Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 04:06 PM EDT

PDB ID	:	3UVF
Title	:	Expanding LAGALIDADG endonuclease scaffold diversity by rapidly surveying evolutionary sequence space
Authors	:	Jacoby, K.; Metzger, M.; Shen, B.; Jarjour, J.; Stoddard, B.; Scharenberg, A.
Deposited on	:	2011-11-29
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

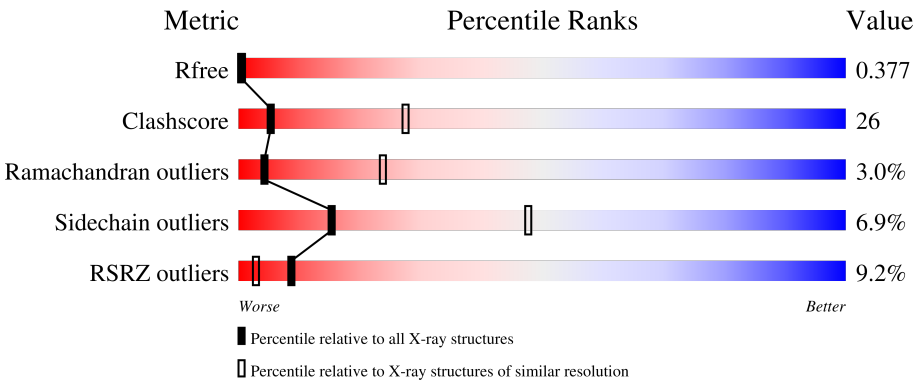
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	255	%, 55%, 41%, .
1	B	255	14%, 48%, 46%, 5%
2	C	28	., 61%, 36%
2	E	28	36%, 11%, 21%, 68%
3	D	28	7%, 43%, 50%

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Mol	Chain	Length	Quality of chain
3	F	28	36% 7% 25% 68%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	B	301	-	-	-	X
5	PEG	A	304	-	-	-	X
5	PEG	B	302	-	-	X	-
5	PEG	E	503	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Intron-encoded DNA endonuclease I-HjeMI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2099	1366	345	383	5	0	1	0
1	B	255	2091	1361	342	383	5	0	0	0

- Molecule 2 is a DNA chain called synthetic oligo.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	28	577	275	106	169	27	0	0	0
2	E	28	577	275	106	169	27	0	0	0

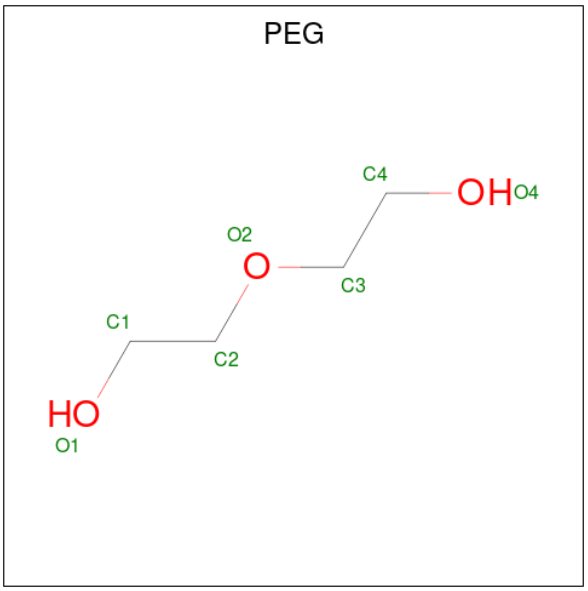
- Molecule 3 is a DNA chain called synthetic oligo.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	28	565	270	105	163	27	0	0	0
3	F	28	565	270	105	163	27	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

