



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:22 AM UTC

PDB ID : 1Q3V / pdb_00001q3v
Title : Crystal structure of a wild-type Cre recombinase-loxP synapse: phosphotyrosine covalent intermediate
Authors : Ennifar, E.; Meyer, J.E.W.; Buchholz, F.; Stewart, A.F.; Suck, D.
Deposited on : 2003-08-01
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

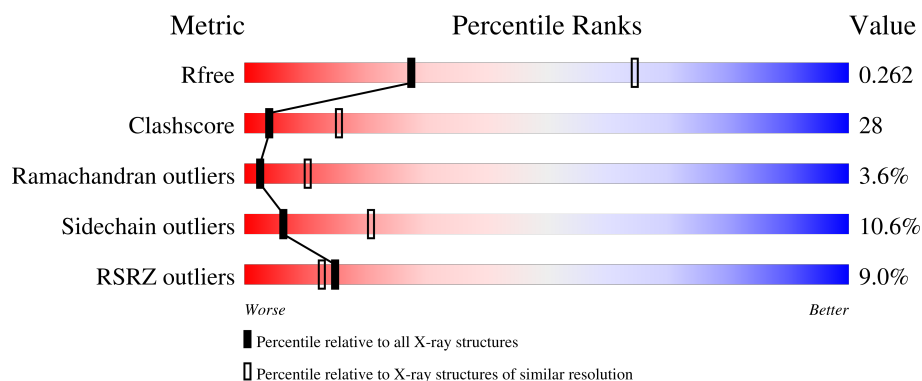
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	C	16	19% 12% 81% 6%
1	G	16	12% 31% 62% 6%
2	X	21	10% 62% 24% 14%
2	Y	21	10% 29% 71%
3	D	37	16% 22% 76% .

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Mol	Chain	Length	Quality of chain
3	H	37	11% 30% 68%
4	A	347	5% 59% 29% 7%
4	B	347	8% 46% 38% 8% 7%
4	E	347	11% 48% 36% 8% 7%
4	F	347	7% 49% 34% 8% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13296 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 loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	16	Total	C	N	O	P	0	0	0
			326	156	59	95	16			
1	G	16	Total	C	N	O	P	0	0	0
			326	156	59	95	16			

- Molecule 2 is a DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	21	Total	C	N	O	P	0	0	0
			428	207	75	126	20			
2	Y	21	Total	C	N	O	P	0	0	0
			428	207	75	126	20			

- Molecule 3 is a DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	37	Total	C	N	O	P	0	0	0
			756	364	137	219	36			
3	H	37	Total	C	N	O	P	0	0	0
			756	364	137	219	36			

- Molecule 4 is a protein called Cre recombinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	332	Total	C	N	O	S	0	0	0
			2620	1629	497	479	15			
4	B	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			
4	E	321	Total	C	N	O	S	0	0	0
			2544	1581	485	463	15			
4	F	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	cloning artifact	UNP P06956
A	-2	GLN	-	cloning artifact	UNP P06956
A	-1	VAL	-	cloning artifact	UNP P06956
A	0	PRO	-	cloning artifact	UNP P06956
B	-3	PHE	-	cloning artifact	UNP P06956
B	-2	GLN	-	cloning artifact	UNP P06956
B	-1	VAL	-	cloning artifact	UNP P06956
B	0	PRO	-	cloning artifact	UNP P06956
E	-3	PHE	-	cloning artifact	UNP P06956
E	-2	GLN	-	cloning artifact	UNP P06956
E	-1	VAL	-	cloning artifact	UNP P06956
E	0	PRO	-	cloning artifact	UNP P06956
F	-3	PHE	-	cloning artifact	UNP P06956
F	-2	GLN	-	cloning artifact	UNP P06956
F	-1	VAL	-	cloning artifact	UNP P06956
F	0	PRO	-	cloning artifact	UNP P06956

- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total I 1 1	0	0
5	F	1	Total I 1 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0
6	A	5	Total Mg 5 5	0	0
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0

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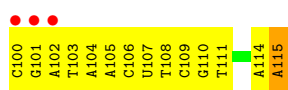
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	O	0	0
			1	1		
7	F	1	Total	O	0	0
			1	1		

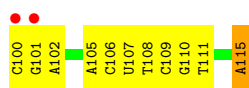
3 Residue-property plots [i](#)

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.

