



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:47 AM EDT

PDB ID : 2GIC / pdb_00002gic
Title : Crystal Structure of a vesicular stomatitis virus nucleocapsid-RNA complex
Authors : Green, T.J.; Zhang, X.; Wertz, G.W.; Luo, M.
Deposited on : 2006-03-28
Resolution : 2.92 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
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

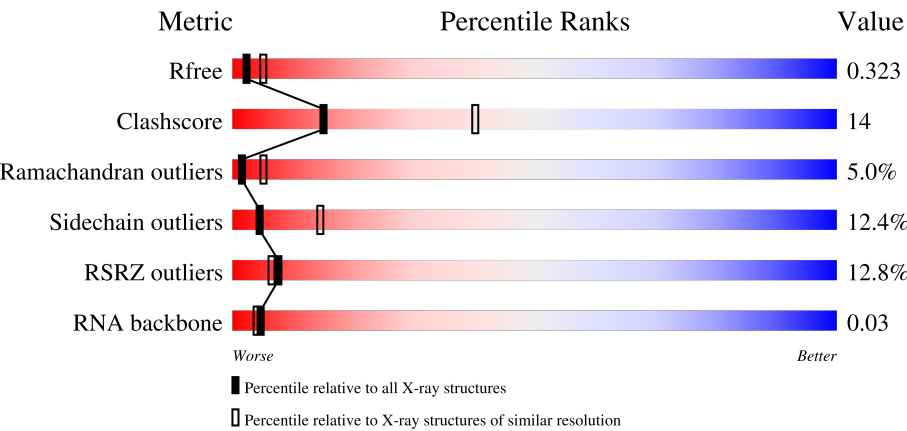
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)
RNA backbone	3983	1016 (3.12-2.72)

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	R	45	
2	A	422	
2	B	422	
2	C	422	

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Mol	Chain	Length	Quality of chain
2	D	422	10% 68% 25% 5%
2	E	422	16% 65% 28% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17432 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.

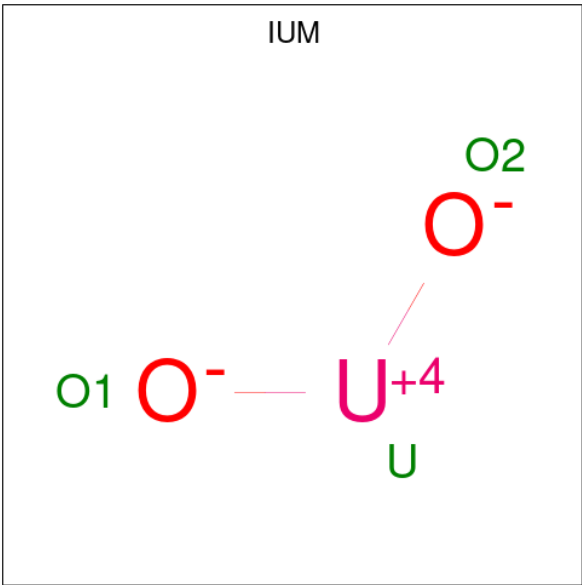
- Molecule 1 is a RNA chain called 45-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			

- Molecule 2 is a protein called Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
2	B	415	Total	C	N	O	S	0	0	0
			3290	2097	552	623	18			
2	C	413	Total	C	N	O	S	0	0	0
			3275	2089	550	618	18			
2	D	416	Total	C	N	O	S	0	0	0
			3298	2103	553	624	18			
2	E	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			

- Molecule 3 is URANYL (VI) ION (CCD ID: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total U 1 1	0	0
3	A	1	Total U 1 1	0	0
3	A	1	Total U 1 1	0	0
3	A	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	C	1	Total U 1 1	0	0
3	C	1	Total U 1 1	0	0
3	C	1	Total U 1 1	0	0
3	D	1	Total U 1 1	0	0
3	D	1	Total U 1 1	0	0
3	E	1	Total U 1 1	0	0
3	E	1	Total U 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	U	0	0
			1	1		

3 Residue-property plots

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

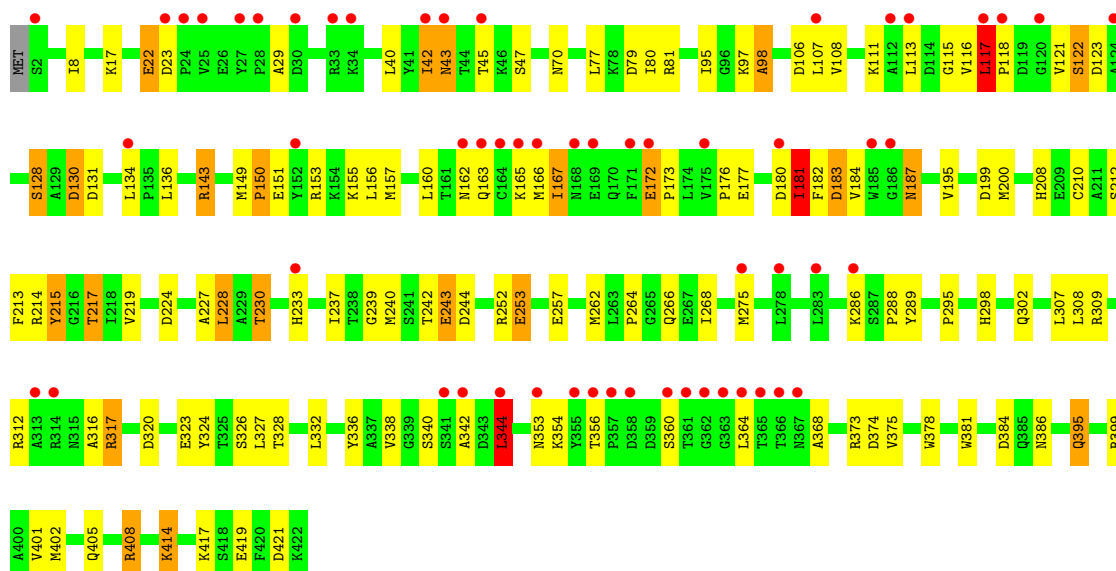
• Molecule 1: 45-MER

Chain R: 



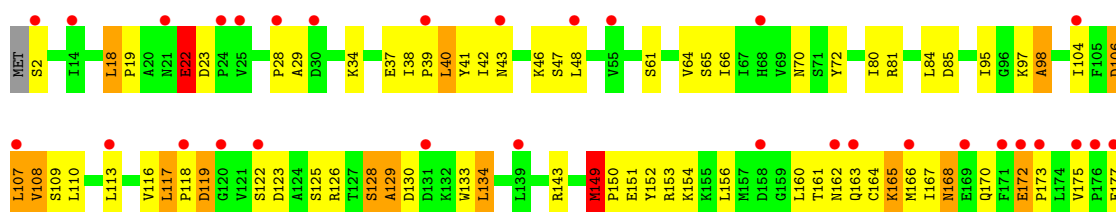
• Molecule 2: Nucleocapsid protein

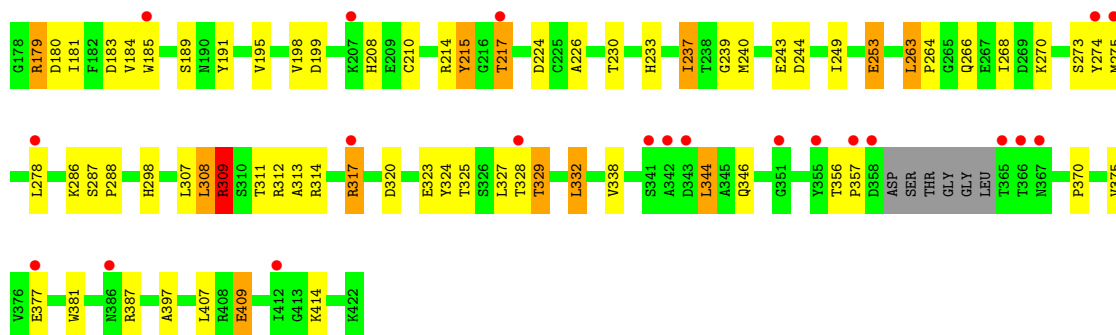
Chain A: 



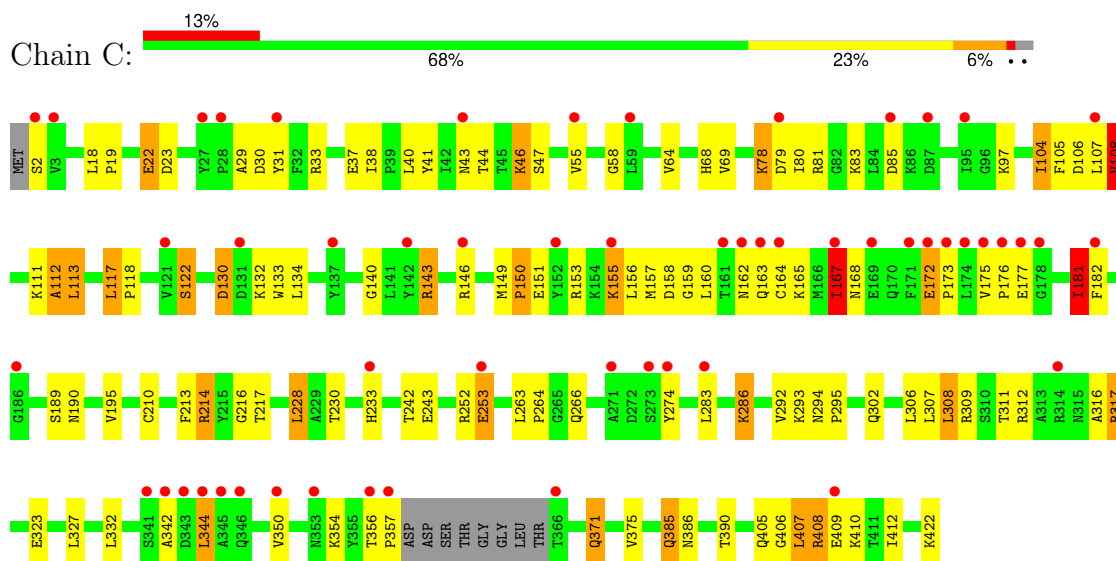
• Molecule 2: Nucleocapsid protein

Chain B: 

