



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:33 AM UTC

PDB ID : 4P0R / pdb_00004p0r
Title : human Mus81-Eme1-3'flap DNA complex
Authors : Gwon, G.H.; Baek, K.; Cho, Y.
Deposited on : 2014-02-22
Resolution : 6.50 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

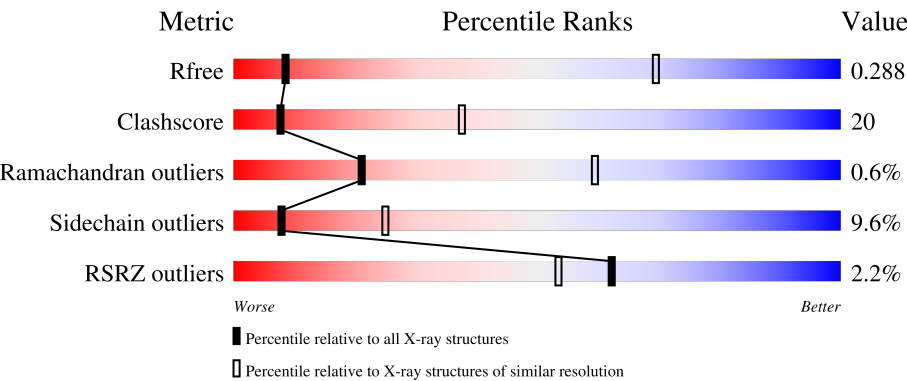
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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.



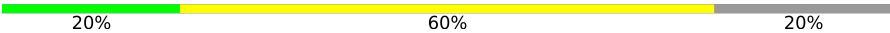
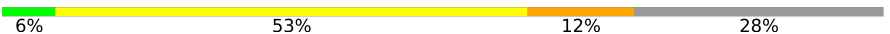
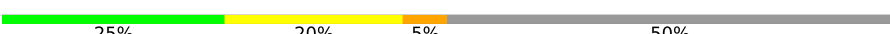
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1162 (9.00-4.00)
Clashscore	190562	1020 (8.98-4.02)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	306	3% 47% 38% 10%
1	C	306	2% 50% 34% 5% 10%
2	B	393	2% 44% 24% 28%
2	D	393	% 44% 24% 28%
3	E	15	33% 47% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	15	 20% 60% 20%
4	F	32	 6% 53% 12% 28%
4	I	32	 9% 50% 12% 28%
5	G	20	 10% 35% 5% 50%
5	J	20	 25% 20% 5% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2173	1364	403	398	8			
1	C	275	Total	C	N	O	S	0	0	0
			2173	1364	403	398	8			

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	0	0	0
			2227	1401	397	415	14			
2	D	284	Total	C	N	O	S	0	0	0
			2227	1401	397	415	14			

- Molecule 3 is a DNA chain called DNA CTGTGTGTAAGCACG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	12	Total	C	N	O	P	0	0	0
			248	118	44	74	12			
3	H	12	Total	C	N	O	P	0	0	0
			248	118	44	74	12			

- Molecule 4 is a DNA chain called DNA ACGTGCTTACACACAGAGGTTAGGGTGAAC TT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	23	Total	C	N	O	P	0	0	0
			478	226	92	137	23			
4	I	23	Total	C	N	O	P	0	0	0
			478	226	92	137	23			

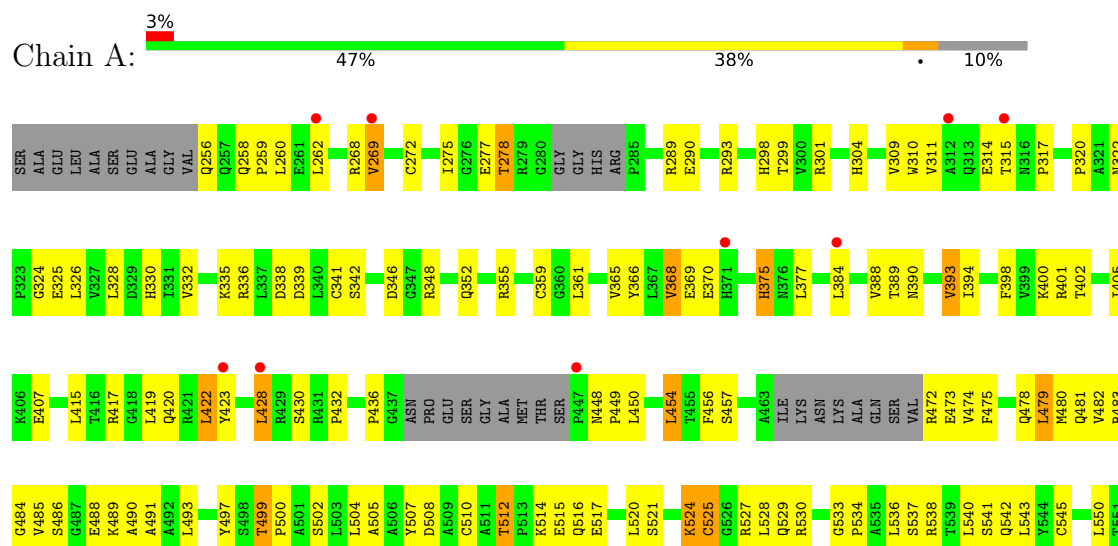
- Molecule 5 is a DNA chain called DNA CAAGTTCACCCTAACCTCAG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	10	Total 197	C 94	N 35	O 58	P 10	0	0	0
5	J	10	Total 197	C 94	N 35	O 58	P 10	0	0	0

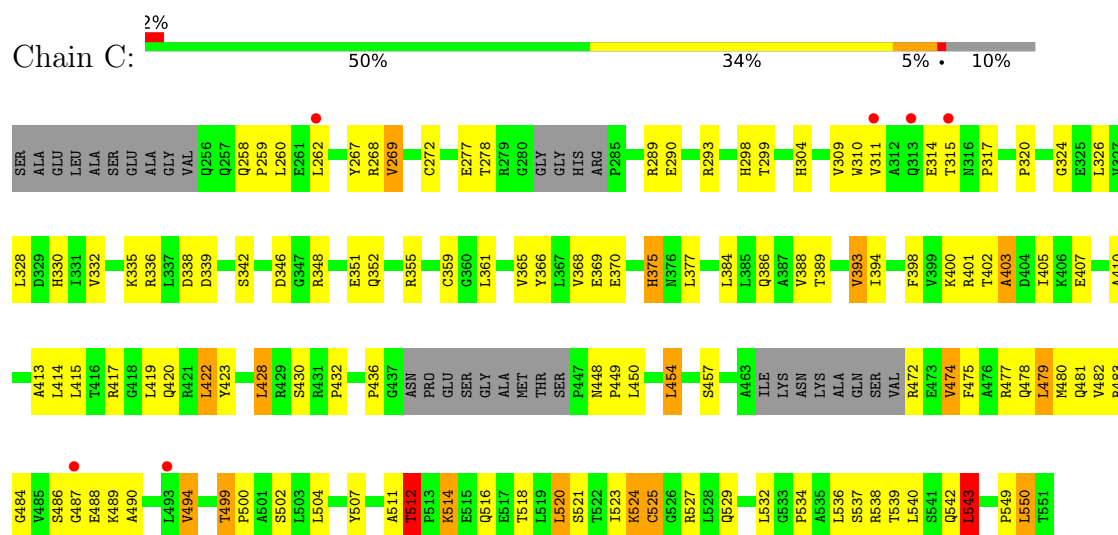
3 Residue-property plots

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.

