 1	0	0
3	H	1	Total K 1 1	0	0
3	A	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	43	Total O 43 43	0	0
4	D	44	Total O 44 44	0	0
4	F	24	Total O 24 24	0	0
4	H	32	Total O 32 32	0	0
4	A	51	Total O 51 51	0	0
4	C	26	Total O 26 26	0	0
4	E	33	Total O 33 33	0	0
4	G	26	Total O 26 26	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.

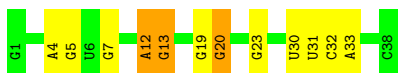
- Molecule 1: mRNA

Chain B: 



- Molecule 1: mRNA

Chain D: 



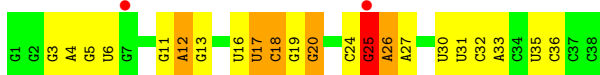
- Molecule 1: mRNA

Chain F: 



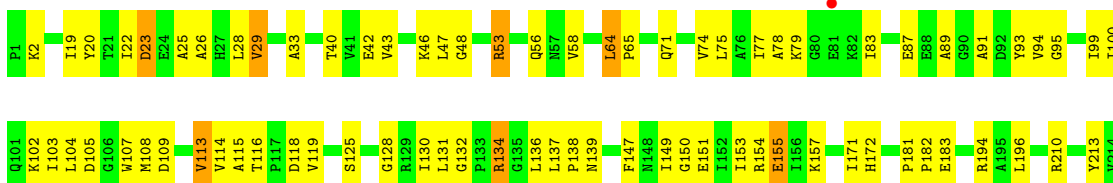
- Molecule 1: mRNA

Chain H: 



- Molecule 2: 50S ribosomal protein L1

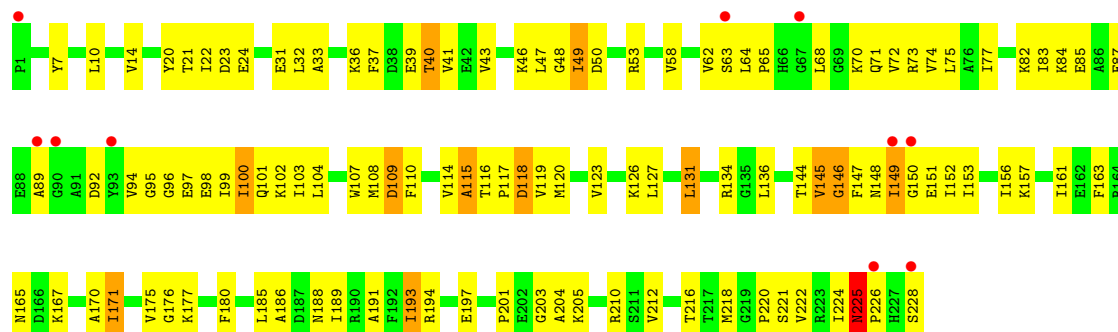
Chain A: 