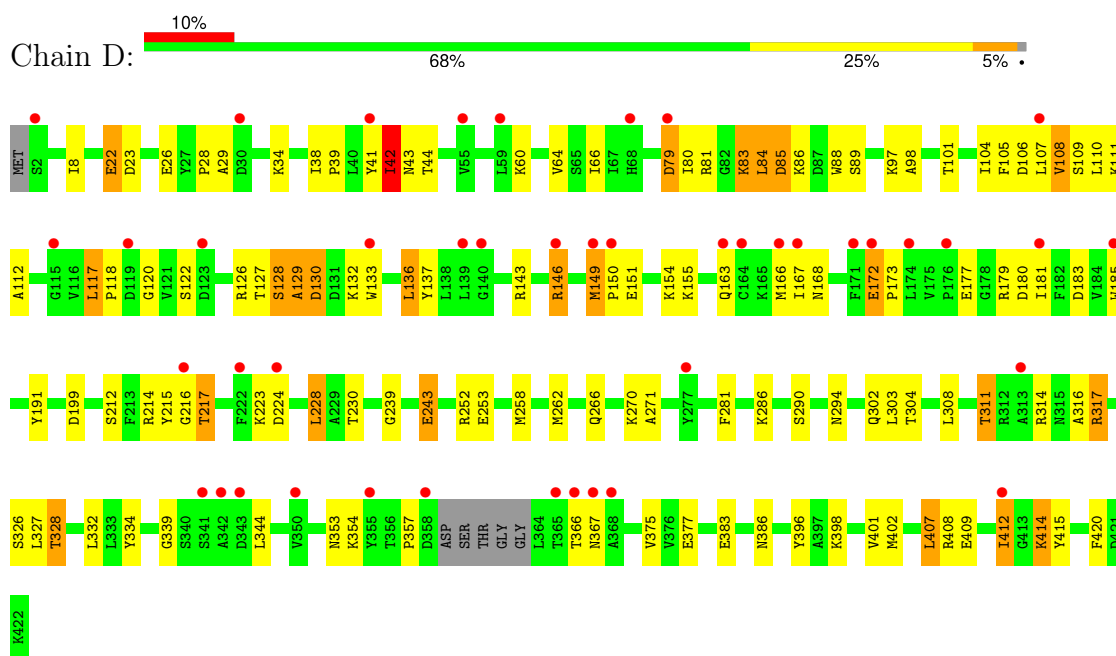




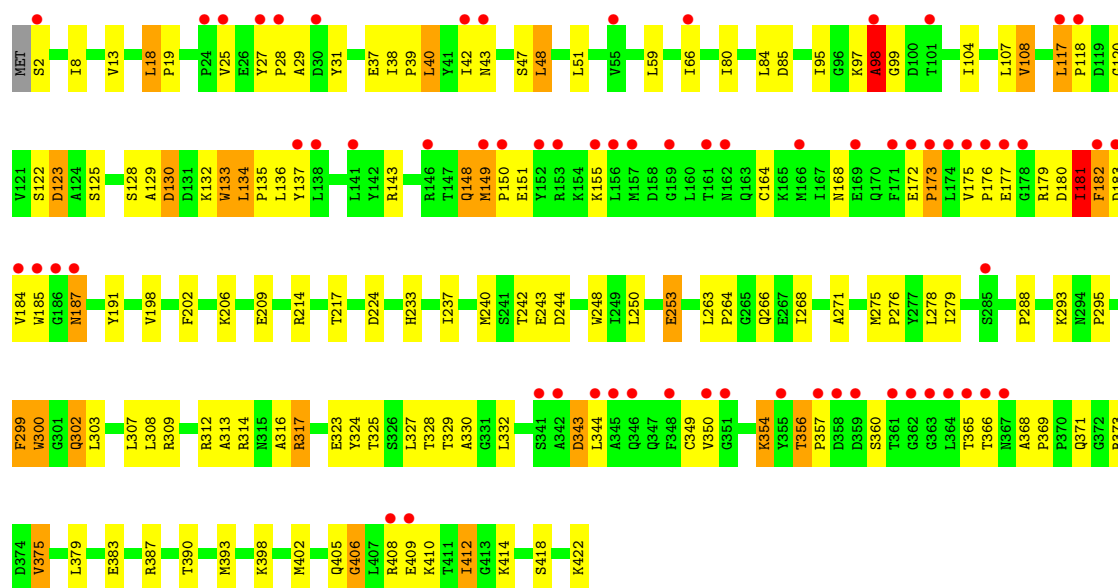
• Molecule 2: Nucleocapsid protein



• Molecule 2: Nucleocapsid protein



• Molecule 2: Nucleocapsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.16Å 236.32Å 75.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.86 – 2.92 44.86 – 2.92	Depositor EDS
% Data completeness (in resolution range)	91.9 (44.86-2.92) 90.5 (44.86-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.255 , 0.306 0.270 , 0.323	Depositor DCC
R_{free} test set	3262 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17432	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	R	0.80	0/989	1.26	6/1526 (0.4%)
2	A	0.51	0/3403	0.85	2/4607 (0.0%)
2	B	0.52	1/3365 (0.0%)	0.87	4/4554 (0.1%)
2	C	0.52	0/3350	0.87	2/4533 (0.0%)
2	D	0.52	1/3373 (0.0%)	0.87	0/4565
2	E	0.53	1/3403 (0.0%)	0.85	3/4607 (0.1%)
All	All	0.54	3/17883 (0.0%)	0.89	17/24392 (0.1%)

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
2	B	0	1
2	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	128	SER	C-N	7.22	1.44	1.33
2	B	64	VAL	C-N	-5.63	1.25	1.33
2	D	106	ASP	C-N	-5.33	1.26	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	20	U	P-O3'-C3'	6.83	130.45	120.20
2	B	263	LEU	CA-C-N	6.47	126.70	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	263	LEU	C-N-CA	6.47	126.70	119.32
1	R	9	U	O4'-C4'-C3'	-6.12	97.88	104.00
2	A	115	GLY	N-CA-C	6.10	118.94	111.93
2	E	224	ASP	N-CA-C	5.77	119.31	111.17
1	R	15	U	N1-C1'-C2'	5.50	120.25	112.00
2	C	112	ALA	N-CA-C	5.46	116.56	108.86
2	A	111	LYS	N-CA-C	5.39	117.51	108.73
2	E	27	TYR	CA-C-N	5.39	124.84	119.24
2	E	27	TYR	C-N-CA	5.39	124.84	119.24
1	R	20	U	C2'-C3'-O3'	5.19	121.49	113.70
2	B	149	MET	CA-C-N	5.17	126.30	119.84
2	B	149	MET	C-N-CA	5.17	126.30	119.84
2	C	113	LEU	N-CA-C	5.16	121.78	110.80
1	R	26	U	C4'-C3'-O3'	-5.11	105.33	113.00
1	R	30	U	C4'-C3'-C2'	-5.07	97.53	102.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106	ASP	Peptide
2	E	98	ALA	Peptide

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	R	900	0	451	61	0
2	A	3327	0	3287	93	0
2	B	3290	0	3253	112	0
2	C	3275	0	3242	82	0
2	D	3298	0	3264	84	0
2	E	3327	0	3287	101	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	0	0
All	All	17432	0	16784	467	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 14.

