



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:46 PM UTC

PDB ID : 2A3V / pdb_00002a3v
Title : Structural basis for broad DNA-specificity in integron recombination
Authors : MacDonald, D.; Demarre, G.; Bouvier, M.; Mazel, D.; Gopaul, D.N.
Deposited on : 2005-06-27
Resolution : 2.80 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:

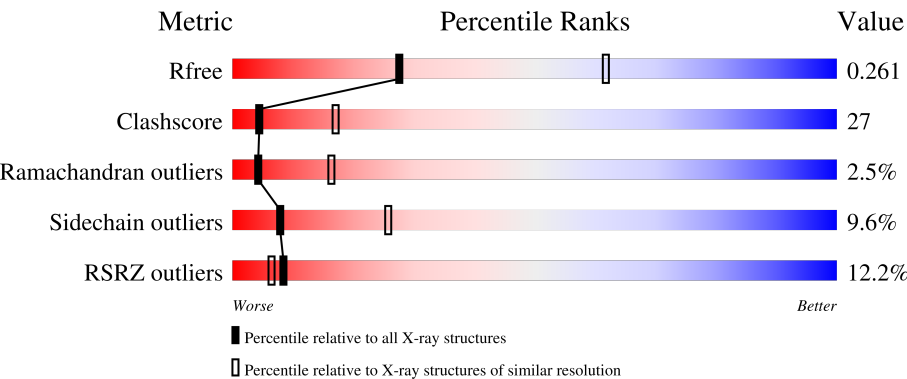
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	E	40	15% 28%42%8%22%
1	G	40	18% 28%38%8%28%
2	F	43	5% 35%40%5%21%
2	H	43	5% 16%51%5%26%
3	A	320	14% 49%40%8%..

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Mol	Chain	Length	Quality of chain
3	B	320	10% 55% 36% 8%
3	C	320	16% 51% 40% 7%
3	D	320	8% 56% 34% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13236 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 DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	31	Total	C	N	O	P	0	0	0
			632	300	120	182	30			
1	G	29	Total	C	N	O	P	0	0	0
			592	281	112	171	28			

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	34	Total	C	N	O	P	0	0	0
			693	332	121	207	33			
2	H	32	Total	C	N	O	P	0	0	0
			651	312	114	194	31			

- Molecule 3 is a protein called site-specific recombinase IntI4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	313	Total	C	N	O	S	0	0	0
			2592	1662	465	457	8			
3	B	320	Total	C	N	O	S	0	0	0
			2643	1693	475	466	9			
3	C	317	Total	C	N	O	S	0	0	0
			2620	1678	472	461	9			
3	D	320	Total	C	N	O	S	0	0	0
			2643	1693	475	466	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	LYS	engineered mutation	GB 9657688
B	2	GLY	LYS	engineered mutation	GB 9657688
C	2	GLY	LYS	engineered mutation	GB 9657688
D	2	GLY	LYS	engineered mutation	GB 9657688

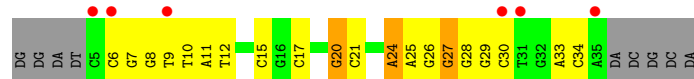
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	7	Total 7	O 7	0	0
4	F	4	Total 4	O 4	0	0
4	G	6	Total 6	O 6	0	0
4	H	4	Total 4	O 4	0	0
4	A	36	Total 36	O 36	0	0
4	B	40	Total 40	O 40	0	0
4	C	32	Total 32	O 32	0	0
4	D	41	Total 41	O 41	0	0

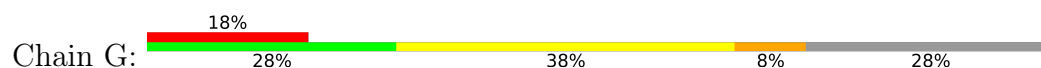
3 Residue-property plots [i](#)

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: DNA (31-MER)



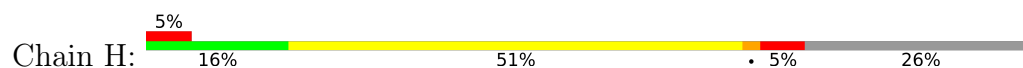
- Molecule 1: DNA (31-MER)



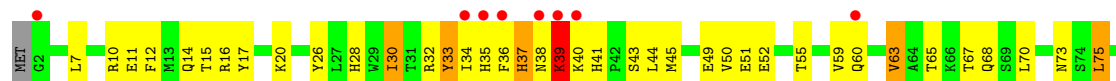
- Molecule 2: DNA (34-MER)

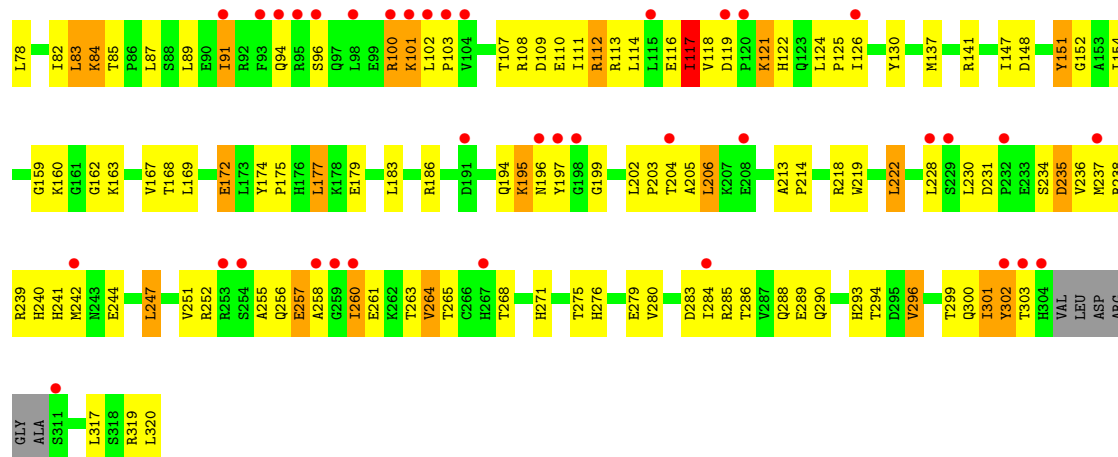


- Molecule 2: DNA (34-MER)