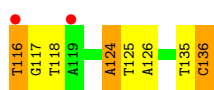
- Molecule 1: loxP DNA



- Molecule 1: loxP DNA



- Molecule 2: loxP DNA



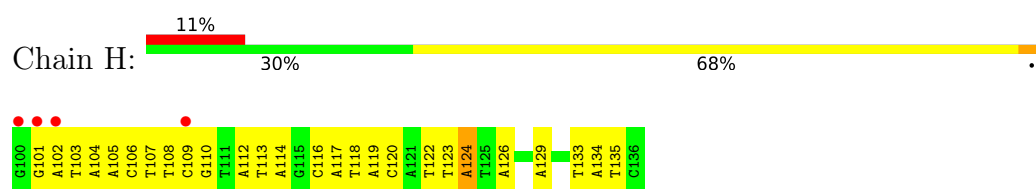
- Molecule 2: loxP DNA



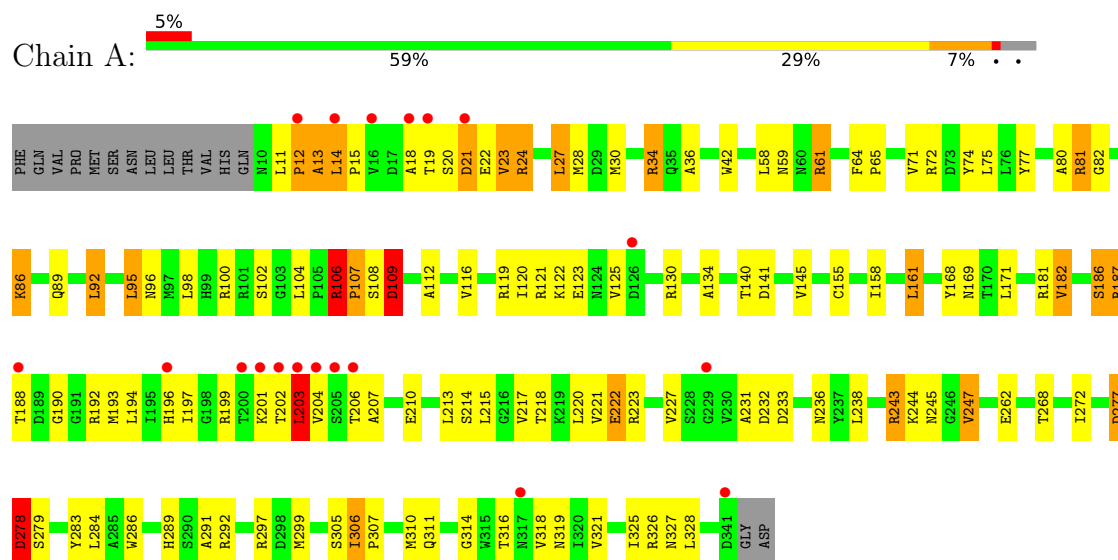
- Molecule 3: loxP DNA



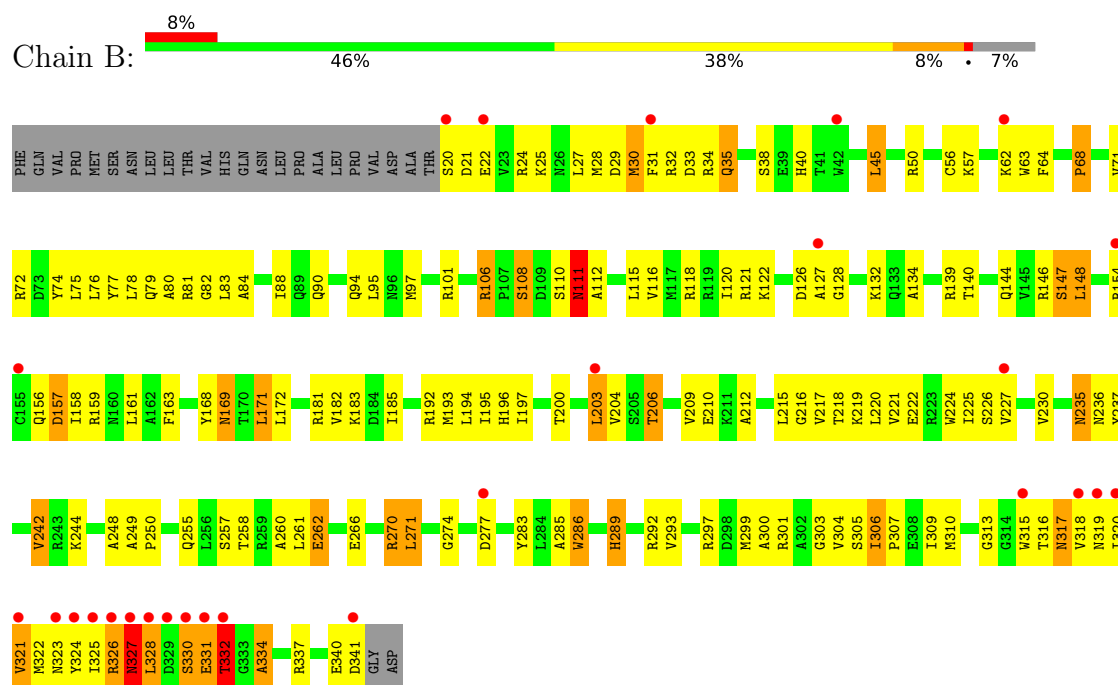
- Molecule 3: loxP DNA



• Molecule 4: Cre recombinase

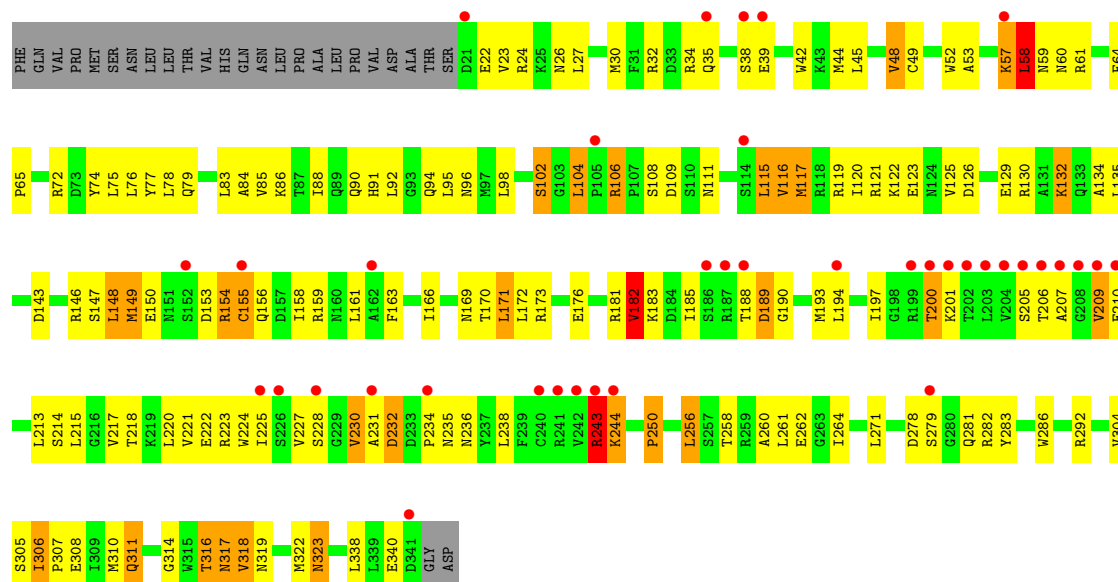


• Molecule 4: Cre recombinase

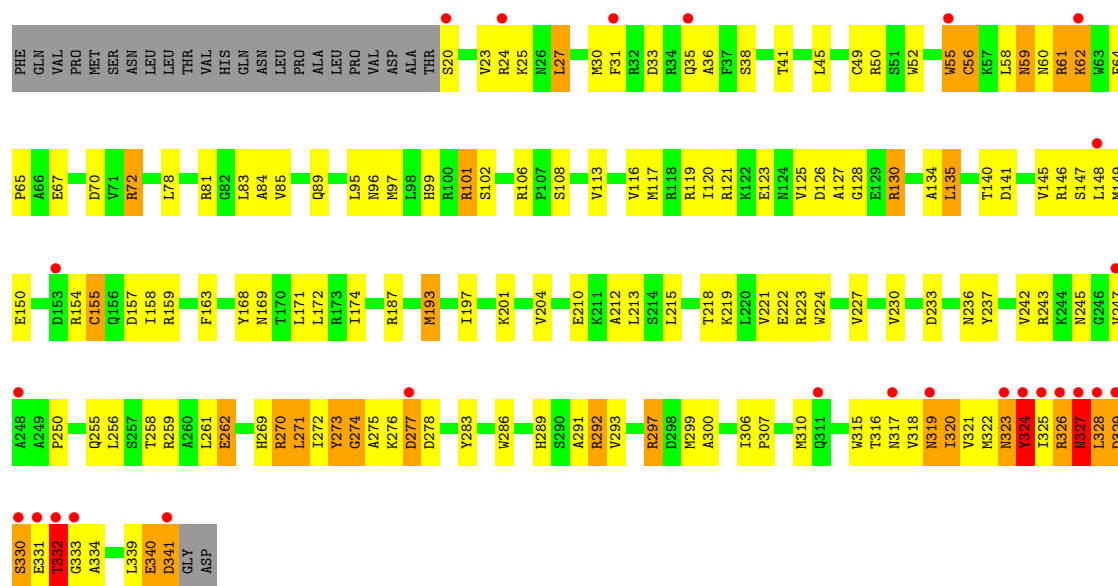


• Molecule 4: Cre recombinase





• Molecule 4: Cre recombinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.94Å 164.16Å 194.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.91 29.92 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.92-2.91) 93.9 (29.92-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.276 0.239 , 0.262	Depositor DCC
R_{free} test set	3694 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13296	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, MG, UMP, A3P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	C	0.37	0/316	0.83	0/483
1	G	0.36	0/316	0.79	0/483
2	X	0.47	0/479	1.23	6/738 (0.8%)
2	Y	0.38	0/479	0.79	0/738
3	D	0.38	0/848	0.83	0/1307
3	H	0.33	0/848	0.76	0/1307
4	A	0.62	1/2663 (0.0%)	1.07	11/3595 (0.3%)
4	B	0.50	0/2591	1.00	8/3493 (0.2%)
4	E	0.47	0/2585	0.97	8/3485 (0.2%)
4	F	0.57	1/2591 (0.0%)	1.01	10/3493 (0.3%)
All	All	0.51	2/13716 (0.0%)	0.98	43/19122 (0.2%)

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
3	D	0	2
3	H	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	324	TYR	N-CA	5.78	1.53	1.46
4	A	306	ILE	CA-CB	-5.21	1.51	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	116	DT	C5'-C4'-O4'	18.32	136.88	109.40
4	F	331	GLU	N-CA-C	-9.66	100.36	113.30
4	E	278	ASP	N-CA-C	-9.14	102.13	113.28
4	E	209	VAL	N-CA-C	-8.60	102.76	111.88
4	B	327	ASN	N-CA-C	7.99	127.83	110.80
2	X	116	DT	C2'-C3'-O3'	-7.78	99.83	111.50
4	A	109	ASP	N-CA-C	-7.68	101.57	113.02
4	A	14	LEU	CA-C-N	7.31	128.98	119.84
4	A	14	LEU	C-N-CA	7.31	128.98	119.84
4	F	327	ASN	N-CA-C	7.04	125.79	110.80
4	B	322	MET	N-CA-C	-6.95	103.71	111.28
2	X	116	DT	N1-C1'-C2'	-6.87	103.19	113.50
4	F	326	ARG	N-CA-C	-6.78	104.33	114.64
4	A	278	ASP	N-CA-C	6.71	121.31	113.18
4	A	23	VAL	N-CA-C	-6.42	104.65	113.00
4	B	79	GLN	N-CA-C	-6.00	104.74	111.28
2	X	116	DT	C4'-C3'-O3'	6.00	119.00	110.00
4	A	203	LEU	N-CA-C	-5.94	104.80	111.28
2	X	136	DC	C2'-C3'-O3'	-5.89	102.67	111.50
4	B	330	SER	CB-CA-C	-5.87	109.79	116.54
2	X	124	DA	C5'-C4'-C3'	-5.76	106.26	114.90
4	F	270	ARG	N-CA-C	-5.73	106.13	113.01
4	E	39	GLU	N-CA-C	-5.66	105.20	111.71
4	B	321	VAL	N-CA-C	-5.64	105.23	110.53
4	E	243	ARG	N-CA-C	5.59	117.76	110.43
4	E	34	ARG	N-CA-C	-5.59	106.30	113.01
4	E	244	LYS	N-CA-C	5.56	119.57	112.34
4	B	306	ILE	CB-CA-C	-5.53	106.76	114.00
4	A	81	ARG	N-CA-C	-5.51	106.53	113.20
4	B	230	VAL	N-CA-C	-5.41	104.98	112.50
4	E	318	VAL	N-CA-C	-5.40	108.24	113.53
4	A	243	ARG	N-CA-C	5.39	118.71	110.36
4	F	341	ASP	CA-C-O	-5.38	111.66	120.80
4	F	36	ALA	N-CA-C	-5.34	106.54	113.16
4	F	262	GLU	N-CA-C	-5.30	105.61	111.71
4	F	332	THR	CB-CA-C	-5.19	110.61	116.63
4	B	262	GLU	N-CA-C	-5.15	105.79	111.71
4	F	212	ALA	N-CA-C	5.15	118.20	109.76
4	A	106	ARG	N-CA-C	5.10	117.33	110.29
4	A	107	PRO	N-CA-C	-5.09	101.98	112.47
4	E	230	VAL	N-CA-C	-5.09	105.43	112.50
4	F	41	THR	N-CA-C	-5.09	105.82	111.36
4	A	24	ARG	N-CA-C	-5.07	105.41	112.45

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	107	DT	Sidechain
3	D	126	DA	Sidechain
3	H	124	DA	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	C	326	0	178	26	0
1	G	326	0	178	14	0
2	X	428	0	241	24	0
2	Y	428	0	241	27	0
3	D	756	0	421	38	0
3	H	756	0	421	38	0
4	A	2620	0	2643	126	0
4	B	2550	0	2570	177	0
4	E	2544	0	2566	164	0
4	F	2550	0	2570	151	0
5	C	1	0	0	1	0
5	F	1	0	0	0	0
6	A	5	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	E	1	0	0	1	0
7	F	1	0	0	0	0
All	All	13296	0	12029	695	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 28.