T215
T216
T217
P220
R223
I224
S228

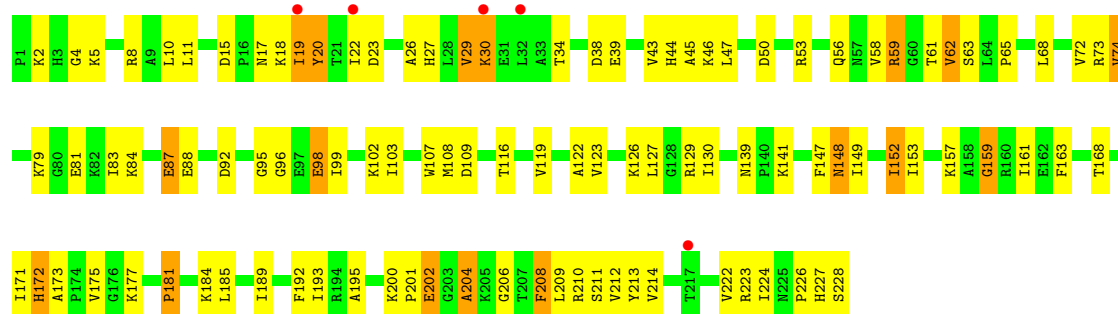
• Molecule 2: 50S ribosomal protein L1

Chain C: 4% 49% 45% 5%



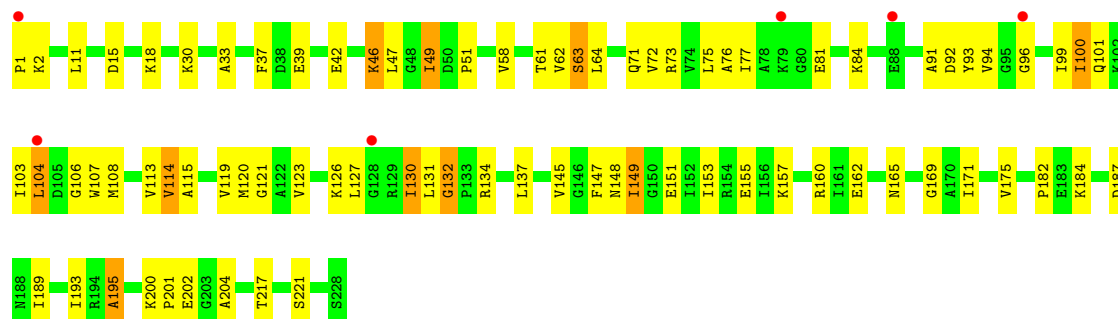
• Molecule 2: 50S ribosomal protein L1

Chain E: 2% 54% 38% 7%



• Molecule 2: 50S ribosomal protein L1

Chain G: 3% 65% 31% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 101.90Å 119.60Å 90.00° 93.66° 90.00°	Depositor
Resolution (Å)	37.06 – 2.60 37.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.7 (37.06-2.60) 96.2 (37.06-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.281 0.219 , 0.281	Depositor DCC
R_{free} test set	2393 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10515	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 20.65 % 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 8.2984e-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:
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	B	0.49	0/912	1.00	6/1419 (0.4%)
1	D	0.43	0/912	0.89	0/1419
1	F	0.38	0/912	0.93	6/1419 (0.4%)
1	H	0.45	0/912	1.08	12/1419 (0.8%)
2	A	0.60	1/1772 (0.1%)	1.14	13/2384 (0.5%)
2	C	0.64	1/1772 (0.1%)	1.20	18/2384 (0.8%)
2	E	0.60	0/1772	1.13	11/2384 (0.5%)
2	G	0.57	0/1772	1.12	11/2384 (0.5%)
All	All	0.55	2/10736 (0.0%)	1.08	77/15212 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	132	GLY	CA-C	5.72	1.56	1.51
2	C	171	ILE	N-CA	-5.06	1.40	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	G	OP1-P-O3'	-10.74	75.77	108.00
1	F	17	U	C2'-C3'-O3'	10.36	125.04	109.50
1	H	18	C	C2'-C3'-O3'	10.23	124.84	109.50
2	G	71	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	B	25	G	OP2-P-O3'	9.52	136.55	108.00
1	H	24	C	P-O3'-C3'	-8.77	107.05	120.20
2	G	126	LYS	N-CA-C	8.33	124.31	111.56
1	H	25	G	OP2-P-O3'	-7.46	85.62	108.00
2	C	100	ILE	N-CA-C	-7.45	103.59	110.82
2	E	59	ARG	N-CA-C	7.24	119.27	107.32
2	A	131	LEU	CA-C-N	7.19	126.38	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	131	LEU	C-N-CA	7.19	126.38	121.13
2	G	46	LYS	N-CA-C	-7.18	97.90	109.96
1	B	26	A	N9-C1'-C2'	7.13	122.70	112.00
2	E	29	VAL	N-CA-C	7.09	117.61	110.23
1	B	26	A	O4'-C4'-C3'	-7.00	97.00	104.00
2	C	148	ASN	N-CA-C	-6.93	101.83	111.81
1	H	25	G	O3'-P-O5'	6.87	114.31	104.00
2	G	71	GLN	CG-CD-NE2	6.67	126.41	116.40
2	C	82	LYS	N-CA-C	-6.64	105.33	113.50
2	A	64	LEU	CA-C-N	6.60	126.85	119.32
2	A	64	LEU	C-N-CA	6.60	126.85	119.32
2	A	155	GLU	N-CA-C	6.55	118.08	111.07
2	C	193	ILE	N-CA-C	-6.52	103.97	110.62
2	E	148	ASN	N-CA-C	-6.47	102.50	111.81
1	H	25	G	OP1-P-O3'	6.46	127.39	108.00
1	H	26	A	P-O5'-C5'	-6.46	111.22	120.90
2	A	181	PRO	N-CA-C	-6.44	103.69	110.58
1	F	18	C	C2'-C3'-O3'	6.40	119.10	109.50
2	A	132	GLY	CA-C-N	6.35	125.92	119.19
2	A	132	GLY	C-N-CA	6.35	125.92	119.19
2	E	206	GLY	CA-C-N	-6.34	112.82	122.21
2	E	206	GLY	C-N-CA	-6.34	112.82	122.21
2	C	23	ASP	N-CA-C	-6.34	104.25	112.68
1	F	16	U	OP1-P-O3'	-6.27	89.19	108.00
1	H	18	C	C4'-C3'-O3'	6.24	118.77	109.40
2	C	224	ILE	N-CA-C	6.24	116.14	108.53
2	G	195	ALA	N-CA-C	-6.07	104.78	111.82
1	H	16	U	OP1-P-O3'	-5.99	90.03	108.00
2	C	221	SER	N-CA-C	5.95	119.25	109.85
2	A	217	THR	N-CA-C	5.81	118.08	111.11
1	F	16	U	OP2-P-O3'	5.79	125.36	108.00
2	C	40	THR	CA-C-N	5.79	130.39	121.71
2	C	40	THR	C-N-CA	5.79	130.39	121.71
2	E	19	ILE	N-CA-C	-5.77	97.34	109.34
2	G	100	ILE	N-CA-C	-5.75	104.90	110.42
2	E	74	VAL	N-CA-C	5.73	116.12	107.75
2	A	181	PRO	CB-CA-C	5.72	116.55	111.17
2	G	148	ASN	N-CA-C	-5.72	106.91	112.97
2	C	203	GLY	CA-C-N	-5.72	113.43	121.72
2	C	203	GLY	C-N-CA	-5.72	113.43	121.72
2	E	152	ILE	N-CA-C	-5.66	105.00	110.72
2	C	225	ASN	CA-C-N	5.64	125.32	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	225	ASN	C-N-CA	5.64	125.32	119.56
2	A	139	ASN	CA-C-N	5.59	125.25	119.05
2	A	139	ASN	C-N-CA	5.59	125.25	119.05
2	C	145	VAL	N-CA-C	5.57	116.30	108.17
1	F	17	U	C4'-C3'-O3'	5.56	117.74	109.40
2	G	121	GLY	N-CA-C	-5.53	100.07	113.18
1	H	16	U	OP2-P-O3'	5.53	124.58	108.00
2	E	206	GLY	N-CA-C	5.52	118.66	110.60
1	H	17	U	C2'-C3'-O3'	5.49	117.73	109.50
1	B	12	A	C4'-C3'-O3'	5.48	117.61	109.40
2	A	125	SER	N-CA-C	5.47	116.93	111.07
2	E	181	PRO	N-CA-C	-5.43	104.07	110.70
2	C	109	ASP	N-CA-C	5.39	117.78	107.75
2	C	115	ALA	N-CA-C	5.35	116.41	108.60
2	G	132	GLY	CA-C-N	5.34	125.01	119.56
2	G	132	GLY	C-N-CA	5.34	125.01	119.56
2	E	87	GLU	N-CA-C	-5.26	105.24	110.97
1	F	12	A	C4'-C3'-O3'	5.16	117.14	109.40
1	B	19	G	N9-C1'-C2'	5.06	119.59	112.00
2	C	146	GLY	N-CA-C	5.06	118.36	110.88
2	C	126	LYS	N-CA-C	5.05	117.56	111.40
1	H	18	C	C4'-C3'-C2'	5.03	107.63	102.60
2	G	126	LYS	CB-CA-C	-5.00	101.67	111.03
1	H	17	U	C4'-C3'-O3'	5.00	116.90	109.40