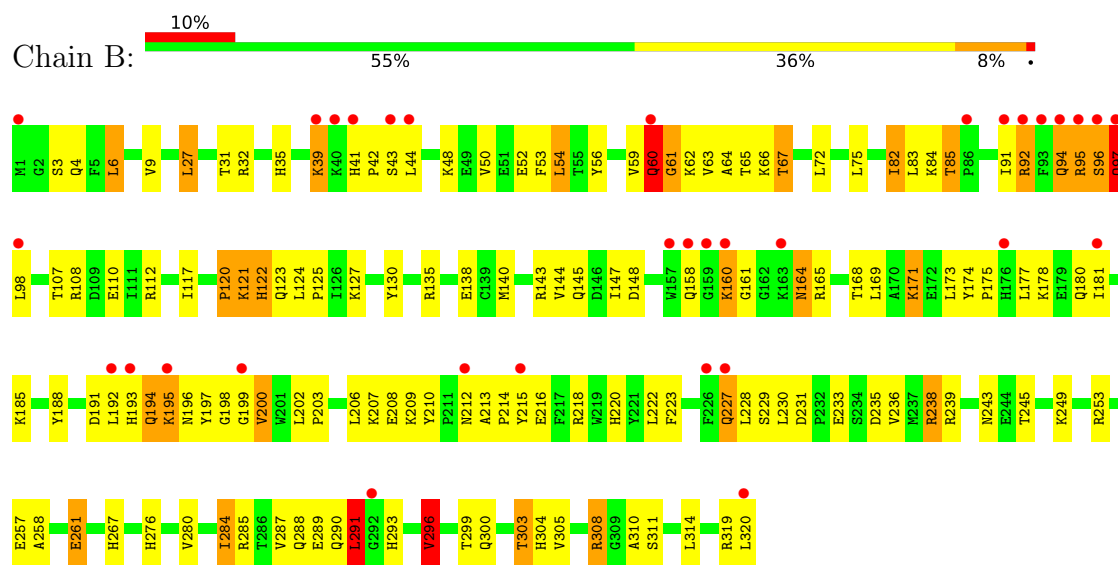


- Molecule 3: site-specific recombinase IntI4

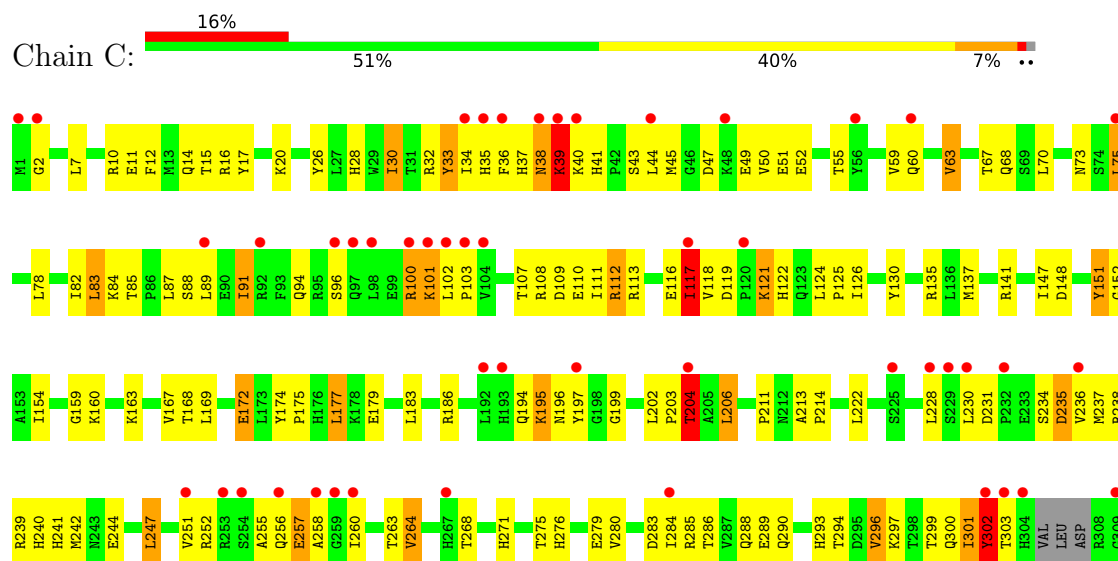


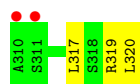


• Molecule 3: site-specific recombinase IntI4

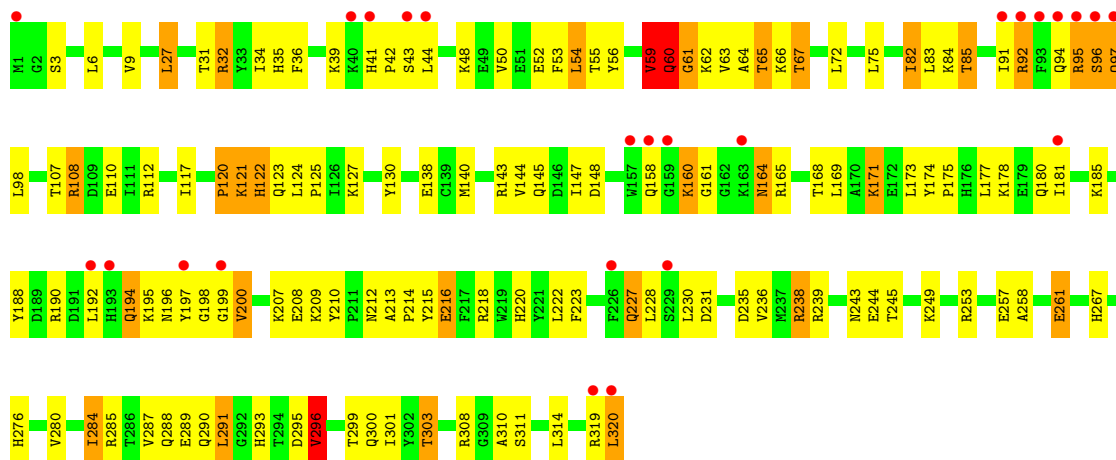


• Molecule 3: site-specific recombinase IntI4





• Molecule 3: site-specific recombinase IntI4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.90Å 170.20Å 209.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.60 – 2.80 44.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (44.60-2.80) 96.4 (44.60-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.262 0.234 , 0.261	Depositor DCC
R_{free} test set	3214 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13236	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.16% 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	E	0.40	0/709	0.77	1/1092 (0.1%)
1	G	0.41	0/664	0.81	2/1023 (0.2%)
2	F	0.42	0/775	0.85	2/1195 (0.2%)
2	H	0.44	0/728	0.93	3/1122 (0.3%)
3	A	0.58	0/2652	0.93	10/3578 (0.3%)
3	B	0.67	0/2704	1.15	27/3649 (0.7%)
3	C	0.57	0/2680	0.94	9/3614 (0.2%)
3	D	0.67	0/2704	1.15	24/3649 (0.7%)
All	All	0.59	0/13616	1.01	78/18922 (0.4%)

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
1	E	0	2
1	G	0	3
2	F	0	3
2	H	0	3
All	All	0	11

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	94	GLN	CA-C-N	-11.48	107.16	123.00
3	D	94	GLN	C-N-CA	-11.48	107.16	123.00
3	D	194	GLN	OE1-CD-NE2	-10.75	111.85	122.60
3	B	94	GLN	CA-C-N	-10.48	105.21	122.81
3	B	94	GLN	C-N-CA	-10.48	105.21	122.81
3	B	97	GLN	OE1-CD-NE2	-10.36	112.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	194	GLN	OE1-CD-NE2	-10.12	112.48	122.60
3	D	94	GLN	OE1-CD-NE2	-9.78	112.82	122.60
3	D	96	SER	CA-C-O	9.58	130.61	120.36
3	B	60	GLN	OE1-CD-NE2	-9.18	113.42	122.60
3	D	97	GLN	OE1-CD-NE2	-9.10	113.50	122.60
3	D	60	GLN	OE1-CD-NE2	-8.92	113.68	122.60
3	B	94	GLN	OE1-CD-NE2	-8.88	113.72	122.60
3	D	98	LEU	N-CA-C	-8.72	100.53	113.61
3	A	39	LYS	CA-C-N	8.56	135.40	122.65
3	A	39	LYS	C-N-CA	8.56	135.40	122.65
3	B	95	ARG	CA-C-N	-8.50	110.30	123.13
3	B	95	ARG	C-N-CA	-8.50	110.30	123.13
3	D	96	SER	CA-C-N	7.93	136.68	121.54
3	D	96	SER	C-N-CA	7.93	136.68	121.54
3	D	96	SER	O-C-N	7.60	131.89	123.22
3	D	94	GLN	CG-CD-NE2	7.34	127.41	116.40
3	D	194	GLN	CG-CD-NE2	7.28	127.31	116.40
3	B	97	GLN	CG-CD-NE2	7.00	126.90	116.40
3	B	94	GLN	CG-CD-NE2	6.99	126.88	116.40
3	D	196	ASN	N-CA-C	-6.92	96.07	110.80
3	D	96	SER	N-CA-C	6.63	119.54	108.73
3	B	122	HIS	N-CA-C	-6.63	106.39	114.75
3	D	97	GLN	CG-CD-NE2	6.62	126.33	116.40
3	B	61	GLY	N-CA-C	-6.58	97.58	113.18
3	D	61	GLY	N-CA-C	-6.56	97.63	113.18
3	A	33	TYR	N-CA-C	-6.49	104.05	112.68
3	D	122	HIS	N-CA-C	-6.47	106.59	114.75
3	B	194	GLN	CG-CD-NE2	6.40	126.00	116.40
1	E	24	DA	C5'-C4'-C3'	-6.31	105.44	114.90
3	C	30	ILE	N-CA-C	-6.31	104.35	110.72
3	A	39	LYS	O-C-N	6.30	130.97	122.59
3	A	30	ILE	N-CA-C	-6.28	104.38	110.72
3	C	33	TYR	N-CA-C	-6.27	104.34	112.68
3	D	60	GLN	CG-CD-NE2	6.24	125.76	116.40
3	B	98	LEU	N-CA-C	-6.18	104.33	113.61
3	B	60	GLN	CG-CD-NE2	6.16	125.64	116.40
3	D	296	VAL	CB-CA-C	-6.12	103.11	112.05
2	H	18	DT	C4'-C3'-O3'	6.08	119.12	110.00
3	B	96	SER	CA-C-N	6.07	133.14	121.54
3	B	96	SER	C-N-CA	6.07	133.14	121.54
3	B	296	VAL	CB-CA-C	-5.98	103.33	112.05
3	C	38	ASN	CB-CA-C	5.93	118.73	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	32	DA	N9-C1'-C2'	-5.86	104.72	113.50
3	B	291	LEU	N-CA-C	-5.84	100.68	109.79
3	B	196	ASN	N-CA-C	-5.75	98.55	110.80
1	G	28	DG	C5'-C4'-C3'	-5.74	106.28	114.90
3	D	308	ARG	N-CA-C	-5.62	105.77	113.30
3	B	195	LYS	CA-C-N	5.62	132.27	121.54
3	B	195	LYS	C-N-CA	5.62	132.27	121.54
3	D	95	ARG	CA-C-N	-5.49	115.47	122.77
3	D	95	ARG	C-N-CA	-5.49	115.47	122.77
2	F	18	DT	C5'-C4'-C3'	-5.49	106.66	114.90
3	C	204	THR	CA-C-N	5.47	131.64	123.05
3	C	204	THR	C-N-CA	5.47	131.64	123.05
3	B	96	SER	CA-C-O	5.45	127.44	120.57
3	B	308	ARG	N-CA-C	-5.44	106.01	113.30
3	C	202	LEU	CA-C-N	5.42	125.72	119.92
3	C	202	LEU	C-N-CA	5.42	125.72	119.92
3	B	82	ILE	N-CA-C	-5.37	102.66	109.80
3	A	39	LYS	CA-C-O	5.33	128.13	120.51
1	G	13	DA	C5'-C4'-C3'	-5.28	106.98	114.90
3	A	202	LEU	CA-C-N	5.27	125.56	119.92
3	A	202	LEU	C-N-CA	5.27	125.56	119.92
2	H	17	DC	N1-C1'-C2'	-5.25	105.62	113.50
3	D	82	ILE	N-CA-C	-5.25	102.81	109.80
3	A	151	TYR	N-CA-C	-5.17	100.27	109.06
2	H	32	DA	N9-C1'-C2'	-5.14	105.80	113.50
3	C	151	TYR	N-CA-C	-5.09	100.40	109.06
3	C	302	TYR	N-CA-C	-5.08	104.81	112.99
3	A	37	HIS	N-CA-C	-5.05	103.86	110.53
3	B	291	LEU	CA-C-N	-5.04	114.64	122.30
3	B	291	LEU	C-N-CA	-5.04	114.64	122.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	20	DG	Sidechain
1	E	27	DG	Sidechain
2	F	17	DC	Sidechain
2	F	19	DT	Sidechain
2	F	29	DG	Sidechain
1	G	16	DG	Sidechain
1	G	20	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	27	DG	Sidechain
2	H	17	DC	Sidechain
2	H	18	DT	Sidechain
2	H	20	DG	Sidechain

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	E	632	0	348	35	0
1	G	592	0	326	15	0
2	F	693	0	387	21	0
2	H	651	0	364	40	0
3	A	2592	0	2637	158	1
3	B	2643	0	2695	152	0
3	C	2620	0	2670	166	0
3	D	2643	0	2695	143	0
4	A	36	0	0	7	0
4	B	40	0	0	3	0
4	C	32	0	0	7	0
4	D	41	0	0	5	0
4	E	7	0	0	4	0
4	F	4	0	0	1	0
4	G	6	0	0	0	0
4	H	4	0	0	0	0
All	All	13236	0	12122	669	1

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 27.