All (695) 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)
4:B:317:ASN:HD21	4:B:320:ILE:HG12	1.08	1.11
4:E:193:MET:HG3	4:E:218:THR:HG23	1.34	1.10
4:B:35:GLN:HE21	4:B:35:GLN:HA	1.10	1.07
1:C:105:DA:H2''	1:C:106:DC:H5''	1.33	1.06
3:H:105:DA:H2''	3:H:106:DC:H5''	1.39	1.04
4:A:72:ARG:HG3	4:A:116:VAL:HG21	1.38	1.02
4:A:15:PRO:HB2	4:A:18:ALA:HB3	1.43	1.00
4:B:315:TRP:HE1	4:B:324:TYR:HE2	1.08	0.97
4:E:200:THR:HG22	4:E:201:LYS:H	1.30	0.97
4:A:188:THR:HG22	4:A:190:GLY:H	1.25	0.96
3:D:132:DT:H2''	3:D:133:DT:H5''	1.46	0.96
4:E:169:ASN:ND2	4:E:213:LEU:HA	1.80	0.95
4:B:315:TRP:NE1	4:B:324:TYR:HE2	1.64	0.94
4:E:154:ARG:HH11	4:E:154:ARG:HB3	1.31	0.94
3:H:134:DA:H2''	3:H:135:DT:H5'	1.50	0.94
4:F:121:ARG:HG3	4:F:121:ARG:HH11	1.34	0.93
4:B:258:THR:HA	4:B:261:LEU:HD12	1.52	0.92
4:E:146:ARG:O	4:E:150:GLU:HB2	1.69	0.91
4:A:181:ARG:HH11	4:A:199:ARG:HH22	1.15	0.90
4:B:317:ASN:HD21	4:B:320:ILE:CG1	1.83	0.90
2:Y:131:DG:H2''	2:Y:132:DT:C5'	2.02	0.89
1:G:105:DA:H2''	1:G:106:DC:H5''	1.55	0.89
4:A:187:ARG:HH11	4:A:187:ARG:HB3	1.39	0.88
1:G:115:A3P:O2P	2:Y:116:DT:H5'	1.75	0.87
4:A:106:ARG:O	4:A:109:ASP:HB2	1.74	0.87
4:A:72:ARG:CG	4:A:116:VAL:HG21	2.05	0.86
2:Y:122:DC:H2''	2:Y:123:DT:H5'	1.57	0.86
4:E:188:THR:HG22	4:E:190:GLY:H	1.41	0.85
1:C:105:DA:C2'	1:C:106:DC:H5''	2.06	0.85
2:X:116:DT:H2''	2:X:117:DG:OP2	1.76	0.84
3:H:105:DA:C2'	3:H:106:DC:H5''	2.06	0.84
4:B:236:ASN:ND2	4:B:250:PRO:HB3	1.93	0.83
3:H:106:DC:H2'	3:H:107:DT:H72	1.61	0.83
4:A:299:MET:HE3	4:B:334:ALA:HB1	1.61	0.83
4:B:185:ILE:HD13	4:B:193:MET:CE	2.09	0.82
4:B:317:ASN:ND2	4:B:320:ILE:HG12	1.92	0.82
4:F:320:ILE:HD12	4:F:320:ILE:H	1.45	0.82
2:Y:131:DG:H2''	2:Y:132:DT:H5'	1.62	0.81
4:A:59:ASN:O	4:A:61:ARG:HD3	1.79	0.81
4:E:48:VAL:HB	7:E:344:HOH:O	1.79	0.80
4:E:117:MET:HE2	4:E:117:MET:HA	1.62	0.79
4:E:121:ARG:O	4:E:125:VAL:HG12	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:148:LEU:O	4:E:149:MET:HB2	1.82	0.79
4:E:271:LEU:HD23	4:E:271:LEU:O	1.82	0.79
4:A:15:PRO:CB	4:A:18:ALA:HB3	2.11	0.79
4:E:317:ASN:H	4:E:317:ASN:HD22	1.29	0.79
3:D:105:DA:H2''	3:D:106:DC:O5'	1.82	0.79
4:B:35:GLN:HA	4:B:35:GLN:NE2	1.92	0.79
4:E:173:ARG:HH11	4:E:173:ARG:HG2	1.48	0.79
4:B:154:ARG:HB2	4:B:157:ASP:HB2	1.65	0.78
4:E:185:ILE:HG21	4:E:193:MET:HE2	1.64	0.78
4:E:316:THR:HG23	4:E:317:ASN:ND2	1.99	0.77
3:H:134:DA:H2''	3:H:135:DT:C5'	2.14	0.77
4:E:169:ASN:HD22	4:E:213:LEU:HA	1.48	0.77
4:E:48:VAL:HG21	4:E:91:HIS:HA	1.66	0.77
4:B:315:TRP:NE1	4:B:324:TYR:CE2	2.51	0.76
4:B:215:LEU:O	4:B:218:THR:HG22	1.86	0.76
4:B:328:LEU:O	4:B:332:THR:HG23	1.86	0.76
4:E:243:ARG:HG2	4:E:243:ARG:HH11	1.52	0.75
4:E:122:LYS:O	4:E:126:ASP:HB2	1.84	0.75
4:E:166:ILE:HG12	4:E:213:LEU:HD11	1.68	0.75
2:Y:131:DG:H2''	2:Y:132:DT:H5''	1.66	0.74
4:B:134:ALA:HA	4:B:283:TYR:CD2	2.22	0.74
4:B:206:THR:HG22	4:E:130:ARG:HA	1.68	0.74
4:E:148:LEU:HD23	4:E:148:LEU:H	1.52	0.74
2:X:117:DG:OP2	4:B:320:ILE:HG13	1.86	0.73
2:X:118:DT:H73	4:B:319:ASN:HB3	1.70	0.73
3:H:102:DA:H2''	3:H:103:DT:O5'	1.88	0.73
4:A:72:ARG:HD2	4:A:116:VAL:HG21	1.71	0.73
4:E:200:THR:HG21	4:E:205:SER:HB2	1.70	0.73
4:E:193:MET:CG	4:E:218:THR:HG23	2.17	0.73
4:A:72:ARG:CD	4:A:116:VAL:HG21	2.17	0.72
2:X:117:DG:H2''	2:X:118:DT:H5'	1.71	0.72
2:Y:117:DG:H5''	4:F:320:ILE:HD11	1.71	0.72
2:Y:122:DC:H2''	2:Y:123:DT:C5'	2.20	0.72
4:E:171:LEU:N	4:E:171:LEU:HD23	2.05	0.71
4:F:230:VAL:HG12	4:F:250:PRO:HB3	1.72	0.71
2:X:117:DG:H5'	4:B:316:THR:OG1	1.89	0.71
4:A:15:PRO:HB2	4:A:18:ALA:CB	2.18	0.71
4:B:315:TRP:CZ2	4:B:324:TYR:CD2	2.78	0.71
4:B:326:ARG:HH11	4:B:326:ARG:HG3	1.55	0.71
4:A:193:MET:HG3	4:A:218:THR:HG23	1.72	0.71
1:C:104:DA:O4'	4:B:244:LYS:HE3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:183:LYS:HG2	4:E:234:PRO:HB2	1.72	0.71
4:F:219:LYS:HD3	4:F:222:GLU:OE1	1.91	0.71
2:Y:118:DT:H71	4:F:319:ASN:ND2	2.06	0.70
4:A:307:PRO:HG3	4:B:306:ILE:CD1	2.21	0.70
4:E:209:VAL:O	4:E:210:GLU:HG3	1.91	0.70
4:F:328:LEU:HD12	4:F:328:LEU:H	1.56	0.70
4:A:326:ARG:HD3	4:F:210:GLU:HG3	1.74	0.70
2:Y:117:DG:H3'	4:F:317:ASN:HB2	1.74	0.69
4:B:320:ILE:O	4:B:323:ASN:HB2	1.92	0.69
4:B:325:ILE:O	4:B:326:ARG:HG3	1.91	0.69
4:B:315:TRP:CZ2	4:B:324:TYR:CE2	2.80	0.69
3:H:106:DC:H2'	3:H:107:DT:C7	2.22	0.69
4:E:154:ARG:HB3	4:E:154:ARG:NH1	2.06	0.69
4:E:193:MET:HG3	4:E:218:THR:CG2	2.20	0.69
4:E:305:SER:OG	4:E:308:GLU:HG3	1.91	0.69
4:F:174:ILE:HD12	4:F:258:THR:HB	1.74	0.68
4:F:243:ARG:HG2	4:F:243:ARG:HH11	1.58	0.68
3:D:132:DT:C2'	3:D:133:DT:H5''	2.22	0.68
4:A:297:ARG:HH12	4:A:327:ASN:HD21	1.42	0.68
4:A:194:LEU:HD21	4:A:210:GLU:OE1	1.93	0.68
4:F:245:ASN:OD1	4:F:247:VAL:HG23	1.93	0.68
4:E:182:VAL:HG23	4:E:234:PRO:O	1.94	0.68
4:A:161:LEU:HD22	4:A:220:LEU:CD1	2.23	0.68
1:C:111:DT:P	4:B:50:ARG:HH12	2.17	0.67
4:A:207:ALA:HB2	4:A:314:GLY:HA3	1.76	0.67
4:B:330:SER:C	4:B:332:THR:H	2.02	0.67
4:B:194:LEU:HD13	4:B:212:ALA:HB2	1.74	0.67
4:F:215:LEU:O	4:F:218:THR:HG22	1.93	0.67
4:A:305:SER:HB2	4:A:307:PRO:HD2	1.77	0.67
4:B:163:PHE:CE1	4:B:261:LEU:HD22	2.30	0.67
3:H:108:DT:H2''	3:H:109:DC:C5'	2.25	0.67
4:B:185:ILE:HG21	4:B:193:MET:HE3	1.77	0.67
4:F:121:ARG:HG3	4:F:121:ARG:NH1	2.10	0.67
4:E:58:LEU:HD12	4:E:58:LEU:O	1.95	0.67
4:E:116:VAL:O	4:E:119:ARG:HB3	1.95	0.67
4:E:74:TYR:CE1	4:E:78:LEU:HD11	2.30	0.66
4:E:53:ALA:O	4:E:57:LYS:HD3	1.94	0.66
4:F:121:ARG:HH11	4:F:121:ARG:CG	2.08	0.66
4:F:130:ARG:HH11	4:F:130:ARG:HB3	1.60	0.66
3:D:116:DC:H4'	3:D:116:DC:OP1	1.96	0.65
4:F:258:THR:O	4:F:262:GLU:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:120:DC:H3'	4:B:106:ARG:HH21	1.59	0.65
4:E:317:ASN:HD22	4:E:317:ASN:N	1.94	0.65
1:G:105:DA:C2'	1:G:106:DC:H5''	2.26	0.65
4:B:147:SER:O	4:B:148:LEU:HB2	1.95	0.65
3:D:119:DA:P	4:B:121:ARG:HH12	2.20	0.65
4:E:134:ALA:HA	4:E:283:TYR:CD2	2.33	0.64
4:F:126:ASP:C	4:F:128:GLY:H	2.05	0.64
4:B:204:VAL:HG22	4:E:125:VAL:HG11	1.78	0.64
4:A:14:LEU:HG	4:A:27:LEU:CD2	2.28	0.64
1:C:103:DT:H2''	1:C:104:DA:C8	2.33	0.64
4:B:315:TRP:CE2	4:B:324:TYR:CE2	2.85	0.64
4:A:310:MET:SD	4:A:318:VAL:HG12	2.38	0.63
4:F:145:VAL:HG22	4:F:272:ILE:HD11	1.80	0.63
1:C:108:DT:H2''	1:C:109:DC:H5'	1.80	0.63
4:A:243:ARG:HG2	4:A:243:ARG:HH11	1.64	0.63
4:E:90:GLN:HE21	4:E:94:GLN:HG2	1.63	0.63
4:A:134:ALA:HA	4:A:283:TYR:CD2	2.33	0.63
4:E:230:VAL:CG1	4:E:236:ASN:HB3	2.29	0.63
4:B:30:MET:SD	4:B:101:ARG:HG2	2.39	0.63
4:E:26:ASN:HB3	4:E:102:SER:HA	1.81	0.63
4:F:78:LEU:HD22	4:F:83:LEU:CD1	2.29	0.63
4:F:204:VAL:O	4:F:204:VAL:HG13	1.97	0.63
4:A:187:ARG:NH2	4:A:222:GLU:OE2	2.31	0.62
4:A:245:ASN:OD1	4:A:247:VAL:HB	1.99	0.62
4:E:74:TYR:O	4:E:77:TYR:HB3	2.00	0.62
4:F:325:ILE:CG2	4:F:327:ASN:ND2	2.62	0.62
4:B:204:VAL:HG13	4:B:204:VAL:O	1.99	0.62
3:H:103:DT:H2''	3:H:104:DA:C8	2.34	0.62
4:B:146:ARG:O	4:B:148:LEU:N	2.33	0.62
4:E:228:SER:OG	4:E:230:VAL:HG23	2.00	0.62
4:F:270:ARG:O	4:F:274:GLY:HA2	2.00	0.62
4:B:204:VAL:CG2	4:E:125:VAL:HG11	2.30	0.62
4:B:206:THR:HG22	4:E:130:ARG:CA	2.30	0.62
4:E:27:LEU:CD2	4:E:102:SER:HB3	2.30	0.62
4:A:192:ARG:HB3	4:A:215:LEU:HD23	1.81	0.62
4:E:230:VAL:HG22	4:E:250:PRO:HG3	1.82	0.61
4:E:159:ARG:HB2	4:E:224:TRP:CZ3	2.35	0.61
4:A:72:ARG:HD2	4:A:116:VAL:CG2	2.30	0.61
4:E:230:VAL:HG13	4:E:236:ASN:HB3	1.83	0.61
4:F:193:MET:HE1	4:F:221:VAL:HB	1.83	0.61
4:E:78:LEU:HD12	4:E:78:LEU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:22:GLU:HG3	4:E:23:VAL:N	2.14	0.61
4:E:143:ASP:O	4:E:146:ARG:HG2	1.99	0.61
3:H:105:DA:H2''	3:H:106:DC:C5'	2.24	0.61
4:A:161:LEU:HD22	4:A:220:LEU:HD11	1.83	0.60
4:F:60:ASN:C	4:F:61:ARG:HD3	2.26	0.60
4:F:72:ARG:HD2	4:F:116:VAL:HB	1.82	0.60
4:E:217:VAL:O	4:E:221:VAL:HG23	2.02	0.60
4:B:325:ILE:HG22	4:B:327:ASN:H	1.66	0.60
4:E:117:MET:HE3	4:E:120:ILE:HD12	1.84	0.60
4:E:169:ASN:HD21	4:E:213:LEU:HA	1.64	0.60
4:E:279:SER:OG	4:E:281:GLN:HG3	2.00	0.60
2:Y:117:DG:H2'	2:Y:118:DT:H72	1.84	0.60
4:E:306:ILE:N	4:E:307:PRO:HD2	2.16	0.60
4:E:318:VAL:O	4:E:322:MET:HG2	2.02	0.60
4:B:317:ASN:ND2	4:B:320:ILE:CG1	2.56	0.60
4:A:161:LEU:HD13	4:A:220:LEU:HD11	1.83	0.59
4:B:74:TYR:O	4:B:77:TYR:HB3	2.01	0.59
4:E:185:ILE:CG2	4:E:193:MET:HE2	2.29	0.59
4:A:72:ARG:NH1	4:F:33:ASP:OD2	2.36	0.59
4:A:243:ARG:HG2	4:A:243:ARG:NH1	2.17	0.59
4:B:172:LEU:HD21	4:B:197:ILE:HG13	1.85	0.59
4:E:197:ILE:HG22	4:E:209:VAL:C	2.27	0.59
3:H:124:DA:H5'	4:F:201:LYS:HG3	1.85	0.59
4:E:304:VAL:HG12	4:E:308:GLU:HB2	1.84	0.59
1:C:115:A3P:O2P	2:X:116:DT:H5'	2.02	0.59
4:B:159:ARG:HB2	4:B:224:TRP:CZ3	2.37	0.59
4:B:325:ILE:HG22	4:B:326:ARG:N	2.16	0.59
3:D:122:DT:H5''	4:B:97:MET:HE2	1.85	0.59
4:E:35:GLN:HB2	4:F:119:ARG:HD2	1.84	0.59
4:B:325:ILE:HG21	4:B:327:ASN:HD22	1.67	0.59
3:D:108:DT:H2''	3:D:109:DC:H5'	1.84	0.58
4:E:117:MET:HA	4:E:117:MET:CE	2.32	0.58
4:F:323:ASN:CG	4:F:324:TYR:N	2.60	0.58
4:B:310:MET:HG2	4:B:321:VAL:HG21	1.84	0.58
4:F:148:LEU:O	4:F:148:LEU:HD23	2.03	0.58
4:F:146:ARG:O	4:F:150:GLU:HB2	2.03	0.58
4:A:306:ILE:HB	4:A:307:PRO:HD3	1.86	0.58
4:F:271:LEU:HD13	4:F:271:LEU:C	2.29	0.58
3:H:122:DT:H5'	4:F:97:MET:HE3	1.85	0.58
4:B:71:VAL:O	4:B:75:LEU:HG	2.03	0.58
4:F:233:ASP:HB3	4:F:236:ASN:ND2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:DT:OP1	4:B:50:ARG:NH1	2.37	0.58
4:E:154:ARG:HH11	4:E:154:ARG:CB	2.12	0.58
4:B:72:ARG:HG3	4:B:116:VAL:HG11	1.86	0.58
4:E:200:THR:HG22	4:E:201:LYS:N	2.10	0.58
1:C:100:DC:H2'	1:C:101:DG:C8	2.39	0.58
4:B:171:LEU:O	4:B:292:ARG:NH1	2.37	0.58
4:F:25:LYS:O	4:F:25:LYS:HD3	2.04	0.57
4:F:78:LEU:HD22	4:F:83:LEU:HD12	1.86	0.57
1:C:115:A3P:C2'	2:X:116:DT:C5'	2.83	0.57
4:E:173:ARG:HG2	4:E:173:ARG:NH1	2.18	0.57
4:A:116:VAL:O	4:A:120:ILE:HG13	2.04	0.57
4:E:48:VAL:HG11	4:E:94:GLN:HB2	1.85	0.57
4:E:209:VAL:O	4:E:209:VAL:HG12	2.05	0.57
1:C:115:A3P:C2'	2:X:116:DT:H5''	2.34	0.57
3:H:117:DA:H2''	3:H:118:DT:H71	1.86	0.57
4:E:316:THR:HG23	4:E:317:ASN:HD22	1.70	0.57
1:C:114:DA:H5''	4:B:132:LYS:O	2.04	0.57
4:E:111:ASN:O	4:E:115:LEU:HB2	2.03	0.57
4:F:67:GLU:HB3	4:F:70:ASP:OD2	2.05	0.57
4:A:188:THR:HG22	4:A:190:GLY:N	2.09	0.57
4:B:148:LEU:O	4:B:148:LEU:HD13	2.04	0.57
4:E:32:ARG:HD2	4:F:72:ARG:HH21	1.69	0.57
4:E:183:LYS:HD3	4:E:235:ASN:ND2	2.19	0.57
1:G:100:DC:H2''	1:G:101:DG:O5'	2.05	0.57