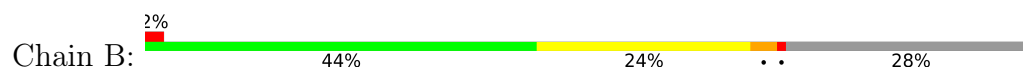
• Molecule 1: Crossover junction endonuclease MUS81

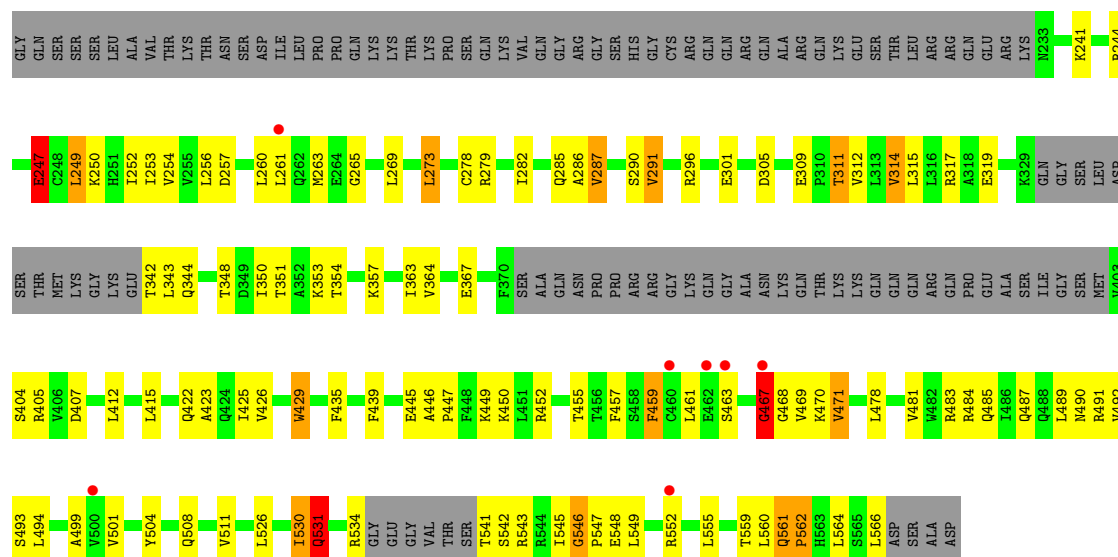


• Molecule 1: Crossover junction endonuclease MUS81

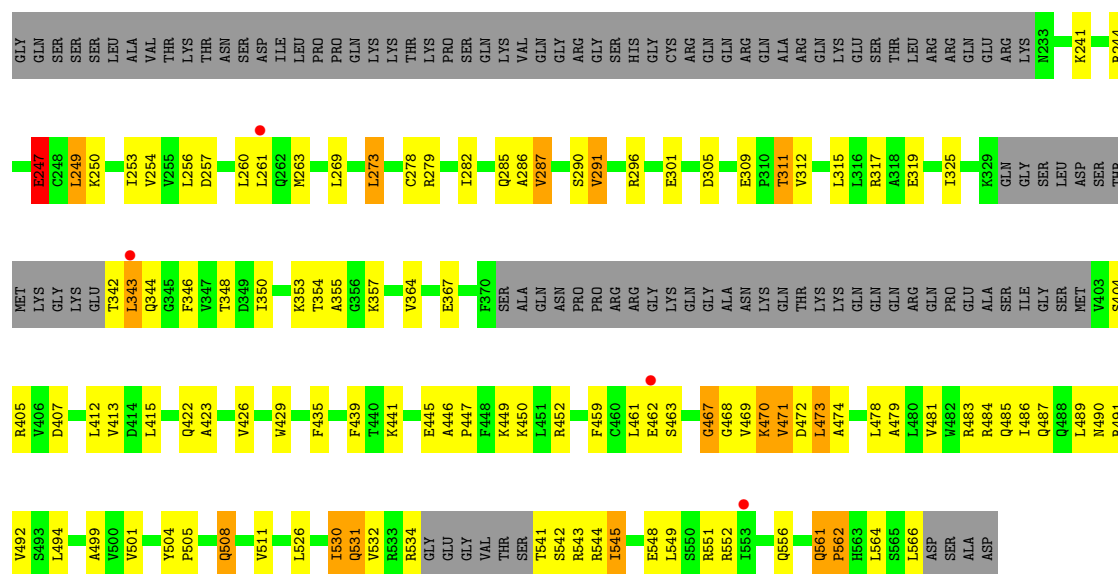
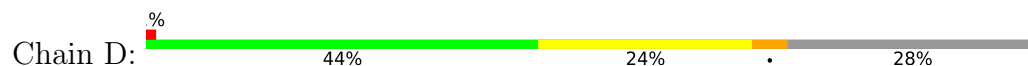


• Molecule 2: Crossover junction endonuclease EME1

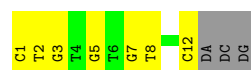




• Molecule 2: Crossover junction endonuclease EME1

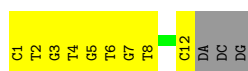


• Molecule 3: DNA CTGTGTGTAAGCAG

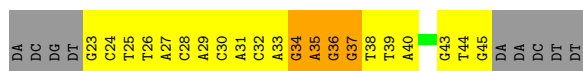


• Molecule 3: DNA CTGTGTGTAAGCAG

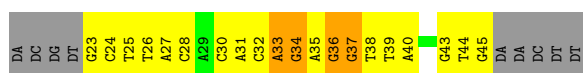




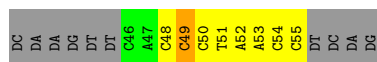
- Molecule 4: DNA ACGTGCTTACACACAGAGGTTAGGGTGAACCTT



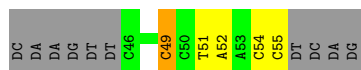
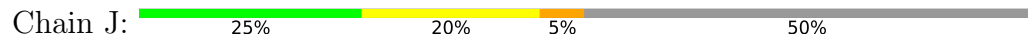
- Molecule 4: DNA ACGTGCTTACACACAGAGGTTAGGGTGAACCTT



- Molecule 5: DNA CAAGTTCACCCTAACCTCAG



- Molecule 5: DNA CAAGTTCACCCTAACCTCAG



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	221.76Å 135.30Å 102.89Å 90.00° 113.27° 90.00°	Depositor
Resolution (Å)	34.86 – 6.50 34.86 – 6.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.86-6.50) 99.0 (34.86-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 6.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.210 , 0.295 0.220 , 0.288	Depositor DCC
R_{free} test set	335 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	371.5	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 101.2	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	0.89	EDS
Total number of atoms	10646	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.75	0/2211	1.06	12/2989 (0.4%)
1	C	0.75	0/2211	1.08	15/2989 (0.5%)
2	B	0.86	0/2258	1.36	30/3054 (1.0%)
2	D	0.89	1/2258 (0.0%)	1.36	29/3054 (0.9%)
3	E	0.31	0/277	0.86	0/426
3	H	0.32	0/277	0.85	0/426
4	F	0.37	0/537	1.10	5/828 (0.6%)
4	I	0.35	0/537	1.04	5/828 (0.6%)
5	G	0.33	0/219	0.93	1/333 (0.3%)
5	J	0.32	0/219	0.96	1/333 (0.3%)
All	All	0.75	1/11004 (0.0%)	1.18	98/15260 (0.6%)