All (467) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:143:ARG:HD2	2:A:155:LYS:CE	1.44	1.45
2:A:143:ARG:CD	2:A:155:LYS:HE2	1.52	1.36
2:B:109:SER:O	2:B:110:LEU:HD23	1.31	1.22
2:D:107:LEU:O	2:D:108:VAL:HG22	1.42	1.18
2:E:133:TRP:CD1	2:E:134:LEU:H	1.62	1.17
2:B:107:LEU:N	2:B:107:LEU:HD23	1.56	1.16
2:B:37:GLU:HB2	2:B:108:VAL:CG2	1.76	1.14
2:B:117:LEU:HB2	2:B:118:PRO:HD3	1.30	1.11
2:C:143:ARG:HH11	2:C:155:LYS:HD3	1.17	1.08
2:B:106:ASP:C	2:B:107:LEU:HD23	1.79	1.06
1:R:22:U:H2'	2:B:317:ARG:HE	1.21	1.06
2:B:37:GLU:HB2	2:B:108:VAL:HG21	1.34	1.05
2:C:214:ARG:HA	2:C:217:THR:HG22	1.36	1.03
2:A:143:ARG:HD2	2:A:155:LYS:HE3	1.41	0.98
2:D:143:ARG:HE	2:D:155:LYS:HE3	1.27	0.96
2:A:117:LEU:HB3	2:A:118:PRO:HD3	1.46	0.94
2:E:133:TRP:CD1	2:E:134:LEU:N	2.36	0.94
2:D:117:LEU:HB2	2:D:118:PRO:HD3	1.48	0.93
2:B:172:GLU:HB3	2:B:173:PRO:HD3	1.49	0.93
2:B:107:LEU:N	2:B:107:LEU:CD2	2.31	0.92
2:E:129:ALA:HB1	2:E:133:TRP:HE1	1.33	0.91
2:A:143:ARG:HD2	2:A:155:LYS:HE2	0.92	0.90
2:B:37:GLU:HB2	2:B:108:VAL:HG22	1.56	0.88
2:D:214:ARG:HA	2:D:217:THR:HG22	1.54	0.88
2:B:320:ASP:HB3	2:C:312:ARG:NH2	1.89	0.88
2:B:109:SER:O	2:B:110:LEU:CD2	2.21	0.87
2:A:324:TYR:O	2:A:328:THR:HG23	1.76	0.86
2:C:117:LEU:HB2	2:C:118:PRO:HD3	1.59	0.85
2:D:146:ARG:HH11	2:D:223:LYS:HE2	1.40	0.85
2:B:107:LEU:HD13	2:B:274:TYR:OH	1.77	0.84
2:B:117:LEU:HB2	2:B:118:PRO:CD	2.07	0.83
2:C:2:SER:HB3	2:D:243:GLU:HG3	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:LEU:HB2	2:E:118:PRO:HD3	1.60	0.82
2:B:106:ASP:C	2:B:107:LEU:CD2	2.53	0.82
1:R:11:U:H3'	1:R:12:U:H5''	1.62	0.81
2:A:253:GLU:CD	2:A:253:GLU:H	1.88	0.81
2:B:37:GLU:CB	2:B:108:VAL:HG21	2.09	0.81
2:A:143:ARG:CG	2:A:155:LYS:HE2	2.09	0.81
2:B:164:CYS:HA	2:B:168:ASN:H	1.46	0.81
2:C:253:GLU:CD	2:C:253:GLU:H	1.89	0.80
2:D:83:LYS:HG3	2:D:101:THR:HG22	1.64	0.79
2:D:107:LEU:C	2:D:108:VAL:HG22	2.06	0.78
2:D:143:ARG:HE	2:D:155:LYS:CE	1.97	0.78
2:E:324:TYR:O	2:E:328:THR:HG23	1.84	0.78
2:A:323:GLU:OE1	2:B:239:GLY:HA3	1.84	0.77
2:C:143:ARG:NH1	2:C:155:LYS:HD3	1.97	0.77
2:D:107:LEU:O	2:D:108:VAL:CG2	2.30	0.77
2:B:320:ASP:HB3	2:C:312:ARG:HH22	1.47	0.76
2:A:215:TYR:N	2:A:215:TYR:HD2	1.83	0.75
2:D:143:ARG:NE	2:D:155:LYS:HE3	1.99	0.74
2:A:354:LYS:HD2	2:E:379:LEU:HB3	1.68	0.74
2:A:214:ARG:HA	2:A:217:THR:HG22	1.68	0.74
2:A:215:TYR:N	2:A:215:TYR:CD2	2.55	0.74
2:C:117:LEU:CB	2:C:118:PRO:HD3	2.17	0.74
2:E:133:TRP:O	2:E:136:LEU:N	2.20	0.74
1:R:3:U:H2'	1:R:4:U:H4'	1.70	0.73
2:A:240:MET:HE2	2:A:244:ASP:HB3	1.70	0.73
2:D:146:ARG:HH11	2:D:223:LYS:CE	2.01	0.73
2:A:215:TYR:HD2	2:A:215:TYR:H	1.36	0.73
2:E:37:GLU:HB2	2:E:108:VAL:HG21	1.68	0.73
1:R:38:U:H3'	1:R:39:U:H5''	1.69	0.73
2:C:44:THR:OG1	2:C:46:LYS:HE3	1.90	0.71
2:C:172:GLU:H	2:C:173:PRO:HD2	1.55	0.71
2:E:129:ALA:HB1	2:E:133:TRP:NE1	2.04	0.71
2:E:253:GLU:CD	2:E:253:GLU:H	1.98	0.71
2:E:133:TRP:HD1	2:E:133:TRP:H	1.35	0.71
2:A:399:ARG:HB3	2:E:422:LYS:NZ	2.06	0.70
1:R:23:U:H5'	2:B:317:ARG:HH21	1.56	0.70
2:B:214:ARG:HA	2:B:217:THR:HG22	1.74	0.70
1:R:44:U:H5''	2:E:143:ARG:NH2	2.07	0.70
1:R:15:U:C4	2:C:408:ARG:HD3	2.28	0.69
2:D:107:LEU:C	2:D:108:VAL:CG2	2.66	0.69
2:E:356:THR:HG23	2:E:357:PRO:HD3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:323:GLU:CD	2:D:239:GLY:HA3	2.18	0.69
2:C:214:ARG:HA	2:C:217:THR:CG2	2.20	0.68
2:B:179:ARG:HA	2:B:183:ASP:CG	2.18	0.68
2:C:37:GLU:HB2	2:C:108:VAL:HG21	1.76	0.68
2:A:399:ARG:HB3	2:E:422:LYS:HZ2	1.57	0.68
2:E:133:TRP:CD1	2:E:133:TRP:H	2.11	0.68
1:R:23:U:H5'	2:B:317:ARG:NH2	2.09	0.68
1:R:44:U:C2'	1:R:45:U:H5''	2.24	0.66
2:C:79:ASP:C	2:C:81:ARG:H	2.03	0.66
2:B:356:THR:HG23	2:B:357:PRO:HD3	1.77	0.66
2:C:172:GLU:H	2:C:173:PRO:CD	2.08	0.66
2:E:133:TRP:CG	2:E:134:LEU:N	2.64	0.66
1:R:12:U:OP2	2:C:286:LYS:NZ	2.28	0.66
2:E:354:LYS:HE3	2:E:356:THR:HA	1.76	0.66
1:R:29:U:OP1	2:A:286:LYS:NZ	2.25	0.65
2:D:66:ILE:HD13	2:D:185:TRP:CD1	2.31	0.65
1:R:44:U:C3'	1:R:45:U:H5''	2.27	0.64
1:R:13:U:H3'	2:C:317:ARG:HH21	1.62	0.64
2:A:364:LEU:HB3	2:A:368:ALA:HB2	1.80	0.64
2:D:28:PRO:HG2	2:D:266:GLN:HE21	1.62	0.64
2:E:151:GLU:CD	2:E:155:LYS:HD2	2.22	0.64
2:C:233:HIS:CE1	2:C:312:ARG:HE	2.16	0.64
1:R:6:U:H5''	1:R:6:U:C6	2.32	0.63
2:B:240:MET:HE2	2:B:244:ASP:HB3	1.78	0.63
2:E:40:LEU:HD22	2:E:42:ILE:HG13	1.80	0.63
2:E:97:LYS:O	2:E:98:ALA:C	2.40	0.63
2:E:379:LEU:O	2:E:383:GLU:HG2	1.99	0.63
1:R:6:U:O4'	2:D:149:MET:HG3	1.99	0.63
2:B:28:PRO:HG2	2:B:266:GLN:HE21	1.64	0.63
1:R:15:U:H5'	2:C:408:ARG:HH22	1.64	0.62
2:A:143:ARG:CD	2:A:155:LYS:CE	2.32	0.62
2:E:317:ARG:H	2:E:317:ARG:NE	1.97	0.62
2:B:325:THR:O	2:B:329:THR:HG22	2.00	0.62
1:R:15:U:H5''	2:C:408:ARG:HH12	1.64	0.62
1:R:2:U:H3'	1:R:3:U:H5''	1.79	0.62
2:A:42:ILE:HG21	2:A:70:ASN:HB3	1.80	0.62
2:A:253:GLU:O	2:A:257:GLU:HG3	2.00	0.62
1:R:44:U:H2'	1:R:45:U:H5''	1.82	0.61
2:D:29:ALA:H	2:D:266:GLN:HE22	1.47	0.61
2:E:104:ILE:HD11	2:E:198:VAL:HG22	1.81	0.61
2:E:133:TRP:HD1	2:E:134:LEU:H	1.42	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:ARG:HH11	2:C:155:LYS:CD	2.05	0.61
2:E:302:GLN:HG2	2:E:316:ALA:CB	2.31	0.61
1:R:44:U:OP2	2:E:155:LYS:NZ	2.33	0.61
1:R:41:U:O5'	2:E:317:ARG:NH2	2.34	0.60
1:R:17:U:H5''	2:C:143:ARG:HH12	1.65	0.60
2:B:149:MET:O	2:B:151:GLU:N	2.33	0.60
2:B:253:GLU:H	2:B:253:GLU:CD	2.09	0.60
2:B:29:ALA:H	2:B:266:GLN:HE22	1.47	0.60
2:A:253:GLU:CD	2:A:253:GLU:N	2.56	0.60
2:A:395:GLN:HE21	2:A:395:GLN:HA	1.65	0.60
2:C:149:MET:HB2	2:C:150:PRO:HD2	1.84	0.60
2:D:143:ARG:HD2	2:D:216:GLY:HA2	1.83	0.60
2:A:130:ASP:CG	2:A:131:ASP:H	2.09	0.59
2:B:298:HIS:NE2	2:B:317:ARG:NH1	2.50	0.59
2:D:146:ARG:NH1	2:D:223:LYS:NZ	2.51	0.59
2:E:350:VAL:HG12	2:E:350:VAL:O	2.03	0.59
2:C:253:GLU:CD	2:C:253:GLU:N	2.60	0.58
2:E:130:ASP:C	2:E:132:LYS:H	2.10	0.58
2:A:136:LEU:HD22	2:A:163:GLN:HE21	1.68	0.58
2:D:89:SER:O	2:D:270:LYS:NZ	2.35	0.58
2:D:128:SER:OG	2:D:129:ALA:N	2.36	0.58
1:R:17:U:H3'	2:C:143:ARG:HH22	1.68	0.58
2:A:317:ARG:CZ	2:A:317:ARG:H	2.16	0.58
2:B:230:THR:HG21	2:B:298:HIS:CE1	2.38	0.58
2:C:385:GLN:HG2	2:C:390:THR:HG22	1.84	0.58
1:R:3:U:H4'	2:D:224:ASP:HB3	1.86	0.58
2:B:233:HIS:CE1	2:B:312:ARG:HD2	2.39	0.58
1:R:17:U:H2'	1:R:18:U:H5''	1.85	0.58
2:D:303:LEU:HA	2:D:412:ILE:HD13	1.86	0.58
2:B:172:GLU:HB3	2:B:173:PRO:CD	2.29	0.58
2:B:106:ASP:O	2:B:107:LEU:HD22	2.05	0.57
2:D:38:ILE:O	2:D:38:ILE:HG13	2.04	0.57
2:A:165:LYS:HA	2:E:184:VAL:HG22	1.86	0.57
2:D:407:LEU:HD13	2:D:414:LYS:HA	1.86	0.57
2:C:155:LYS:HA	2:C:155:LYS:HE3	1.87	0.57
2:E:390:THR:OG1	2:E:393:MET:HG2	2.04	0.57
2:A:149:MET:C	2:A:151:GLU:H	2.13	0.57
2:B:317:ARG:CZ	2:B:317:ARG:H	2.18	0.57
2:C:55:VAL:HG12	2:C:69:VAL:HG12	1.87	0.57
2:D:179:ARG:HA	2:D:183:ASP:CG	2.29	0.57
1:R:20:U:OP1	2:B:286:LYS:NZ	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ARG:CD	2:D:216:GLY:HA2	2.35	0.56
2:B:104:ILE:HD11	2:B:198:VAL:HG22	1.87	0.56