There are no chirality outliers.

There are no planarity outliers.

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	B	816	0	413	7	0
1	D	816	0	413	11	0
1	F	816	0	413	17	0
1	H	816	0	412	15	0
2	A	1742	0	1796	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1742	0	1796	85	0
2	E	1742	0	1796	95	0
2	G	1742	0	1796	59	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
4	A	51	0	0	4	0
4	B	43	0	0	1	0
4	C	26	0	0	2	0
4	D	44	0	0	1	0
4	E	33	0	0	2	0
4	F	24	0	0	0	0
4	G	26	0	0	0	0
4	H	32	0	0	0	0
All	All	10515	0	8835	329	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 17.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:A:H4'	2:G:46:LYS:HD3	1.42	0.99
2:E:8:ARG:HA	2:E:11:LEU:HD12	1.42	0.99
2:E:30:LYS:H	2:E:30:LYS:HD2	1.26	0.98
2:E:99:ILE:HD12	2:E:102:LYS:HD2	1.52	0.92
2:C:115:ALA:HB3	2:C:120:MSE:HE1	1.57	0.87
2:E:30:LYS:H	2:E:30:LYS:CD	1.92	0.83
2:E:99:ILE:HA	2:E:102:LYS:HD2	1.59	0.81
2:C:10:LEU:HD22	2:C:32:LEU:HA	1.64	0.79
2:C:21:THR:HG23	2:C:228:SER:HB2	1.63	0.79
2:G:123:VAL:HG13	2:G:127:LEU:HD12	1.64	0.78
2:E:149:ILE:O	2:E:153:ILE:HG13	1.83	0.78
2:C:116:THR:O	2:C:119:VAL:HG22	1.84	0.77
2:C:120:MSE:HE3	2:C:145:VAL:HG13	1.69	0.74
2:E:201:PRO:HG2	2:E:204:ALA:HB2	1.69	0.74
2:A:83:ILE:O	2:A:87:GLU:HG3	1.88	0.74
2:A:113:VAL:HG22	2:A:138:PRO:HG3	1.70	0.74
1:F:12:A:H4'	1:F:13:G:O5'	1.88	0.73
2:A:78:ALA:HB3	2:A:83:ILE:HD13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:ILE:HG21	2:C:226:PRO:HB3	1.69	0.72
2:G:132:GLY:HA2	2:G:137:LEU:HB2	1.72	0.72
2:G:153:ILE:O	2:G:157:LYS:HG2	1.89	0.71
2:C:47:LEU:HD13	2:C:58:VAL:HG21	1.72	0.71
2:E:103:ILE:HD12	2:E:127:LEU:HD21	1.72	0.71
2:A:42:GLU:HG3	2:A:215:THR:HG23	1.73	0.70
2:C:47:LEU:HB2	2:C:49:ILE:HD12	1.72	0.70
2:G:151:GLU:O	2:G:155:GLU:HG3	1.91	0.70
2:C:201:PRO:HG2	2:C:204:ALA:HB2	1.74	0.70
2:A:134:ARG:HB3	2:A:136:LEU:HG	1.73	0.70
2:E:98:GLU:O	2:E:102:LYS:HG3	1.91	0.69
2:C:33:ALA:HB1	4:C:229:HOH:O	1.92	0.69
2:G:189:ILE:O	2:G:193:ILE:HG12	1.94	0.68
1:F:31:U:H2'	1:F:32:C:C6	2.29	0.68
2:E:30:LYS:HD2	2:E:30:LYS:N	2.05	0.68
2:G:108:MSE:HE1	2:G:134:ARG:HG3	1.76	0.67
2:G:30:LYS:HE2	2:G:182:PRO:HD3	1.77	0.67
2:G:201:PRO:HG2	2:G:204:ALA:HB2	1.75	0.67
1:F:33:A:H4'	2:E:46:LYS:HD3	1.76	0.67
2:C:127:LEU:HD13	2:C:131:LEU:HD11	1.76	0.67
2:A:87:GLU:HG2	2:A:94:VAL:HG11	1.76	0.66
2:G:103:ILE:HA	2:G:107:TRP:O	1.96	0.66
2:A:95:GLY:HA3	2:A:99:ILE:HD11	1.78	0.66
2:E:96:GLY:O	2:E:99:ILE:HG22	1.95	0.66
1:F:15:C:H5''	2:E:4:GLY:HA3	1.78	0.66
2:C:189:ILE:O	2:C:193:ILE:HG12	1.95	0.66
2:A:149:ILE:O	2:A:153:ILE:HG13	1.94	0.65
2:E:46:LYS:HB3	2:E:210:ARG:HB2	1.78	0.65
2:C:114:VAL:HG12	2:C:144:THR:HG22	1.79	0.65
2:E:47:LEU:HD13	2:E:58:VAL:HG21	1.79	0.64
2:G:75:LEU:HD12	2:G:93:TYR:HB2	1.80	0.64
2:G:77:ILE:HG22	2:G:119:VAL:HG11	1.80	0.64
2:C:165:ASN:HA	2:C:170:ALA:O	1.97	0.64
2:C:212:VAL:HG21	2:C:226:PRO:HG3	1.80	0.64
2:E:148:ASN:O	2:E:152:ILE:HG13	1.98	0.64
2:G:47:LEU:HB2	2:G:49:ILE:HD12	1.80	0.63
2:C:83:ILE:HG23	2:C:94:VAL:CG1	2.28	0.63
2:C:77:ILE:O	2:C:119:VAL:HG21	1.99	0.63