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	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	532	VAL	CA-CB	6.12	1.61	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	467	GLY	N-CA-C	8.63	123.64	110.18
2	B	467	GLY	CA-C-N	8.54	133.14	121.01
2	B	467	GLY	C-N-CA	8.54	133.14	121.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	512	THR	CA-C-N	-7.56	110.39	119.84
1	C	512	THR	C-N-CA	-7.56	110.39	119.84
2	D	467	GLY	N-CA-C	7.50	130.95	113.18
4	F	37	DG	C5'-C4'-C3'	-7.49	103.66	114.90
2	B	531	GLN	CA-C-N	7.32	130.94	120.98
2	B	531	GLN	C-N-CA	7.32	130.94	120.98
2	B	350	ILE	N-CA-C	7.32	117.45	110.42
2	D	468	GLY	CA-C-N	-7.29	113.64	123.12
2	D	468	GLY	C-N-CA	-7.29	113.64	123.12
2	B	247	GLU	N-CA-C	7.27	120.25	111.82
1	C	514	LYS	N-CA-C	-7.21	104.29	113.23
2	B	468	GLY	CA-C-N	-7.16	113.76	123.14
2	B	468	GLY	C-N-CA	-7.16	113.76	123.14
2	D	531	GLN	CA-C-N	7.14	131.89	121.18
2	D	531	GLN	C-N-CA	7.14	131.89	121.18
2	D	350	ILE	N-CA-C	7.12	117.25	110.42
2	D	305	ASP	N-CA-C	-7.02	105.06	112.93
1	C	298	HIS	N-CA-C	6.83	119.32	109.14
2	B	542	SER	N-CA-C	6.82	118.65	110.19
1	A	298	HIS	N-CA-C	6.77	119.23	109.14
2	D	543	ARG	N-CA-C	-6.71	105.08	113.20
2	D	405	ARG	N-CA-C	6.70	119.59	111.82
2	B	305	ASP	N-CA-C	-6.67	105.46	112.93
2	B	531	GLN	N-CA-C	6.60	120.00	109.24
2	B	530	ILE	CA-C-N	-6.60	113.61	122.72
2	B	530	ILE	C-N-CA	-6.60	113.61	122.72
5	J	49	DC	C5'-C4'-C3'	6.48	124.63	114.90
2	D	531	GLN	N-CA-C	6.46	119.76	109.24
2	D	545	ILE	N-CA-C	-6.38	105.52	111.45
2	D	348	THR	N-CA-C	-6.33	104.46	111.36
2	D	467	GLY	CA-C-N	-6.31	117.73	122.33
2	D	467	GLY	C-N-CA	-6.31	117.73	122.33
1	A	448	ASN	N-CA-C	6.21	117.90	110.07
2	B	405	ARG	N-CA-C	6.20	119.01	111.82
2	D	530	ILE	N-CA-C	-6.18	100.73	108.89
4	F	34	DG	C2'-C3'-O3'	6.11	120.66	111.50
2	D	247	GLU	N-CA-C	6.06	118.85	111.82
4	I	33	DA	O5'-C5'-C4'	-6.01	101.79	110.80
4	I	36	DG	C2'-C3'-O3'	5.93	120.39	111.50
2	B	530	ILE	N-CA-C	-5.92	101.07	108.89
1	C	525	CYS	N-CA-C	5.86	118.28	108.73
2	D	530	ILE	CA-C-N	-5.83	114.68	122.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	530	ILE	C-N-CA	-5.83	114.68	122.72
1	C	448	ASN	N-CA-C	5.79	117.37	110.07
4	I	34	DG	C2'-C3'-O3'	5.76	120.14	111.50
1	C	277	GLU	N-CA-C	-5.73	106.26	113.20
2	D	423	ALA	N-CA-C	5.72	117.80	108.76
4	I	37	DG	C2'-C3'-O3'	5.72	120.07	111.50
4	I	37	DG	P-O5'-C5'	5.71	128.57	120.00
1	A	258	GLN	CA-C-N	5.70	126.96	119.84
1	A	258	GLN	C-N-CA	5.70	126.96	119.84
2	D	350	ILE	CB-CA-C	-5.65	104.73	111.97
2	B	350	ILE	CB-CA-C	-5.62	104.77	111.97
1	C	543	LEU	N-CA-C	-5.60	105.26	111.36
2	B	423	ALA	N-CA-C	5.57	117.56	108.76
2	B	348	THR	N-CA-C	-5.57	105.29	111.36
4	F	36	DG	C4'-C3'-O3'	5.50	118.26	110.00
2	B	252	ILE	N-CA-C	5.49	115.79	108.11
1	A	277	GLU	N-CA-C	-5.47	106.68	113.19
1	A	388	VAL	CB-CA-C	-5.46	104.98	111.97
5	G	49	DC	C5'-C4'-C3'	5.42	123.04	114.90
1	C	388	VAL	CB-CA-C	-5.42	105.03	111.97
2	D	473	LEU	N-CA-C	-5.42	105.54	111.82
1	C	524	LYS	N-CA-C	5.38	117.52	107.99
1	C	258	GLN	CA-C-N	5.36	126.54	119.84
1	C	258	GLN	C-N-CA	5.36	126.54	119.84
1	C	511	ALA	N-CA-C	-5.35	106.92	113.50
2	D	551	ARG	N-CA-C	5.34	116.91	111.14
1	A	485	VAL	N-CA-C	5.32	115.52	107.80
4	F	33	DA	O5'-C5'-C4'	-5.32	102.82	110.80
2	B	546	GLY	CA-C-N	5.25	124.95	119.64
2	B	546	GLY	C-N-CA	5.25	124.95	119.64
2	B	314	VAL	N-CA-C	5.25	115.41	107.75
1	A	368	VAL	CB-CA-C	-5.23	103.72	110.84
2	D	561	GLN	CA-C-N	5.22	126.36	119.84
2	D	561	GLN	C-N-CA	5.22	126.36	119.84
2	B	561	GLN	CA-C-N	5.17	126.30	119.84
2	B	561	GLN	C-N-CA	5.17	126.30	119.84
2	B	351	THR	N-CA-C	-5.17	105.77	111.71
4	F	35	DA	C2'-C3'-O3'	5.16	119.24	111.50
2	D	504	TYR	CA-C-N	5.16	126.29	119.84
2	D	504	TYR	C-N-CA	5.16	126.29	119.84
2	B	429	TRP	N-CA-C	-5.16	106.25	112.54
2	B	504	TYR	CA-C-N	5.16	126.29	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	TYR	C-N-CA	5.16	126.29	119.84
2	B	548	GLU	N-CA-C	-5.10	105.63	111.14
1	C	403	ALA	N-CA-C	5.10	116.52	111.07
2	D	548	GLU	N-CA-C	-5.07	105.66	111.14
2	D	429	TRP	N-CA-C	-5.07	106.35	112.54
1	A	525	CYS	N-CA-C	5.05	117.79	109.76
1	A	524	LYS	N-CA-C	5.03	117.52	107.62
1	C	488	GLU	N-CA-C	-5.01	107.33	113.50
2	D	508	GLN	CA-CB-CG	-5.01	104.07	114.10
1	A	533	GLY	CA-C-N	5.00	124.72	119.82
1	A	533	GLY	C-N-CA	5.00	124.72	119.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	467	GLY	Peptide
2	D	544	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2173	0	2203	100	0
1	C	2173	0	2203	104	0
2	B	2227	0	2265	88	0
2	D	2227	0	2265	97	0
3	E	248	0	137	11	0
3	H	248	0	137	13	0
4	F	478	0	259	34	0
4	I	478	0	259	33	0
5	G	197	0	112	15	0
5	J	197	0	112	11	0
All	All	10646	0	9952	403	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 20.