All (669) 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)
3:B:35:HIS:ND1	3:B:39:LYS:HD3	1.38	1.36
3:B:35:HIS:CE1	3:B:39:LYS:HD3	1.81	1.13
3:B:35:HIS:CE1	3:B:39:LYS:CD	2.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:DT:H2''	1:E:10:DT:H5''	1.35	1.08
3:D:65:THR:HG21	3:D:95:ARG:HD2	1.28	1.08
3:B:35:HIS:ND1	3:B:39:LYS:CD	2.16	1.08
1:G:24:DA:H2''	1:G:25:DA:H5''	1.37	1.06
2:F:19:DT:H2'	3:B:67:THR:HG22	1.46	0.97
3:B:320:LEU:HD23	3:C:112:ARG:HH21	1.29	0.96
3:B:35:HIS:CE1	3:B:39:LYS:HE2	2.01	0.95
3:B:35:HIS:CE1	3:B:39:LYS:CE	2.51	0.94
2:F:19:DT:OP2	3:B:67:THR:HG21	1.67	0.93
3:A:16:ARG:HD2	3:D:92:ARG:HB3	1.50	0.93
3:D:65:THR:CG2	3:D:95:ARG:HD2	1.99	0.93
1:E:17:DC:H5''	4:E:47:HOH:O	1.71	0.90
3:D:65:THR:HG21	3:D:95:ARG:CD	2.00	0.90
3:A:34:ILE:HD12	3:A:39:LYS:HE3	1.53	0.89
3:C:168:THR:H	3:C:290:GLN:HE22	1.19	0.87
3:A:168:THR:H	3:A:290:GLN:HE22	1.19	0.85
3:B:95:ARG:HB2	3:B:97:GLN:NE2	1.91	0.85
3:C:34:ILE:HD12	3:C:39:LYS:HE2	1.56	0.85
3:B:6:LEU:HD11	3:B:31:THR:HG22	1.59	0.83
3:A:137:MET:HE1	3:A:244:GLU:HG2	1.61	0.83
3:C:137:MET:HE1	3:C:244:GLU:HG2	1.61	0.83
3:C:300:GLN:O	3:C:303:THR:HG22	1.79	0.82
3:B:59:VAL:O	3:B:60:GLN:C	2.17	0.82
3:A:300:GLN:O	3:A:303:THR:HG22	1.78	0.82
3:A:59:VAL:O	3:A:60:GLN:HG2	1.79	0.82
3:C:59:VAL:O	3:C:60:GLN:HG2	1.80	0.82
1:E:24:DA:C2'	1:E:25:DA:H5''	2.08	0.81
1:E:24:DA:H2''	1:E:25:DA:H5''	1.61	0.81
3:D:6:LEU:HD11	3:D:31:THR:HG22	1.61	0.81
3:B:92:ARG:HB3	3:C:16:ARG:HD2	1.62	0.81
3:C:101:LYS:H	3:C:101:LYS:HZ2	1.29	0.80
2:H:19:DT:H2'	3:D:67:THR:HG22	1.62	0.80
3:B:35:HIS:ND1	3:B:39:LYS:CE	2.45	0.80
3:B:320:LEU:HD23	3:C:112:ARG:NH2	1.97	0.80
3:B:60:GLN:O	3:B:60:GLN:HG2	1.80	0.79
3:B:32:ARG:HG2	3:B:32:ARG:HH11	1.48	0.79
3:C:38:ASN:O	3:C:40:LYS:N	2.16	0.78
2:F:13:DC:H41	3:B:245:THR:HG21	1.48	0.78
1:E:9:DT:H2''	1:E:10:DT:C5'	2.10	0.78
2:H:13:DC:H41	3:D:245:THR:HG21	1.48	0.78
3:D:160:LYS:HG3	3:D:161:GLY:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:101:LYS:H	3:A:101:LYS:HZ2	1.31	0.77
3:B:160:LYS:HG3	3:B:161:GLY:H	1.49	0.77
3:B:168:THR:H	3:B:290:GLN:HE22	1.31	0.77
2:H:23:DG:H4'	2:H:23:DG:OP1	1.87	0.75
3:B:92:ARG:HH11	3:B:92:ARG:HA	1.50	0.75
3:D:32:ARG:HH11	3:D:32:ARG:HG2	1.48	0.75
3:D:59:VAL:HG22	3:D:60:GLN:H	1.50	0.75
3:D:168:THR:H	3:D:290:GLN:HE22	1.34	0.75
3:D:95:ARG:C	3:D:97:GLN:HE21	1.95	0.75
3:D:92:ARG:HA	3:D:92:ARG:HH11	1.51	0.75
3:B:35:HIS:HE1	3:B:39:LYS:HE2	1.50	0.74
1:G:24:DA:C2'	1:G:25:DA:H5''	2.16	0.74
3:D:59:VAL:O	3:D:60:GLN:C	2.30	0.73
3:A:32:ARG:HA	3:A:35:HIS:HB3	1.70	0.73
3:C:63:VAL:HG13	3:C:67:THR:HB	1.70	0.73
3:C:320:LEU:HD22	3:D:112:ARG:HG3	1.70	0.73
3:B:261:GLU:H	3:B:261:GLU:CD	1.97	0.73
3:D:41:HIS:HB3	3:D:44:LEU:HD13	1.70	0.72
2:F:28:DT:H4'	3:A:73:ASN:ND2	2.05	0.72
3:B:41:HIS:HB3	3:B:44:LEU:HD13	1.71	0.72
2:H:18:DT:H4'	2:H:19:DT:OP1	1.89	0.72
2:F:19:DT:OP1	3:C:204:THR:O	2.08	0.72
3:B:95:ARG:C	3:B:97:GLN:HE21	1.97	0.72
1:E:28:DG:H2''	1:E:29:DG:H5''	1.72	0.71
3:D:222:LEU:HD12	3:D:223:PHE:CE1	2.26	0.71
3:A:63:VAL:HG13	3:A:67:THR:HB	1.71	0.71
3:C:124:LEU:HB3	3:C:125:PRO:HD3	1.73	0.71
3:A:320:LEU:HD22	3:B:112:ARG:HG3	1.71	0.70
3:B:59:VAL:CG1	3:B:60:GLN:H	2.03	0.70
3:C:32:ARG:HA	3:C:35:HIS:HB3	1.71	0.70
2:H:29:DG:H2''	2:H:30:DT:H5''	1.72	0.70
3:B:95:ARG:CB	3:B:97:GLN:NE2	2.55	0.69
2:H:37:DC:H2''	2:H:38:DG:N7	2.06	0.69
3:B:222:LEU:HD12	3:B:223:PHE:CE1	2.26	0.69
3:A:124:LEU:HB3	3:A:125:PRO:HD3	1.73	0.69
3:B:280:VAL:HG12	3:B:280:VAL:O	1.93	0.69
3:D:261:GLU:CD	3:D:261:GLU:H	1.98	0.69
3:D:280:VAL:O	3:D:280:VAL:HG12	1.93	0.69
3:B:59:VAL:HG12	3:B:60:GLN:N	2.09	0.68
3:B:300:GLN:O	3:B:303:THR:HB	1.94	0.68
3:A:204:THR:OG1	3:D:62:LYS:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:PRO:HG2	4:C:327:HOH:O	1.92	0.68
3:D:60:GLN:O	3:D:60:GLN:HG2	1.93	0.68
3:B:164:ASN:N	3:B:164:ASN:HD22	1.91	0.68
3:D:107:THR:HG23	3:D:110:GLU:OE1	1.93	0.68
3:A:41:HIS:HB3	3:A:44:LEU:HD23	1.74	0.68
3:C:230:LEU:HB2	3:C:237:MET:HE3	1.76	0.68
3:B:59:VAL:HG12	3:B:60:GLN:H	1.58	0.67
3:D:35:HIS:CE1	3:D:39:LYS:HE2	2.29	0.67
1:E:24:DA:C3'	1:E:25:DA:H5''	2.23	0.67
3:C:41:HIS:HB3	3:C:44:LEU:HD23	1.76	0.67
3:A:230:LEU:HB2	3:A:237:MET:HE3	1.77	0.67
3:D:59:VAL:HG22	3:D:60:GLN:N	2.09	0.67
3:C:51:GLU:HB3	3:C:91:ILE:HG23	1.76	0.67
3:A:137:MET:CE	3:A:244:GLU:HG2	2.25	0.67
3:D:164:ASN:N	3:D:164:ASN:HD22	1.92	0.67
3:D:231:ASP:HB2	3:D:238:ARG:HD2	1.77	0.67
3:A:110:GLU:HG2	3:A:260:ILE:HD11	1.77	0.67
3:B:107:THR:HG23	3:B:110:GLU:OE1	1.95	0.67
3:B:140:MET:HE2	3:B:140:MET:HA	1.77	0.67
3:D:55:THR:O	3:D:59:VAL:HG12	1.95	0.67
3:D:284:ILE:HD12	3:D:285:ARG:H	1.59	0.67
3:B:284:ILE:HD12	3:B:285:ARG:H	1.60	0.66
3:A:83:LEU:O	3:A:85:THR:N	2.29	0.66
3:A:283:ASP:OD2	3:A:285:ARG:HG2	1.95	0.66
3:D:300:GLN:O	3:D:303:THR:HB	1.95	0.66
3:A:87:LEU:HB3	3:A:91:ILE:HD11	1.78	0.66
1:E:20:DG:H2''	1:E:21:DC:O5'	1.95	0.66
3:A:34:ILE:CD1	3:A:39:LYS:HE3	2.25	0.66
3:A:51:GLU:HB3	3:A:91:ILE:HG23	1.77	0.66
3:B:62:LYS:O	3:C:204:THR:OG1	2.13	0.65
3:C:137:MET:CE	3:C:244:GLU:HG2	2.25	0.65
3:D:140:MET:HA	3:D:140:MET:HE2	1.77	0.65
3:A:195:LYS:HD3	3:A:195:LYS:N	2.11	0.65
3:B:231:ASP:HB2	3:B:238:ARG:HD2	1.77	0.65
3:C:34:ILE:HD12	3:C:39:LYS:CE	2.24	0.65
3:B:164:ASN:HD22	3:B:164:ASN:H	1.45	0.65
3:C:83:LEU:O	3:C:85:THR:N	2.30	0.65
3:B:320:LEU:HD13	3:C:108:ARG:HD2	1.78	0.65
2:H:14:DC:H2''	2:H:15:DC:H5'	1.79	0.64
3:D:147:ILE:HG21	3:D:177:LEU:HD23	1.79	0.64
3:C:195:LYS:HD3	3:C:195:LYS:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:325:HOH:O	3:D:171:LYS:HG3	1.96	0.64
2:H:28:DT:H4'	3:C:73:ASN:ND2	2.13	0.64
3:B:59:VAL:CG1	3:B:60:GLN:N	2.60	0.64
3:C:87:LEU:HB3	3:C:91:ILE:HD11	1.78	0.64
2:H:29:DG:H2''	2:H:30:DT:C5'	2.28	0.64
2:F:11:DG:H2''	2:F:13:DC:O4'	1.97	0.63
3:A:162:GLY:HA3	3:D:95:ARG:HH12	1.62	0.63
3:C:283:ASP:OD2	3:C:285:ARG:HG2	1.97	0.63
2:H:23:DG:H2''	2:H:24:DC:C6	2.34	0.63
3:B:147:ILE:HG21	3:B:177:LEU:HD23	1.79	0.63
3:D:164:ASN:HD22	3:D:164:ASN:H	1.47	0.63
3:B:41:HIS:HD2	3:B:43:SER:HB3	1.63	0.63
3:A:102:LEU:H	3:A:102:LEU:HD23	1.64	0.63
3:D:41:HIS:HD2	3:D:43:SER:HB3	1.64	0.63
3:C:2:GLY:HA3	3:C:39:LYS:NZ	2.14	0.63
2:H:35:DA:H2''	2:H:36:DC:H5''	1.79	0.62
1:E:28:DG:H2''	1:E:29:DG:C5'	2.28	0.62
3:A:101:LYS:H	3:A:101:LYS:NZ	1.98	0.62
2:F:19:DT:OP2	3:B:67:THR:CG2	2.46	0.62
1:G:7:DG:H2''	1:G:8:DG:C8	2.34	0.62
3:B:41:HIS:CD2	3:B:43:SER:HB3	2.35	0.62
3:C:100:ARG:NH2	3:C:102:LEU:HA	2.15	0.62
3:C:55:THR:HG23	3:C:94:GLN:HB2	1.80	0.62
3:D:227:GLN:HA	3:D:239:ARG:HH12	1.64	0.62
3:A:100:ARG:NH2	3:A:102:LEU:HA	2.15	0.61
3:B:59:VAL:O	3:B:61:GLY:N	2.33	0.61
3:D:41:HIS:CD2	3:D:43:SER:HB3	2.35	0.61
3:C:102:LEU:H	3:C:102:LEU:HD23	1.65	0.61
3:B:284:ILE:HD12	3:B:285:ARG:N	2.16	0.61
1:E:24:DA:H2''	1:E:25:DA:O4'	2.01	0.61
3:B:227:GLN:HA	3:B:239:ARG:HH12	1.65	0.61
3:C:204:THR:O	3:C:204:THR:HG23	2.00	0.61
3:B:95:ARG:HB2	3:B:97:GLN:HE21	1.65	0.60
2:F:16:DT:H5'	3:B:31:THR:OG1	2.02	0.60
2:H:19:DT:OP1	3:A:205:ALA:O	2.19	0.60
3:A:110:GLU:HG2	3:A:260:ILE:CD1	2.31	0.60
3:A:55:THR:HG23	3:A:94:GLN:HB2	1.82	0.60
3:A:38:ASN:O	3:A:40:LYS:N	2.33	0.60
3:A:285:ARG:HH11	3:B:285:ARG:HH21	1.50	0.60
3:D:59:VAL:CG2	3:D:60:GLN:H	2.14	0.60
3:D:66:LYS:HE2	3:D:97:GLN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:DC:H2''	2:F:15:DC:O5'	2.01	0.60
3:B:285:ARG:NH1	4:B:345:HOH:O	2.33	0.60
3:D:6:LEU:HD12	3:D:27:LEU:HG	1.84	0.60
3:A:183:LEU:HD23	3:A:186:ARG:HH21	1.67	0.59
3:C:183:LEU:HD23	3:C:186:ARG:HH21	1.66	0.59
3:B:222:LEU:HD12	3:B:223:PHE:CZ	2.38	0.59
3:B:95:ARG:CB	3:B:97:GLN:HE21	2.15	0.59
3:D:284:ILE:HD12	3:D:285:ARG:N	2.16	0.59
3:B:27:LEU:O	3:B:31:THR:HG23	2.03	0.59
3:A:228:LEU:HD11	3:A:239:ARG:HH12	1.67	0.59
3:B:6:LEU:HD12	3:B:27:LEU:HG	1.85	0.59
2:H:29:DG:C8	2:H:30:DT:H72	2.37	0.59
4:A:349:HOH:O	3:B:285:ARG:HG3	2.02	0.59
3:C:26:TYR:O	3:C:30:ILE:HG12	2.03	0.59
1:E:29:DG:H2''	1:E:30:DC:H5'	1.83	0.59
3:A:124:LEU:HD21	3:A:177:LEU:HD13	1.85	0.59
3:D:222:LEU:HD12	3:D:223:PHE:CZ	2.38	0.59
3:B:83:LEU:O	3:B:85:THR:N	2.36	0.58
3:D:243:ASN:OD1	3:D:245:THR:HB	2.03	0.58
2:F:7:DG:H2''	2:F:8:DA:C8	2.38	0.58
1:E:28:DG:C2'	1:E:29:DG:H5''	2.34	0.58
3:A:10:ARG:O	3:A:14:GLN:HG3	2.03	0.58
3:C:101:LYS:H	3:C:101:LYS:NZ	1.98	0.58
3:C:124:LEU:HD21	3:C:177:LEU:HD13	1.85	0.58
3:A:299:THR:O	3:A:302:TYR:HB2	2.03	0.58
3:C:228:LEU:HD11	3:C:239:ARG:HH12	1.67	0.58
3:D:27:LEU:O	3:D:31:THR:HG23	2.04	0.58
3:D:32:ARG:HG2	3:D:32:ARG:NH1	2.19	0.58
3:D:83:LEU:O	3:D:85:THR:N	2.36	0.58
3:B:32:ARG:HG2	3:B:32:ARG:NH1	2.18	0.58
3:B:230:LEU:HD11	3:B:235:ASP:HA	1.85	0.58
3:C:50:VAL:HG13	3:C:75:LEU:HD23	1.86	0.58
2:F:13:DC:N4	3:B:245:THR:HG21	2.16	0.57
3:D:65:THR:HG23	4:D:322:HOH:O	2.03	0.57
3:B:6:LEU:CD1	3:B:31:THR:HG22	2.34	0.57
3:B:243:ASN:OD1	3:B:245:THR:HB	2.03	0.57
2:F:24:DC:H2''	2:F:25:DG:O5'	2.03	0.57
2:H:17:DC:H2'	2:H:18:DT:H71	1.87	0.57
3:A:196:ASN:ND2	3:A:236:VAL:HA	2.20	0.57
3:C:100:ARG:NH2	3:C:103:PRO:HD3	2.19	0.57
3:C:137:MET:SD	3:C:244:GLU:HG2	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:227:GLN:HE21	3:D:227:GLN:C	2.13	0.57
3:A:148:ASP:O	3:A:151:TYR:O	2.22	0.57
3:C:10:ARG:O	3:C:14:GLN:HG3	2.03	0.57
3:D:230:LEU:HD11	3:D:235:ASP:HA	1.86	0.57
2:H:28:DT:H72	3:C:89:LEU:O	2.05	0.57
3:A:100:ARG:HH22	3:A:103:PRO:HD3	1.70	0.57
3:A:100:ARG:NH2	3:A:103:PRO:HD3	2.19	0.57
3:B:200:VAL:HG11	3:B:220:HIS:HA	1.86	0.57
3:A:26:TYR:O	3:A:30:ILE:HG12	2.05	0.57
3:A:34:ILE:HD12	3:A:39:LYS:CE	2.31	0.57
3:C:100:ARG:HH22	3:C:103:PRO:HD3	1.70	0.57
3:C:196:ASN:ND2	3:C:236:VAL:HA	2.20	0.57
3:D:65:THR:HG21	3:D:95:ARG:CG	2.35	0.57
3:D:120:PRO:O	3:D:121:LYS:HG3	2.04	0.57