4:F:121:ARG:NH1	4:F:121:ARG:CG	2.67	0.57
3:H:108:DT:C2'	3:H:109:DC:H5''	2.34	0.57
4:B:258:THR:O	4:B:262:GLU:HG3	2.05	0.56
4:E:96:ASN:ND2	4:E:108:SER:OG	2.36	0.56
4:F:325:ILE:HG21	4:F:327:ASN:ND2	2.20	0.56
3:H:122:DT:C5'	4:F:97:MET:HE3	2.35	0.56
4:B:236:ASN:HD21	4:B:250:PRO:HB3	1.70	0.56
4:E:154:ARG:C	4:E:156:GLN:H	2.13	0.56
4:F:163:PHE:CE1	4:F:261:LEU:HD13	2.39	0.56
4:E:78:LEU:HB3	4:E:83:LEU:HD12	1.87	0.56
2:X:117:DG:OP2	2:X:117:DG:H8	1.88	0.56
4:E:256:LEU:HD22	4:E:260:ALA:HB3	1.87	0.56
1:C:115:A3P:O1P	4:B:292:ARG:CZ	2.53	0.56
1:C:115:A3P:O1P	4:B:292:ARG:NH2	2.38	0.56
4:A:187:ARG:HH11	4:A:187:ARG:CB	2.14	0.56
3:D:134:DA:H2''	3:D:135:DT:O5'	2.05	0.55
3:H:108:DT:H2''	3:H:109:DC:H5''	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:330:SER:O	4:B:332:THR:N	2.38	0.55
4:F:64:PHE:HA	4:F:65:PRO:C	2.31	0.55
4:A:204:VAL:HG23	4:B:326:ARG:NH2	2.21	0.55
4:B:31:PHE:O	4:B:34:ARG:HB3	2.06	0.55
4:A:121:ARG:O	4:A:125:VAL:HG23	2.05	0.55
4:A:169:ASN:OD1	4:A:213:LEU:HA	2.05	0.55
4:B:325:ILE:HG21	4:B:327:ASN:ND2	2.22	0.55
1:C:115:A3P:O1P	4:B:292:ARG:NE	2.40	0.55
4:B:45:LEU:C	4:B:45:LEU:HD23	2.31	0.55
4:E:310:MET:HE3	4:E:317:ASN:O	2.06	0.55
4:E:317:ASN:ND2	4:E:317:ASN:N	2.55	0.55
4:A:307:PRO:HG3	4:B:306:ILE:HD11	1.89	0.55
4:B:106:ARG:HH12	4:B:108:SER:HB3	1.70	0.55
4:E:74:TYR:CD1	4:E:78:LEU:HD11	2.41	0.55
4:A:161:LEU:HD22	4:A:220:LEU:HD12	1.88	0.55
4:E:64:PHE:CD1	4:E:64:PHE:C	2.85	0.55
4:F:243:ARG:HG2	4:F:243:ARG:NH1	2.19	0.55
4:E:96:ASN:HD21	4:E:108:SER:HG	1.53	0.54
3:D:108:DT:H1'	3:D:109:DC:H5''	1.90	0.54
4:F:277:ASP:OD1	4:F:278:ASP:N	2.40	0.54
3:H:107:DT:H2''	3:H:108:DT:O5'	2.08	0.54
4:B:156:GLN:HB3	4:B:242:VAL:HG11	1.87	0.54
4:F:55:TRP:CD1	4:F:55:TRP:C	2.85	0.54
3:H:113:DT:O4	4:E:44:MET:HE2	2.08	0.54
3:D:119:DA:OP1	4:B:121:ARG:NH1	2.39	0.54
4:A:30:MET:HE3	4:A:42:TRP:HH2	1.73	0.54
4:F:193:MET:HE1	4:F:221:VAL:CB	2.38	0.54
4:F:320:ILE:O	4:F:323:ASN:N	2.40	0.54
4:A:30:MET:HE3	4:A:42:TRP:CH2	2.41	0.54
4:F:320:ILE:H	4:F:320:ILE:CD1	2.19	0.54
4:A:145:VAL:HG22	4:A:272:ILE:CD1	2.38	0.54
4:A:197:ILE:O	4:A:197:ILE:HG13	2.08	0.54
4:E:182:VAL:O	4:E:183:LYS:C	2.49	0.54
4:F:145:VAL:HG12	4:F:149:MET:HE2	1.89	0.54
3:D:120:DC:H3'	4:B:106:ARG:NH2	2.23	0.53
4:B:306:ILE:HG22	4:B:310:MET:HE2	1.89	0.53
4:B:313:GLY:HA3	4:B:315:TRP:CZ3	2.44	0.53
4:A:15:PRO:CG	4:A:18:ALA:HB3	2.38	0.53
4:F:242:VAL:HG23	4:F:242:VAL:O	2.06	0.53
2:X:135:DT:H2''	2:X:136:DC:OP2	2.08	0.53
4:E:78:LEU:HD12	4:E:78:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:121:ARG:NH1	4:F:204:VAL:HG13	2.24	0.53
4:E:215:LEU:HG	4:F:340:GLU:OE1	2.08	0.53
4:F:126:ASP:C	4:F:128:GLY:N	2.66	0.53
4:B:237:TYR:CE1	4:B:255:GLN:HG2	2.44	0.53
4:F:116:VAL:O	4:F:120:ILE:HG13	2.07	0.53
3:D:118:DT:H2''	3:D:119:DA:N7	2.24	0.53
4:F:316:THR:O	4:F:316:THR:HG22	2.07	0.53
3:D:101:DG:H2''	3:D:102:DA:C8	2.44	0.53
4:A:145:VAL:HG22	4:A:272:ILE:HD11	1.91	0.53
4:B:320:ILE:C	4:B:323:ASN:HB2	2.34	0.53
4:E:72:ARG:HG3	4:E:116:VAL:HG11	1.91	0.53
4:A:161:LEU:HD13	4:A:220:LEU:CD1	2.39	0.53
1:C:107:UMP:OP2	4:B:257:SER:HB3	2.09	0.52
2:Y:131:DG:C2'	2:Y:132:DT:H5''	2.39	0.52
4:B:77:TYR:O	4:B:80:ALA:HB3	2.09	0.52
4:B:326:ARG:HG3	4:B:326:ARG:NH1	2.21	0.52
4:F:306:ILE:N	4:F:307:PRO:HD2	2.24	0.52
4:A:112:ALA:O	4:A:116:VAL:HG23	2.09	0.52
4:E:154:ARG:NH1	4:E:154:ARG:CB	2.71	0.52
2:Y:117:DG:H5'	4:F:316:THR:HB	1.91	0.52
3:H:108:DT:H2''	3:H:109:DC:H5'	1.91	0.52
2:Y:117:DG:C8	2:Y:118:DT:H72	2.44	0.52
4:E:159:ARG:HB2	4:E:224:TRP:CE3	2.44	0.52
4:F:58:LEU:O	4:F:58:LEU:HD23	2.09	0.52
3:D:103:DT:O2	4:A:244:LYS:HE3	2.09	0.52
3:D:112:DA:OP1	4:A:81:ARG:NH2	2.43	0.52
3:D:115:DG:H2''	3:D:116:DC:C6	2.45	0.52
3:D:115:DG:H2''	3:D:116:DC:H6	1.75	0.52
4:A:277:ASP:OD1	4:A:278:ASP:N	2.43	0.52
4:E:163:PHE:CE2	4:E:261:LEU:HD22	2.45	0.52
2:X:117:DG:H3'	4:B:317:ASN:HB3	1.92	0.52
4:A:106:ARG:C	4:A:107:PRO:O	2.49	0.52
4:A:192:ARG:NH1	4:B:331:GLU:HG2	2.25	0.52
4:B:182:VAL:HG23	4:B:236:ASN:O	2.09	0.52
4:E:79:GLN:NE2	4:E:120:ILE:HG23	2.25	0.52
4:E:231:ALA:O	4:E:232:ASP:C	2.53	0.52
4:A:24:ARG:O	4:A:28:MET:HB2	2.10	0.51
4:B:80:ALA:C	4:B:82:GLY:H	2.18	0.51
4:B:97:MET:O	4:B:101:ARG:HB2	2.09	0.51
2:X:135:DT:H2''	2:X:136:DC:C6	2.45	0.51
4:E:116:VAL:O	4:E:120:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:117:DG:OP2	2:X:117:DG:C8	2.63	0.51
4:A:187:ARG:HB3	4:A:187:ARG:NH1	2.17	0.51
4:E:258:THR:O	4:E:262:GLU:HG3	2.10	0.51
4:F:154:ARG:HD3	4:F:157:ASP:OD2	2.10	0.51
4:B:330:SER:C	4:B:332:THR:N	2.66	0.51
4:F:159:ARG:HB2	4:F:224:TRP:CZ3	2.46	0.51
1:G:110:DG:H2''	1:G:111:DT:OP2	2.10	0.51
1:G:101:DG:H2''	1:G:102:DA:O5'	2.11	0.51
2:Y:118:DT:H3	3:H:119:DA:H61	1.57	0.51
4:A:202:THR:HG22	4:A:203:LEU:N	2.25	0.51
4:B:236:ASN:HD22	4:B:250:PRO:HB3	1.73	0.51
4:F:339:LEU:O	4:F:341:ASP:N	2.44	0.51
3:H:109:DC:H2''	3:H:110:DG:C8	2.46	0.51
2:X:117:DG:P	4:B:320:ILE:HG13	2.51	0.51
4:B:45:LEU:C	4:B:45:LEU:CD2	2.84	0.51
4:F:52:TRP:O	4:F:56:CYS:HB2	2.11	0.51
4:A:12:PRO:O	4:A:13:ALA:HB2	2.11	0.50
4:F:187:ARG:NH2	4:F:222:GLU:OE2	2.45	0.50
4:B:94:GLN:OE1	4:B:97:MET:HE3	2.11	0.50
4:E:32:ARG:CZ	4:F:72:ARG:HE	2.25	0.50
1:C:102:DA:H1'	1:C:103:DT:H5''	1.92	0.50
1:G:108:DT:H2''	1:G:109:DC:C5'	2.41	0.50
1:G:111:DT:OP2	4:F:50:ARG:NH1	2.44	0.50
4:A:27:LEU:HD13	4:A:102:SER:HB2	1.93	0.50
4:B:118:ARG:HG3	4:B:118:ARG:HH11	1.75	0.50
4:B:169:ASN:C	4:B:169:ASN:HD22	2.19	0.50
1:C:102:DA:H2''	1:C:103:DT:H5'	1.92	0.50
3:D:125:DT:H71	4:B:40:HIS:CD2	2.46	0.50
4:A:74:TYR:O	4:A:77:TYR:HB3	2.12	0.50
4:A:119:ARG:O	4:A:123:GLU:HG3	2.11	0.50
4:B:33:ASP:C	4:B:35:GLN:H	2.20	0.50
4:B:235:ASN:N	4:B:235:ASN:HD22	2.10	0.50
4:E:197:ILE:HG23	4:E:197:ILE:O	2.11	0.50
2:Y:118:DT:H73	4:F:319:ASN:CG	2.37	0.50
4:A:168:TYR:HA	4:A:291:ALA:HB1	1.94	0.50
1:G:106:DC:H2''	1:G:107:UMP:O5'	2.12	0.49
4:B:299:MET:O	4:B:304:VAL:HG23	2.12	0.49
4:F:320:ILE:HD12	4:F:320:ILE:N	2.22	0.49
3:D:117:DA:OP1	4:A:201:LYS:HD3	2.12	0.49
2:Y:123:DT:H3'	4:E:38:SER:OG	2.12	0.49
4:A:20:SER:O	4:A:21:ASP:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:270:ARG:HG2	4:B:274:GLY:O	2.12	0.49
3:D:124:DA:H2'	3:D:125:DT:C7	2.41	0.49
4:E:243:ARG:HH11	4:E:243:ARG:CG	2.22	0.49
4:F:30:MET:SD	4:F:101:ARG:HG2	2.51	0.49
4:B:237:TYR:CZ	4:B:255:GLN:HG2	2.48	0.49
4:F:169:ASN:C	4:F:169:ASN:HD22	2.20	0.49
4:F:62:LYS:NZ	4:F:62:LYS:HB2	2.27	0.49
4:F:119:ARG:O	4:F:123:GLU:HG3	2.12	0.49
4:F:145:VAL:CG1	4:F:149:MET:HE2	2.43	0.49
3:H:116:DC:OP1	4:E:292:ARG:NH2	2.45	0.49
4:A:72:ARG:NH1	4:A:116:VAL:HG22	2.28	0.49
4:A:14:LEU:HB3	4:A:19:THR:OG1	2.13	0.49
4:A:107:PRO:O	4:A:108:SER:HB3	2.13	0.49
4:E:23:VAL:HG23	4:E:24:ARG:N	2.27	0.49
4:E:132:LYS:NZ	4:E:132:LYS:HB3	2.28	0.49
4:F:147:SER:HA	4:F:150:GLU:OE2	2.13	0.49
4:F:215:LEU:C	4:F:218:THR:HG22	2.38	0.49
4:B:194:LEU:CD1	4:B:212:ALA:HB2	2.42	0.48
4:E:161:LEU:HD23	4:E:220:LEU:HD21	1.94	0.48
4:E:221:VAL:O	4:E:225:ILE:HG13	2.13	0.48
4:A:19:THR:CG2	4:A:23:VAL:HG23	2.42	0.48
4:A:193:MET:HE1	4:A:221:VAL:HB	1.94	0.48
2:X:124:DA:H2'	2:X:125:DT:C7	2.43	0.48
4:B:181:ARG:HD3	4:B:183:LYS:HE2	1.95	0.48
4:B:200:THR:OG1	4:B:203:LEU:HD23	2.13	0.48
4:B:216:GLY:O	4:B:219:LYS:HB3	2.13	0.48
4:F:96:ASN:HD21	4:F:108:SER:HB2	1.78	0.48
4:F:146:ARG:O	4:F:150:GLU:N	2.43	0.48
4:A:72:ARG:HH12	4:F:33:ASP:CG	2.21	0.48
4:E:117:MET:CE	4:E:120:ILE:HD12	2.43	0.48
4:B:227:VAL:O	4:B:227:VAL:HG12	2.13	0.48
4:E:188:THR:C	4:E:190:GLY:N	2.72	0.48
4:A:64:PHE:HA	4:A:65:PRO:C	2.39	0.48
4:F:134:ALA:HA	4:F:283:TYR:CD2	2.49	0.48
3:D:106:DC:H2'	3:D:107:DT:H71	1.95	0.48
4:B:320:ILE:HA	4:B:323:ASN:HB2	1.96	0.48
4:E:213:LEU:N	4:E:213:LEU:HD22	2.29	0.48
4:F:158:ILE:HG12	4:F:223:ARG:NH1	2.29	0.48
4:F:163:PHE:HE1	4:F:261:LEU:HD13	1.79	0.48
4:F:297:ARG:NH1	4:F:297:ARG:HG2	2.28	0.48
4:A:158:ILE:HD11	4:A:223:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:78:LEU:HD22	4:B:83:LEU:HD12	1.96	0.48
4:A:158:ILE:HD11	4:A:223:ARG:CZ	2.44	0.47
4:F:27:LEU:O	4:F:31:PHE:HD1	1.95	0.47
4:F:193:MET:HE1	4:F:221:VAL:CG1	2.44	0.47
4:B:33:ASP:C	4:B:35:GLN:N	2.70	0.47
4:E:59:ASN:O	4:E:60:ASN:HB2	2.13	0.47
4:E:261:LEU:HA	4:E:264:ILE:HD12	1.94	0.47
4:E:304:VAL:CG1	4:E:308:GLU:HB2	2.43	0.47
4:F:340:GLU:O	4:F:341:ASP:C	2.57	0.47
4:B:306:ILE:N	4:B:307:PRO:HD2	2.29	0.47
4:E:106:ARG:HG2	4:E:109:ASP:OD2	2.15	0.47
4:B:328:LEU:HD12	4:B:328:LEU:H	1.79	0.47
3:D:106:DC:H2''	3:D:107:DT:H5'	1.96	0.47
4:B:319:ASN:ND2	4:B:323:ASN:OD1	2.45	0.47
4:F:96:ASN:HD21	4:F:108:SER:CB	2.27	0.47
1:C:115:A3P:O2P	2:X:116:DT:C5'	2.62	0.47
4:B:25:LYS:O	4:B:28:MET:N	2.48	0.47
4:B:221:VAL:O	4:B:225:ILE:HG13	2.14	0.47
4:E:26:ASN:CB	4:E:102:SER:HA	2.44	0.47
4:F:84:ALA:O	4:F:85:VAL:C	2.58	0.47
4:F:329:ASP:O	4:F:330:SER:C	2.57	0.47
1:C:109:DC:H2''	1:C:110:DG:C8	2.50	0.47
4:A:71:VAL:O	4:A:75:LEU:HG	2.15	0.47
4:B:317:ASN:OD1	4:B:319:ASN:HB3	2.15	0.47
3:D:100:DG:H2''	3:D:101:DG:O5'	2.14	0.47
3:D:107:DT:H2''	3:D:108:DT:H5'	1.96	0.47
2:Y:125:DT:H2''	2:Y:126:DA:H5'	1.96	0.47
4:E:23:VAL:HA	4:E:26:ASN:HD22	1.80	0.47
4:F:237:TYR:CE1	4:F:255:GLN:HB3	2.50	0.47
5:C:200:IOD:I	4:B:260:ALA:HA	2.85	0.47
3:H:101:DG:H2''	3:H:102:DA:OP2	2.14	0.47
3:H:112:DA:H1'	3:H:113:DT:H5''	1.96	0.47
4:B:249:ALA:N	4:B:250:PRO:HD3	2.29	0.47
4:F:310:MET:HE3	4:F:316:THR:C	2.40	0.47
4:A:306:ILE:N	4:A:307:PRO:CD	2.77	0.46
4:E:188:THR:C	4:E:190:GLY:H	2.23	0.46
4:E:311:GLN:C	4:E:311:GLN:CD	2.84	0.46
4:A:27:LEU:HD13	4:A:102:SER:CB	2.45	0.46
4:B:192:ARG:NH1	4:E:340:GLU:OE2	2.49	0.46
1:C:110:DG:H2''	1:C:111:DT:OP2	2.15	0.46
4:A:307:PRO:HG3	4:B:306:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:94:GLN:OE1	4:B:94:GLN:HA	2.15	0.46
4:B:217:VAL:O	4:B:221:VAL:HG23	2.15	0.46
4:B:319:ASN:C	4:B:323:ASN:OD1	2.59	0.46
4:F:135:LEU:HD23	4:F:283:TYR:O	2.15	0.46
4:F:326:ARG:HG2	4:F:326:ARG:HH11	1.80	0.46
4:F:269:HIS:HB2	4:F:286:TRP:CE3	2.51	0.46
4:B:22:GLU:O	4:B:25:LYS:N	2.48	0.46
4:E:74:TYR:O	4:E:78:LEU:HD12	2.15	0.46
4:E:92:LEU:O	4:E:92:LEU:HD23	2.16	0.46
4:F:20:SER:O	4:F:24:ARG:HG2	2.16	0.46
4:F:272:ILE:HB	4:F:273:TYR:CD1	2.51	0.46
4:A:158:ILE:HD13	4:A:223:ARG:HG2	1.96	0.46
4:E:171:LEU:N	4:E:171:LEU:CD2	2.75	0.46