All (403) 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:C:486:SER:H	1:C:489:LYS:HB2	1.34	0.92
2:D:490:ASN:O	2:D:552:ARG:NH2	2.05	0.90
1:C:472:ARG:HB2	2:D:562:PRO:HB3	1.55	0.88
2:B:490:ASN:O	2:B:552:ARG:NH2	2.06	0.87
2:B:493:SER:HB3	5:G:50:DC:H3'	1.56	0.87
2:D:542:SER:OG	4:I:45:DG:O3'	1.92	0.86
1:A:472:ARG:HD3	2:B:562:PRO:HB3	1.57	0.85
2:B:534:ARG:NH1	5:G:49:DC:OP1	2.09	0.84
2:D:449:LYS:NZ	3:H:1:DC:OP2	2.10	0.84
1:C:534:PRO:HA	1:C:537:SER:HB3	1.61	0.83
2:B:541:THR:HB	5:G:49:DC:H5'	1.61	0.82
1:A:499:THR:HG21	2:B:560:LEU:HA	1.62	0.81
3:E:5:DG:H1	4:F:30:DC:H42	1.32	0.78
4:F:37:DG:N1	5:G:54:DC:N3	2.31	0.77
1:A:417:ARG:NH1	1:A:420:GLN:OE1	2.18	0.76
1:C:472:ARG:HB2	2:D:562:PRO:CB	2.15	0.75
4:F:37:DG:N2	5:G:54:DC:O2	2.17	0.74
4:F:34:DG:H2''	4:F:35:DA:H5'	1.68	0.73
4:I:34:DG:H2''	4:I:35:DA:H5'	1.70	0.73
2:D:552:ARG:HD2	2:D:566:LEU:HB3	1.71	0.72
2:B:541:THR:OG1	5:G:48:DC:O2	2.08	0.71
1:A:486:SER:H	1:A:489:LYS:HB2	1.54	0.71
1:C:472:ARG:N	2:D:562:PRO:O	2.23	0.71
1:C:474:VAL:HG21	2:D:566:LEU:HD11	1.73	0.70
4:F:36:DG:P	4:F:36:DG:H3'	2.32	0.70
1:C:472:ARG:HB2	2:D:562:PRO:CA	2.22	0.70
2:D:541:THR:CB	5:J:49:DC:H4'	2.20	0.70
2:B:541:THR:HB	5:G:49:DC:C5'	2.22	0.69
1:A:269:VAL:HG13	1:A:420:GLN:HG2	1.75	0.69
1:A:474:VAL:HG21	2:B:566:LEU:HD12	1.74	0.68
2:D:445:GLU:OE1	3:H:2:DT:OP2	2.11	0.68
1:C:269:VAL:HG13	1:C:420:GLN:HG2	1.74	0.68
2:B:241:LYS:NZ	4:F:28:DC:OP2	2.25	0.68
1:C:483:ARG:HH11	4:I:31:DA:H4'	1.59	0.68
1:C:472:ARG:CD	2:D:562:PRO:HB3	2.24	0.68
1:C:417:ARG:NH1	1:C:420:GLN:OE1	2.27	0.68
1:A:480:MET:HE2	1:A:490:ALA:HB3	1.74	0.67
1:C:477:ARG:NH1	2:D:462:GLU:OE1	2.27	0.67
2:B:552:ARG:HD2	2:B:566:LEU:HB3	1.77	0.66
1:A:474:VAL:HG21	2:B:566:LEU:CD1	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:THR:HG23	1:A:502:SER:HB2	1.77	0.65
1:A:512:THR:HG22	1:A:514:LYS:H	1.61	0.65
4:I:37:DG:H2''	4:I:38:DT:OP2	1.95	0.65
2:B:483:ARG:NH1	2:B:487:GLN:OE1	2.30	0.65
1:C:262:LEU:HD22	1:C:314:GLU:HB3	1.79	0.65
1:C:499:THR:HG23	1:C:502:SER:HB2	1.78	0.65
4:I:43:DG:N2	5:J:49:DC:O2	2.30	0.64
1:C:521:SER:HB2	1:C:534:PRO:HD3	1.78	0.64
1:C:472:ARG:HD3	2:D:562:PRO:HB3	1.78	0.64
2:D:541:THR:HB	5:J:49:DC:H4'	1.78	0.64
4:I:39:DT:H2''	4:I:40:DA:C8	2.33	0.64
1:C:500:PRO:HG2	2:D:556:GLN:O	1.97	0.64
4:I:36:DG:H1'	4:I:37:DG:H5'	1.80	0.64
2:D:241:LYS:HB3	2:D:244:ARG:HH11	1.64	0.63
1:C:368:VAL:HB	1:C:401:ARG:HA	1.79	0.63
3:H:5:DG:H1	4:I:30:DC:H42	1.47	0.63
1:A:474:VAL:HG11	2:B:489:LEU:HG	1.80	0.63
4:I:26:DT:H2''	4:I:27:DA:H5'	1.82	0.62
1:C:474:VAL:HB	2:D:556:GLN:CD	2.25	0.62
2:D:309:GLU:O	2:D:357:LYS:NZ	2.32	0.62
1:A:314:GLU:HG2	1:A:324:GLY:H	1.65	0.62
1:C:335:LYS:HZ1	1:C:348:ARG:HH21	1.48	0.61
1:C:474:VAL:HB	2:D:556:GLN:NE2	2.14	0.61
4:F:25:DT:H2'	4:F:26:DT:C6	2.35	0.61
4:I:25:DT:H2''	4:I:26:DT:H5'	1.82	0.61
1:A:262:LEU:HD22	1:A:314:GLU:HB3	1.81	0.61
2:B:241:LYS:HB3	2:B:244:ARG:HH11	1.66	0.61
2:B:353:LYS:HG2	2:D:355:ALA:HB2	1.83	0.60
4:F:26:DT:H2''	4:F:27:DA:H5'	1.82	0.60
1:A:368:VAL:HB	1:A:401:ARG:HA	1.82	0.60
2:B:263:MET:HE1	2:B:315:LEU:HD22	1.83	0.60
2:B:309:GLU:O	2:B:357:LYS:NZ	2.34	0.60
4:F:23:DG:H2'	4:F:24:DC:C6	2.37	0.60
4:F:39:DT:H2''	4:F:40:DA:C8	2.37	0.60
1:A:499:THR:HG23	1:A:502:SER:H	1.67	0.60
1:A:534:PRO:HA	1:A:537:SER:HB3	1.84	0.60
2:D:312:VAL:HG11	2:D:354:THR:HG21	1.84	0.59
1:A:473:GLU:HG3	2:B:459:PHE:CE1	2.37	0.59
1:A:474:VAL:O	1:A:478:GLN:NE2	2.35	0.59
1:A:488:GLU:OE1	2:B:455:THR:HG21	2.02	0.59
4:I:25:DT:H2'	4:I:26:DT:C6	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:483:ARG:NH1	2:D:487:GLN:OE1	2.36	0.59
1:C:486:SER:OG	4:I:30:DC:OP1	2.17	0.59
1:C:481:GLN:HB2	2:D:481:VAL:HG13	1.84	0.58
3:H:3:DG:H1	4:I:32:DC:H42	1.50	0.58
1:A:510:CYS:HB2	1:A:516:GLN:HE21	1.67	0.58
1:C:483:ARG:HH21	2:D:470:LYS:HB2	1.68	0.58
1:C:314:GLU:HG2	1:C:324:GLY:H	1.68	0.58
2:B:353:LYS:CG	2:D:355:ALA:HB2	2.33	0.58
2:D:263:MET:HE1	2:D:315:LEU:HD22	1.86	0.58
4:I:23:DG:H2'	4:I:24:DC:C6	2.39	0.58
2:B:534:ARG:HH12	5:G:49:DC:P	2.26	0.58
1:A:326:LEU:HD12	1:A:428:LEU:HB3	1.85	0.58
1:C:394:ILE:HG23	2:D:450:LYS:HE3	1.84	0.58
2:B:249:LEU:HD22	2:B:278:CYS:HB3	1.85	0.57
3:E:3:DG:H1	4:F:32:DC:H42	1.51	0.57
1:A:483:ARG:HD3	4:F:31:DA:H4'	1.87	0.57
1:A:335:LYS:HZ1	1:A:348:ARG:HH21	1.51	0.57
1:A:507:TYR:OH	1:A:520:LEU:HD11	2.04	0.57
2:B:534:ARG:HE	2:B:534:ARG:HA	1.68	0.57
2:B:312:VAL:HG11	2:B:354:THR:HG21	1.87	0.57
2:B:449:LYS:NZ	3:E:1:DC:OP2	2.29	0.57
1:C:472:ARG:HB2	2:D:562:PRO:HA	1.86	0.57