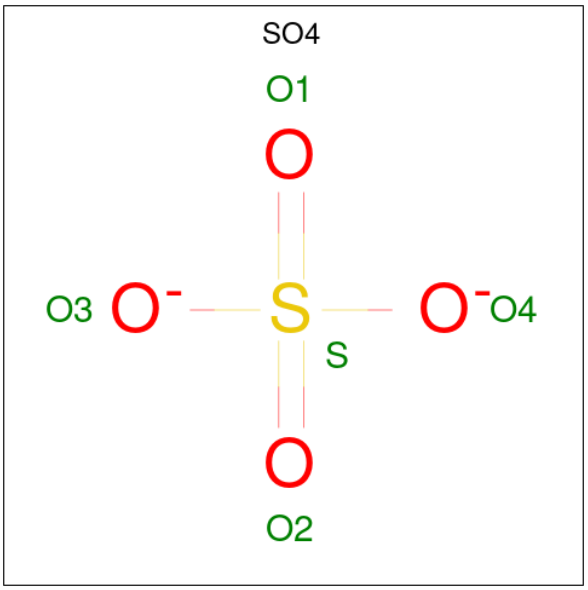
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	3	3	3	0	0
4	B	1	1	1	0	0
4	E	2	2	2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			7	4	3			
5	B	1	Total	C	O		0	0
			7	4	3			
5	E	1	Total	C	O		0	0
			7	4	3			
5	F	1	Total	C	O		0	0
			7	4	3			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	B	1	5	4	1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	B	1	1	1	0	0

- Molecule 8 is water.

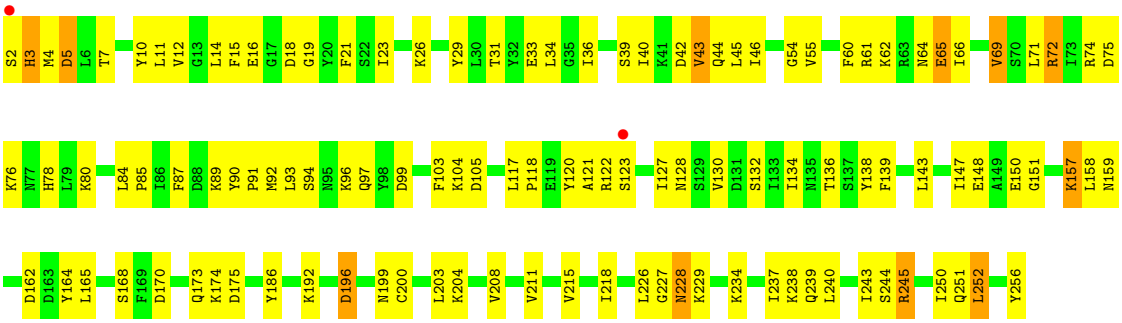
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	43	43	43	0	0
			Total	O		
8	C	26	26	26	0	0
			Total	O		
8	D	9	9	9	0	0
			Total	O		
8	B	44	44	44	0	0
			Total	O		
8	E	26	26	26	0	0
			Total	O		
8	F	26	26	26	0	0

3 Residue-property plots (i)

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

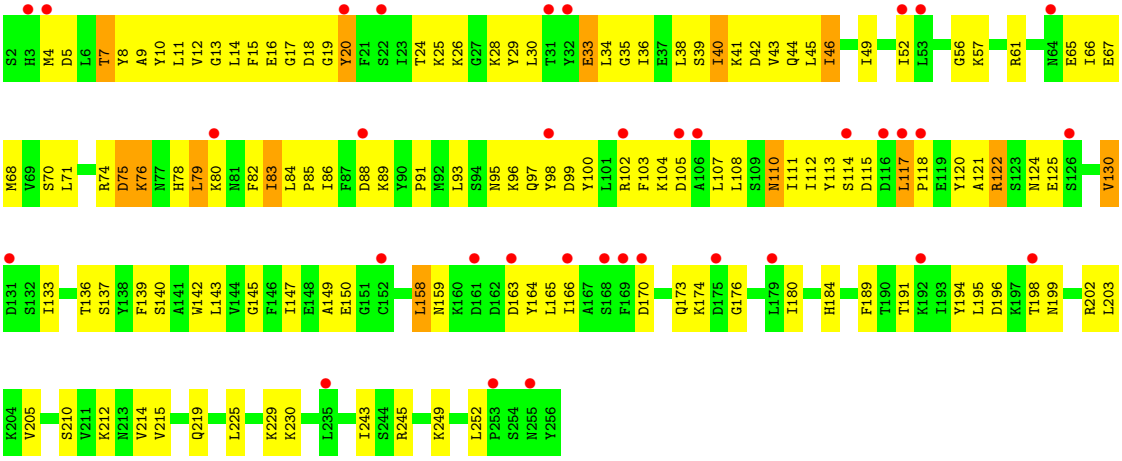
• Molecule 1: Intron-encoded DNA endonuclease I-HjeMI

Chain A:



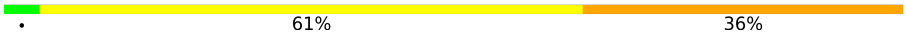
• Molecule 1: Intron-encoded DNA endonuclease I-HjeMI

Chain B:



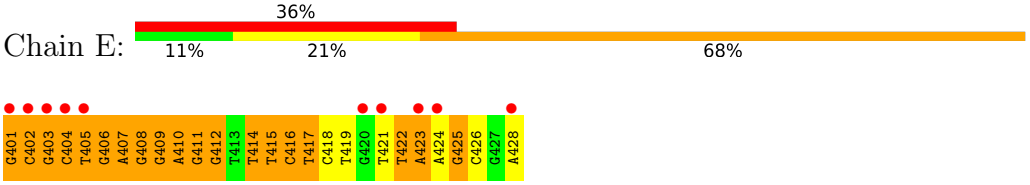
• Molecule 2: synthetic oligo

Chain C:



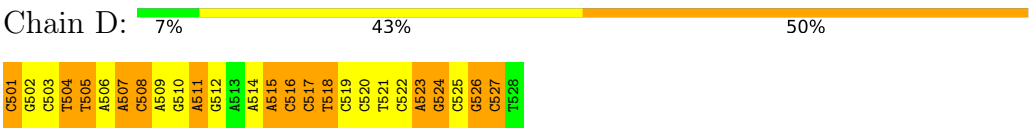
- Molecule 2: synthetic oligo

Chain E:



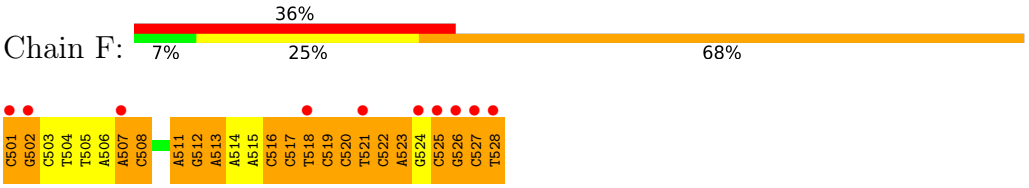
- Molecule 3: synthetic oligo

Chain D:



- Molecule 3: synthetic oligo

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	181.59Å 73.59Å 82.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 3.00 48.71 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.71-3.00) 99.3 (48.71-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	12.14 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.280 , 0.378 0.277 , 0.377	Depositor DCC
R_{free} test set	1155 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	1.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6688	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0079e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PEG, CA, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.72	0/2144	0.84	1/2883 (0.0%)
1	B	0.68	0/2133	0.80	1/2869 (0.0%)
2	C	1.26	2/647 (0.3%)	2.18	28/999 (2.8%)
2	E	1.19	1/647 (0.2%)	2.17	41/999 (4.1%)
3	D	1.18	0/633	2.19	37/973 (3.8%)
3	F	1.24	1/633 (0.2%)	2.21	41/973 (4.2%)
All	All	0.93	4/6837 (0.1%)	1.53	149/9696 (1.5%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	417	DT	C1'-N1	5.80	1.56	1.49
3	F	528	DT	C1'-N1	5.53	1.56	1.49
2	C	426	DC	C3'-O3'	-5.47	1.36	1.44
2	C	407	DA	C3'-O3'	-5.24	1.37	1.44