4:F:193:MET:HE1	4:F:221:VAL:HG11	1.98	0.46
2:X:124:DA:H2'	2:X:125:DT:C6	2.51	0.46
4:A:22:GLU:C	4:A:24:ARG:N	2.72	0.46
4:B:325:ILE:CG2	4:B:326:ARG:N	2.79	0.46
4:E:243:ARG:HG2	4:E:243:ARG:NH1	2.27	0.46
4:F:168:TYR:HA	4:F:291:ALA:HB1	1.96	0.46
2:Y:134:DA:C8	2:Y:135:DT:H72	2.51	0.46
4:B:35:GLN:HE21	4:B:35:GLN:CA	1.98	0.46
4:B:106:ARG:HB2	4:B:106:ARG:HH11	1.80	0.46
4:B:337:ARG:O	4:B:341:ASP:HB2	2.16	0.46
4:F:97:MET:O	4:F:101:ARG:HB2	2.16	0.46
4:F:273:TYR:CD1	4:F:273:TYR:N	2.84	0.46
4:F:276:LYS:O	4:F:277:ASP:O	2.34	0.46
4:B:315:TRP:CE2	4:B:324:TYR:CD2	3.04	0.45
2:X:117:DG:C2'	2:X:118:DT:H5'	2.44	0.45
4:E:75:LEU:HA	4:E:78:LEU:HD13	1.97	0.45
4:E:222:GLU:O	4:E:223:ARG:C	2.60	0.45
4:F:272:ILE:C	4:F:273:TYR:CD1	2.95	0.45
2:X:118:DT:H73	4:B:319:ASN:CB	2.42	0.45
3:D:105:DA:C2	3:D:106:DC:C2	3.04	0.45
4:B:161:LEU:HG	4:B:220:LEU:HD13	1.97	0.45
4:B:226:SER:OG	4:B:227:VAL:N	2.49	0.45
3:D:104:DA:H2''	3:D:105:DA:O5'	2.17	0.45
4:B:285:ALA:O	4:B:286:TRP:C	2.59	0.45
4:E:154:ARG:C	4:E:156:GLN:N	2.74	0.45
4:E:155:CYS:SG	4:E:227:VAL:HG12	2.56	0.45
3:D:118:DT:H3'	4:B:121:ARG:NH1	2.32	0.45
4:A:318:VAL:O	4:A:319:ASN:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:305:SER:HB2	4:E:307:PRO:HD2	1.98	0.45
4:F:81:ARG:HG3	4:F:81:ARG:HH11	1.81	0.45
3:D:114:DA:N7	4:A:86:LYS:HD2	2.31	0.45
4:B:62:LYS:HE3	4:B:62:LYS:HB2	1.78	0.45
4:B:325:ILE:C	4:B:326:ARG:HG3	2.41	0.45
4:E:42:TRP:CE3	4:E:45:LEU:HD23	2.52	0.45
4:E:64:PHE:HA	4:E:65:PRO:C	2.41	0.45
4:B:270:ARG:HA	4:B:274:GLY:O	2.17	0.45
4:E:282:ARG:O	4:E:283:TYR:HB2	2.16	0.45
4:B:209:VAL:HG22	4:B:210:GLU:N	2.31	0.45
1:G:107:UMP:OP2	4:F:256:LEU:HD12	2.17	0.45
2:Y:118:DT:C7	4:F:319:ASN:ND2	2.76	0.45
3:H:108:DT:H1'	3:H:109:DC:H5''	1.99	0.45
4:B:195:ILE:HG22	4:B:196:HIS:N	2.31	0.44
4:E:154:ARG:H	4:E:154:ARG:HG2	1.48	0.44
3:H:133:DT:H2''	3:H:134:DA:C8	2.53	0.44
4:B:310:MET:HG2	4:B:321:VAL:CG2	2.47	0.44
4:E:306:ILE:N	4:E:307:PRO:CD	2.80	0.44
4:F:60:ASN:O	4:F:61:ARG:HD3	2.17	0.44
4:F:297:ARG:HG2	4:F:297:ARG:HH11	1.81	0.44
4:E:207:ALA:HB2	4:E:314:GLY:HA3	2.00	0.44
1:C:105:DA:H2''	1:C:106:DC:C5'	2.24	0.44
4:A:20:SER:O	4:A:21:ASP:CB	2.65	0.44
4:B:22:GLU:O	4:B:25:LYS:HB3	2.17	0.44
4:B:320:ILE:CA	4:B:323:ASN:HB2	2.47	0.44
4:E:78:LEU:HD21	4:E:91:HIS:ND1	2.33	0.44
4:E:200:THR:HG21	4:E:205:SER:CB	2.43	0.44
4:E:213:LEU:HD22	4:E:213:LEU:H	1.83	0.44
4:F:320:ILE:O	4:F:321:VAL:C	2.59	0.44
4:A:11:LEU:HD13	4:A:14:LEU:HD21	2.00	0.44
4:B:116:VAL:O	4:B:120:ILE:HG13	2.18	0.44
4:B:218:THR:O	4:B:222:GLU:HG3	2.18	0.44
4:E:171:LEU:HD23	4:E:171:LEU:H	1.77	0.44
4:F:155:CYS:SG	4:F:227:VAL:HG12	2.57	0.44
4:F:158:ILE:HG12	4:F:223:ARG:HH12	1.82	0.44
3:D:108:DT:H1'	3:D:109:DC:C5'	2.47	0.44
2:Y:128:DG:H1	3:H:109:DC:H42	1.65	0.44
4:A:92:LEU:HD22	4:A:96:ASN:HD21	1.82	0.44
4:A:231:ALA:O	4:A:233:ASP:N	2.50	0.44
4:B:185:ILE:HD13	4:B:193:MET:HE1	1.95	0.44
4:B:315:TRP:HZ2	4:B:324:TYR:CE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:59:ASN:HB3	4:E:61:ARG:NH1	2.32	0.44
4:F:55:TRP:O	4:F:59:ASN:HB2	2.18	0.44
2:X:117:DG:C5'	4:B:316:THR:OG1	2.63	0.44
2:Y:118:DT:C7	4:F:319:ASN:CG	2.90	0.44
3:D:117:DA:OP1	4:A:201:LYS:CE	2.66	0.44
3:D:135:DT:H1'	4:B:244:LYS:HD3	1.98	0.44
4:A:14:LEU:HG	4:A:27:LEU:HD23	1.99	0.44
4:A:72:ARG:HH11	4:A:116:VAL:CG2	2.30	0.44
4:E:185:ILE:HG21	4:E:193:MET:CE	2.42	0.44
4:F:172:LEU:HD21	4:F:197:ILE:HG13	2.00	0.44
4:F:310:MET:HG3	4:F:321:VAL:HG21	1.99	0.44
4:A:100:ARG:C	4:A:102:SER:H	2.26	0.44
4:A:193:MET:CE	4:A:221:VAL:HB	2.47	0.44
4:B:45:LEU:HD23	4:B:45:LEU:O	2.18	0.44
4:F:299:MET:O	4:F:300:ALA:C	2.60	0.44
4:E:65:PRO:HB3	4:E:104:LEU:HD21	1.99	0.43
4:F:89:GLN:HG2	4:F:117:MET:HE2	1.99	0.43
4:F:315:TRP:CZ2	4:F:324:TYR:CE1	3.05	0.43
1:G:105:DA:H4'	4:F:242:VAL:O	2.18	0.43
3:H:126:DA:OP2	4:F:262:GLU:OE2	2.36	0.43
4:A:181:ARG:HB2	4:A:236:ASN:O	2.18	0.43
4:E:169:ASN:OD1	4:F:339:LEU:HD12	2.18	0.43
2:Y:131:DG:C2'	2:Y:132:DT:C5'	2.86	0.43
4:A:23:VAL:O	4:A:27:LEU:HB2	2.18	0.43
4:B:331:GLU:O	4:B:332:THR:C	2.61	0.43
3:H:122:DT:C6	3:H:123:DT:H72	2.53	0.43
4:A:213:LEU:N	4:A:213:LEU:HD23	2.34	0.43
4:B:122:LYS:O	4:B:126:ASP:HB2	2.18	0.43
4:E:306:ILE:HG22	4:F:306:ILE:HD11	2.00	0.43
4:F:49:CYS:O	4:F:50:ARG:C	2.59	0.43
4:F:297:ARG:HH11	4:F:297:ARG:CG	2.30	0.43
3:D:124:DA:H2'	3:D:125:DT:H72	1.99	0.43
4:A:171:LEU:O	4:A:292:ARG:NH1	2.52	0.43
4:B:29:ASP:O	4:B:32:ARG:HB3	2.19	0.43
4:B:110:SER:O	4:B:112:ALA:N	2.52	0.43
4:B:139:ARG:HB2	4:B:168:TYR:OH	2.19	0.43
4:F:171:LEU:O	4:F:292:ARG:HG3	2.18	0.43
1:C:115:A3P:C2'	2:X:116:DT:H5'	2.49	0.43
4:F:20:SER:HB3	4:F:23:VAL:HG23	2.01	0.43
4:F:272:ILE:HB	4:F:273:TYR:HD1	1.82	0.43
4:A:72:ARG:HH11	4:A:116:VAL:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:156:GLN:C	4:E:158:ILE:N	2.74	0.43
1:G:115:A3P:O3'	2:Y:116:DT:C5'	2.67	0.43
4:A:122:LYS:O	4:A:123:GLU:C	2.61	0.43
4:B:319:ASN:C	4:B:319:ASN:HD22	2.27	0.43
4:A:277:ASP:HB3	4:A:284:LEU:HD13	2.00	0.43
4:B:159:ARG:HB2	4:B:224:TRP:CE3	2.54	0.43
4:E:74:TYR:O	4:E:78:LEU:CD1	2.67	0.43
4:E:305:SER:C	4:E:307:PRO:HD2	2.44	0.43
4:F:126:ASP:O	4:F:128:GLY:N	2.51	0.43
4:F:121:ARG:O	4:F:125:VAL:HG23	2.18	0.43
3:D:133:DT:H2''	3:D:134:DA:C8	2.54	0.42
1:G:108:DT:H2''	1:G:109:DC:O5'	2.19	0.42
4:A:169:ASN:C	4:A:169:ASN:HD22	2.27	0.42
4:F:61:ARG:HG2	4:F:70:ASP:OD1	2.19	0.42
4:F:326:ARG:O	4:F:326:ARG:HG3	2.18	0.42
2:X:126:DA:OP2	4:A:262:GLU:OE1	2.38	0.42
3:H:118:DT:H2''	3:H:119:DA:N7	2.33	0.42
4:A:121:ARG:HH11	4:F:204:VAL:HG13	1.83	0.42
4:E:243:ARG:CG	4:E:243:ARG:NH1	2.81	0.42
3:D:128:DG:H2''	3:D:129:DA:H5'	2.00	0.42
3:H:122:DT:OP2	4:F:101:ARG:NH1	2.51	0.42
4:A:65:PRO:HG3	4:A:104:LEU:HD13	2.00	0.42
2:X:118:DT:C7	4:B:319:ASN:HB3	2.45	0.42
4:E:200:THR:CG2	4:E:201:LYS:H	2.11	0.42
4:F:61:ARG:HG2	4:F:61:ARG:NH1	2.34	0.42
4:F:332:THR:HB	4:F:333:GLY:H	1.56	0.42
4:A:202:THR:HG22	4:A:204:VAL:H	1.85	0.42
4:E:57:LYS:O	4:E:58:LEU:HB2	2.20	0.42
4:E:92:LEU:HD21	4:E:108:SER:OG	2.18	0.42
4:E:119:ARG:O	4:E:123:GLU:HB2	2.20	0.42
4:E:181:ARG:O	4:E:182:VAL:C	2.63	0.42
4:E:215:LEU:O	4:E:218:THR:HB	2.20	0.42
3:H:129:DA:C8	3:H:129:DA:H5'	2.55	0.42
4:A:141:ASP:O	4:A:145:VAL:HG23	2.20	0.42
4:B:118:ARG:HG3	4:B:118:ARG:NH1	2.35	0.42
4:B:154:ARG:O	4:B:158:ILE:HG12	2.20	0.42
4:E:317:ASN:HB3	4:E:319:ASN:OD1	2.18	0.42
4:F:270:ARG:HG3	4:F:270:ARG:HH11	1.85	0.42
3:H:123:DT:C2	3:H:124:DA:C8	3.08	0.42
4:A:22:GLU:C	4:A:24:ARG:H	2.27	0.42
4:A:268:THR:HG22	4:A:286:TRP:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:20:SER:O	4:B:24:ARG:HD2	2.20	0.42
4:B:20:SER:OG	4:B:21:ASP:N	2.50	0.42
4:F:99:HIS:O	4:F:102:SER:HB2	2.19	0.42
3:H:124:DA:OP2	4:F:38:SER:OG	2.35	0.42
4:A:107:PRO:C	4:A:109:ASP:N	2.75	0.42
4:B:90:GLN:HE21	4:B:94:GLN:HG2	1.85	0.42
3:D:119:DA:P	4:B:121:ARG:NH1	2.89	0.41
4:A:34:ARG:C	4:A:36:ALA:H	2.26	0.41
4:E:84:ALA:O	4:E:88:ILE:HG13	2.20	0.41
4:E:223:ARG:HG3	4:E:223:ARG:HH11	1.85	0.41
4:E:235:ASN:N	4:E:235:ASN:HD22	2.18	0.41
4:F:55:TRP:CD1	4:F:56:CYS:N	2.88	0.41
2:X:135:DT:H5'	2:X:135:DT:H6	1.85	0.41
4:A:215:LEU:HG	4:B:340:GLU:OE1	2.20	0.41
4:E:52:TRP:HZ3	4:E:74:TYR:HB2	1.85	0.41
4:E:78:LEU:H	4:E:78:LEU:CD1	2.30	0.41
4:F:140:THR:HG22	4:F:141:ASP:N	2.35	0.41
4:A:243:ARG:O	4:A:244:LYS:C	2.64	0.41
4:B:63:TRP:O	4:B:64:PHE:HB2	2.19	0.41
4:B:301:ARG:C	4:B:303:GLY:N	2.78	0.41
2:Y:119:DA:H2''	2:Y:120:DT:O5'	2.20	0.41
2:Y:135:DT:H2''	2:Y:136:DC:C6	2.55	0.41
4:B:111:ASN:O	4:B:115:LEU:HG	2.20	0.41
4:A:106:ARG:O	4:A:109:ASP:CB	2.57	0.41
4:A:318:VAL:HG13	4:B:318:VAL:HG11	2.02	0.41
4:A:325:ILE:HB	4:A:328:LEU:HD12	2.03	0.41
4:B:76:LEU:HD23	4:B:76:LEU:HA	1.73	0.41
4:B:305:SER:O	4:B:309:ILE:HG13	2.21	0.41
4:E:48:VAL:O	4:E:49:CYS:C	2.64	0.41
4:F:259:ARG:HA	4:F:259:ARG:HD2	1.89	0.41
3:H:134:DA:C8	3:H:135:DT:H72	2.56	0.41
4:A:19:THR:HG23	4:A:23:VAL:HG23	2.01	0.41
4:E:57:LYS:H	4:E:57:LYS:CD	2.33	0.41
4:E:323:ASN:HD22	4:E:323:ASN:HA	1.62	0.41
4:F:145:VAL:HG12	4:F:145:VAL:O	2.20	0.41
1:C:105:DA:H4'	4:B:242:VAL:O	2.20	0.41
3:D:123:DT:H3'	4:B:38:SER:HB2	2.03	0.41
3:H:113:DT:H2''	3:H:114:DA:H8	1.86	0.41
4:E:49:CYS:SG	4:E:98:LEU:HD22	2.61	0.41
4:E:173:ARG:NH1	4:E:173:ARG:CG	2.81	0.41
1:C:106:DC:H2''	1:C:107:UMP:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:DC:H2''	1:G:107:UMP:C6	2.56	0.41
4:A:80:ALA:C	4:A:82:GLY:H	2.29	0.41
4:A:92:LEU:HD21	4:A:108:SER:HB2	2.02	0.41
4:A:204:VAL:HG13	4:A:204:VAL:O	2.20	0.41
4:B:80:ALA:C	4:B:82:GLY:N	2.79	0.41
4:B:110:SER:O	4:B:111:ASN:C	2.64	0.41
4:B:206:THR:HG21	4:E:129:GLU:HG2	2.03	0.41
4:B:227:VAL:O	4:B:227:VAL:CG1	2.68	0.41
4:B:289:HIS:CD2	4:B:292:ARG:HD3	2.56	0.41
4:E:173:ARG:O	4:E:176:GLU:HB2	2.21	0.41
4:F:96:ASN:O	4:F:97:MET:C	2.64	0.41
4:F:193:MET:HB3	4:F:213:LEU:HD12	2.03	0.41
4:F:333:GLY:O	4:F:334:ALA:HB3	2.21	0.41
4:B:84:ALA:O	4:B:88:ILE:HG13	2.21	0.41
4:B:327:ASN:OD1	4:B:328:LEU:HD12	2.20	0.41
2:Y:118:DT:OP2	4:F:317:ASN:CG	2.64	0.40
4:A:188:THR:C	4:A:190:GLY:N	2.76	0.40
4:F:163:PHE:CZ	4:F:261:LEU:HB3	2.56	0.40
3:D:124:DA:H8	3:D:124:DA:H5'	1.87	0.40
4:A:95:LEU:HA	4:A:95:LEU:HD12	1.79	0.40
4:A:181:ARG:O	4:A:182:VAL:C	2.64	0.40
4:B:74:TYR:CZ	4:B:78:LEU:HD11	2.56	0.40
4:B:297:ARG:O	4:B:300:ALA:N	2.53	0.40
4:B:319:ASN:ND2	4:B:319:ASN:O	2.55	0.40
4:F:322:MET:HE3	4:F:322:MET:HA	2.04	0.40
1:C:100:DC:C2'	1:C:101:DG:C8	3.05	0.40
4:A:207:ALA:HA	4:A:314:GLY:HA2	2.03	0.40
4:E:85:VAL:HG23	4:E:129:GLU:OE2	2.21	0.40
4:E:170:THR:C	4:E:172:LEU:N	2.79	0.40
4:A:15:PRO:HB2	4:A:18:ALA:H	1.86	0.40
4:A:217:VAL:O	4:A:221:VAL:HG23	2.20	0.40
4:F:27:LEU:HD12	4:F:27:LEU:HA	1.82	0.40
2:Y:117:DG:O6	3:H:120:DC:N3	2.54	0.40
3:H:123:DT:O2	4:F:201:LYS:HE2	2.22	0.40
4:A:72:ARG:NH1	4:F:33:ASP:CG	2.80	0.40
4:A:186:SER:OG	4:A:196:HIS:HE1	2.05	0.40
4:E:197:ILE:O	4:E:197:ILE:HG12	2.21	0.40
4:F:113:VAL:O	4:F:116:VAL:HG12	2.21	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	
4	A	330/347 (95%)	297 (90%)	25 (8%)	8 (2%)	4	17
4	B	320/347 (92%)	265 (83%)	39 (12%)	16 (5%)	1	5
4	E	319/347 (92%)	265 (83%)	42 (13%)	12 (4%)	2	9
4	F	320/347 (92%)	278 (87%)	32 (10%)	10 (3%)	3	12
All	All	1289/1388 (93%)	1105 (86%)	138 (11%)	46 (4%)	2	10