2:A:262:MET:HA	2:A:262:MET:HE2	1.86	0.56
2:C:143:ARG:HG2	2:C:216:GLY:HA2	1.87	0.56
1:R:24:U:H6	1:R:24:U:H5'	1.70	0.56
2:C:302:GLN:HG2	2:C:316:ALA:CB	2.35	0.56
2:E:278:LEU:HD12	2:E:279:ILE:HG12	1.87	0.56
2:A:17:LYS:HG3	2:B:268:ILE:HD11	1.87	0.56
2:A:187:ASN:N	2:A:187:ASN:HD22	2.02	0.56
2:A:342:ALA:N	2:E:387:ARG:HH12	2.04	0.56
2:B:38:ILE:HD11	2:B:107:LEU:HD12	1.87	0.56
2:C:155:LYS:O	2:C:155:LYS:HG3	2.05	0.56
2:D:105:PHE:C	2:D:107:LEU:H	2.14	0.56
2:C:157:MET:HG3	2:C:158:ASP:H	1.71	0.56
2:B:37:GLU:OE2	2:B:108:VAL:HG11	2.06	0.56
2:B:226:ALA:O	2:B:230:THR:HG23	2.06	0.56
2:C:41:TYR:HB2	2:C:190:ASN:HD21	1.69	0.56
2:E:253:GLU:CD	2:E:253:GLU:N	2.65	0.55
2:D:212:SER:O	2:D:215:TYR:HD1	1.90	0.55
2:E:133:TRP:O	2:E:134:LEU:C	2.48	0.55
1:R:3:U:C2'	1:R:4:U:H4'	2.36	0.55
2:A:166:MET:C	2:A:167:ILE:HG13	2.32	0.55
2:A:336:TYR:O	2:A:340:SER:HB2	2.07	0.55
2:C:149:MET:O	2:C:151:GLU:N	2.38	0.55
2:E:133:TRP:CD1	2:E:133:TRP:N	2.67	0.55
2:A:233:HIS:CE1	2:A:312:ARG:HD2	2.42	0.55
1:R:22:U:H2'	2:B:317:ARG:NE	2.06	0.55
2:E:202:PHE:HB2	2:E:214:ARG:HD3	1.89	0.55
2:B:106:ASP:O	2:B:107:LEU:CD2	2.54	0.55
2:D:136:LEU:HD22	2:D:163:GLN:HG3	1.89	0.54
2:E:240:MET:HE2	2:E:244:ASP:HB3	1.88	0.54
2:A:106:ASP:C	2:A:107:LEU:HD12	2.33	0.54
2:A:399:ARG:HA	2:A:402:MET:HE3	1.90	0.54
2:C:149:MET:C	2:C:151:GLU:H	2.14	0.54
2:C:106:ASP:C	2:C:107:LEU:HD12	2.33	0.54
2:D:258:MET:HE3	2:D:262:MET:CG	2.38	0.54
2:D:328:THR:HG21	2:D:415:TYR:HE1	1.71	0.54
2:B:356:THR:CG2	2:B:357:PRO:HD3	2.37	0.54
2:C:146:ARG:O	2:C:146:ARG:HD3	2.08	0.54
1:R:18:U:H4'	1:R:18:U:OP1	2.08	0.54
2:A:77:LEU:C	2:A:79:ASP:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:257:GLU:OE1	2:A:295:PRO:HD2	2.08	0.54
2:B:118:PRO:O	2:B:119:ASP:HB2	2.08	0.53
2:B:324:TYR:O	2:B:328:THR:HG22	2.07	0.53
2:E:268:ILE:HG22	2:E:275:MET:HG3	1.89	0.53
2:A:117:LEU:HB3	2:A:118:PRO:CD	2.29	0.53
2:B:109:SER:C	2:B:110:LEU:HD23	2.24	0.53
1:R:6:U:H5''	1:R:6:U:H6	1.72	0.53
2:A:149:MET:O	2:A:151:GLU:N	2.41	0.53
2:B:317:ARG:NH1	2:B:317:ARG:H	2.06	0.53
2:B:208:HIS:HD1	2:B:210:CYS:H	1.56	0.53
2:E:97:LYS:O	2:E:99:GLY:N	2.42	0.53
1:R:30:U:H2'	1:R:31:U:O4'	2.09	0.53
2:A:302:GLN:HG2	2:A:316:ALA:CB	2.39	0.53
2:C:29:ALA:H	2:C:266:GLN:HE22	1.57	0.53
2:C:38:ILE:HG13	2:C:38:ILE:O	2.08	0.53
2:E:149:MET:O	2:E:151:GLU:N	2.38	0.53
2:C:210:CYS:HB3	2:C:213:PHE:CE1	2.44	0.52
1:R:41:U:C4	2:E:312:ARG:HG3	2.44	0.52
2:E:129:ALA:O	2:E:133:TRP:CD1	2.62	0.52
2:A:23:ASP:HB2	2:A:286:LYS:NZ	2.24	0.52
2:B:66:ILE:HD13	2:B:185:TRP:CD1	2.44	0.52
2:C:43:ASN:CG	2:C:112:ALA:HB3	2.35	0.52
2:D:304:THR:HG21	2:D:334:TYR:CD2	2.45	0.52
1:R:14:U:H5''	2:C:317:ARG:HH22	1.74	0.52
2:D:149:MET:C	2:D:151:GLU:H	2.18	0.52
2:E:151:GLU:OE2	2:E:155:LYS:HD2	2.09	0.52
2:B:320:ASP:CB	2:C:312:ARG:HH22	2.22	0.52
2:D:43:ASN:HB2	2:D:112:ALA:N	2.25	0.52
1:R:4:U:OP2	2:D:290:SER:HB2	2.10	0.52
2:D:107:LEU:HD11	2:D:281:PHE:CZ	2.45	0.52
2:D:317:ARG:H	2:D:317:ARG:NE	2.08	0.52
2:A:298:HIS:NE2	2:A:317:ARG:NH1	2.58	0.51
2:B:149:MET:C	2:B:151:GLU:H	2.18	0.51
1:R:4:U:C6	2:D:317:ARG:HG3	2.44	0.51
2:A:29:ALA:H	2:A:266:GLN:HE22	1.57	0.51
2:E:233:HIS:O	2:E:237:ILE:HG12	2.11	0.51
1:R:8:U:P	2:D:155:LYS:NZ	2.83	0.51
1:R:26:U:H5''	2:B:143:ARG:HH21	1.76	0.51
2:B:66:ILE:HD13	2:B:185:TRP:CG	2.46	0.51
2:B:104:ILE:HD11	2:B:198:VAL:HA	1.92	0.51
2:D:149:MET:O	2:D:151:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:LEU:CD1	2:D:281:PHE:CZ	2.93	0.51
2:A:143:ARG:HG3	2:A:155:LYS:HE2	1.92	0.51
1:R:23:U:C5'	2:B:317:ARG:NH2	2.74	0.50
2:C:133:TRP:HB3	2:C:167:ILE:HD12	1.92	0.50
1:R:44:U:H5''	2:E:143:ARG:HH22	1.76	0.50
2:C:293:LYS:C	2:C:295:PRO:HD3	2.36	0.50
2:B:270:LYS:HE3	2:B:273:SER:HB2	1.93	0.50
2:B:160:LEU:HD12	2:B:161:THR:HG23	1.94	0.50
2:B:253:GLU:CD	2:B:253:GLU:N	2.70	0.50
2:D:146:ARG:NH1	2:D:223:LYS:CE	2.74	0.50
2:E:343:ASP:OD2	2:E:373:ARG:NH2	2.45	0.50
1:R:13:U:H3'	2:C:317:ARG:NH2	2.25	0.50
2:A:143:ARG:HD3	2:A:219:VAL:HG11	1.94	0.50
2:D:117:LEU:HB2	2:D:118:PRO:CD	2.32	0.50
2:A:324:TYR:HD1	2:B:237:ILE:HD11	1.76	0.50
2:B:65:SER:HB2	2:B:117:LEU:HD11	1.94	0.50
2:D:133:TRP:HB3	2:D:167:ILE:HD13	1.94	0.50
1:R:2:U:OP1	2:D:286:LYS:NZ	2.34	0.49
2:A:214:ARG:HA	2:A:217:THR:CG2	2.38	0.49
2:B:268:ILE:HG22	2:B:275:MET:HE3	1.93	0.49
2:A:143:ARG:HH11	2:A:155:LYS:HE3	1.77	0.49
2:D:328:THR:HG21	2:D:415:TYR:CE1	2.46	0.49
2:E:66:ILE:HD13	2:E:185:TRP:CD1	2.47	0.49
2:A:136:LEU:HD21	2:A:162:ASN:HD22	1.77	0.49
2:B:128:SER:O	2:B:129:ALA:C	2.56	0.49
2:B:38:ILE:HG13	2:B:38:ILE:O	2.13	0.48
2:C:79:ASP:C	2:C:81:ARG:N	2.68	0.48
2:A:320:ASP:HA	2:A:324:TYR:OH	2.14	0.48
2:A:338:VAL:HG13	2:A:373:ARG:NH1	2.28	0.48
2:B:107:LEU:CD1	2:B:274:TYR:HE2	2.26	0.48
2:E:149:MET:C	2:E:151:GLU:H	2.21	0.48
2:B:107:LEU:HD23	2:B:107:LEU:H	1.66	0.48
2:B:123:ASP:C	2:B:125:SER:H	2.21	0.48
2:D:172:GLU:HB3	2:D:173:PRO:HD3	1.96	0.48
1:R:6:U:H3'	2:D:408:ARG:HH22	1.79	0.48
2:D:109:SER:O	2:D:110:LEU:HD23	2.14	0.47
2:A:210:CYS:HB3	2:A:213:PHE:CE1	2.49	0.47
2:C:117:LEU:CB	2:C:118:PRO:CD	2.90	0.47
2:E:29:ALA:H	2:E:266:GLN:HE22	1.62	0.47
1:R:4:U:H3'	2:D:317:ARG:NE	2.28	0.47
2:C:342:ALA:HB1	2:C:344:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:27:U:O2'	1:R:29:U:OP2	2.32	0.47
2:A:239:GLY:HA3	2:E:323:GLU:CD	2.40	0.47
2:A:166:MET:H	2:E:184:VAL:HG13	1.80	0.47
1:R:8:U:P	2:D:155:LYS:HZ1	2.38	0.47
2:A:414:LYS:HE3	2:A:414:LYS:HA	1.95	0.47
2:A:81:ARG:HD2	2:A:208:HIS:HE2	1.80	0.47
2:B:107:LEU:CD1	2:B:274:TYR:CE2	2.98	0.47
2:B:172:GLU:CB	2:B:173:PRO:HD3	2.33	0.47
1:R:21:U:H4'	2:B:224:ASP:CG	2.40	0.47
2:B:66:ILE:O	2:B:70:ASN:ND2	2.48	0.47
2:B:184:VAL:HG13	2:C:165:LYS:HA	1.96	0.47
2:C:19:PRO:HD3	2:D:228:LEU:HD22	1.97	0.47
2:C:105:PHE:C	2:C:107:LEU:H	2.22	0.47
2:A:42:ILE:CG2	2:A:70:ASN:HB3	2.45	0.46
2:B:107:LEU:HD13	2:B:274:TYR:CZ	2.50	0.46
2:E:117:LEU:CB	2:E:118:PRO:HD3	2.36	0.46
2:E:250:LEU:HD22	2:E:379:LEU:HD21	1.98	0.46
2:E:368:ALA:HB1	2:E:369:PRO:HD2	1.96	0.46
2:B:41:TYR:HA	2:B:110:LEU:O	2.15	0.46
2:B:332:LEU:HD21	2:B:397:ALA:HB2	1.98	0.46
2:E:325:THR:O	2:E:329:THR:HG22	2.15	0.46
2:A:268:ILE:HG22	2:A:275:MET:SD	2.56	0.46
2:D:66:ILE:HD11	2:D:191:TYR:HB2	1.97	0.46
2:D:84:LEU:HD11	2:D:88:TRP:HB2	1.96	0.46
2:A:419:GLU:OE1	2:B:309:ARG:NH1	2.48	0.46
1:R:23:U:C5'	2:B:317:ARG:HH21	2.26	0.46
2:B:409:GLU:N	2:B:409:GLU:OE2	2.48	0.46
2:D:339:GLY:HA3	2:D:396:TYR:OH	2.16	0.46
1:R:8:U:OP1	2:D:154:LYS:NZ	2.46	0.46
2:B:152:TYR:HD1	2:B:153:ARG:H	1.63	0.46
2:B:199:ASP:OD1	2:B:214:ARG:HD2	2.16	0.46
2:A:97:LYS:O	2:A:98:ALA:C	2.59	0.46
2:D:199:ASP:OD1	2:D:217:THR:HG23	2.16	0.46
2:E:130:ASP:O	2:E:132:LYS:N	2.49	0.46
2:B:72:TYR:CE1	2:B:134:LEU:HD12	2.51	0.46
2:B:317:ARG:O	2:B:317:ARG:HG2	2.16	0.46
2:E:130:ASP:C	2:E:132:LYS:N	2.73	0.46
2:A:43:ASN:ND2	2:A:45:THR:OG1	2.48	0.45
2:B:133:TRP:HB3	2:B:167:ILE:HG21	1.99	0.45