1:C:472:ARG:CB	2:D:562:PRO:HB3	2.31	0.57
2:D:541:THR:OG1	5:J:49:DC:H4'	2.04	0.57
1:C:486:SER:N	1:C:489:LYS:HB2	2.14	0.56
1:C:328:LEU:HD23	1:C:419:LEU:HD22	1.87	0.56
2:D:241:LYS:NZ	4:I:28:DC:OP2	2.39	0.56
2:D:249:LEU:HD22	2:D:278:CYS:HB3	1.87	0.56
2:D:541:THR:HB	5:J:49:DC:H5''	1.86	0.56
1:C:326:LEU:HD12	1:C:428:LEU:HB3	1.87	0.56
2:D:489:LEU:HB3	2:D:552:ARG:HH21	1.71	0.56
1:C:389:THR:O	1:C:393:VAL:HG23	2.06	0.56
1:C:549:PRO:HA	2:D:505:PRO:HB2	1.87	0.56
2:B:296:ARG:HH22	2:B:301:GLU:HB2	1.71	0.56
1:C:332:VAL:HG22	1:C:365:VAL:HB	1.87	0.56
2:B:354:THR:HB	2:B:357:LYS:HD2	1.87	0.56
2:B:545:ILE:HG23	2:B:549:LEU:HD23	1.88	0.56
2:D:254:VAL:HG11	2:D:273:LEU:HD21	1.88	0.56
2:D:241:LYS:HB3	2:D:244:ARG:NH1	2.21	0.55
2:B:508:GLN:HA	2:B:511:VAL:HG12	1.88	0.55
4:F:24:DC:H2''	4:F:25:DT:H5'	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LYS:HD3	1:A:525:CYS:SG	2.46	0.55
4:F:25:DT:H2''	4:F:26:DT:H5'	1.87	0.55
4:I:43:DG:H2''	4:I:44:DT:C5	2.42	0.55
1:C:475:PHE:CD1	1:C:500:PRO:HG3	2.42	0.55
1:A:336:ARG:NH2	1:A:370:GLU:OE2	2.40	0.55
2:B:261:LEU:HD11	2:B:282:ILE:HD12	1.88	0.55
1:A:472:ARG:N	2:B:562:PRO:O	2.40	0.55
3:H:3:DG:H2'	3:H:4:DT:H71	1.89	0.55
1:C:483:ARG:NH1	4:I:31:DA:H4'	2.22	0.54
1:C:436:PRO:HB3	1:C:450:LEU:HD11	1.89	0.54
1:A:481:GLN:HB2	2:B:481:VAL:HG13	1.89	0.54
1:A:489:LYS:HA	1:A:525:CYS:SG	2.48	0.54
1:A:489:LYS:O	1:A:493:LEU:HG	2.07	0.54
2:B:241:LYS:HB3	2:B:244:ARG:NH1	2.23	0.54
2:D:483:ARG:HA	2:D:501:VAL:HG21	1.89	0.54
1:C:475:PHE:O	1:C:479:LEU:HD22	2.07	0.54
2:D:441:LYS:HE2	3:H:2:DT:OP1	2.07	0.54
2:B:296:ARG:NH2	2:B:301:GLU:HB2	2.22	0.54
3:E:5:DG:H1	4:F:30:DC:N4	2.02	0.54
3:H:12:DC:N3	4:I:23:DG:N2	2.53	0.54
4:I:36:DG:P	4:I:36:DG:H3'	2.48	0.54
1:C:550:LEU:HB3	2:D:479:ALA:HB2	1.90	0.53
2:D:354:THR:HB	2:D:357:LYS:HD2	1.90	0.53
2:B:547:PRO:HD2	4:F:45:DG:P	2.49	0.53
2:B:531:GLN:HG3	2:B:543:ARG:O	2.09	0.53
1:A:521:SER:HB2	1:A:534:PRO:HD3	1.91	0.53
5:J:54:DC:H1'	5:J:55:DC:H5'	1.91	0.53
2:D:296:ARG:HH22	2:D:301:GLU:HB2	1.73	0.53
1:C:310:TRP:HB2	1:C:328:LEU:HB2	1.91	0.53
4:I:43:DG:H2''	4:I:44:DT:C6	2.44	0.53
2:B:445:GLU:OE1	3:E:2:DT:OP2	2.26	0.53
1:C:262:LEU:CD2	1:C:314:GLU:HB3	2.38	0.52
1:A:389:THR:O	1:A:393:VAL:HG23	2.09	0.52
2:B:286:ALA:O	2:B:353:LYS:HD3	2.09	0.52
1:C:542:GLN:OE1	2:D:478:LEU:HD11	2.09	0.52
1:A:481:GLN:O	2:B:469:VAL:HB	2.10	0.52
1:A:505:ALA:HA	1:A:508:ASP:HB3	1.90	0.52
2:D:446:ALA:HB3	2:D:447:PRO:HD3	1.92	0.52
2:D:545:ILE:HG23	2:D:549:LEU:HD23	1.91	0.52
4:F:38:DT:O2	5:G:53:DA:N1	2.43	0.52
2:B:257:ASP:O	2:B:260:LEU:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:HG22	1:A:365:VAL:HB	1.90	0.52
2:D:241:LYS:HA	2:D:244:ARG:HD3	1.91	0.52
1:A:512:THR:HG22	1:A:514:LYS:N	2.25	0.52
1:C:521:SER:HB2	1:C:534:PRO:CD	2.39	0.52
1:A:389:THR:HG23	2:B:435:PHE:CE1	2.45	0.51
1:A:472:ARG:HB2	2:B:562:PRO:CA	2.40	0.51
1:A:499:THR:CG2	1:A:502:SER:HB2	2.40	0.51
2:B:446:ALA:HB3	2:B:447:PRO:HD3	1.91	0.51
1:C:348:ARG:O	1:C:352:GLN:HG3	2.11	0.51
2:D:296:ARG:NH2	2:D:301:GLU:HB2	2.25	0.51
1:C:484:GLY:HA3	1:C:536:LEU:HD21	1.92	0.51
3:H:7:DG:H2'	3:H:8:DT:C6	2.45	0.51
1:A:262:LEU:CD2	1:A:314:GLU:HB3	2.40	0.51
1:A:541:SER:O	1:A:545:CYS:HB2	2.09	0.51
2:B:499:ALA:HB1	2:B:530:ILE:HG22	1.92	0.51
5:G:54:DC:H1'	5:G:55:DC:H5'	1.93	0.51
4:F:36:DG:O6	5:G:55:DC:H1'	2.09	0.51
1:C:538:ARG:NH1	2:D:473:LEU:O	2.41	0.51
2:D:534:ARG:HA	2:D:534:ARG:HE	1.76	0.51
2:B:546:GLY:HA3	4:F:45:DG:OP1	2.11	0.51
1:C:504:LEU:HD22	2:D:508:GLN:NE2	2.26	0.51
1:A:328:LEU:HD23	1:A:419:LEU:HD22	1.93	0.50
2:B:254:VAL:HG11	2:B:273:LEU:HD21	1.93	0.50
2:D:492:VAL:HG22	2:D:549:LEU:HD11	1.94	0.50
1:C:398:PHE:HA	2:D:422:GLN:OE1	2.11	0.50
1:A:497:TYR:HB3	1:A:502:SER:HB3	1.93	0.50
1:C:317:PRO:HG2	1:C:320:PRO:HA	1.93	0.50
3:E:12:DC:N3	4:F:23:DG:N2	2.51	0.50
1:A:394:ILE:HG23	2:B:450:LYS:HE3	1.93	0.50
1:C:398:PHE:CE2	2:D:422:GLN:HA	2.47	0.50
1:A:436:PRO:HB3	1:A:450:LEU:HD11	1.93	0.50
1:A:472:ARG:HD3	2:B:562:PRO:CB	2.36	0.50
4:F:37:DG:H2''	4:F:38:DT:O5'	2.10	0.50
1:A:422:LEU:HD22	1:A:449:PRO:HB3	1.94	0.50
2:B:467:GLY:HA2	2:B:484:ARG:HH22	1.76	0.50
1:C:402:THR:HG23	1:C:407:GLU:HB2	1.93	0.50
1:C:543:LEU:HD23	2:D:478:LEU:HB3	1.92	0.50
1:C:489:LYS:HD3	1:C:525:CYS:SG	2.52	0.49
4:F:38:DT:H2''	4:F:39:DT:H5'	1.93	0.49
3:H:3:DG:O6	4:I:32:DC:N4	2.45	0.49
2:D:261:LEU:HD11	2:D:282:ILE:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:ASP:O	2:D:260:LEU:HB3	2.12	0.49
4:F:25:DT:H2''	4:F:26:DT:C5'	2.42	0.49