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	402	DC	O4'-C1'-N1	-13.70	98.41	108.00
2	E	409	DG	O4'-C1'-N9	13.28	117.30	108.00
3	F	518	DT	O4'-C4'-C3'	-11.04	99.38	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	526	DG	O4'-C1'-N9	10.90	115.63	108.00
3	F	519	DC	O4'-C1'-N1	10.86	115.60	108.00
2	C	418	DC	C1'-O4'-C4'	-10.13	99.97	110.10
3	F	511	DA	O4'-C1'-N9	10.04	115.03	108.00
3	D	518	DT	O4'-C4'-C3'	-9.99	100.01	106.00
3	D	516	DC	O5'-P-OP2	-9.63	97.04	105.70
3	D	504	DT	O4'-C4'-C3'	-9.45	100.33	106.00
3	F	523	DA	P-O3'-C3'	9.42	131.00	119.70
3	D	510	DG	O4'-C1'-N9	-9.21	101.56	108.00
3	F	520	DC	O4'-C1'-N1	9.20	114.44	108.00
2	C	418	DC	P-O3'-C3'	9.12	130.64	119.70
2	E	423	DA	O4'-C1'-N9	9.12	114.38	108.00
2	C	426	DC	O4'-C1'-C2'	-8.90	98.78	105.90
3	F	522	DC	O4'-C1'-N1	8.84	114.19	108.00
2	C	409	DG	O4'-C1'-N9	8.66	114.06	108.00
3	D	509	DA	O4'-C1'-N9	8.54	113.98	108.00
3	F	524	DG	O4'-C1'-N9	8.44	113.91	108.00
3	D	505	DT	C4-C5-C7	8.40	124.04	119.00
2	E	415	DT	P-O3'-C3'	8.39	129.77	119.70
3	F	517	DC	O4'-C1'-N1	8.37	113.86	108.00
3	F	516	DC	O4'-C1'-N1	8.35	113.84	108.00
2	C	422	DT	C6-C5-C7	-8.34	117.90	122.90
2	C	410	DA	O4'-C4'-C3'	-8.23	101.06	106.00
2	E	405	DT	O4'-C4'-C3'	-7.95	101.23	106.00
3	D	504	DT	C1'-O4'-C4'	-7.93	102.17	110.10
3	F	518	DT	C6-C5-C7	-7.92	118.15	122.90
3	F	525	DC	O4'-C1'-N1	7.91	113.54	108.00
2	E	404	DC	P-O3'-C3'	7.84	129.10	119.70
2	C	422	DT	C4-C5-C7	7.76	123.66	119.00
2	C	425	DG	N3-C4-C5	-7.64	124.78	128.60
2	E	419	DT	O4'-C1'-N1	7.64	113.35	108.00
3	D	505	DT	C6-C5-C7	-7.63	118.32	122.90
2	C	415	DT	O4'-C1'-N1	-7.63	102.66	108.00
2	E	417	DT	O4'-C1'-N1	7.60	113.32	108.00
2	C	406	DG	O4'-C1'-N9	-7.53	102.73	108.00
2	E	403	DG	O4'-C1'-N9	-7.51	102.75	108.00
3	F	519	DC	C1'-O4'-C4'	-7.50	102.60	110.10
3	D	509	DA	C1'-O4'-C4'	-7.49	102.61	110.10
3	F	527	DC	P-O3'-C3'	7.47	128.67	119.70
2	E	415	DT	O4'-C1'-N1	-7.47	102.77	108.00
3	F	528	DT	O4'-C1'-N1	7.41	113.19	108.00
3	F	518	DT	C4-C5-C7	7.27	123.36	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	509	DA	O4'-C1'-C2'	-7.25	100.10	105.90
3	F	501	DC	O4'-C1'-N1	-7.20	102.96	108.00
2	C	427	DG	P-O3'-C3'	7.09	128.21	119.70
2	E	404	DC	O4'-C1'-N1	6.96	112.87	108.00
3	F	521	DT	P-O3'-C3'	6.94	128.03	119.70
3	D	518	DT	N3-C4-O4	6.87	124.02	119.90
2	E	409	DG	C1'-O4'-C4'	-6.86	103.24	110.10
3	F	524	DG	C1'-O4'-C4'	-6.85	103.25	110.10
3	F	507	DA	O4'-C1'-N9	-6.77	103.26	108.00
3	D	506	DA	O4'-C1'-C2'	-6.55	100.66	105.90
3	F	508	DC	C1'-O4'-C4'	-6.53	103.57	110.10
3	F	513	DA	P-O3'-C3'	6.53	127.53	119.70
3	D	503	DC	P-O3'-C3'	6.48	127.47	119.70
2	E	401	DG	N1-C6-O6	6.46	123.78	119.90