2:D:317:ARG:H	2:D:317:ARG:CD	2.28	0.45
2:E:175:VAL:HB	2:E:176:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:GLU:N	2:C:173:PRO:HD2	2.27	0.45
2:A:374:ASP:O	2:A:378:TRP:HD1	1.98	0.45
2:B:128:SER:C	2:B:130:ASP:N	2.70	0.45
2:E:263:LEU:HA	2:E:264:PRO:HD3	1.83	0.45
2:E:299:PHE:O	2:E:300:TRP:C	2.59	0.45
1:R:11:U:H3'	1:R:12:U:C5'	2.42	0.45
2:B:18:LEU:HD21	2:C:242:THR:HG22	1.97	0.45
2:A:128:SER:C	2:A:130:ASP:H	2.23	0.45
2:A:149:MET:C	2:A:151:GLU:N	2.75	0.45
2:B:313:ALA:O	2:B:314:ARG:C	2.58	0.45
2:C:31:TYR:CD2	2:C:283:LEU:HA	2.51	0.45
2:E:129:ALA:O	2:E:133:TRP:HD1	1.99	0.45
2:B:37:GLU:CG	2:B:108:VAL:HG21	2.46	0.45
2:E:233:HIS:HB2	2:E:312:ARG:CZ	2.47	0.45
1:R:31:U:H3'	2:A:317:ARG:NE	2.30	0.45
2:A:354:LYS:HE3	2:A:356:THR:HA	1.99	0.45
2:B:81:ARG:HD3	2:B:208:HIS:CE1	2.52	0.45
2:B:128:SER:O	2:B:130:ASP:N	2.49	0.45
2:C:41:TYR:HB2	2:C:190:ASN:ND2	2.31	0.45
2:C:140:GLY:HA2	2:C:216:GLY:HA3	1.97	0.45
2:E:299:PHE:HE1	2:E:328:THR:HG22	1.82	0.45
2:A:228:LEU:HD12	2:E:19:PRO:HD3	1.98	0.45
2:C:104:ILE:HD12	2:C:104:ILE:N	2.32	0.45
2:B:152:TYR:HD1	2:B:153:ARG:N	2.14	0.45
2:B:287:SER:HA	2:B:288:PRO:HD3	1.88	0.45
2:D:146:ARG:NH1	2:D:223:LYS:HE2	2.20	0.45
2:B:66:ILE:HD11	2:B:191:TYR:HB2	1.99	0.44
2:C:68:HIS:HE1	2:C:117:LEU:H	1.66	0.44
1:R:14:U:C5'	2:C:317:ARG:HH22	2.30	0.44
2:A:182:PHE:C	2:A:184:VAL:H	2.26	0.44
2:B:308:LEU:O	2:B:309:ARG:HB2	2.16	0.44
2:C:405:GLN:O	2:C:407:LEU:HG	2.16	0.44
2:A:417:LYS:HE2	2:A:421:ASP:OD2	2.18	0.44
2:B:38:ILE:H	2:B:108:VAL:HG23	1.82	0.44
2:C:317:ARG:H	2:C:317:ARG:NH1	2.16	0.44
2:E:179:ARG:HA	2:E:183:ASP:CG	2.43	0.44
2:E:398:LYS:HG2	2:E:402:MET:HE2	2.00	0.44
1:R:2:U:H3'	1:R:3:U:C5'	2.46	0.44
2:D:117:LEU:CB	2:D:118:PRO:HD3	2.34	0.44
2:B:346:GLN:O	2:E:8:ILE:HD11	2.18	0.44
2:E:48:LEU:HA	2:E:51:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:17:U:C5'	2:C:155:LYS:HZ3	2.31	0.44
2:C:162:ASN:C	2:C:164:CYS:H	2.24	0.44
2:C:306:LEU:HD22	2:C:412:ILE:HD12	1.99	0.44
2:A:122:SER:OG	2:A:123:ASP:N	2.50	0.43
2:B:215:TYR:CD2	2:B:215:TYR:N	2.86	0.43
2:C:308:LEU:O	2:C:309:ARG:HB2	2.17	0.43
2:E:172:GLU:H	2:E:173:PRO:CD	2.31	0.43
2:D:28:PRO:HG2	2:D:266:GLN:NE2	2.31	0.43
2:E:172:GLU:H	2:E:173:PRO:HD2	1.84	0.43
2:E:148:GLN:HG2	2:E:179:ARG:HD2	2.00	0.43
2:D:214:ARG:HA	2:D:217:THR:CG2	2.37	0.43
2:E:123:ASP:C	2:E:125:SER:H	2.26	0.43
1:R:14:U:O5'	2:C:317:ARG:NH2	2.51	0.43
2:C:263:LEU:HA	2:C:264:PRO:HD3	1.84	0.43
2:D:128:SER:C	2:D:130:ASP:N	2.76	0.43
2:D:302:GLN:HG2	2:D:316:ALA:CB	2.48	0.43
2:A:227:ALA:HA	2:A:230:THR:HG23	2.01	0.43
2:E:28:PRO:O	2:E:31:TYR:HB3	2.19	0.43
2:E:66:ILE:HD11	2:E:191:TYR:HB2	2.00	0.43
2:E:172:GLU:N	2:E:173:PRO:CD	2.81	0.43
2:E:59:LEU:HD11	2:E:137:TYR:CE2	2.53	0.43
2:E:233:HIS:HB2	2:E:312:ARG:NH1	2.34	0.43
2:E:366:THR:C	2:E:368:ALA:H	2.27	0.43
2:A:228:LEU:HD23	2:A:289:TYR:HB3	2.00	0.43
2:E:25:VAL:HG11	2:E:288:PRO:HA	2.01	0.43
2:E:303:LEU:HA	2:E:412:ILE:HD13	2.00	0.43
2:B:22:GLU:O	2:B:23:ASP:C	2.62	0.43
2:D:258:MET:HE3	2:D:262:MET:HG3	1.99	0.43
2:A:288:PRO:HG2	2:A:289:TYR:CE2	2.53	0.43
2:E:181:ILE:HB	2:E:182:PHE:H	1.72	0.43
2:D:85:ASP:OD1	2:D:86:LYS:HE3	2.19	0.42
2:B:97:LYS:O	2:B:98:ALA:C	2.61	0.42
2:C:107:LEU:HD23	2:C:274:TYR:HE2	1.84	0.42
1:R:6:U:O5'	2:D:149:MET:HE3	2.20	0.42
2:E:38:ILE:HA	2:E:39:PRO:HD3	1.84	0.42
2:A:408:ARG:H	2:A:408:ARG:HG2	1.65	0.42
2:A:212:SER:O	2:A:215:TYR:CD2	2.72	0.42
2:B:152:TYR:C	2:B:154:LYS:H	2.27	0.42
2:D:303:LEU:HD22	2:D:328:THR:HG22	2.01	0.42
2:D:130:ASP:C	2:D:132:LYS:N	2.75	0.42
2:E:38:ILE:HD11	2:E:107:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:248:TRP:CD1	2:E:375:VAL:HG22	2.55	0.42
2:A:344:LEU:HD21	2:E:330:ALA:HB2	2.01	0.42
2:B:19:PRO:HD3	2:C:228:LEU:HD22	2.02	0.42
2:B:152:TYR:CD1	2:B:153:ARG:N	2.88	0.42
2:B:263:LEU:HA	2:B:264:PRO:HD3	1.82	0.42
2:D:137:TYR:OH	2:D:173:PRO:HD3	2.20	0.42
2:E:302:GLN:HG3	2:E:313:ALA:HB1	2.00	0.42
2:A:181:ILE:N	2:A:183:ASP:OD1	2.53	0.42
2:A:199:ASP:OD1	2:A:217:THR:HG23	2.19	0.42
2:B:81:ARG:HD3	2:B:208:HIS:NE2	2.34	0.42
2:B:199:ASP:CG	2:B:214:ARG:HH11	2.27	0.42
2:E:409:GLU:HA	2:E:414:LYS:HD2	2.01	0.42
1:R:27:U:H4'	1:R:29:U:C5	2.54	0.42
2:E:172:GLU:N	2:E:173:PRO:HD2	2.34	0.42
2:C:78:LYS:HA	2:C:78:LYS:HD3	1.81	0.42
2:D:105:PHE:C	2:D:107:LEU:N	2.78	0.42
2:B:149:MET:C	2:B:151:GLU:N	2.78	0.41
2:C:409:GLU:O	2:C:410:LYS:HB2	2.19	0.41
2:D:398:LYS:O	2:D:402:MET:HG2	2.20	0.41
1:R:23:U:H2'	1:R:25:U:H5''	2.02	0.41
2:A:149:MET:HE3	2:A:150:PRO:HD2	2.02	0.41
2:A:172:GLU:CB	2:A:173:PRO:HD3	2.50	0.41
2:B:40:LEU:HD13	2:B:42:ILE:HD11	2.02	0.41
2:A:342:ALA:H	2:E:387:ARG:HH12	1.68	0.41
2:D:43:ASN:ND2	2:D:111:LYS:HD3	2.35	0.41
2:A:130:ASP:CG	2:A:131:ASP:N	2.77	0.41
2:A:342:ALA:HB2	2:E:329:THR:HG21	2.02	0.41
2:A:381:TRP:O	2:A:384:ASP:HB2	2.20	0.41
2:B:370:PRO:HD3	2:B:381:TRP:CG	2.56	0.41
2:D:79:ASP:HB2	2:D:81:ARG:HG3	2.02	0.41
2:D:290:SER:O	2:D:294:ASN:ND2	2.50	0.41
1:R:31:U:H2'	2:A:317:ARG:HE	1.84	0.41
2:E:187:ASN:HD22	2:E:187:ASN:HA	1.70	0.41
2:E:275:MET:HB3	2:E:276:PRO:HD3	2.01	0.41
2:C:175:VAL:O	2:C:181:ILE:HG12	2.20	0.41
2:C:293:LYS:HD2	2:C:293:LYS:HA	1.91	0.41
2:E:214:ARG:HA	2:E:217:THR:OG1	2.21	0.41
2:C:294:ASN:N	2:C:295:PRO:HD3	2.36	0.41
2:E:133:TRP:O	2:E:135:PRO:N	2.54	0.41
2:A:107:LEU:HD21	2:A:200:MET:HE1	2.02	0.41
2:A:199:ASP:OD1	2:A:214:ARG:NE	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:243:GLU:HG3	2:E:2:SER:HB3	2.02	0.41
2:A:401:VAL:HG23	2:A:421:ASP:HB2	2.03	0.41
2:D:41:TYR:C	2:D:42:ILE:HG13	2.45	0.41
2:D:128:SER:C	2:D:130:ASP:H	2.29	0.41
2:D:311:THR:O	2:D:314:ARG:HG2	2.21	0.41
2:E:405:GLN:O	2:E:406:GLY:C	2.64	0.41
2:E:18:LEU:HB2	2:E:19:PRO:HD2	2.03	0.40
2:B:28:PRO:HG2	2:B:266:GLN:NE2	2.34	0.40
2:B:38:ILE:HA	2:B:39:PRO:HD3	1.88	0.40
2:C:181:ILE:HB	2:C:182:PHE:H	1.51	0.40
2:D:401:VAL:HG21	2:D:420:PHE:HB2	2.03	0.40
2:E:293:LYS:C	2:E:295:PRO:HD3	2.46	0.40
2:E:302:GLN:HG3	2:E:313:ALA:CB	2.51	0.40
1:R:13:U:H5'	1:R:14:U:OP2	2.21	0.40
2:A:395:GLN:HA	2:A:395:GLN:NE2	2.35	0.40
2:D:43:ASN:HD22	2:D:111:LYS:HD3	1.85	0.40
1:R:20:U:H2'	1:R:21:U:O4'	2.21	0.40
2:B:166:MET:C	2:B:167:ILE:HG13	2.45	0.40
2:C:22:GLU:HB3	2:C:23:ASP:H	1.55	0.40
2:C:356:THR:N	2:C:357:PRO:HD3	2.36	0.40
2:D:38:ILE:HA	2:D:39:PRO:HD3	1.91	0.40
2:B:118:PRO:O	2:B:119:ASP:CB	2.70	0.40
2:C:58:GLY:HA3	2:C:64:VAL:HB	2.03	0.40
2:C:130:ASP:C	2:C:132:LYS:H	2.30	0.40
2:D:130:ASP:C	2:D:132:LYS:H	2.29	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	419/422 (99%)	354 (84%)	46 (11%)	19 (4%)	2 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	411/422 (97%)	344 (84%)	45 (11%)	22 (5%)	1	4
2	C	409/422 (97%)	340 (83%)	49 (12%)	20 (5%)	1	5
2	D	412/422 (98%)	343 (83%)	48 (12%)	21 (5%)	1	5
2	E	419/422 (99%)	349 (83%)	48 (12%)	22 (5%)	1	4
All	All	2070/2110 (98%)	1730 (84%)	236 (11%)	104 (5%)	1	5