3:A:137:MET:SD	3:A:244:GLU:HG2	2.45	0.56
3:A:183:LEU:HD13	3:A:183:LEU:C	2.31	0.56
3:D:171:LYS:C	3:D:173:LEU:H	2.12	0.56
2:H:18:DT:O3'	3:D:67:THR:HG21	2.03	0.56
2:H:18:DT:H2'	2:H:19:DT:H71	1.88	0.56
3:A:147:ILE:HD13	3:A:177:LEU:HG	1.87	0.56
3:B:145:GLN:HB2	3:B:218:ARG:HG2	1.88	0.56
3:C:89:LEU:N	3:C:89:LEU:HD22	2.21	0.56
3:A:50:VAL:HG13	3:A:75:LEU:HD23	1.87	0.56
3:B:120:PRO:O	3:B:121:LYS:HG3	2.05	0.56
3:B:35:HIS:HE1	3:B:39:LYS:CD	2.12	0.56
3:C:299:THR:O	3:C:302:TYR:HB2	2.05	0.56
3:D:199:GLY:O	3:D:238:ARG:HB3	2.06	0.56
3:A:213:ALA:N	3:A:214:PRO:HD2	2.21	0.56
3:D:200:VAL:HG11	3:D:220:HIS:HA	1.86	0.56
1:G:31:DT:H2''	1:G:32:DG:C8	2.41	0.55
3:C:280:VAL:HG12	3:C:280:VAL:O	2.06	0.55
3:A:7:LEU:HD13	3:A:7:LEU:O	2.06	0.55
3:A:263:THR:N	4:A:348:HOH:O	2.29	0.55
2:H:35:DA:C2'	2:H:36:DC:H5''	2.37	0.55
3:B:227:GLN:HE21	3:B:227:GLN:C	2.13	0.55
3:C:147:ILE:HD13	3:C:177:LEU:HG	1.87	0.55
3:C:196:ASN:HD21	3:C:236:VAL:HA	1.72	0.55
3:D:145:GLN:HB2	3:D:218:ARG:HG2	1.89	0.55
3:D:253:ARG:O	3:D:257:GLU:HG3	2.06	0.55
3:B:199:GLY:O	3:B:238:ARG:HB3	2.06	0.55
3:D:59:VAL:CG2	3:D:60:GLN:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:DG:H2''	1:G:28:DG:C8	2.42	0.55
3:B:171:LYS:C	3:B:173:LEU:H	2.14	0.55
3:C:7:LEU:HD13	3:C:7:LEU:O	2.07	0.55
3:C:30:ILE:HD12	3:C:78:LEU:HD22	1.88	0.55
3:C:183:LEU:HD13	3:C:183:LEU:C	2.31	0.55
3:B:253:ARG:O	3:B:257:GLU:HG3	2.07	0.55
3:A:196:ASN:HD21	3:A:236:VAL:HA	1.72	0.54
3:A:255:ALA:HB1	3:A:264:VAL:CG1	2.37	0.54
3:C:213:ALA:N	3:C:214:PRO:HD2	2.22	0.54
3:C:148:ASP:O	3:C:151:TYR:O	2.24	0.54
3:D:213:ALA:N	3:D:214:PRO:HD2	2.21	0.54
3:A:30:ILE:HD12	3:A:78:LEU:HD22	1.89	0.54
3:A:152:GLY:HA3	3:D:310:ALA:HB2	1.89	0.54
3:C:255:ALA:HB1	3:C:264:VAL:HG13	1.88	0.54
3:A:194:GLN:HB3	3:A:197:TYR:HB2	1.90	0.54
3:B:94:GLN:HG3	3:B:94:GLN:O	2.07	0.54
3:D:6:LEU:CD1	3:D:31:THR:HG22	2.35	0.54
3:D:124:LEU:N	3:D:125:PRO:HD2	2.23	0.54
3:C:255:ALA:HB1	3:C:264:VAL:CG1	2.38	0.54
3:C:285:ARG:HH11	3:D:285:ARG:HH21	1.54	0.54
3:A:280:VAL:HG12	3:A:280:VAL:O	2.08	0.54
3:B:213:ALA:N	3:B:214:PRO:HD2	2.22	0.54
3:A:89:LEU:HD22	3:A:89:LEU:N	2.22	0.54
3:B:320:LEU:CD2	3:C:112:ARG:HH21	2.12	0.54
3:D:158:GLN:HB2	4:D:347:HOH:O	2.06	0.54
3:A:255:ALA:HB1	3:A:264:VAL:HG13	1.89	0.53
3:B:130:TYR:OH	3:B:276:HIS:HD2	1.91	0.53
3:D:35:HIS:ND1	3:D:39:LYS:HE2	2.23	0.53
3:A:194:GLN:HG3	3:A:195:LYS:HD3	1.90	0.53
3:A:301:ILE:O	3:A:301:ILE:HG22	2.09	0.53
1:E:33:DA:H4'	1:E:34:DC:OP1	2.09	0.53
3:B:212:ASN:C	3:B:214:PRO:HD2	2.34	0.53
3:C:50:VAL:C	3:C:52:GLU:H	2.17	0.53
1:E:10:DT:H5''	1:E:10:DT:H6	1.73	0.53
2:H:8:DA:H2''	2:H:9:DC:O5'	2.08	0.53
3:C:194:GLN:HG3	3:C:195:LYS:HD3	1.90	0.53
3:D:210:TYR:HB2	3:D:213:ALA:HB2	1.91	0.53
3:D:147:ILE:N	3:D:147:ILE:HD12	2.24	0.53
3:B:288:GLN:OE1	3:B:296:VAL:HG13	2.09	0.53
2:H:22:DG:H2''	2:H:23:DG:O5'	2.09	0.52
3:B:124:LEU:N	3:B:125:PRO:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:210:TYR:HB2	3:B:213:ALA:HB2	1.90	0.52
3:C:301:ILE:O	3:C:301:ILE:HG22	2.09	0.52
3:D:95:ARG:O	3:D:97:GLN:NE2	2.36	0.52
1:E:6:DC:H2''	1:E:7:DG:C8	2.45	0.52
3:C:68:GLN:HE22	3:C:96:SER:H	1.57	0.52
3:D:280:VAL:O	3:D:280:VAL:CG1	2.58	0.52
3:A:12:PHE:O	3:A:16:ARG:HG2	2.09	0.52
3:B:280:VAL:O	3:B:280:VAL:CG1	2.58	0.52
3:C:194:GLN:HB3	3:C:197:TYR:HB2	1.91	0.52
1:E:10:DT:H5'	3:A:28:HIS:CD2	2.45	0.52
3:A:50:VAL:C	3:A:52:GLU:H	2.18	0.51
3:A:68:GLN:HE22	3:A:96:SER:H	1.57	0.51
4:E:46:HOH:O	3:A:65:THR:HG22	2.09	0.51
3:A:33:TYR:O	3:A:36:PHE:HB3	2.10	0.51
3:D:130:TYR:OH	3:D:276:HIS:HD2	1.93	0.51
3:D:319:ARG:CB	3:D:320:LEU:HD12	2.41	0.51
3:A:163:LYS:NZ	3:A:294:THR:HG22	2.26	0.51
3:D:212:ASN:C	3:D:214:PRO:HD2	2.34	0.51
2:H:27:DT:H5''	2:H:27:DT:H6	1.75	0.51
3:D:145:GLN:NE2	3:D:218:ARG:HE	2.08	0.51
3:A:302:TYR:N	4:A:352:HOH:O	2.43	0.51
1:E:10:DT:H2''	1:E:11:DA:C8	2.46	0.51
3:C:174:TYR:N	3:C:175:PRO:HD2	2.26	0.51
1:G:11:DA:C2	2:H:34:DA:C2	2.99	0.51
3:D:64:ALA:HB3	3:D:67:THR:HG23	1.92	0.51
3:B:66:LYS:HE2	3:B:97:GLN:HB3	1.92	0.50
3:C:12:PHE:O	3:C:16:ARG:HG2	2.10	0.50
3:D:55:THR:O	3:D:59:VAL:CG1	2.58	0.50
3:C:293:HIS:HD2	3:C:299:THR:OG1	1.94	0.50
3:A:293:HIS:HD2	3:A:299:THR:OG1	1.94	0.50
3:D:123:GLN:NE2	3:D:127:LYS:HE3	2.26	0.50
3:B:222:LEU:HD13	3:B:222:LEU:O	2.11	0.50
3:C:2:GLY:HA3	3:C:39:LYS:HZ1	1.74	0.50
1:E:8:DG:H2''	1:E:9:DT:C6	2.47	0.50
3:A:174:TYR:N	3:A:175:PRO:HD2	2.26	0.50
3:B:123:GLN:NE2	3:B:127:LYS:HE3	2.26	0.50
3:D:230:LEU:HD22	3:D:236:VAL:O	2.11	0.50
3:B:145:GLN:NE2	3:B:218:ARG:HE	2.09	0.50
3:B:147:ILE:HD12	3:B:147:ILE:N	2.26	0.50
3:A:122:HIS:O	3:A:126:ILE:HG12	2.11	0.50
3:B:230:LEU:HD22	3:B:236:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:LYS:HB2	3:C:122:HIS:ND1	2.27	0.50
3:A:121:LYS:HB2	3:A:122:HIS:ND1	2.26	0.49
3:C:33:TYR:O	3:C:36:PHE:HB3	2.11	0.49
3:D:230:LEU:HD22	3:D:236:VAL:C	2.37	0.49
3:D:314:LEU:HD23	3:D:319:ARG:NH1	2.27	0.49
3:B:64:ALA:HB3	3:B:67:THR:HG23	1.93	0.49
3:C:122:HIS:O	3:C:126:ILE:HG12	2.11	0.49
3:D:222:LEU:HD13	3:D:222:LEU:O	2.12	0.49
2:F:28:DT:H4'	3:A:73:ASN:HD21	1.77	0.49
3:A:112:ARG:HH21	3:D:320:LEU:HD23	1.77	0.49
3:A:195:LYS:HD3	3:A:196:ASN:H	1.78	0.49
3:A:252:ARG:NH1	3:A:263:THR:HG23	2.27	0.49
3:C:51:GLU:HB3	3:C:91:ILE:CG2	2.40	0.49
3:A:252:ARG:HH12	3:A:263:THR:HG23	1.76	0.49
3:B:308:ARG:HG3	4:C:324:HOH:O	2.11	0.49
3:B:314:LEU:HD23	3:B:319:ARG:NH1	2.27	0.49
3:C:252:ARG:HH12	3:C:263:THR:HG23	1.77	0.49
3:C:296:VAL:HG21	4:D:352:HOH:O	2.12	0.49
3:D:288:GLN:OE1	3:D:296:VAL:HG13	2.12	0.49
3:B:261:GLU:CD	3:B:261:GLU:N	2.70	0.49
2:H:29:DG:C2'	2:H:30:DT:H5''	2.42	0.48
3:C:163:LYS:NZ	3:C:294:THR:HG22	2.27	0.48
3:D:284:ILE:HG13	4:D:359:HOH:O	2.12	0.48
1:E:27:DG:H2''	1:E:28:DG:C8	2.48	0.48
1:G:8:DG:H1'	1:G:9:DT:H5''	1.95	0.48
3:A:111:ILE:HD12	3:A:276:HIS:HE1	1.78	0.48
3:A:230:LEU:HD21	3:A:235:ASP:OD2	2.13	0.48
3:C:55:THR:HG23	3:C:94:GLN:CB	2.43	0.48
3:C:195:LYS:HD3	3:C:196:ASN:H	1.78	0.48
1:G:8:DG:H2''	1:G:9:DT:C5'	2.43	0.48
3:A:219:TRP:NE1	4:A:333:HOH:O	2.46	0.48
3:C:252:ARG:NH1	3:C:263:THR:HG23	2.28	0.48
3:A:275:THR:O	3:A:279:GLU:HG3	2.12	0.48
3:B:230:LEU:HD22	3:B:236:VAL:C	2.38	0.48
3:B:319:ARG:CB	3:B:320:LEU:HD12	2.42	0.48
3:D:120:PRO:C	3:D:121:LYS:HG3	2.39	0.48
3:A:34:ILE:HD12	3:A:39:LYS:CG	2.44	0.48
3:A:55:THR:HG23	3:A:94:GLN:CB	2.44	0.48
3:B:185:LYS:HA	3:B:188:TYR:HB3	1.96	0.48
3:B:245:THR:O	3:B:249:LYS:HG3	2.13	0.48
3:C:102:LEU:HD23	3:C:102:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:DC:C5'	4:E:47:HOH:O	2.46	0.48
3:B:160:LYS:HA	3:B:160:LYS:HE3	1.96	0.48
3:C:203:PRO:O	3:C:206:LEU:HB2	2.14	0.48
3:C:296:VAL:HG23	4:C:346:HOH:O	2.12	0.48
3:D:160:LYS:HA	3:D:160:LYS:HE3	1.95	0.48
1:G:10:DT:H5''	3:C:28:HIS:NE2	2.27	0.48
1:G:31:DT:H2''	1:G:32:DG:N7	2.29	0.48
2:H:32:DA:H2'	2:H:33:DT:C6	2.49	0.48
3:C:30:ILE:HD13	3:C:75:LEU:HD12	1.96	0.48
3:C:230:LEU:HD21	3:C:235:ASP:OD2	2.13	0.48
3:C:256:GLN:C	3:C:258:ALA:H	2.21	0.48
3:C:275:THR:O	3:C:279:GLU:HG3	2.14	0.48
2:H:23:DG:H2''	2:H:24:DC:C5	2.49	0.48
3:A:30:ILE:HD13	3:A:75:LEU:HD12	1.96	0.48
3:B:287:VAL:O	3:B:291:LEU:HD22	2.14	0.48
2:F:19:DT:P	3:B:67:THR:HG21	2.54	0.47
3:A:109:ASP:O	3:A:113:ARG:HG3	2.13	0.47
3:A:154:ILE:HB	3:A:167:VAL:HG12	1.96	0.47
3:C:34:ILE:O	3:C:37:HIS:O	2.32	0.47
3:A:256:GLN:C	3:A:258:ALA:H	2.22	0.47
3:D:124:LEU:HD23	3:D:180:GLN:HG3	1.96	0.47
2:H:13:DC:N4	3:D:245:THR:HG21	2.23	0.47
3:A:255:ALA:CB	3:A:264:VAL:HG13	2.44	0.47
3:C:255:ALA:CB	3:C:264:VAL:HG13	2.45	0.47
3:C:83:LEU:HD22	3:C:83:LEU:H	1.80	0.47
3:C:317:LEU:HD12	3:C:320:LEU:HD12	1.96	0.47
3:A:102:LEU:HD23	3:A:102:LEU:N	2.28	0.47
3:A:119:ASP:OD2	3:A:119:ASP:N	2.46	0.47
3:A:163:LYS:HB3	4:A:337:HOH:O	2.13	0.47
3:C:7:LEU:HD13	3:C:7:LEU:C	2.40	0.47
1:G:16:DG:H2''	1:G:17:DC:O5'	2.14	0.47
2:H:27:DT:H3	3:C:68:GLN:NE2	2.13	0.47
3:A:7:LEU:HD13	3:A:7:LEU:C	2.40	0.47
3:A:152:GLY:N	4:A:336:HOH:O	2.47	0.47
3:C:10:ARG:HG2	3:C:14:GLN:HE21	1.80	0.47
3:C:109:ASP:O	3:C:113:ARG:HG3	2.14	0.47
3:C:111:ILE:HD12	3:C:276:HIS:HE1	1.79	0.47
3:C:300:GLN:HE22	3:D:288:GLN:HE22	1.62	0.47
3:D:287:VAL:O	3:D:291:LEU:HD22	2.14	0.47
3:A:203:PRO:O	3:A:206:LEU:HB2	2.14	0.47
3:C:16:ARG:HG2	3:C:16:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:GLU:CD	3:D:261:GLU:N	2.70	0.47
3:A:112:ARG:HG2	3:A:112:ARG:HH11	1.80	0.47
3:A:163:LYS:HZ3	3:A:294:THR:HG22	1.80	0.47
3:B:120:PRO:C	3:B:121:LYS:HG3	2.39	0.47
3:C:117:ILE:HG12	3:C:257:GLU:O	2.15	0.47
3:D:50:VAL:HG13	3:D:75:LEU:HD12	1.97	0.47
3:A:218:ARG:NH1	3:D:261:GLU:O	2.49	0.46
2:H:24:DC:H4'	2:H:25:DG:OP1	2.16	0.46
3:B:50:VAL:HG13	3:B:75:LEU:HD12	1.97	0.46
3:C:112:ARG:HH11	3:C:112:ARG:HG2	1.80	0.46
3:D:296:VAL:O	3:D:300:GLN:HG3	2.14	0.46
3:D:185:LYS:HA	3:D:188:TYR:HB3	1.98	0.46
2:F:34:DA:H3'	3:A:265:THR:HG21	1.98	0.46
3:A:51:GLU:HB3	3:A:91:ILE:CG2	2.41	0.46
3:C:168:THR:HG22	3:C:290:GLN:NE2	2.31	0.46
1:E:25:DA:H2'	1:E:26:DG:C8	2.51	0.46
3:A:45:MET:SD	3:A:49:GLU:HG2	2.56	0.46
3:A:159:GLY:O	3:A:160:LYS:C	2.56	0.46
3:C:119:ASP:OD2	3:C:119:ASP:N	2.47	0.46
3:C:195:LYS:HE2	3:C:196:ASN:HB3	1.98	0.46
3:C:116:GLU:C	3:C:118:VAL:H	2.24	0.46
3:C:300:GLN:NE2	3:D:288:GLN:HE22	2.14	0.46
3:D:59:VAL:O	3:D:61:GLY:N	2.48	0.46
3:B:293:HIS:HD2	3:B:299:THR:OG1	1.99	0.46
3:C:154:ILE:HB	3:C:167:VAL:HG12	1.97	0.46
3:C:240:HIS:ND1	3:C:241:HIS:N	2.64	0.46
3:D:207:LYS:NZ	3:D:238:ARG:HH22	2.14	0.46
3:A:111:ILE:HD12	3:A:276:HIS:CE1	2.51	0.46
3:A:206:LEU:HD22	3:A:206:LEU:HA	1.81	0.46
3:A:300:GLN:C	3:A:302:TYR:H	2.24	0.46
3:A:317:LEU:HD12	3:A:320:LEU:HD12	1.96	0.46
1:E:10:DT:H2''	1:E:11:DA:H8	1.80	0.45
3:C:41:HIS:CE1	3:C:43:SER:HB2	2.51	0.45