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	13	ALA
4	A	182	VAL
4	B	148	LEU
4	B	248	ALA
4	B	327	ASN
4	E	58	LEU
4	E	147	SER
4	E	149	MET
4	E	182	VAL
4	E	232	ASP
4	F	277	ASP
4	F	327	ASN
4	F	328	LEU
4	F	330	SER
4	A	21	ASP
4	A	214	SER
4	A	232	ASP
4	A	279	SER
4	B	81	ARG
4	B	111	ASN
4	B	286	TRP
4	B	328	LEU

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Mol	Chain	Res	Type
4	B	331	GLU
4	E	155	CYS
4	F	59	ASN
4	F	275	ALA
4	F	340	GLU
4	B	128	GLY
4	B	147	SER
4	B	271	LEU
4	B	332	THR
4	B	334	ALA
4	E	286	TRP
4	F	324	TYR
4	A	206	THR
4	E	200	THR
4	E	214	SER
4	E	244	LYS
4	F	127	ALA
4	B	127	ALA
4	B	326	ARG
4	E	189	ASP
4	E	250	PRO
4	F	274	GLY
4	B	68	PRO
4	A	12	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	
4	A	277/291 (95%)	249 (90%)	28 (10%)	7	23
4	B	269/291 (92%)	241 (90%)	28 (10%)	7	21
4	E	268/291 (92%)	236 (88%)	32 (12%)	5	16
4	F	269/291 (92%)	242 (90%)	27 (10%)	7	23
All	All	1083/1164 (93%)	968 (89%)	115 (11%)	6	21