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	47	SER
2	A	98	ALA
2	A	113	LEU
2	A	172	GLU
2	B	98	ALA
2	B	117	LEU
2	B	122	SER
2	B	128	SER
2	B	150	PRO
2	B	168	ASN
2	C	113	LEU
2	C	117	LEU
2	C	122	SER
2	C	172	GLU
2	C	181	ILE
2	D	98	ALA
2	D	122	SER
2	D	357	PRO
2	E	98	ALA
2	A	150	PRO
2	A	181	ILE
2	A	344	LEU
2	B	22	GLU
2	B	47	SER
2	B	119	ASP
2	B	129	ALA
2	B	172	GLU
2	B	177	GLU
2	B	344	LEU
2	C	130	ASP
2	C	150	PRO
2	C	344	LEU

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Mol	Chain	Res	Type
2	C	371	GLN
2	D	120	GLY
2	D	130	ASP
2	D	168	ASN
2	D	344	LEU
2	D	366	THR
2	D	386	ASN
2	E	47	SER
2	E	120	GLY
2	E	122	SER
2	E	177	GLU
2	E	343	ASP
2	E	344	LEU
2	E	360	SER
2	E	371	GLN
2	E	406	GLY
2	A	22	GLU
2	A	176	PRO
2	A	180	ASP
2	A	386	ASN
2	B	43	ASN
2	B	61	SER
2	B	113	LEU
2	B	170	GLN
2	B	180	ASP
2	D	79	ASP
2	D	127	THR
2	D	150	PRO
2	D	172	GLU
2	D	180	ASP
2	E	150	PRO
2	E	299	PHE
2	E	300	TRP
2	A	117	LEU
2	A	122	SER
2	A	130	ASP
2	B	165	LYS
2	C	22	GLU
2	C	168	ASN
2	C	176	PRO
2	C	386	ASN
2	C	406	GLY