3:D:108:ARG:HD3	4:D:329:HOH:O	2.17	0.45
3:D:174:TYR:N	3:D:175:PRO:HD2	2.31	0.45
1:E:11:DA:H1'	1:E:12:DT:H5''	1.98	0.45
2:H:24:DC:H2''	2:H:25:DG:C8	2.51	0.45
3:A:34:ILE:O	3:A:37:HIS:O	2.34	0.45
3:A:240:HIS:ND1	3:A:241:HIS:N	2.64	0.45
3:D:245:THR:O	3:D:249:LYS:HG3	2.15	0.45
3:A:15:THR:C	3:A:17:TYR:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:16:ARG:HG2	3:A:16:ARG:HH11	1.80	0.45
3:A:10:ARG:HG2	3:A:14:GLN:HE21	1.79	0.45
3:A:83:LEU:HD22	3:A:83:LEU:H	1.81	0.45
3:A:117:ILE:HG12	3:A:257:GLU:O	2.16	0.45
3:A:152:GLY:HA3	3:D:310:ALA:CB	2.47	0.45
3:B:53:PHE:O	3:B:56:TYR:HB3	2.17	0.45
3:C:59:VAL:CG2	3:C:94:GLN:HG2	2.46	0.45
3:C:107:THR:H	3:C:110:GLU:HB2	1.81	0.45
3:C:288:GLN:NE2	3:C:296:VAL:HG22	2.31	0.45
1:E:33:DA:H1'	1:E:34:DC:C6	2.52	0.45
1:G:8:DG:H2''	1:G:9:DT:H5''	1.98	0.45
3:A:107:THR:H	3:A:110:GLU:HB2	1.81	0.45
3:B:296:VAL:O	3:B:300:GLN:HG3	2.16	0.45
2:H:27:DT:H4'	2:H:28:DT:OP1	2.15	0.45
3:B:207:LYS:NZ	3:B:238:ARG:HH22	2.14	0.45
3:B:310:ALA:CB	3:C:152:GLY:HA3	2.47	0.45
3:C:135:ARG:HD3	4:C:349:HOH:O	2.16	0.45
1:G:8:DG:C2'	1:G:9:DT:H5''	2.46	0.45
2:H:28:DT:H3	3:C:91:ILE:HD12	1.82	0.45
2:H:37:DC:H2''	2:H:38:DG:C8	2.52	0.45
3:D:117:ILE:HD12	3:D:258:ALA:CA	2.47	0.45
2:F:12:DT:H5'	3:B:229:SER:OG	2.17	0.45
3:A:168:THR:N	3:A:290:GLN:HE22	2.01	0.45
3:B:48:LYS:O	3:B:52:GLU:HG3	2.17	0.45
4:C:337:HOH:O	3:D:296:VAL:HG22	2.17	0.45
3:A:168:THR:HG22	3:A:290:GLN:NE2	2.31	0.45
3:B:82:ILE:HG22	3:B:83:LEU:CD1	2.47	0.45
3:C:141:ARG:HG3	3:C:141:ARG:HH11	1.82	0.45
3:D:124:LEU:HD11	3:D:177:LEU:CD1	2.47	0.45
1:E:33:DA:H1'	1:E:34:DC:H5'	1.99	0.44
3:A:41:HIS:CE1	3:A:43:SER:HB2	2.51	0.44
3:A:116:GLU:C	3:A:118:VAL:H	2.24	0.44
3:A:195:LYS:HD3	3:A:195:LYS:H	1.81	0.44
3:B:124:LEU:HD23	3:B:180:GLN:HG3	1.98	0.44
3:D:143:ARG:O	3:D:144:VAL:C	2.60	0.44
1:E:24:DA:H2''	1:E:25:DA:C5'	2.41	0.44
3:D:293:HIS:HD2	3:D:299:THR:OG1	1.99	0.44
1:E:11:DA:C2	2:F:34:DA:C2	3.05	0.44
3:B:147:ILE:CG2	3:B:177:LEU:HD23	2.47	0.44
3:C:111:ILE:HD12	3:C:276:HIS:CE1	2.52	0.44
3:D:82:ILE:HG22	3:D:83:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:20:LYS:HD3	3:A:20:LYS:HA	1.77	0.44
3:A:234:SER:O	3:A:236:VAL:HG22	2.17	0.44
3:C:159:GLY:O	3:C:160:LYS:C	2.58	0.44
2:H:36:DC:H5'	2:H:36:DC:H6	1.82	0.44
3:B:143:ARG:O	3:B:144:VAL:C	2.60	0.44
3:B:171:LYS:C	3:B:173:LEU:N	2.76	0.44
3:B:320:LEU:HD22	3:C:108:ARG:HB3	1.98	0.44
3:A:84:LYS:H	3:A:84:LYS:HG2	1.55	0.44
3:D:53:PHE:O	3:D:56:TYR:HB3	2.17	0.44
3:D:198:GLY:HA2	3:D:215:TYR:OH	2.18	0.44
3:A:195:LYS:HE2	3:A:196:ASN:HB3	1.98	0.44
3:A:288:GLN:NE2	3:A:296:VAL:HG22	2.32	0.44
3:B:174:TYR:N	3:B:175:PRO:HD2	2.33	0.44
3:C:285:ARG:HA	3:C:288:GLN:HE21	1.82	0.44
3:A:320:LEU:HD23	3:A:320:LEU:HA	1.89	0.44
3:B:117:ILE:HD12	3:B:258:ALA:CA	2.48	0.44
3:C:195:LYS:HD3	3:C:195:LYS:H	1.82	0.44
3:C:45:MET:SD	3:C:49:GLU:HG2	2.58	0.44
3:C:59:VAL:C	3:C:60:GLN:HG2	2.43	0.44
3:D:138:GLU:HG2	3:D:158:GLN:NE2	2.33	0.44
3:C:15:THR:C	3:C:17:TYR:H	2.25	0.43
3:C:47:ASP:OD2	3:C:47:ASP:N	2.51	0.43
3:C:234:SER:O	3:C:236:VAL:HG22	2.18	0.43
3:D:3:SER:OG	3:D:6:LEU:HD23	2.17	0.43
1:E:28:DG:C5'	3:C:211:PRO:HG2	2.48	0.43
2:H:16:DT:H5'	3:D:31:THR:OG1	2.18	0.43
3:C:20:LYS:HD3	3:C:20:LYS:HA	1.77	0.43
3:C:300:GLN:C	3:C:302:TYR:H	2.26	0.43
3:D:92:ARG:HA	3:D:92:ARG:NH1	2.27	0.43
1:G:22:DC:H2'	1:G:23:DT:H71	2.01	0.43
3:A:59:VAL:CG2	3:A:94:GLN:HG2	2.48	0.43
3:B:198:GLY:HA2	3:B:215:TYR:OH	2.19	0.43
1:G:15:DC:H2''	1:G:16:DG:O5'	2.18	0.43
3:A:107:THR:O	3:A:108:ARG:C	2.62	0.43
3:A:111:ILE:HD13	3:A:130:TYR:CE1	2.54	0.43
3:A:285:ARG:O	3:A:289:GLU:HG3	2.19	0.43
1:E:29:DG:C2'	1:E:30:DC:H5'	2.47	0.43
3:B:135:ARG:HD3	4:B:334:HOH:O	2.17	0.43
3:B:138:GLU:HG2	3:B:158:GLN:NE2	2.33	0.43
3:D:48:LYS:O	3:D:52:GLU:HG3	2.19	0.43
3:D:54:LEU:HD21	3:D:72:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:276:HIS:O	3:A:280:VAL:HG23	2.18	0.43
3:B:124:LEU:HD11	3:B:177:LEU:CD1	2.49	0.43
2:F:29:DG:C8	2:F:30:DT:H72	2.53	0.43
4:F:45:HOH:O	3:B:66:LYS:HB2	2.18	0.43
3:A:7:LEU:O	3:A:11:GLU:HG2	2.18	0.43
2:H:14:DC:C4	2:H:15:DC:N4	2.87	0.43
3:A:285:ARG:HA	3:A:288:GLN:HE21	1.83	0.43
3:B:4:GLN:HG2	4:B:347:HOH:O	2.19	0.43
3:B:319:ARG:CZ	3:C:280:VAL:HG11	2.49	0.43
3:C:231:ASP:OD1	3:C:238:ARG:NH1	2.52	0.43
3:D:320:LEU:HD12	3:D:320:LEU:N	2.34	0.43
3:A:261:GLU:HA	3:A:261:GLU:OE2	2.18	0.43
3:C:141:ARG:HG3	3:C:141:ARG:NH1	2.34	0.43
1:E:10:DT:H5'	3:A:28:HIS:NE2	2.33	0.43
3:C:38:ASN:O	3:C:39:LYS:C	2.61	0.43
3:C:107:THR:O	3:C:108:ARG:C	2.61	0.43
3:D:287:VAL:HG12	3:D:291:LEU:HD22	2.00	0.43
3:B:287:VAL:HG12	3:B:291:LEU:HD22	2.00	0.42
3:C:297:LYS:HE2	3:D:295:ASP:HB2	2.00	0.42
3:D:41:HIS:ND1	3:D:42:PRO:HD2	2.34	0.42
3:D:147:ILE:CG2	3:D:177:LEU:HD23	2.48	0.42
3:C:7:LEU:O	3:C:11:GLU:HG2	2.19	0.42
3:C:168:THR:N	3:C:290:GLN:HE22	2.01	0.42
3:D:124:LEU:HD11	3:D:177:LEU:HD12	2.01	0.42
1:E:10:DT:C2'	1:E:11:DA:C8	3.02	0.42
3:A:228:LEU:HD12	3:A:228:LEU:N	2.34	0.42
3:A:280:VAL:HG11	3:D:319:ARG:CZ	2.49	0.42
3:B:124:LEU:N	3:B:125:PRO:CD	2.83	0.42
3:B:191:ASP:C	3:B:193:HIS:N	2.77	0.42
3:D:138:GLU:OE2	3:D:165:ARG:NH2	2.52	0.42
3:A:101:LYS:HZ2	3:A:101:LYS:N	2.09	0.42
3:A:108:ARG:HG3	3:A:108:ARG:HH11	1.84	0.42
3:A:141:ARG:NH1	3:A:141:ARG:HG3	2.34	0.42
3:B:92:ARG:HA	3:B:92:ARG:NH1	2.26	0.42
3:B:168:THR:H	3:B:290:GLN:NE2	2.09	0.42
1:E:28:DG:H5'	3:C:211:PRO:HG2	2.01	0.42
3:B:94:GLN:CB	3:C:16:ARG:O	2.68	0.42
3:C:28:HIS:ND1	3:C:28:HIS:C	2.77	0.42
3:C:247:LEU:O	3:C:251:VAL:HG12	2.18	0.42
3:D:301:ILE:H	3:D:301:ILE:HG13	1.69	0.42
3:A:172:GLU:CD	3:A:172:GLU:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9:VAL:HG13	3:B:82:ILE:CD1	2.50	0.42
3:C:264:VAL:HG23	3:C:268:THR:OG1	2.20	0.42
1:E:9:DT:H2''	1:E:10:DT:OP1	2.19	0.42
3:A:231:ASP:OD1	3:A:238:ARG:NH1	2.52	0.42
3:B:35:HIS:CE1	3:B:39:LYS:HD2	2.44	0.42
3:B:194:GLN:O	3:B:195:LYS:C	2.60	0.42
3:C:276:HIS:O	3:C:280:VAL:HG23	2.19	0.42
3:C:101:LYS:HZ2	3:C:101:LYS:N	2.07	0.42
3:A:301:ILE:C	4:A:352:HOH:O	2.63	0.42
3:B:138:GLU:OE2	3:B:165:ARG:NH2	2.53	0.42
3:C:163:LYS:HZ3	3:C:294:THR:HG22	1.85	0.42
3:A:141:ARG:HG3	3:A:141:ARG:HH11	1.83	0.42
3:C:121:LYS:NZ	3:C:121:LYS:HB3	2.35	0.42
3:D:171:LYS:C	3:D:173:LEU:N	2.74	0.42
3:D:178:LYS:O	3:D:181:ILE:HG12	2.20	0.42
2:H:28:DT:C4	3:C:88:SER:O	2.73	0.41
3:B:35:HIS:HE1	3:B:39:LYS:CE	2.11	0.41
3:B:120:PRO:O	3:B:121:LYS:CG	2.68	0.41
3:B:124:LEU:HD11	3:B:177:LEU:HD12	2.02	0.41
3:C:271:HIS:HA	3:C:302:TYR:HE1	1.85	0.41
3:D:120:PRO:O	3:D:121:LYS:CG	2.68	0.41
3:D:200:VAL:HG13	3:D:220:HIS:CE1	2.55	0.41
2:H:18:DT:C2'	2:H:19:DT:H71	2.48	0.41
2:H:28:DT:C4	3:C:89:LEU:HA	2.55	0.41
3:A:137:MET:HE1	3:A:244:GLU:CG	2.42	0.41
3:A:271:HIS:HA	3:A:302:TYR:HE1	1.85	0.41
3:B:41:HIS:ND1	3:B:42:PRO:HD2	2.35	0.41
3:C:285:ARG:O	3:C:289:GLU:HG3	2.20	0.41
3:D:124:LEU:N	3:D:125:PRO:CD	2.83	0.41
3:D:148:ASP:OD1	3:D:148:ASP:C	2.63	0.41
3:D:216:GLU:H	3:D:216:GLU:HG2	1.69	0.41
3:C:50:VAL:C	3:C:52:GLU:N	2.78	0.41
3:C:228:LEU:HD12	3:C:228:LEU:N	2.36	0.41
1:E:9:DT:H1'	1:E:10:DT:OP1	2.20	0.41
3:C:44:LEU:N	3:C:44:LEU:HD22	2.35	0.41
3:C:108:ARG:HH11	3:C:108:ARG:HG3	1.86	0.41
3:D:197:TYR:HD1	3:D:228:LEU:HD21	1.85	0.41
2:F:12:DT:H72	3:B:238:ARG:HG3	2.02	0.41
3:A:113:ARG:NH2	3:A:260:ILE:HD11	2.35	0.41
3:A:199:GLY:O	3:A:238:ARG:HB3	2.20	0.41
3:A:283:ASP:O	3:A:286:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:LEU:HD23	3:C:186:ARG:NH2	2.34	0.41
3:D:9:VAL:HG13	3:D:82:ILE:CD1	2.49	0.41
3:A:59:VAL:C	3:A:60:GLN:HG2	2.43	0.41
3:D:140:MET:HE2	3:D:140:MET:CA	2.49	0.41
3:B:304:HIS:O	3:B:305:VAL:C	2.61	0.41
3:C:172:GLU:CD	3:C:172:GLU:H	2.27	0.41
2:F:15:DC:H6	2:F:15:DC:H2'	1.61	0.41
3:A:264:VAL:HG23	3:A:268:THR:OG1	2.21	0.41
3:B:54:LEU:HD21	3:B:72:LEU:HD23	2.02	0.41
3:B:148:ASP:OD1	3:B:148:ASP:C	2.63	0.41
3:C:37:HIS:NE2	3:C:49:GLU:HB3	2.36	0.41
3:D:82:ILE:H	3:D:82:ILE:HG13	1.61	0.41
3:D:194:GLN:O	3:D:195:LYS:C	2.63	0.41
2:H:29:DG:H2'	2:H:30:DT:C7	2.51	0.41
3:A:30:ILE:O	3:A:33:TYR:HB3	2.21	0.41
3:A:121:LYS:HB3	3:A:121:LYS:NZ	2.35	0.41
3:B:200:VAL:HG13	3:B:220:HIS:CE1	2.55	0.41
3:B:310:ALA:HB2	3:C:152:GLY:HA3	2.03	0.41
3:C:285:ARG:NH1	3:D:285:ARG:HH21	2.18	0.41
3:C:319:ARG:O	3:C:320:LEU:C	2.63	0.41
3:D:200:VAL:HG13	3:D:220:HIS:ND1	2.35	0.41
3:A:247:LEU:O	3:A:251:VAL:HG12	2.21	0.41
3:A:285:ARG:NH1	3:B:285:ARG:HH21	2.18	0.41
3:C:199:GLY:O	3:C:238:ARG:HB3	2.20	0.41
3:D:190:ARG:HG2	3:D:190:ARG:O	2.21	0.41
3:B:178:LYS:O	3:B:181:ILE:HG12	2.21	0.40
3:C:152:GLY:N	4:C:345:HOH:O	2.54	0.40
3:D:230:LEU:CD1	3:D:235:ASP:HA	2.51	0.40
3:B:230:LEU:CD1	3:B:235:ASP:HA	2.51	0.40
3:C:111:ILE:HD13	3:C:130:TYR:CE1	2.56	0.40
3:C:121:LYS:C	3:C:122:HIS:ND1	2.79	0.40
1:E:15:DC:C5'	4:E:41:HOH:O	2.69	0.40
2:F:10:DA:H2''	2:F:11:DG:C8	2.57	0.40
2:H:23:DG:C2'	2:H:24:DC:C5	3.03	0.40
3:A:28:HIS:ND1	3:A:28:HIS:C	2.79	0.40
3:B:200:VAL:HG13	3:B:220:HIS:ND1	2.35	0.40
3:B:231:ASP:OD2	3:B:231:ASP:C	2.64	0.40
3:D:34:ILE:C	3:D:36:PHE:H	2.30	0.40
3:D:82:ILE:O	3:D:83:LEU:HB2	2.21	0.40
3:A:319:ARG:CZ	3:B:280:VAL:HG11	2.51	0.40
3:B:197:TYR:HD1	3:B:228:LEU:HD21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:202:LEU:HA	3:B:203:PRO:HD3	1.98	0.40
3:B:203:PRO:HD2	3:B:206:LEU:HD12	2.04	0.40
3:C:283:ASP:O	3:C:286:THR:HB	2.22	0.40
3:A:114:LEU:O	3:A:118:VAL:HG23	2.22	0.40
3:A:147:ILE:HD11	3:A:222:LEU:HD11	2.04	0.40
3:B:231:ASP:OD2	3:B:233:GLU:HG2	2.22	0.40
3:C:30:ILE:O	3:C:33:TYR:HB3	2.22	0.40
3:C:68:GLN:NE2	3:C:96:SER:H	2.19	0.40
3:C:101:LYS:H	3:C:101:LYS:CE	2.35	0.40
3:D:244:GLU:HG2	3:D:245:THR:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:HIS:CE1	3:A:35:HIS:CE1[3_656]	1.78	0.42