1:A:512:THR:CG2	1:A:514:LYS:H	2.24	0.49
1:C:483:ARG:HB2	2:D:469:VAL:O	2.13	0.48
1:C:539:THR:HG21	2:D:471:VAL:HG11	1.94	0.48
2:B:287:VAL:HG13	2:B:290:SER:OG	2.12	0.48
2:B:435:PHE:CZ	2:B:439:PHE:HD2	2.30	0.48
2:D:499:ALA:HB1	2:D:530:ILE:HG22	1.95	0.48
1:C:518:THR:HG22	1:C:534:PRO:HB3	1.96	0.48
2:D:542:SER:H	4:I:45:DG:H4'	1.78	0.48
1:A:398:PHE:HA	2:B:422:GLN:OE1	2.13	0.48
4:I:25:DT:H2''	4:I:26:DT:C5'	2.43	0.48
1:C:520:LEU:O	1:C:532:LEU:HD23	2.14	0.48
2:D:260:LEU:HD12	2:D:263:MET:HE2	1.96	0.48
5:J:51:DT:H2''	5:J:52:DA:C8	2.48	0.48
1:A:304:HIS:O	1:A:355:ARG:NH2	2.44	0.48
2:B:241:LYS:HA	2:B:244:ARG:HD3	1.94	0.48
2:D:435:PHE:CZ	2:D:439:PHE:HD2	2.31	0.48
2:B:469:VAL:CG2	2:B:484:ARG:NH1	2.77	0.48
3:E:3:DG:O6	4:F:32:DC:N4	2.47	0.48
1:A:359:CYS:C	1:A:361:LEU:H	2.22	0.48
2:B:260:LEU:HD12	2:B:263:MET:HE2	1.94	0.47
2:B:492:VAL:N	5:G:51:DT:OP1	2.47	0.47
1:C:304:HIS:O	1:C:355:ARG:NH2	2.47	0.47
2:D:541:THR:HG22	2:D:542:SER:O	2.14	0.47
1:A:512:THR:HG22	1:A:515:GLU:H	1.80	0.47
1:C:480:MET:HE2	1:C:487:GLY:HA2	1.96	0.47
2:D:452:ARG:HE	2:D:452:ARG:HB3	1.59	0.47
1:C:478:GLN:O	2:D:485:GLN:NE2	2.47	0.47
1:C:539:THR:HG22	2:D:478:LEU:HD21	1.96	0.47
1:A:475:PHE:O	1:A:479:LEU:HD22	2.15	0.47
2:B:483:ARG:NH1	2:B:494:LEU:HD12	2.29	0.47
2:B:555:LEU:O	2:B:559:THR:HG22	2.14	0.47
4:I:43:DG:N2	5:J:49:DC:C2	2.82	0.47
1:A:310:TRP:HB2	1:A:328:LEU:HB2	1.96	0.47
2:B:483:ARG:HA	2:B:501:VAL:HG21	1.97	0.47
2:D:286:ALA:O	2:D:353:LYS:HD3	2.15	0.47
2:D:491:ARG:HH21	2:D:552:ARG:NH1	2.13	0.47
4:I:38:DT:H2''	4:I:39:DT:H5'	1.97	0.47
1:A:484:GLY:HA3	1:A:536:LEU:HD21	1.97	0.47
1:A:491:ALA:HB2	2:B:457:PHE:HE1	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLU:O	2:B:250:LYS:HB2	2.14	0.47
1:C:483:ARG:HD3	4:I:31:DA:H5"	1.97	0.47
1:A:504:LEU:HD22	2:B:508:GLN:NE2	2.29	0.47
1:A:402:THR:HG23	1:A:407:GLU:HB2	1.96	0.47
1:A:475:PHE:CD1	1:A:500:PRO:HG3	2.50	0.47
3:E:5:DG:N2	4:F:30:DC:N3	2.52	0.47
2:D:508:GLN:HA	2:D:511:VAL:HG12	1.95	0.46
5:J:51:DT:C4	5:J:52:DA:C6	3.03	0.46
1:C:290:GLU:OE2	1:C:293:ARG:NE	2.34	0.46
1:A:369:GLU:HA	1:A:402:THR:O	2.14	0.46
2:B:260:LEU:HD12	2:B:263:MET:CE	2.45	0.46
2:D:247:GLU:O	2:D:250:LYS:HB2	2.15	0.46
1:C:539:THR:HG21	2:D:471:VAL:CG1	2.46	0.46
1:A:536:LEU:O	1:A:540:LEU:HG	2.16	0.46
1:A:472:ARG:HB2	2:B:562:PRO:HA	1.97	0.46
1:A:478:GLN:HB3	2:B:485:GLN:HG2	1.97	0.46
1:A:346:ASP:OD1	1:A:348:ARG:HB2	2.16	0.46
1:C:348:ARG:NH1	5:J:54:DC:C5	2.84	0.46
1:C:512:THR:HG23	1:C:514:LYS:H	1.81	0.46
1:C:534:PRO:O	1:C:538:ARG:HB2	2.16	0.46
2:D:256:LEU:HD23	2:D:291:VAL:HB	1.98	0.46
2:D:469:VAL:CG2	2:D:484:ARG:NH1	2.79	0.46
1:A:375:HIS:HA	1:A:377:LEU:HG	1.98	0.45
1:C:375:HIS:HA	1:C:377:LEU:HG	1.99	0.45
2:B:265:GLY:HA3	2:B:429:TRP:CE3	2.51	0.45
3:H:3:DG:H2"	3:H:4:DT:C6	2.51	0.45
1:A:486:SER:N	1:A:489:LYS:HB2	2.26	0.45
1:C:474:VAL:HG21	2:D:566:LEU:CD1	2.43	0.45
1:C:479:LEU:HD12	1:C:479:LEU:HA	1.74	0.45
2:D:260:LEU:HD12	2:D:263:MET:CE	2.46	0.45
1:A:260:LEU:HD23	1:A:326:LEU:HD21	1.99	0.45
1:A:524:LYS:HG3	1:A:529:GLN:OE1	2.17	0.45
2:B:469:VAL:HG22	2:B:484:ARG:NH1	2.32	0.45
1:C:366:TYR:N	1:C:398:PHE:O	2.45	0.45
1:C:422:LEU:HD22	1:C:449:PRO:HB3	1.98	0.45
1:C:486:SER:O	1:C:490:ALA:N	2.42	0.45
2:D:287:VAL:HG13	2:D:290:SER:OG	2.17	0.45
1:C:369:GLU:HA	1:C:402:THR:O	2.16	0.45
1:A:272:CYS:HB3	1:A:309:VAL:HG23	1.99	0.45
1:A:475:PHE:CG	1:A:500:PRO:HD3	2.51	0.45
1:C:512:THR:CG2	1:C:514:LYS:H	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:7:DG:H2'	3:E:8:DT:C6	2.51	0.45
4:F:38:DT:H3	5:G:53:DA:H61	1.65	0.45
2:B:452:ARG:HE	2:B:452:ARG:HB3	1.62	0.45
1:C:520:LEU:HA	1:C:523:ILE:HG12	1.99	0.45
2:D:483:ARG:NH1	2:D:494:LEU:HD12	2.32	0.45
1:C:346:ASP:OD1	1:C:348:ARG:HB2	2.17	0.45
1:C:410:ALA:O	1:C:413:ALA:HB3	2.16	0.45
2:D:561:GLN:HG3	2:D:564:LEU:HB2	1.99	0.45
1:A:317:PRO:HG2	1:A:320:PRO:HA	1.98	0.44
1:A:335:LYS:HG3	1:A:339:ASP:HB2	1.98	0.44
1:C:454:LEU:HD12	1:C:454:LEU:HA	1.72	0.44
2:B:364:VAL:HA	2:B:426:VAL:HG23	1.99	0.44
2:B:415:LEU:HA	2:B:415:LEU:HD12	1.60	0.44
1:C:414:LEU:HB3	2:D:413:VAL:HG21	1.99	0.44
2:D:364:VAL:HA	2:D:426:VAL:HG23	1.98	0.44
2:B:561:GLN:HG3	2:B:564:LEU:HB2	2.00	0.44
1:C:524:LYS:HD2	1:C:529:GLN:HB3	2.00	0.44
1:A:422:LEU:HB3	1:A:423:TYR:CD1	2.53	0.44
1:C:268:ARG:NH2	1:C:315:THR:HG22	2.33	0.44
1:C:368:VAL:O	1:C:402:THR:HB	2.17	0.44
1:C:536:LEU:O	1:C:540:LEU:HG	2.17	0.44
4:F:43:DG:N2	5:G:49:DC:O2	2.51	0.44
1:A:336:ARG:HH21	1:A:370:GLU:CD	2.25	0.44
1:C:336:ARG:NH2	1:C:370:GLU:OE2	2.49	0.44