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Mol	Chain	Res	Type
2	D	22	GLU
2	D	129	ALA
2	E	108	VAL
2	E	164	CYS
2	E	168	ASN
2	E	365	THR
2	A	128	SER
2	A	360	SER
2	C	47	SER
2	C	83	LYS
2	C	108	VAL
2	C	159	GLY
2	D	117	LEU
2	D	128	SER
2	D	271	ALA
2	E	173	PRO
2	E	271	ALA
2	B	179	ARG
2	B	309	ARG
2	C	167	ILE
2	E	80	ILE
2	E	117	LEU
2	A	121	VAL
2	A	264	PRO
2	C	80	ILE
2	E	181	ILE
2	B	80	ILE
2	D	42	ILE
2	D	80	ILE
2	A	108	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	362/363 (100%)	317 (88%)	45 (12%)	4 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	358/363 (99%)	310 (87%)	48 (13%)	4	12
2	C	356/363 (98%)	310 (87%)	46 (13%)	4	13
2	D	359/363 (99%)	314 (88%)	45 (12%)	4	14
2	E	362/363 (100%)	323 (89%)	39 (11%)	6	20
All	All	1797/1815 (99%)	1574 (88%)	223 (12%)	4	14

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	8	ILE
2	A	22	GLU
2	A	40	LEU
2	A	42	ILE
2	A	43	ASN
2	A	80	ILE
2	A	95	ILE
2	A	116	VAL
2	A	117	LEU
2	A	134	LEU
2	A	143	ARG
2	A	153	ARG
2	A	156	LEU
2	A	157	MET
2	A	160	LEU
2	A	167	ILE
2	A	177	GLU
2	A	181	ILE
2	A	183	ASP
2	A	187	ASN
2	A	195	VAL
2	A	215	TYR
2	A	217	THR
2	A	224	ASP
2	A	228	LEU
2	A	230	THR
2	A	237	ILE
2	A	242	THR
2	A	243	GLU
2	A	252	ARG
2	A	253	GLU
2	A	307	LEU

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Mol	Chain	Res	Type
2	A	308	LEU
2	A	309	ARG
2	A	317	ARG
2	A	326	SER
2	A	327	LEU
2	A	332	LEU
2	A	344	LEU
2	A	353	ASN
2	A	375	VAL
2	A	395	GLN
2	A	405	GLN
2	A	408	ARG
2	A	414	LYS
2	B	2	SER
2	B	18	LEU
2	B	22	GLU
2	B	34	LYS
2	B	40	LEU
2	B	46	LYS
2	B	48	LEU
2	B	84	LEU
2	B	85	ASP
2	B	95	ILE
2	B	107	LEU
2	B	108	VAL
2	B	116	VAL
2	B	126	ARG
2	B	134	LEU
2	B	149	MET
2	B	156	LEU
2	B	162	ASN
2	B	163	GLN
2	B	165	LYS
2	B	175	VAL
2	B	181	ILE
2	B	189	SER
2	B	195	VAL
2	B	215	TYR
2	B	217	THR
2	B	237	ILE
2	B	243	GLU
2	B	249	ILE

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Mol	Chain	Res	Type
2	B	253	GLU
2	B	278	LEU
2	B	307	LEU
2	B	308	LEU
2	B	309	ARG
2	B	311	THR
2	B	317	ARG
2	B	323	GLU
2	B	327	LEU
2	B	329	THR
2	B	332	LEU
2	B	338	VAL
2	B	344	LEU
2	B	375	VAL
2	B	377	GLU
2	B	387	ARG
2	B	407	LEU
2	B	409	GLU
2	B	414	LYS
2	C	18	LEU
2	C	30	ASP
2	C	33	ARG
2	C	40	LEU
2	C	46	LYS
2	C	78	LYS
2	C	85	ASP
2	C	97	LYS
2	C	104	ILE
2	C	108	VAL
2	C	111	LYS
2	C	122	SER
2	C	134	LEU
2	C	143	ARG
2	C	153	ARG
2	C	155	LYS
2	C	156	LEU
2	C	160	LEU
2	C	163	GLN
2	C	167	ILE
2	C	177	GLU
2	C	181	ILE
2	C	189	SER

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Mol	Chain	Res	Type
2	C	195	VAL
2	C	214	ARG
2	C	228	LEU
2	C	230	THR
2	C	243	GLU
2	C	252	ARG
2	C	253	GLU
2	C	286	LYS
2	C	292	VAL
2	C	307	LEU
2	C	308	LEU
2	C	311	THR
2	C	317	ARG
2	C	327	LEU
2	C	332	LEU
2	C	350	VAL
2	C	354	LYS
2	C	371	GLN
2	C	375	VAL
2	C	385	GLN
2	C	407	LEU
2	C	408	ARG
2	C	422	LYS
2	D	8	ILE
2	D	22	GLU
2	D	23	ASP
2	D	26	GLU
2	D	34	LYS
2	D	42	ILE
2	D	44	THR
2	D	60	LYS
2	D	64	VAL
2	D	83	LYS
2	D	84	LEU
2	D	85	ASP
2	D	97	LYS
2	D	104	ILE
2	D	108	VAL
2	D	126	ARG
2	D	136	LEU
2	D	146	ARG
2	D	149	MET

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Mol	Chain	Res	Type
2	D	166	MET
2	D	177	GLU
2	D	181	ILE
2	D	217	THR
2	D	228	LEU
2	D	230	THR
2	D	243	GLU
2	D	252	ARG
2	D	253	GLU
2	D	308	LEU
2	D	311	THR
2	D	317	ARG
2	D	326	SER
2	D	327	LEU
2	D	328	THR
2	D	332	LEU
2	D	353	ASN
2	D	354	LYS
2	D	367	ASN
2	D	375	VAL
2	D	377	GLU
2	D	383	GLU
2	D	407	LEU
2	D	409	GLU
2	D	412	ILE
2	D	414	LYS
2	E	13	VAL
2	E	18	LEU
2	E	40	LEU
2	E	43	ASN
2	E	48	LEU
2	E	84	LEU
2	E	85	ASP
2	E	95	ILE
2	E	123	ASP
2	E	130	ASP
2	E	133	TRP
2	E	134	LEU
2	E	148	GLN
2	E	149	MET
2	E	180	ASP
2	E	181	ILE

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Mol	Chain	Res	Type
2	E	182	PHE
2	E	187	ASN
2	E	206	LYS
2	E	209	GLU
2	E	242	THR
2	E	243	GLU
2	E	253	GLU
2	E	302	GLN
2	E	307	LEU
2	E	308	LEU
2	E	309	ARG
2	E	314	ARG
2	E	317	ARG
2	E	327	LEU
2	E	332	LEU
2	E	349	CYS
2	E	354	LYS
2	E	356	THR
2	E	375	VAL
2	E	408	ARG
2	E	410	LYS
2	E	412	ILE
2	E	418	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	43	ASN
2	A	70	ASN
2	A	162	ASN
2	A	163	GLN
2	A	187	ASN
2	A	190	ASN
2	A	251	ASN
2	A	260	GLN
2	A	266	GLN
2	A	347	GLN
2	A	395	GLN
2	B	70	ASN
2	B	148	GLN
2	B	163	GLN
2	B	168	ASN

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Mol	Chain	Res	Type
2	B	251	ASN
2	B	266	GLN
2	B	385	GLN
2	C	70	ASN
2	C	168	ASN
2	C	190	ASN
2	C	266	GLN
2	C	346	GLN
2	C	371	GLN
2	C	395	GLN
2	D	43	ASN
2	D	57	GLN
2	D	63	ASN
2	D	68	HIS
2	D	94	ASN
2	D	162	ASN
2	D	163	GLN
2	D	203	HIS
2	D	266	GLN
2	D	371	GLN
2	D	386	ASN
2	D	395	GLN
2	E	187	ASN
2	E	251	ASN
2	E	266	GLN
2	E	315	ASN
2	E	347	GLN
2	E	385	GLN
2	E	395	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	44/45 (97%)	36 (81%)	8 (18%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	3	U
1	R	4	U

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Mol	Chain	Res	Type
1	R	5	U
1	R	6	U
1	R	7	U
1	R	8	U
1	R	9	U
1	R	10	U
1	R	11	U
1	R	12	U
1	R	13	U
1	R	14	U
1	R	15	U
1	R	17	U
1	R	18	U
1	R	19	U
1	R	21	U
1	R	23	U
1	R	24	U
1	R	25	U
1	R	26	U
1	R	27	U
1	R	28	U
1	R	29	U
1	R	30	U
1	R	32	U
1	R	33	U
1	R	36	U
1	R	37	U
1	R	38	U
1	R	39	U
1	R	40	U
1	R	41	U
1	R	42	U
1	R	45	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	4	U
1	R	5	U
1	R	6	U
1	R	12	U
1	R	14	U

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Mol	Chain	Res	Type
1	R	20	U
1	R	32	U
1	R	39	U