2:G:115:ALA:O	2:G:145:VAL:HA	1.99	0.63
2:E:81:GLU:HA	4:E:252:HOH:O	1.99	0.62
2:E:211:SER:HB2	2:E:213:TYR:HE1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:49:ILE:HD13	2:G:49:ILE:H	1.63	0.62
2:C:73:ARG:HA	2:C:92:ASP:OD1	1.99	0.62
2:E:62:VAL:HG13	2:E:195:ALA:HB2	1.80	0.62
2:C:127:LEU:CD1	2:C:131:LEU:HD11	2.30	0.62
2:G:75:LEU:HD21	2:G:103:ILE:HD11	1.81	0.62
2:E:189:ILE:O	2:E:193:ILE:HG13	1.99	0.61
2:C:96:GLY:O	2:C:99:ILE:HG22	1.99	0.61
1:B:31:U:H2'	1:B:32:C:C6	2.35	0.61
2:C:180:PHE:HB3	2:C:185:LEU:HG	1.83	0.61
2:E:119:VAL:O	2:E:123:VAL:HG23	2.02	0.60
2:E:99:ILE:HA	2:E:102:LYS:CD	2.31	0.60
2:E:122:ALA:O	2:E:126:LYS:HG2	2.01	0.60
2:G:73:ARG:HA	2:G:92:ASP:OD2	2.01	0.60
2:A:194:ARG:HD2	4:A:232:HOH:O	2.02	0.59
2:G:63:SER:HA	2:G:160:ARG:HA	1.85	0.59
2:G:15:ASP:OD2	2:G:18:LYS:HB2	2.03	0.59
2:E:62:VAL:HG22	2:E:163:PHE:HE2	1.68	0.58
2:C:83:ILE:HG23	2:C:94:VAL:HG12	1.86	0.58
2:E:2:LYS:HE2	2:E:8:ARG:HH12	1.68	0.58
2:A:91:ALA:HB2	2:A:153:ILE:HD13	1.84	0.57
2:G:75:LEU:HD11	2:G:99:ILE:HD11	1.86	0.57
2:E:72:VAL:O	2:E:74:VAL:HG23	2.04	0.57
2:C:72:VAL:HG21	2:C:156:ILE:HG22	1.87	0.56
2:E:214:VAL:HG23	2:E:224:ILE:HD13	1.87	0.56
2:C:40:THR:O	2:C:216:THR:HA	2.05	0.56
2:C:22:ILE:HG22	2:C:22:ILE:O	2.06	0.56
2:C:14:VAL:HG13	2:C:222:VAL:HG12	1.86	0.55
2:E:98:GLU:HB2	2:E:102:LYS:HE3	1.87	0.55
2:E:47:LEU:HA	2:E:208:PHE:O	2.07	0.55
1:D:12:A:H4'	1:D:13:G:H5'	1.89	0.55
2:E:10:LEU:HD21	2:E:34:THR:CG2	2.37	0.55
2:G:91:ALA:HB3	2:G:94:VAL:HG22	1.89	0.55
2:C:102:LYS:O	2:C:107:TRP:HB3	2.07	0.55
2:A:100:ILE:O	2:A:104:LEU:HG	2.06	0.55
2:A:105:ASP:O	2:C:205:LYS:HB2	2.06	0.55
2:C:95:GLY:HA3	2:C:99:ILE:HB	1.89	0.55
1:H:31:U:O2'	1:H:32:C:H5'	2.07	0.54
2:E:10:LEU:HD21	2:E:34:THR:HG21	1.89	0.54
2:A:116:THR:O	2:A:119:VAL:HG22	2.06	0.54
2:E:84:LYS:O	2:E:88:GLU:HB3	2.08	0.54
2:E:95:GLY:HA3	2:E:99:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:PRO:HB2	2:E:184:LYS:HG2	1.89	0.54
2:E:129:ARG:HG3	2:E:130:ILE:HD12	1.89	0.54
2:C:77:ILE:HD13	2:C:100:ILE:HD13	1.90	0.53
2:G:75:LEU:HA	2:G:93:TYR:O	2.07	0.53
1:H:35:U:H2'	1:H:36:C:O4'	2.08	0.53
2:C:43:VAL:HG23	2:C:175:VAL:HG11	1.90	0.53
1:D:33:A:HA4'	2:C:46:LYS:HD3	1.89	0.53
2:A:48:GLY:HA2	2:A:210:ARG:HE	1.72	0.53
2:E:72:VAL:HG12	4:E:234:HOH:O	2.07	0.53
2:G:119:VAL:O	2:G:123:VAL:HG23	2.08	0.53
2:C:194:ARG:HD3	2:E:65:PRO:HB3	1.91	0.53
2:E:5:LYS:HB3	2:E:8:ARG:HH21	1.74	0.53
2:E:212:VAL:HG21	2:E:226:PRO:HG3	1.91	0.53
1:H:25:G:O2'	1:H:27:A:N7	2.35	0.53
2:G:130:ILE:HG13	2:G:131:LEU:H	1.74	0.53
2:A:53:ARG:HG2	2:A:56:GLN:HG3	1.90	0.52
2:C:120:MSE:HE3	2:C:145:VAL:CG1	2.38	0.52
2:C:48:GLY:HA2	2:C:210:ARG:HH21	1.73	0.52
1:H:12:A:HA4'	1:H:13:G:O5'	2.09	0.52
2:G:131:LEU:HA	2:G:134:ARG:HB2	1.90	0.52
1:F:1:G:H2'	1:F:2:G:O4'	2.10	0.52
2:G:120:MSE:HE3	2:G:145:VAL:HG13	1.91	0.52
1:H:20:G:O2'	2:A:128:GLY:HA3	2.09	0.52
1:H:31:U:H2'	1:H:32:C:C6	2.45	0.52
2:C:77:ILE:HG12	2:C:99:ILE:HG21	1.92	0.52
2:E:99:ILE:HD12	2:E:102:LYS:CD	2.33	0.52
2:A:113:VAL:HG22	2:A:138:PRO:CG	2.38	0.52
2:C:20:TYR:HB3	2:C:24:GLU:HB3	1.91	0.51