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	
3	A	309/320 (97%)	270 (87%)	29 (9%)	10 (3%)	3	11
3	B	318/320 (99%)	282 (89%)	31 (10%)	5 (2%)	7	27
3	C	313/320 (98%)	276 (88%)	26 (8%)	11 (4%)	3	10
3	D	318/320 (99%)	280 (88%)	33 (10%)	5 (2%)	7	27
All	All	1258/1280 (98%)	1108 (88%)	119 (10%)	31 (2%)	4	16

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	39	LYS
3	A	84	LYS
3	A	117	ILE
3	A	235	ASP
3	B	84	LYS
3	C	39	LYS
3	C	84	LYS
3	C	117	ILE
3	C	235	ASP
3	D	84	LYS
3	A	91	ILE
3	B	60	GLN
3	B	97	GLN
3	C	91	ILE
3	D	60	GLN
3	A	242	MET
3	C	204	THR
3	A	257	GLU
3	A	260	ILE
3	C	242	MET
3	C	257	GLU
3	C	260	ILE
3	A	301	ILE
3	C	301	ILE
3	B	120	PRO
3	D	120	PRO
3	C	82	ILE
3	D	59	VAL
3	A	82	ILE
3	B	91	ILE
3	D	91	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	282/287 (98%)	260 (92%)	22 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	287/287 (100%)	254 (88%)	33 (12%)	5	18
3	C	284/287 (99%)	262 (92%)	22 (8%)	12	36
3	D	287/287 (100%)	254 (88%)	33 (12%)	5	18
All	All	1140/1148 (99%)	1030 (90%)	110 (10%)	8	26