1:C:402:THR:HG23	1:C:407:GLU:CB	2.48	0.44
3:E:3:DG:H1	4:F:32:DC:N4	2.15	0.44
4:F:37:DG:H2''	4:F:38:DT:H6	1.83	0.44
2:B:481:VAL:O	2:B:485:GLN:HG3	2.18	0.44
3:H:7:DG:H2'	3:H:8:DT:H6	1.83	0.44
1:A:268:ARG:NH2	1:A:315:THR:HG22	2.33	0.44
1:C:359:CYS:C	1:C:361:LEU:H	2.25	0.43
1:C:422:LEU:HB3	1:C:423:TYR:CD1	2.53	0.43
1:A:341:CYS:SG	1:A:377:LEU:HB3	2.59	0.43
2:B:491:ARG:HH21	2:B:552:ARG:NH1	2.17	0.43
4:I:39:DT:OP2	4:I:39:DT:H6	2.02	0.43
2:B:354:THR:HB	2:B:357:LYS:HB2	2.00	0.43
2:D:481:VAL:O	2:D:485:GLN:HG3	2.19	0.43
2:B:309:GLU:C	2:B:311:THR:H	2.27	0.43
2:B:363:ILE:HB	2:B:425:ILE:HG12	2.00	0.43
2:B:489:LEU:HB3	2:B:552:ARG:HH21	1.83	0.43
2:D:489:LEU:HD12	2:D:489:LEU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:O	1:A:352:GLN:HG3	2.19	0.43
1:A:402:THR:HG23	1:A:407:GLU:CB	2.49	0.43
3:H:3:DG:H1	4:I:32:DC:N4	2.15	0.43
2:B:253:ILE:HG22	2:B:279:ARG:HB2	2.00	0.43
2:D:404:SER:OG	2:D:407:ASP:OD2	2.35	0.43
1:C:260:LEU:HD23	1:C:326:LEU:HD21	2.01	0.43
4:F:26:DT:C2'	4:F:27:DA:H5'	2.48	0.43
2:D:343:LEU:O	2:D:346:PHE:HB3	2.18	0.43
1:A:272:CYS:SG	1:A:301:ARG:HD2	2.59	0.42
2:D:317:ARG:HG2	2:D:319:GLU:HG3	2.00	0.42
2:D:561:GLN:HA	2:D:562:PRO:HD2	1.71	0.42
4:F:43:DG:H2''	4:F:44:DT:C6	2.54	0.42
4:I:32:DC:H2''	4:I:33:DA:OP2	2.19	0.42
1:A:289:ARG:HA	1:A:289:ARG:HD3	1.69	0.42
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.91	0.42
2:D:309:GLU:C	2:D:311:THR:H	2.27	0.42
1:A:275:ILE:HD12	1:A:278:THR:CG2	2.49	0.42
1:A:290:GLU:OE2	1:A:293:ARG:NE	2.37	0.42
1:A:390:ASN:O	1:A:394:ILE:HB	2.19	0.42
4:F:43:DG:H2''	4:F:44:DT:C5	2.55	0.42
1:A:369:GLU:HG2	1:A:370:GLU:H	1.83	0.42
1:A:524:LYS:HA	1:A:530:ARG:O	2.19	0.42
2:D:486:ILE:HG22	2:D:492:VAL:HG11	2.01	0.42
1:A:514:LYS:HA	1:A:514:LYS:HD3	1.84	0.42
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.66	0.42
1:C:534:PRO:O	1:C:538:ARG:N	2.40	0.42
2:D:415:LEU:HA	2:D:415:LEU:HD12	1.62	0.42
2:B:260:LEU:HA	2:B:263:MET:HE2	2.02	0.42
2:D:260:LEU:HA	2:D:263:MET:HE2	2.02	0.42
2:D:472:ASP:CG	2:D:474:ALA:H	2.28	0.42
2:D:471:VAL:HG21	2:D:478:LEU:HD21	2.02	0.41
1:A:538:ARG:O	1:A:542:GLN:HG3	2.19	0.41
2:B:312:VAL:HG12	2:B:357:LYS:HB3	2.02	0.41
4:I:39:DT:OP2	4:I:39:DT:C6	2.73	0.41
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.81	0.41
1:C:370:GLU:HA	1:C:403:ALA:O	2.19	0.41
4:I:37:DG:H3'	4:I:37:DG:P	2.60	0.41
1:A:325:GLU:O	1:A:456:PHE:N	2.47	0.41
1:A:524:LYS:HB3	1:A:529:GLN:HB3	2.01	0.41
1:C:330:HIS:O	1:C:361:LEU:HD23	2.20	0.41
1:C:352:GLN:HG3	1:C:352:GLN:H	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:PHE:HD2	1:C:494:VAL:HG22	1.84	0.41
2:D:325:ILE:HG22	2:D:343:LEU:HD12	2.02	0.41
2:D:469:VAL:HG22	2:D:484:ARG:NH1	2.34	0.41
1:A:328:LEU:C	1:A:330:HIS:H	2.29	0.41
1:C:507:TYR:O	1:C:516:GLN:NE2	2.52	0.41
2:D:253:ILE:HG22	2:D:279:ARG:HB2	2.03	0.41
4:F:24:DC:C2'	4:F:25:DT:H5'	2.48	0.41
3:H:6:DT:H2''	3:H:7:DG:C8	2.56	0.41
2:B:404:SER:OG	2:B:407:ASP:OD2	2.35	0.41
1:C:335:LYS:HG3	1:C:339:ASP:HB2	2.02	0.41
4:I:36:DG:O6	5:J:55:DC:H1'	2.20	0.41
1:A:534:PRO:O	1:A:538:ARG:HB2	2.20	0.41
2:B:317:ARG:HG2	2:B:319:GLU:HG3	2.02	0.41
1:C:262:LEU:HB3	1:C:267:TYR:HB3	2.01	0.41
1:C:369:GLU:HG2	1:C:370:GLU:H	1.85	0.41
3:E:7:DG:N2	4:F:29:DA:C2	2.88	0.41
5:G:51:DT:H2''	5:G:52:DA:C8	2.55	0.41
1:A:275:ILE:HD12	1:A:278:THR:HG21	2.03	0.41
1:C:272:CYS:HB3	1:C:309:VAL:HG23	2.02	0.41
1:C:289:ARG:HD3	1:C:289:ARG:HA	1.69	0.41
1:C:386:GLN:NE2	2:D:441:LYS:HB3	2.36	0.41
1:A:314:GLU:HG2	1:A:324:GLY:N	2.33	0.41
2:B:265:GLY:HA3	2:B:429:TRP:CD2	2.56	0.41
2:B:290:SER:HB3	2:B:314:VAL:HG22	2.03	0.41
1:A:330:HIS:O	1:A:361:LEU:HD23	2.21	0.40
4:I:37:DG:H1'	4:I:38:DT:O4'	2.21	0.40
1:C:475:PHE:CD2	1:C:494:VAL:HG22	2.57	0.40
1:A:528:LEU:HA	1:A:529:GLN:HA	1.90	0.40
2:B:481:VAL:O	2:B:485:GLN:N	2.53	0.40
1:A:517:GLU:HG2	1:A:538:ARG:HG3	2.04	0.40
2:B:471:VAL:HG21	2:B:478:LEU:CD2	2.52	0.40
1:A:256:GLN:HG3	1:A:322:ASN:HD22	1.87	0.40
1:A:366:TYR:N	1:A:398:PHE:O	2.49	0.40
2:B:256:LEU:HD23	2:B:291:VAL:HB	2.03	0.40
1:C:328:LEU:C	1:C:330:HIS:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/306 (87%)	243 (91%)	22 (8%)	2 (1%)	18	56
1	C	267/306 (87%)	244 (91%)	21 (8%)	2 (1%)	18	56
2	B	276/393 (70%)	261 (95%)	14 (5%)	1 (0%)	30	67
2	D	276/393 (70%)	260 (94%)	14 (5%)	2 (1%)	18	56
All	All	1086/1398 (78%)	1008 (93%)	71 (6%)	7 (1%)	21	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	PRO
1	C	259	PRO
2	D	562	PRO
2	D	467	GLY
1	C	432	PRO
1	A	432	PRO
2	B	562	PRO