2:E:45:ALA:HA	2:E:211:SER:O	2.09	0.51
2:A:171:ILE:HD13	2:A:196:LEU:HD21	1.92	0.51
2:E:116:THR:O	2:E:119:VAL:HG22	2.10	0.51
1:D:4:A:H2'	1:D:5:G:H8	1.74	0.51
1:F:16:U:H2'	1:F:18:C:C4	2.45	0.51
2:E:62:VAL:CG1	2:E:195:ALA:HB2	2.40	0.51
2:G:114:VAL:HG13	2:G:149:ILE:CD1	2.40	0.51
1:F:16:U:H2'	1:F:18:C:C5	2.44	0.51
2:C:153:ILE:O	2:C:157:LYS:HG2	2.11	0.51
2:G:73:ARG:HA	2:G:92:ASP:CG	2.35	0.51
1:H:30:U:O2'	1:H:31:U:H5'	2.11	0.51
2:C:131:LEU:HB3	2:C:136:LEU:HB2	1.93	0.51
2:C:14:VAL:CG2	2:C:32:LEU:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:A:H4'	2:A:46:LYS:HD3	1.91	0.51
2:E:29:VAL:HG21	2:E:185:LEU:HD13	1.93	0.51
2:E:62:VAL:HG22	2:E:163:PHE:CE2	2.45	0.51
2:A:154:ARG:HG2	2:A:154:ARG:HH11	1.75	0.50
2:A:114:VAL:HG21	2:A:153:ILE:HG12	1.94	0.50
2:E:211:SER:HB2	2:E:213:TYR:CE1	2.46	0.50
2:E:214:VAL:CG2	2:E:224:ILE:HD13	2.41	0.50
2:C:73:ARG:HB2	2:C:110:PHE:HA	1.93	0.50
2:E:147:PHE:C	2:E:149:ILE:H	2.20	0.50
2:C:68:LEU:HD11	2:C:161:ILE:HG22	1.93	0.50
2:E:83:ILE:O	2:E:87:GLU:HG3	2.12	0.50
2:G:33:ALA:HB1	2:G:39:GLU:HB2	1.94	0.50
1:B:4:A:H4'	2:C:118:ASP:HA	1.94	0.50
2:G:114:VAL:HG13	2:G:149:ILE:HD11	1.93	0.49
2:E:22:ILE:HD12	2:E:228:SER:C	2.37	0.49
2:E:107:TRP:O	2:E:108:MSE:HG2	2.13	0.49
2:C:85:GLU:O	2:C:85:GLU:HG2	2.11	0.49
2:A:137:LEU:HD12	2:A:138:PRO:HD2	1.93	0.49
2:C:163:PHE:HB2	2:C:171:ILE:HD11	1.95	0.49
2:A:87:GLU:CG	2:A:94:VAL:HG11	2.41	0.49
2:A:171:ILE:HD13	2:A:196:LEU:CD2	2.43	0.49
1:D:12:A:H4'	1:D:13:G:C5'	2.43	0.49
2:C:14:VAL:CG1	2:C:222:VAL:HG12	2.43	0.49
2:E:47:LEU:CD1	2:E:58:VAL:HG21	2.42	0.49
2:E:17:ASN:O	2:E:19:ILE:HD12	2.13	0.49
2:E:222:VAL:HG23	2:E:222:VAL:O	2.11	0.49
2:E:202:GLU:HA	2:E:202:GLU:OE1	2.11	0.48
1:D:4:A:H2'	1:D:5:G:C8	2.48	0.48
2:G:96:GLY:O	2:G:99:ILE:HG22	2.13	0.48
1:F:31:U:O2'	1:F:32:C:H5'	2.13	0.48
1:H:31:U:O3'	2:G:221:SER:HB3	2.13	0.48
2:C:127:LEU:HB3	2:C:131:LEU:HG	1.95	0.48
2:G:81:GLU:O	2:G:84:LYS:HB3	2.14	0.48
1:B:20:G:H2'	1:B:21:C:C6	2.49	0.48
2:A:75:LEU:HD12	2:A:93:TYR:O	2.13	0.48
1:B:5:G:O2'	1:B:6:U:H5'	2.14	0.48
2:C:177:LYS:O	2:C:180:PHE:HB2	2.13	0.48
2:E:163:PHE:HB2	2:E:171:ILE:HD11	1.95	0.48
1:B:27:A:H2'	4:B:73:HOH:O	2.14	0.47
2:E:19:ILE:HG13	2:E:223:ARG:HD3	1.96	0.47
2:E:200:LYS:HE3	2:E:208:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:C:H4'	1:B:19:G:H5''	1.95	0.47
2:A:137:LEU:HB3	4:A:254:HOH:O	2.12	0.47
2:G:149:ILE:O	2:G:153:ILE:HG13	2.14	0.47
2:A:89:ALA:HB2	2:A:150:GLY:HA2	1.96	0.47
2:C:152:ILE:O	2:C:156:ILE:HG13	2.14	0.47
2:A:99:ILE:O	2:A:103:ILE:HG13	2.15	0.47
1:D:12:A:N1	1:D:23:G:O2'	2.42	0.47
2:A:147:PHE:C	2:A:149:ILE:H	2.22	0.47
2:C:83:ILE:HG23	2:C:94:VAL:HG11	1.95	0.47
2:E:50:ASP:HB3	2:E:53:ARG:HG2	1.97	0.47
2:A:102:LYS:HE2	2:A:107:TRP:CD2	2.50	0.47
2:C:149:ILE:O	2:C:153:ILE:HG13	2.15	0.47
2:C:150:GLY:HA2	2:C:153:ILE:HD12	1.97	0.47
1:F:17:U:O3'	1:F:18:C:H6	1.98	0.47
2:C:108:MSE:HG3	2:C:134:ARG:NH2	2.30	0.46
2:E:61:THR:HA	2:E:161:ILE:O	2.15	0.46
2:E:38:ASP:OD2	2:E:177:LYS:HB3	2.15	0.46
2:E:208:PHE:CD2	2:E:209:LEU:HG	2.51	0.46
1:F:35:U:O2'	1:F:36:C:H5'	2.15	0.46