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	39	LYS
3	A	63	VAL
3	A	70	LEU
3	A	75	LEU
3	A	83	LEU
3	A	100	ARG
3	A	101	LYS
3	A	112	ARG
3	A	117	ILE
3	A	121	LYS
3	A	169	LEU
3	A	172	GLU
3	A	177	LEU
3	A	179	GLU
3	A	195	LYS
3	A	206	LEU
3	A	222	LEU
3	A	247	LEU
3	A	264	VAL
3	A	284	ILE
3	A	296	VAL
3	A	302	TYR
3	B	3	SER
3	B	6	LEU
3	B	27	LEU
3	B	39	LYS
3	B	54	LEU
3	B	63	VAL
3	B	65	THR
3	B	67	THR
3	B	85	THR
3	B	92	ARG
3	B	96	SER

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Mol	Chain	Res	Type
3	B	108	ARG
3	B	121	LYS
3	B	122	HIS
3	B	160	LYS
3	B	164	ASN
3	B	169	LEU
3	B	171	LYS
3	B	192	LEU
3	B	200	VAL
3	B	208	GLU
3	B	209	LYS
3	B	216	GLU
3	B	227	GLN
3	B	238	ARG
3	B	261	GLU
3	B	267	HIS
3	B	284	ILE
3	B	289	GLU
3	B	291	LEU
3	B	296	VAL
3	B	303	THR
3	B	311	SER
3	C	39	LYS
3	C	63	VAL
3	C	70	LEU
3	C	75	LEU
3	C	83	LEU
3	C	100	ARG
3	C	101	LYS
3	C	112	ARG
3	C	117	ILE
3	C	121	LYS
3	C	169	LEU
3	C	172	GLU
3	C	177	LEU
3	C	179	GLU
3	C	195	LYS
3	C	206	LEU
3	C	222	LEU
3	C	247	LEU
3	C	264	VAL
3	C	284	ILE