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
4	A	34	ARG
4	A	58	LEU
4	A	61	ARG
4	A	86	LYS
4	A	89	GLN
4	A	92	LEU
4	A	95	LEU
4	A	98	LEU
4	A	106	ARG
4	A	109	ASP
4	A	130	ARG
4	A	140	THR
4	A	155	CYS
4	A	161	LEU
4	A	186	SER
4	A	187	ARG
4	A	203	LEU
4	A	222	GLU
4	A	227	VAL
4	A	238	LEU
4	A	247	VAL
4	A	277	ASP
4	A	278	ASP
4	A	289	HIS
4	A	311	GLN
4	A	316	THR
4	A	321	VAL
4	B	27	LEU
4	B	30	MET
4	B	35	GLN
4	B	45	LEU
4	B	56	CYS
4	B	57	LYS
4	B	68	PRO
4	B	95	LEU
4	B	106	ARG
4	B	108	SER
4	B	111	ASN
4	B	140	THR
4	B	144	GLN
4	B	157	ASP

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Mol	Chain	Res	Type
4	B	169	ASN
4	B	171	LEU
4	B	203	LEU
4	B	206	THR
4	B	235	ASN
4	B	242	VAL
4	B	266	GLU
4	B	270	ARG
4	B	271	LEU
4	B	277	ASP
4	B	289	HIS
4	B	293	VAL
4	B	317	ASN
4	B	332	THR
4	E	30	MET
4	E	48	VAL
4	E	57	LYS
4	E	58	LEU
4	E	76	LEU
4	E	86	LYS
4	E	95	LEU
4	E	102	SER
4	E	104	LEU
4	E	106	ARG
4	E	115	LEU
4	E	116	VAL
4	E	117	MET
4	E	132	LYS
4	E	135	LEU
4	E	148	LEU
4	E	153	ASP
4	E	154	ARG
4	E	171	LEU
4	E	182	VAL
4	E	189	ASP
4	E	194	LEU
4	E	206	THR
4	E	238	LEU
4	E	243	ARG
4	E	256	LEU
4	E	306	ILE
4	E	311	GLN