2:E:53:ARG:HG3	2:E:56:GLN:HB2	1.97	0.46
2:G:47:LEU:HD13	2:G:58:VAL:HG21	1.97	0.46
2:G:101:GLN:O	2:G:104:LEU:HB3	2.15	0.46
2:G:147:PHE:C	2:G:149:ILE:H	2.23	0.46
1:F:15:C:O2'	1:F:16:U:H5'	2.15	0.46
1:H:11:G:H2'	1:H:12:A:C8	2.51	0.46
1:D:4:A:H1'	4:D:40:HOH:O	2.15	0.46
2:A:47:LEU:HD13	2:A:58:VAL:HG21	1.98	0.46
2:G:51:PRO:HG3	2:G:169:GLY:HA2	1.97	0.46
1:D:19:G:H2'	1:D:20:G:O4'	2.15	0.46
2:A:79:LYS:HB3	2:A:118:ASP:OD2	2.15	0.46
2:C:119:VAL:O	2:C:123:VAL:HG23	2.15	0.46
2:E:68:LEU:HD11	2:E:161:ILE:HG22	1.97	0.46
2:E:98:GLU:C	2:E:102:LYS:HE3	2.41	0.46
2:E:171:ILE:O	2:E:171:ILE:HG23	2.16	0.46
2:G:75:LEU:HD11	2:G:99:ILE:CD1	2.46	0.46
2:G:37:PHE:HZ	2:G:217:THR:HG21	1.81	0.45
2:A:87:GLU:CD	2:A:94:VAL:HG11	2.41	0.45
2:E:46:LYS:HE3	2:E:168:THR:O	2.16	0.45
2:E:130:ILE:HD12	2:E:130:ILE:N	2.31	0.45
2:G:119:VAL:HG12	2:G:123:VAL:HG23	1.99	0.45
2:G:96:GLY:H	2:G:99:ILE:HG22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:77:ILE:HD13	2:C:100:ILE:CD1	2.47	0.45
2:C:101:GLN:O	2:C:104:LEU:HB2	2.17	0.45
1:F:16:U:OP1	2:E:5:LYS:HG2	2.17	0.45
2:C:194:ARG:HA	2:C:197:GLU:HG2	1.99	0.45
1:D:31:U:H2'	1:D:32:C:C6	2.52	0.45
1:H:35:U:H2'	1:H:36:C:C6	2.51	0.45
2:C:87:GLU:C	2:C:89:ALA:H	2.25	0.45
2:C:39:GLU:HG3	4:C:229:HOH:O	2.15	0.44
2:C:40:THR:HG22	2:C:41:VAL:O	2.17	0.44
2:C:117:PRO:HD3	2:C:146:GLY:CA	2.47	0.44
2:E:26:ALA:O	2:E:30:LYS:NZ	2.50	0.44
2:E:84:LYS:HA	2:E:87:GLU:OE1	2.16	0.44
2:E:173:ALA:HB3	2:E:192:PHE:CZ	2.53	0.44
2:G:2:LYS:O	2:G:2:LYS:HG3	2.17	0.44
2:A:77:ILE:O	2:A:115:ALA:HA	2.18	0.44
2:C:22:ILE:HG22	2:C:186:ALA:HB1	1.99	0.44
1:H:4:A:H2'	1:H:5:G:O4'	2.18	0.44
2:E:29:VAL:HB	2:E:30:LYS:NZ	2.33	0.44
2:A:151:GLU:O	2:A:155:GLU:HG3	2.18	0.44
2:E:18:LYS:HB3	2:E:20:TYR:CE1	2.52	0.44
2:C:43:VAL:HG23	2:C:175:VAL:CG1	2.47	0.44
2:A:20:TYR:CE2	2:A:28:LEU:HD11	2.52	0.44
2:A:89:ALA:HB2	2:A:150:GLY:CA	2.48	0.44
2:C:107:TRP:CD1	2:C:109:ASP:H	2.36	0.44
2:C:193:ILE:CG2	2:C:226:PRO:HB3	2.44	0.44
2:E:139:ASN:OD1	2:E:141:LYS:N	2.50	0.44
1:F:24:C:H6	1:F:24:C:O5'	2.01	0.44
2:E:175:VAL:O	2:E:175:VAL:HG23	2.18	0.44
1:F:37:C:O2'	1:F:38:C:H5'	2.18	0.44
2:E:127:LEU:N	2:E:127:LEU:CD1	2.80	0.44
2:G:165:ASN:N	2:G:171:ILE:HD12	2.33	0.44
2:E:29:VAL:HB	2:E:30:LYS:HZ1	1.83	0.44
2:E:208:PHE:HD2	2:E:209:LEU:HG	1.83	0.44
2:A:74:VAL:HG11	2:A:153:ILE:HG23	1.99	0.43
2:C:41:VAL:HG23	2:C:176:GLY:O	2.18	0.43
2:E:43:VAL:HB	2:E:192:PHE:CE2	2.53	0.43
2:A:25:ALA:O	2:A:29:VAL:HG23	2.18	0.43
2:A:64:LEU:HA	2:A:65:PRO:HD3	1.81	0.43
2:E:44:HIS:O	2:E:212:VAL:HA	2.18	0.43
2:E:127:LEU:HA	2:E:130:ILE:HD13	2.00	0.43
2:G:75:LEU:HD13	2:G:107:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:22:ILE:HG13	2:A:228:SER:HB2	2.00	0.43
2:E:59:ARG:O	2:E:59:ARG:HG2	2.17	0.43
2:G:61:THR:HG22	2:G:162:GLU:HA	2.00	0.43
1:D:30:U:H4'	2:C:218:MSE:O	2.19	0.43
2:G:200:LYS:HE3	2:G:204:ALA:HB3	2.00	0.43
2:C:21:THR:H	2:C:24:GLU:CB	2.31	0.43
2:C:225:ASN:HA	2:C:226:PRO:HD3	1.88	0.42
2:E:18:LYS:HB3	2:E:20:TYR:HE1	1.84	0.42
1:H:3:G:OP2	2:G:1:PRO:HA	2.19	0.42
2:A:89:ALA:CB	2:A:150:GLY:HA2	2.50	0.42