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	
1	A	237/259 (92%)	213 (90%)	24 (10%)	7	23
1	C	237/259 (92%)	209 (88%)	28 (12%)	5	18
2	B	242/334 (72%)	222 (92%)	20 (8%)	10	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	242/334 (72%)	222 (92%)	20 (8%)	10	30
All	All	958/1186 (81%)	866 (90%)	92 (10%)	8	25

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	VAL
1	A	278	THR
1	A	299	THR
1	A	311	VAL
1	A	338	ASP
1	A	342	SER
1	A	375	HIS
1	A	384	LEU
1	A	393	VAL
1	A	400	LYS
1	A	405	ILE
1	A	415	LEU
1	A	422	LEU
1	A	428	LEU
1	A	430	SER
1	A	454	LEU
1	A	457	SER
1	A	479	LEU
1	A	482	VAL
1	A	499	THR
1	A	512	THR
1	A	527	ARG
1	A	543	LEU
1	A	550	LEU
2	B	247	GLU
2	B	249	LEU
2	B	269	LEU
2	B	273	LEU
2	B	285	GLN
2	B	287	VAL
2	B	291	VAL
2	B	311	THR
2	B	342	THR
2	B	343	LEU
2	B	344	GLN
2	B	367	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	412	LEU
2	B	459	PHE
2	B	461	LEU
2	B	463	SER
2	B	470	LYS
2	B	471	VAL
2	B	526	LEU
2	B	531	GLN
1	C	269	VAL
1	C	278	THR
1	C	299	THR
1	C	311	VAL
1	C	338	ASP
1	C	342	SER
1	C	351	GLU
1	C	375	HIS
1	C	384	LEU
1	C	393	VAL
1	C	400	LYS
1	C	405	ILE
1	C	415	LEU
1	C	422	LEU
1	C	428	LEU
1	C	430	SER
1	C	454	LEU
1	C	457	SER
1	C	474	VAL
1	C	479	LEU
1	C	482	VAL
1	C	494	VAL
1	C	499	THR
1	C	512	THR
1	C	520	LEU
1	C	527	ARG
1	C	543	LEU
1	C	550	LEU
2	D	247	GLU
2	D	249	LEU
2	D	269	LEU
2	D	273	LEU
2	D	285	GLN
2	D	287	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	291	VAL
2	D	311	THR
2	D	342	THR
2	D	343	LEU
2	D	344	GLN
2	D	367	GLU
2	D	412	LEU
2	D	459	PHE
2	D	461	LEU
2	D	463	SER
2	D	470	LYS
2	D	471	VAL
2	D	526	LEU
2	D	531	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	A	330	HIS
1	A	352	GLN
1	A	516	GLN
2	B	327	ASN
2	B	563	HIS
1	C	295	HIS
1	C	322	ASN
1	C	330	HIS
1	C	352	GLN
1	C	481	GLN
2	D	262	GLN
2	D	327	ASN
2	D	485	GLN
2	D	488	GLN
2	D	508	GLN
2	D	556	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	275/306 (89%)	-0.22	9 (3%)	49	45	57, 134, 185, 227	0
1	C	275/306 (89%)	-0.19	6 (2%)	62	53	67, 120, 183, 239	0
2	B	284/393 (72%)	-0.25	7 (2%)	58	50	70, 151, 222, 269	0
2	D	284/393 (72%)	-0.23	4 (1%)	73	62	48, 147, 225, 278	0
3	E	12/15 (80%)	-0.19	0	100	100	228, 256, 291, 293	0
3	H	12/15 (80%)	-0.20	0	100	100	177, 251, 313, 317	0
4	F	23/32 (71%)	-0.31	0	100	100	228, 268, 310, 313	0
4	I	23/32 (71%)	-0.17	0	100	100	234, 278, 315, 345	0
5	G	10/20 (50%)	-0.28	0	100	100	240, 273, 285, 287	0
5	J	10/20 (50%)	-0.19	0	100	100	225, 266, 281, 284	0
All	All	1208/1532 (78%)	-0.22	26 (2%)	62	53	48, 143, 259, 345	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	261	LEU	4.2
2	B	463	SER	4.1
1	A	428	LEU	4.0
2	B	261	LEU	3.1
2	B	467	GLY	3.0
1	A	384	LEU	2.9
2	D	462	GLU	2.9
1	C	313	GLN	2.8
1	A	312	ALA	2.6
1	A	262	LEU	2.6
1	C	315	THR	2.6
1	A	371	HIS	2.6
2	B	552	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	VAL	2.5
2	B	462	GLU	2.5
2	B	460	CYS	2.4
2	D	343	LEU	2.4
1	A	447	PRO	2.3
1	A	423	TYR	2.3
2	B	500	VAL	2.3
1	C	262	LEU	2.2
1	C	493	LEU	2.2
2	D	553	ILE	2.2
1	C	311	VAL	2.2
1	A	315	THR	2.1
1	C	487	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.