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 15 ligands modelled in this entry, 15 are modelled with single atom - 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	R	45/45 (100%)	0.72	0	100	100	29, 44, 53, 58	0
2	A	421/422 (99%)	0.82	57 (13%)	7	5	23, 27, 35, 40	0
2	B	415/422 (98%)	0.87	52 (12%)	8	7	23, 27, 33, 42	0
2	C	413/422 (97%)	0.90	55 (13%)	7	6	23, 27, 33, 39	0
2	D	416/422 (98%)	0.83	43 (10%)	12	10	23, 27, 34, 43	0
2	E	421/422 (99%)	0.91	66 (15%)	5	4	23, 27, 36, 45	0
All	All	2131/2155 (98%)	0.86	273 (12%)	7	6	23, 27, 37, 58	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2	SER	9.6
2	C	169	GLU	8.5
2	B	2	SER	7.8
2	C	163	GLN	6.9
2	A	2	SER	6.7
2	C	59	LEU	6.2
2	D	166	MET	6.1
2	D	172	GLU	6.0
2	A	361	THR	5.9
2	C	356	THR	5.6
2	E	185	TRP	5.6
2	B	163	GLN	5.6
2	B	169	GLU	5.5
2	C	173	PRO	5.3
2	B	172	GLU	5.2
2	E	186	GLY	5.1
2	E	365	THR	5.1
2	B	55	VAL	5.1
2	C	342	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	A	172	GLU	4.9
2	A	353	ASN	4.9
2	A	358	ASP	4.9
2	A	362	GLY	4.8
2	A	363	GLY	4.8
2	A	367	ASN	4.8
2	C	172	GLU	4.7
2	E	175	VAL	4.7
2	E	367	ASN	4.6
2	C	2	SER	4.5
2	B	162	ASN	4.5
2	B	386	ASN	4.3
2	B	185	TRP	4.3
2	E	184	VAL	4.2
2	B	171	PHE	4.2
2	E	178	GLY	4.1
2	E	101	THR	4.1
2	C	175	VAL	4.1
2	E	350	VAL	4.1
2	A	342	ALA	4.1
2	B	342	ALA	4.1
2	D	342	ALA	4.1
2	B	358	ASP	4.0
2	A	357	PRO	4.0
2	D	171	PHE	4.0
2	E	366	THR	4.0
2	C	162	ASN	4.0
2	E	152	TYR	4.0
2	E	171	PHE	4.0
2	C	55	VAL	3.9
2	A	30	ASP	3.9
2	E	162	ASN	3.9
2	B	176	PRO	3.9
2	C	167	ILE	3.9
2	E	169	GLU	3.8
2	B	166	MET	3.8
2	C	171	PHE	3.8
2	D	185	TRP	3.7
2	B	355	TYR	3.7
2	C	178	GLY	3.7
2	D	68	HIS	3.7
2	B	120	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	365	THR	3.7
2	C	43	ASN	3.7
2	D	216	GLY	3.7
2	B	175	VAL	3.7
2	C	107	LEU	3.6
2	E	150	PRO	3.6
2	E	357	PRO	3.6
2	A	166	MET	3.6
2	B	412	ILE	3.6
2	D	368	ALA	3.6
2	E	174	LEU	3.6
2	B	341	SER	3.5
2	D	174	LEU	3.5
2	C	164	CYS	3.5
2	A	366	THR	3.5
2	D	163	GLN	3.5
2	D	164	CYS	3.5
2	D	107	LEU	3.5
2	C	357	PRO	3.5
2	D	149	MET	3.4
2	E	149	MET	3.4
2	A	364	LEU	3.4
2	E	30	ASP	3.4
2	D	41	TYR	3.4
2	D	366	THR	3.4
2	C	177	GLU	3.4
2	B	365	THR	3.4
2	E	362	GLY	3.4
2	A	233	HIS	3.4
2	A	164	CYS	3.3
2	E	161	THR	3.3
2	B	131	ASP	3.3
2	E	55	VAL	3.3
2	E	361	THR	3.3
2	A	355	TYR	3.3
2	A	162	ASN	3.3
2	C	121	VAL	3.3
2	D	350	VAL	3.2
2	E	155	LYS	3.2
2	B	377	GLU	3.2
2	B	173	PRO	3.2
2	E	118	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
2	A	169	GLU	3.2
2	B	367	ASN	3.1
2	E	176	PRO	3.1
2	E	138	LEU	3.1
2	B	351	GLY	3.1
2	C	409	GLU	3.1
2	C	346	GLN	3.1
2	E	25	VAL	3.1
2	B	317	ARG	3.1
2	A	25	VAL	3.0
2	E	358	ASP	3.0
2	E	166	MET	3.0
2	C	271	ALA	3.0
2	E	182	PHE	3.0
2	C	137	TYR	3.0
2	C	142	TYR	3.0
2	E	146	ARG	3.0
2	C	233	HIS	3.0
2	E	27	TYR	3.0
2	E	159	GLY	3.0
2	B	39	PRO	3.0
2	E	177	GLU	3.0
2	B	48	LEU	2.9
2	D	30	ASP	2.9
2	E	24	PRO	2.9
2	C	366	THR	2.9
2	E	173	PRO	2.9
2	D	341	SER	2.9
2	A	286	LYS	2.9
2	D	412	ILE	2.9
2	E	117	LEU	2.9
2	A	120	GLY	2.9
2	B	24	PRO	2.9
2	C	350	VAL	2.9
2	C	174	LEU	2.9
2	B	158	ASP	2.8
2	A	278	LEU	2.8
2	B	366	THR	2.8
2	A	171	PHE	2.8
2	C	341	SER	2.8
2	E	348	PHE	2.8
2	C	95	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	344	LEU	2.8
2	E	156	LEU	2.8
2	E	359	ASP	2.8
2	E	172	GLU	2.7
2	B	122	SER	2.7
2	D	139	LEU	2.7
2	B	43	ASN	2.7
2	C	353	ASN	2.7
2	B	278	LEU	2.7
2	A	341	SER	2.7
2	D	167	ILE	2.6
2	C	161	THR	2.6
2	A	163	GLN	2.6
2	E	141	LEU	2.6
2	A	112	ALA	2.6
2	C	182	PHE	2.6
2	E	157	MET	2.6
2	D	355	TYR	2.6
2	A	24	PRO	2.6
2	E	363	GLY	2.6
2	B	275	MET	2.6
2	E	153	ARG	2.6
2	C	155	LYS	2.6
2	E	28	PRO	2.6
2	E	43	ASN	2.6
2	A	28	PRO	2.5
2	A	185	TRP	2.5
2	C	28	PRO	2.5
2	A	175	VAL	2.5
2	D	313	ALA	2.5
2	B	21	ASN	2.5
2	C	131	ASP	2.5
2	A	314	ARG	2.5
2	C	273	SER	2.5
2	B	113	LEU	2.5
2	A	165	LYS	2.5
2	B	30	ASP	2.5
2	D	2	SER	2.5
2	D	115	GLY	2.5
2	A	42	ILE	2.4
2	B	28	PRO	2.4
2	E	66	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	43	ASN	2.4
2	A	107	LEU	2.4
2	D	367	ASN	2.4
2	A	118	PRO	2.4
2	B	104	ILE	2.4
2	D	343	ASP	2.4
2	D	146	ARG	2.4
2	B	357	PRO	2.4
2	E	342	ALA	2.4
2	A	356	THR	2.4
2	E	351	GLY	2.3
2	D	222	PHE	2.3
2	B	177	GLU	2.3
2	A	113	LEU	2.3
2	C	152	TYR	2.3
2	C	283	LEU	2.3
2	E	355	TYR	2.3
2	A	34	LYS	2.3
2	C	176	PRO	2.3
2	C	85	ASP	2.3
2	D	224	ASP	2.3
2	C	27	TYR	2.3
2	E	137	TYR	2.3
2	A	117	LEU	2.3
2	B	107	LEU	2.3
2	A	152	TYR	2.3
2	C	314	ARG	2.3
2	D	150	PRO	2.3
2	C	186	GLY	2.3
2	A	124	ALA	2.3
2	B	118	PRO	2.3
2	C	274	TYR	2.3
2	A	186	GLY	2.3
2	E	98	ALA	2.2
2	A	283	LEU	2.2
2	E	183	ASP	2.2
2	B	274	TYR	2.2
2	A	275	MET	2.2
2	D	59	LEU	2.2
2	E	409	GLU	2.2
2	E	42	ILE	2.2
2	C	87	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	27	TYR	2.2
2	A	23	ASP	2.2
2	B	343	ASP	2.2
2	C	79	ASP	2.2
2	D	119	ASP	2.2
2	A	313	ALA	2.2
2	C	3	VAL	2.2
2	D	358	ASP	2.2
2	D	140	GLY	2.2
2	A	360	SER	2.2
2	D	181	ILE	2.1
2	D	176	PRO	2.1
2	A	344	LEU	2.1
2	A	33	ARG	2.1
2	E	346	GLN	2.1
2	B	139	LEU	2.1
2	D	133	TRP	2.1
2	C	345	ALA	2.1
2	E	285	SER	2.1
2	B	25	VAL	2.1
2	D	365	THR	2.1
2	B	14	ILE	2.1
2	C	146	ARG	2.1
2	D	277	TYR	2.1
2	D	55	VAL	2.0
2	A	134	LEU	2.0
2	E	187	ASN	2.0
2	E	408	ARG	2.0
2	A	45	THR	2.0
2	A	180	ASP	2.0
2	C	343	ASP	2.0
2	C	253	GLU	2.0
2	C	31	TYR	2.0
2	B	68	HIS	2.0
2	E	341	SER	2.0
2	E	344	LEU	2.0
2	E	364	LEU	2.0
2	A	168	ASN	2.0
2	B	217	THR	2.0
2	B	328	THR	2.0
2	E	345	ALA	2.0
2	D	79	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	123	ASP	2.0
2	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IUM	E	425	1/3	0.91	0.13	192,192,192,192	0
3	IUM	E	423	1/3	0.92	0.13	107,107,107,107	0
3	IUM	B	425	1/3	0.92	0.12	184,184,184,184	0
3	IUM	B	423	1/3	0.93	0.13	129,129,129,129	0
3	IUM	A	425	1/3	0.94	0.07	129,129,129,129	0
3	IUM	D	423	1/3	0.95	0.16	120,120,120,120	0
3	IUM	A	423	1/3	0.96	0.13	92,92,92,92	0
3	IUM	A	426	1/3	0.96	0.14	114,114,114,114	0
3	IUM	C	425	1/3	0.96	0.09	123,123,123,123	0
3	IUM	C	423	1/3	0.98	0.17	54,54,54,54	0
3	IUM	A	424	1/3	0.99	0.19	21,21,21,21	0
3	IUM	E	424	1/3	0.99	0.19	21,21,21,21	0
3	IUM	D	424	1/3	0.99	0.18	17,17,17,17	0
3	IUM	B	424	1/3	1.00	0.19	15,15,15,15	0
3	IUM	C	424	1/3	1.00	0.19	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.