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Mol	Chain	Res	Type
4	E	316	THR
4	E	317	ASN
4	E	323	ASN
4	E	338	LEU
4	F	27	LEU
4	F	35	GLN
4	F	45	LEU
4	F	55	TRP
4	F	56	CYS
4	F	61	ARG
4	F	62	LYS
4	F	72	ARG
4	F	95	LEU
4	F	101	ARG
4	F	106	ARG
4	F	130	ARG
4	F	135	LEU
4	F	155	CYS
4	F	193	MET
4	F	271	LEU
4	F	273	TYR
4	F	289	HIS
4	F	292	ARG
4	F	293	VAL
4	F	297	ARG
4	F	318	VAL
4	F	319	ASN
4	F	320	ILE
4	F	323	ASN
4	F	329	ASP
4	F	332	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	40	HIS
4	A	79	GLN
4	A	89	GLN
4	A	90	GLN
4	A	96	ASN
4	A	124	ASN
4	A	133	GLN

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Mol	Chain	Res	Type
4	A	196	HIS
4	A	255	GLN
4	A	311	GLN
4	B	35	GLN
4	B	40	HIS
4	B	60	ASN
4	B	79	GLN
4	B	90	GLN
4	B	133	GLN
4	B	156	GLN
4	B	235	ASN
4	B	236	ASN
4	B	255	GLN
4	B	289	HIS
4	E	26	ASN
4	E	35	GLN
4	E	79	GLN
4	E	89	GLN
4	E	90	GLN
4	E	94	GLN
4	E	96	ASN
4	E	144	GLN
4	E	169	ASN
4	E	235	ASN
4	E	289	HIS
4	E	317	ASN
4	E	323	ASN
4	F	35	GLN
4	F	91	HIS
4	F	96	ASN
4	F	133	GLN
4	F	156	GLN
4	F	255	GLN
4	F	281	GLN
4	F	319	ASN
4	F	327	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	UMP	C	107	3,1	17,20,21	0.49	0	23,28,31	0.38	0
1	A3P	G	115	3,4,1	20,26,29	0.83	1 (5%)	28,37,45	1.12	1 (3%)
1	UMP	G	107	3,1	17,20,21	0.42	0	23,28,31	0.47	0
1	A3P	C	115	3,4,1	20,26,29	0.77	0	28,37,45	1.64	6 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UMP	C	107	3,1	-	0/7/21/22	0/2/2/2
1	A3P	G	115	3,4,1	-	0/9/25/31	0/3/3/3
1	UMP	G	107	3,1	-	1/7/21/22	0/2/2/2
1	A3P	C	115	3,4,1	-	3/9/25/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	115	A3P	O3'-C3'	-2.35	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	A3P	C2'-C1'-N9	4.89	126.12	114.63
1	C	115	A3P	C2'-C3'-C4'	4.65	111.97	102.93
1	G	115	A3P	C2'-C1'-N9	4.15	124.37	114.63
1	C	115	A3P	O3'-C3'-C4'	-2.45	101.51	108.66
1	C	115	A3P	O4'-C1'-N9	-2.29	103.86	107.96
1	C	115	A3P	C3'-C2'-C1'	-2.27	98.56	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	A3P	O3'-C3'-C2'	2.07	120.37	113.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	115	A3P	O4'-C4'-C5'-O5'
1	C	115	A3P	C3'-C4'-C5'-O5'
1	C	115	A3P	C2'-C1'-N9-C4
1	G	107	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	107	UMP	2	0
1	G	115	A3P	2	0
1	G	107	UMP	3	0
1	C	115	A3P	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	14/16 (87%)	1.16	3 (21%) 2 2	39, 71, 89, 93	0
1	G	14/16 (87%)	0.57	2 (14%) 6 5	45, 61, 114, 131	0
2	X	21/21 (100%)	0.37	2 (9%) 14 11	35, 56, 95, 99	0
2	Y	21/21 (100%)	1.01	2 (9%) 14 11	49, 77, 115, 120	0
3	D	37/37 (100%)	0.68	6 (16%) 4 4	34, 57, 92, 96	0
3	H	37/37 (100%)	0.88	4 (10%) 11 9	44, 74, 104, 115	0
4	A	332/347 (95%)	0.29	19 (5%) 29 23	29, 54, 93, 134	0
4	B	322/347 (92%)	0.65	27 (8%) 17 14	42, 73, 104, 139	0
4	E	321/347 (92%)	0.87	38 (11%) 9 7	48, 82, 114, 150	0
4	F	322/347 (92%)	0.56	26 (8%) 18 15	36, 65, 99, 139	0
All	All	1441/1536 (93%)	0.61	129 (8%) 15 13	29, 69, 106, 150	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	328	LEU	6.7
4	F	319	ASN	6.6
4	F	328	LEU	6.1
4	B	330	SER	6.1
4	F	330	SER	6.0
4	A	201	LYS	6.0
4	E	204	VAL	5.9
4	E	202	THR	5.8
3	D	100	DG	5.7
4	E	203	LEU	5.7
4	A	204	VAL	5.6
4	F	329	ASP	5.5
4	F	323	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
4	E	205	SER	5.4
3	H	100	DG	5.4
4	E	201	LYS	5.2
4	F	326	ARG	4.8
2	Y	117	DG	4.6
4	A	203	LEU	4.5
4	A	202	THR	4.5
4	F	332	THR	4.4
4	E	200	THR	4.4
4	B	331	GLU	4.3
4	E	210	GLU	4.2
4	B	324	TYR	4.2
4	F	331	GLU	4.2
4	B	319	ASN	4.1
4	B	327	ASN	4.1
4	B	318	VAL	4.1
4	B	326	ARG	4.0
2	Y	116	DT	3.9
4	E	206	THR	3.9
4	F	325	ILE	3.9
4	A	196	HIS	3.8
4	F	324	TYR	3.7
4	E	21	ASP	3.7
4	F	62	LYS	3.7
4	B	332	THR	3.6
4	A	205	SER	3.6
4	B	323	ASN	3.6
4	E	155	CYS	3.5
4	E	208	GLY	3.5
4	A	200	THR	3.4
4	F	327	ASN	3.4
1	G	100	DC	3.3
4	A	206	THR	3.3
3	D	101	DG	3.2
4	B	20	SER	3.2
4	B	127	ALA	3.2
1	G	101	DG	3.2
4	E	242	VAL	3.2
4	F	20	SER	3.1
4	F	341	ASP	3.1
4	E	244	LYS	3.1
4	A	19	THR	3.1

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Mol	Chain	Res	Type	RSRZ
4	E	188	THR	3.1
4	A	126	ASP	3.0
4	B	329	ASP	3.0
4	E	241	ARG	3.0
2	X	116	DT	3.0
4	F	333	GLY	3.0
4	A	229	GLY	2.9
4	E	186	SER	2.9
4	E	279	SER	2.9
4	E	243	ARG	2.8
3	H	101	DG	2.8
4	E	341	ASP	2.8
4	E	152	SER	2.8
4	F	277	ASP	2.8
4	B	341	ASP	2.8
3	D	116	DC	2.7
4	E	194	LEU	2.7
3	D	136	DC	2.7
4	E	187	ARG	2.6
4	F	31	PHE	2.6
4	B	31	PHE	2.6
4	E	240	CYS	2.6
4	B	321	VAL	2.6
4	A	14	LEU	2.5
4	F	248	ALA	2.5
4	E	199	ARG	2.5
4	A	21	ASP	2.5
4	A	12	PRO	2.5
4	B	320	ILE	2.4
3	D	117	DA	2.4
1	C	101	DG	2.4
4	F	247	VAL	2.4
4	E	228	SER	2.4
4	E	231	ALA	2.4
4	E	162	ALA	2.4
4	A	341	ASP	2.4
4	B	154	ARG	2.4
4	E	38	SER	2.4
4	E	225	ILE	2.4
4	E	39	GLU	2.3
4	E	114	SER	2.3
2	X	119	DA	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	134	DA	2.3
4	B	22	GLU	2.3
4	A	16	VAL	2.3
4	F	153	ASP	2.3
4	F	148	LEU	2.3
4	F	317	ASN	2.3
4	E	57	LYS	2.3
4	A	188	THR	2.3
4	E	209	VAL	2.2
4	B	325	ILE	2.2
4	F	55	TRP	2.2
4	E	207	ALA	2.2
4	A	317	ASN	2.2
4	B	155	CYS	2.2
4	B	203	LEU	2.2
4	F	35	GLN	2.2
4	E	226	SER	2.2
4	F	24	ARG	2.1
4	B	62	LYS	2.1
4	E	105	PRO	2.1
4	B	42	TRP	2.1
4	A	18	ALA	2.1
3	H	109	DC	2.1
1	C	102	DA	2.1
4	B	277	ASP	2.1
4	B	315	TRP	2.1
4	E	35	GLN	2.0
4	F	311	GLN	2.0
4	E	234	PRO	2.0
3	H	102	DA	2.0
1	C	100	DC	2.0
4	B	227	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	A3P	C	115	24/27	0.86	0.19	42,55,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	UMP	C	107	19/20	0.90	0.15	61,69,75,78	0
1	A3P	G	115	24/27	0.90	0.12	31,40,73,74	0
1	UMP	G	107	19/20	0.93	0.12	58,62,66,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	347	1/1	0.78	0.15	49,49,49,49	0
6	MG	F	345	1/1	0.86	0.29	69,69,69,69	0
6	MG	A	348	1/1	0.89	0.16	44,44,44,44	1
6	MG	A	344	1/1	0.89	0.11	51,51,51,51	0
5	IOD	C	200	1/1	0.92	0.13	74,74,74,74	1
6	MG	D	310	1/1	0.92	0.59	47,47,47,47	1
6	MG	A	345	1/1	0.93	0.19	47,47,47,47	0
6	MG	A	346	1/1	0.94	0.38	50,50,50,50	0
5	IOD	F	344	1/1	0.96	0.10	73,73,73,73	1

6.5 Other polymers [i](#)

There are no such residues in this entry.