2:G:100:ILE:O	2:G:104:LEU:HB2	2.20	0.42
2:E:15:ASP:C	2:E:17:ASN:H	2.27	0.42
1:H:5:G:H2'	1:H:6:U:O4'	2.18	0.42
2:C:114:VAL:HA	2:C:144:THR:O	2.20	0.42
2:E:18:LYS:O	2:E:20:TYR:HD1	2.02	0.42
2:G:76:ALA:HB3	2:G:94:VAL:HG13	2.01	0.42
2:E:92:ASP:OD2	2:E:157:LYS:HE2	2.18	0.42
2:A:19:ILE:HD12	2:A:19:ILE:N	2.34	0.42
2:A:153:ILE:O	2:A:157:LYS:HG2	2.19	0.42
2:C:75:LEU:HD21	2:C:103:ILE:HD11	2.01	0.42
1:F:15:C:H2'	1:F:16:U:O4'	2.19	0.42
2:A:53:ARG:HG2	2:A:56:GLN:HE21	1.84	0.42
2:C:20:TYR:HD2	2:C:24:GLU:HG2	1.85	0.42
2:G:115:ALA:HB3	2:G:120:MSE:HE1	2.02	0.42
1:F:30:U:H2'	1:F:31:U:C6	2.55	0.42
2:C:147:PHE:C	2:C:149:ILE:H	2.28	0.42
2:E:23:ASP:O	2:E:27:HIS:HD2	2.03	0.42
2:A:79:LYS:HE2	2:A:119:VAL:HG12	2.02	0.42
2:A:108:MSE:CE	2:A:130:ILE:HG12	2.50	0.42
2:C:37:PHE:HZ	2:C:218:MSE:HE2	1.84	0.41
2:C:65:PRO:HD2	2:C:188:ASN:OD1	2.19	0.41
2:C:149:ILE:HG23	2:C:150:GLY:H	1.85	0.41
2:G:96:GLY:H	2:G:99:ILE:CG2	2.34	0.41
2:G:107:TRP:O	2:G:108:MSE:HG3	2.21	0.41
2:G:184:LYS:O	2:G:187:ASP:HB2	2.20	0.41
2:C:72:VAL:HG23	2:C:74:VAL:HG23	2.02	0.41
2:E:22:ILE:O	2:E:26:ALA:HB2	2.20	0.41
2:C:50:ASP:HB3	2:C:53:ARG:HD3	2.01	0.41
2:E:227:HIS:CD2	2:E:227:HIS:N	2.87	0.41
2:A:40:THR:O	2:A:216:THR:HA	2.20	0.41
2:E:173:ALA:HB3	2:E:192:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:G:O4'	2:C:167:LYS:HE2	2.21	0.41
1:F:11:G:H8	1:F:11:G:O5'	2.04	0.41
2:A:83:ILE:HG23	2:A:94:VAL:HG22	2.02	0.41
2:A:23:ASP:HB2	4:A:233:HOH:O	2.21	0.41
2:A:20:TYR:O	2:A:224:ILE:HA	2.21	0.41
2:C:62:VAL:HG21	2:C:191:ALA:O	2.21	0.41
2:C:117:PRO:HD3	2:C:146:GLY:HA2	2.01	0.41
2:G:175:VAL:O	2:G:175:VAL:HG23	2.21	0.41
2:A:26:ALA:HB1	2:A:182:PRO:O	2.21	0.41
2:C:7:TYR:CE1	2:C:220:PRO:HB3	2.56	0.41
2:C:64:LEU:HA	2:C:65:PRO:HD3	1.90	0.41
2:C:84:LYS:O	2:C:84:LYS:HD3	2.21	0.41
2:G:62:VAL:HG21	2:G:195:ALA:HB2	2.02	0.40
2:A:43:VAL:HA	2:A:213:TYR:O	2.21	0.40
2:E:10:LEU:HD11	2:E:34:THR:OG1	2.21	0.40
2:G:130:ILE:O	2:G:134:ARG:HG2	2.22	0.40
2:E:44:HIS:CE1	2:E:172:HIS:HB3	2.56	0.40
2:E:157:LYS:C	2:E:159:GLY:H	2.29	0.40
2:G:75:LEU:O	2:G:113:VAL:HA	2.21	0.40
1:H:3:G:H2'	1:H:4:A:C8	2.56	0.40
2:A:33:ALA:HB1	4:A:266:HOH:O	2.21	0.40
2:C:77:ILE:HG12	2:C:99:ILE:CG2	2.51	0.40
2:E:73:ARG:HE	2:E:109:ASP:C	2.29	0.40
2:G:64:LEU:HD23	2:G:64:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	226/228 (99%)	212 (94%)	12 (5%)	2 (1%)	14 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	14	30
2	E	226/228 (99%)	191 (84%)	30 (13%)	5 (2%)	5	10
2	G	226/228 (99%)	185 (82%)	38 (17%)	3 (1%)	9	21
All	All	904/912 (99%)	789 (87%)	103 (11%)	12 (1%)	9	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	208	PHE
2	E	20	TYR
2	G	202	GLU
2	C	36	LYS
2	E	39	GLU
2	E	159	GLY
2	E	204	ALA
2	C	118	ASP
2	A	220	PRO
2	G	104	LEU
2	G	106	GLY
2	A	29	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/177 (102%)	170 (94%)	10 (6%)	19	40
2	C	180/177 (102%)	169 (94%)	11 (6%)	17	37
2	E	180/177 (102%)	173 (96%)	7 (4%)	28	55
2	G	180/177 (102%)	172 (96%)	8 (4%)	25	50
All	All	720/708 (102%)	684 (95%)	36 (5%)	22	46