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Mol	Chain	Res	Type
3	C	296	VAL
3	C	302	TYR
3	D	27	LEU
3	D	32	ARG
3	D	54	LEU
3	D	59	VAL
3	D	63	VAL
3	D	65	THR
3	D	67	THR
3	D	85	THR
3	D	92	ARG
3	D	96	SER
3	D	108	ARG
3	D	121	LYS
3	D	122	HIS
3	D	160	LYS
3	D	164	ASN
3	D	169	LEU
3	D	171	LYS
3	D	192	LEU
3	D	200	VAL
3	D	208	GLU
3	D	209	LYS
3	D	216	GLU
3	D	227	GLN
3	D	238	ARG
3	D	261	GLU
3	D	267	HIS
3	D	284	ILE
3	D	289	GLU
3	D	291	LEU
3	D	296	VAL
3	D	303	THR
3	D	311	SER
3	D	320	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	38	ASN
3	A	68	GLN
3	A	73	ASN

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Mol	Chain	Res	Type
3	A	123	GLN
3	A	145	GLN
3	A	158	GLN
3	A	180	GLN
3	A	194	GLN
3	A	196	ASN
3	A	256	GLN
3	A	267	HIS
3	A	288	GLN
3	A	290	GLN
3	A	293	HIS
3	A	300	GLN
3	B	14	GLN
3	B	38	ASN
3	B	41	HIS
3	B	60	GLN
3	B	97	GLN
3	B	122	HIS
3	B	123	GLN
3	B	145	GLN
3	B	158	GLN
3	B	164	ASN
3	B	176	HIS
3	B	212	ASN
3	B	220	HIS
3	B	227	GLN
3	B	256	GLN
3	B	276	HIS
3	B	290	GLN
3	B	293	HIS
3	C	4	GLN
3	C	38	ASN
3	C	68	GLN
3	C	73	ASN
3	C	145	GLN
3	C	176	HIS
3	C	180	GLN
3	C	194	GLN
3	C	196	ASN
3	C	256	GLN
3	C	267	HIS
3	C	288	GLN

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Mol	Chain	Res	Type
3	C	290	GLN
3	C	293	HIS
3	D	14	GLN
3	D	38	ASN
3	D	41	HIS
3	D	97	GLN
3	D	122	HIS
3	D	123	GLN
3	D	145	GLN
3	D	158	GLN
3	D	164	ASN
3	D	176	HIS
3	D	212	ASN
3	D	220	HIS
3	D	227	GLN
3	D	276	HIS
3	D	288	GLN
3	D	290	GLN
3	D	293	HIS
3	D	304	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	E	31/40 (77%)	0.68	6 (19%) 3 2	38, 62, 154, 171	0
1	G	29/40 (72%)	0.86	7 (24%) 2 1	33, 63, 132, 160	0
2	F	34/43 (79%)	0.28	2 (5%) 28 21	35, 58, 164, 175	0
2	H	32/43 (74%)	0.42	2 (6%) 26 19	35, 57, 119, 169	0
3	A	313/320 (97%)	0.80	45 (14%) 6 5	30, 60, 107, 125	0
3	B	320/320 (100%)	0.66	33 (10%) 12 9	27, 54, 93, 131	0
3	C	317/320 (99%)	0.87	50 (15%) 5 4	30, 61, 108, 125	0
3	D	320/320 (100%)	0.63	25 (7%) 19 14	26, 54, 93, 131	0
All	All	1396/1446 (96%)	0.72	170 (12%) 8 6	26, 57, 108, 175	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	39	LYS	6.5
3	C	39	LYS	6.0
3	B	97	GLN	6.0
3	D	97	GLN	5.9
3	B	193	HIS	5.5
3	D	95	ARG	5.4
3	D	193	HIS	5.2
3	C	98	LEU	5.1
3	A	98	LEU	4.9
3	C	258	ALA	4.7
3	D	320	LEU	4.7
3	D	93	PHE	4.6
3	B	93	PHE	4.4
3	B	95	ARG	4.3
3	A	259	GLY	4.3
3	D	1	MET	4.3

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Mol	Chain	Res	Type	RSRZ
3	B	320	LEU	4.3
3	B	91	ILE	4.2
3	A	260	ILE	4.2
3	D	96	SER	4.2
3	A	2	GLY	4.1
3	B	158	GLN	4.0
3	B	159	GLY	3.9
3	C	228	LEU	3.9
3	A	204	THR	3.9
3	C	38	ASN	3.8
3	D	192	LEU	3.7
1	E	5	DC	3.6
1	G	6	DC	3.6
3	C	254	SER	3.6
2	F	6	DT	3.6
3	B	195	LYS	3.5
3	B	192	LEU	3.5
3	C	1	MET	3.4
3	C	303	THR	3.4
3	B	39	LYS	3.4
3	D	199	GLY	3.3
3	C	96	SER	3.3
3	B	157	TRP	3.3
3	C	259	GLY	3.2
3	A	96	SER	3.2
3	B	41	HIS	3.2
3	D	92	ARG	3.2
3	C	193	HIS	3.2
3	C	101	LYS	3.2
3	C	102	LEU	3.2
2	F	39	DG	3.1
3	B	94	GLN	3.1
3	C	309	GLY	3.1
3	C	100	ARG	3.1
3	D	319	ARG	3.1
3	B	92	ARG	3.1
3	A	267	HIS	3.1
3	A	100	ARG	3.0
3	C	34	ILE	3.0
3	C	60	GLN	3.0
3	D	157	TRP	3.0
3	A	228	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	36	PHE	3.0
3	B	160	LYS	3.0
3	A	60	GLN	3.0
3	D	158	GLN	2.9
3	C	204	THR	2.9
3	C	267	HIS	2.9
3	C	89	LEU	2.9
3	C	225	SER	2.9
1	E	6	DC	2.9
1	G	34	DC	2.9
3	D	159	GLY	2.9
3	B	212	ASN	2.9
3	D	40	LYS	2.9
3	C	260	ILE	2.9
3	B	1	MET	2.8
3	D	226	PHE	2.8
3	A	198	GLY	2.8
3	C	2	GLY	2.8
3	A	36	PHE	2.8
3	D	229	SER	2.8
1	G	32	DG	2.8
3	A	34	ILE	2.7
3	A	93	PHE	2.7
3	B	292	GLY	2.7
3	A	229	SER	2.7
3	C	311	SER	2.7
3	B	44	LEU	2.7
3	C	251	VAL	2.7
3	C	284	ILE	2.7
3	C	92	ARG	2.7
3	C	35	HIS	2.6
3	C	304	HIS	2.6
3	C	230	LEU	2.6
3	D	43	SER	2.6
3	A	101	LYS	2.6
3	B	215	TYR	2.6
3	C	44	LEU	2.6
3	B	181	ILE	2.6
3	A	208	GLU	2.6
3	D	94	GLN	2.6
3	B	96	SER	2.5
3	D	197	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	40	LYS	2.5
1	E	9	DT	2.5
3	A	302	TYR	2.5
3	C	310	ALA	2.5
3	C	40	LYS	2.5
3	A	304	HIS	2.5
3	A	237	MET	2.4
3	A	94	GLN	2.4
3	D	41	HIS	2.4
3	C	48	LYS	2.4
3	A	104	VAL	2.4
3	A	95	ARG	2.4
3	B	199	GLY	2.4
3	C	229	SER	2.4
3	C	232	PRO	2.4
3	A	119	ASP	2.3
1	G	11	DA	2.3
3	B	176	HIS	2.3
3	A	38	ASN	2.3
3	A	102	LEU	2.3
3	A	115	LEU	2.3
3	D	91	ILE	2.3
3	A	232	PRO	2.3
3	B	227	GLN	2.3
3	A	284	ILE	2.3
3	A	197	TYR	2.3
3	B	226	PHE	2.3
3	B	163	LYS	2.3
3	A	303	THR	2.3
3	A	196	ASN	2.2
3	B	98	LEU	2.2
3	C	75	LEU	2.2
3	A	253	ARG	2.2
3	A	103	PRO	2.2
3	C	302	TYR	2.2
3	A	242	MET	2.2
1	G	33	DA	2.2
3	A	91	ILE	2.2
3	A	126	ILE	2.2
3	A	35	HIS	2.2
1	G	31	DT	2.2
3	B	86	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	258	ALA	2.2
1	G	12	DT	2.2
2	H	7	DG	2.2
3	C	253	ARG	2.2
3	C	236	VAL	2.2
3	B	43	SER	2.2
1	E	30	DC	2.2
3	B	60	GLN	2.1
3	C	117	ILE	2.1
3	C	103	PRO	2.1
3	A	191	ASP	2.1
3	C	192	LEU	2.1
3	A	311	SER	2.1
3	C	97	GLN	2.1
3	A	120	PRO	2.1
3	C	120	PRO	2.1
1	E	31	DT	2.1
2	H	8	DA	2.1
3	C	104	VAL	2.1
3	D	163	LYS	2.1
3	D	181	ILE	2.1
3	C	197	TYR	2.1
3	C	256	GLN	2.0
1	E	35	DA	2.0
3	B	40	LYS	2.0
3	C	56	TYR	2.0
3	A	254	SER	2.0
3	D	44	LEU	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.