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	LYS
2	A	23	ASP
2	A	53	ARG
2	A	71	GLN
2	A	109	ASP
2	A	113	VAL
2	A	134	ARG
2	A	172	HIS
2	A	183	GLU
2	A	223	ARG
2	C	31	GLU
2	C	49	ILE
2	C	63	SER
2	C	70	LYS
2	C	71	GLN
2	C	97	GLU
2	C	98	GLU
2	C	131	LEU
2	C	149	ILE
2	C	151	GLU
2	C	225	ASN
2	E	30	LYS
2	E	62	VAL
2	E	63	SER
2	E	79	LYS
2	E	98	GLU
2	E	172	HIS
2	E	202	GLU
2	G	11	LEU
2	G	42	GLU
2	G	49	ILE
2	G	63	SER
2	G	72	VAL
2	G	114	VAL
2	G	130	ILE
2	G	149	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	56	GLN
2	A	57	ASN
2	C	66	HIS

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Mol	Chain	Res	Type
2	C	71	GLN
2	E	27	HIS
2	E	56	GLN
2	E	57	ASN
2	E	227	HIS
2	G	56	GLN
2	G	57	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	37/38 (97%)	3 (8%)	1 (2%)
1	D	37/38 (97%)	3 (8%)	0
1	F	37/38 (97%)	6 (16%)	3 (8%)
1	H	37/38 (97%)	6 (16%)	2 (5%)
All	All	148/152 (97%)	18 (12%)	6 (4%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	12	A
1	B	13	G
1	B	18	C
1	D	12	A
1	D	13	G
1	D	20	G
1	F	12	A
1	F	13	G
1	F	17	U
1	F	18	C
1	F	19	G
1	F	25	G
1	H	12	A
1	H	18	C
1	H	19	G
1	H	20	G
1	H	25	G
1	H	26	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	12	A
1	F	12	A
1	F	17	U
1	F	18	C
1	H	17	U
1	H	18	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	38/38 (100%)	0.12	0  	26, 40, 55, 58	0
1	D	38/38 (100%)	0.02	0  	29, 39, 52, 60	0
1	F	38/38 (100%)	0.61	2 (5%)  	34, 50, 82, 88	0
1	H	38/38 (100%)	0.78	2 (5%)  	40, 50, 61, 70	0
2	A	225/228 (98%)	0.14	1 (0%)  	23, 45, 60, 69	0
2	C	225/228 (98%)	0.56	10 (4%)  	34, 51, 69, 80	0
2	E	225/228 (98%)	0.51	5 (2%)  	30, 54, 73, 78	0
2	G	225/228 (98%)	0.42	6 (2%)  	31, 50, 81, 92	0
All	All	1052/1064 (98%)	0.40	26 (2%)  	23, 49, 70, 92	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1	PRO	4.3
2	C	1	PRO	3.3
2	C	226	PRO	3.2
2	E	22	ILE	3.1
2	E	32	LEU	3.1
2	G	104	LEU	3.0
2	C	90	GLY	2.9
2	G	96	GLY	2.9
2	C	149	ILE	2.5
2	E	19	ILE	2.5
1	F	17	U	2.3
2	G	128	GLY	2.3
2	C	89	ALA	2.2
1	H	25	G	2.2
1	H	7	G	2.2
2	G	79	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	67	GLY	2.1
2	E	217	THR	2.1
2	A	81	GLU	2.1
2	C	93	TYR	2.1
2	C	63	SER	2.0
2	C	228	SER	2.0
2	G	88	GLU	2.0
2	E	30	LYS	2.0
1	F	18	C	2.0
2	C	150	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	K	E	229	1/1	0.82	0.20	66,66,66,66	0
3	K	H	39	1/1	0.90	0.13	61,61,61,61	0
3	K	D	39	1/1	0.95	0.07	41,41,41,41	0
3	K	A	229	1/1	0.98	0.06	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.