2	E	403	DG	N3-C4-N9	6.43	129.86	126.00
3	D	507	DA	O4'-C1'-N9	-6.39	103.52	108.00
3	F	524	DG	O4'-C1'-C2'	-6.29	100.87	105.90
2	E	409	DG	C3'-C2'-C1'	-6.26	94.99	102.50
3	F	525	DC	O4'-C1'-C2'	-6.26	100.89	105.90
3	F	508	DC	O4'-C4'-C3'	-6.24	102.00	104.50
3	D	517	DC	C1'-O4'-C4'	-6.23	103.87	110.10
3	D	511	DA	O4'-C1'-N9	6.23	112.36	108.00
3	F	526	DG	C5-C6-O6	-6.21	124.87	128.60
2	C	420	DG	C8-N9-C4	-6.15	103.94	106.40
3	D	517	DC	C6-N1-C2	6.15	122.76	120.30
3	F	501	DC	N1-C2-O2	6.13	122.58	118.90
3	D	523	DA	C4'-C3'-C2'	6.11	108.60	103.10
3	F	523	DA	O4'-C1'-C2'	-6.08	101.04	105.90
2	E	410	DA	C1'-O4'-C4'	-6.06	104.04	110.10
3	F	525	DC	N1-C2-O2	6.06	122.53	118.90
2	C	414	DT	C3'-C2'-C1'	-6.04	95.25	102.50
2	E	416	DC	P-O3'-C3'	6.01	126.91	119.70
2	E	415	DT	N3-C4-O4	5.99	123.49	119.90
2	E	412	DG	N9-C1'-C2'	5.98	123.97	112.60
3	D	516	DC	O4'-C1'-C2'	-5.93	101.16	105.90
2	E	406	DG	O4'-C1'-N9	-5.87	103.89	108.00
2	C	408	DG	C1'-O4'-C4'	-5.85	104.25	110.10
2	E	410	DA	P-O3'-C3'	5.83	126.70	119.70
3	F	523	DA	O4'-C4'-C3'	-5.80	102.18	104.50
2	E	425	DG	C1'-O4'-C4'	-5.79	104.31	110.10
2	E	423	DA	P-O3'-C3'	5.72	126.56	119.70
2	C	413	DT	N1-C2-N3	5.70	118.02	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	ASP	CB-CG-OD2	5.68	123.41	118.30
2	E	422	DT	C3'-C2'-C1'	-5.67	95.69	102.50
3	D	523	DA	O4'-C1'-N9	5.66	111.97	108.00
3	D	520	DC	O4'-C1'-N1	5.61	111.93	108.00
3	F	524	DG	C3'-C2'-C1'	-5.60	95.78	102.50
3	D	508	DC	N1-C2-O2	-5.57	115.56	118.90
2	E	412	DG	O4'-C1'-C2'	-5.57	101.45	105.90
2	E	407	DA	O4'-C1'-N9	-5.57	104.11	108.00
2	C	414	DT	O4'-C1'-N1	-5.56	104.11	108.00
3	D	505	DT	O4'-C1'-C2'	-5.53	101.47	105.90
2	C	425	DG	N3-C4-N9	5.51	129.31	126.00
2	E	401	DG	C5-C6-O6	-5.51	125.30	128.60
2	E	410	DA	O4'-C1'-N9	5.50	111.85	108.00
2	C	416	DC	N1-C1'-C2'	5.49	123.03	112.60
3	F	528	DT	C6-N1-C2	-5.47	118.56	121.30
2	E	405	DT	O4'-C1'-N1	5.46	111.82	108.00
3	D	524	DG	C3'-C2'-C1'	-5.46	95.95	102.50
3	D	512	DG	C3'-C2'-C1'	-5.46	95.95	102.50
2	E	418	DC	P-O3'-C3'	5.44	126.23	119.70
2	E	425	DG	O4'-C1'-C2'	-5.43	101.56	105.90
2	C	405	DT	C4-C5-C7	-5.42	115.75	119.00
3	F	523	DA	C1'-O4'-C4'	-5.42	104.69	110.10
3	D	523	DA	P-O3'-C3'	5.39	126.17	119.70
3	F	502	DG	O4'-C1'-N9	5.39	111.78	108.00
2	C	416	DC	O4'-C1'-C2'	-5.35	101.62	105.90
3	D	517	DC	N3-C4-C5	5.34	124.03	121.90
2	E	402	DC	P-O3'-C3'	5.33	126.10	119.70
3	F	526	DG	N3-C4-N9	5.33	129.20	126.00
2	E	414	DT	C4-C5-C7	5.30	122.18	119.00
2	C	411	DG	C6-C5-N7	-5.30	127.22	130.40
3	F	515	DA	P-O3'-C3'	5.30	126.06	119.70
2	C	421	DT	O4'-C1'-N1	-5.28	104.30	108.00
2	E	408	DG	P-O3'-C3'	5.27	126.03	119.70
3	D	518	DT	P-O3'-C3'	-5.25	113.40	119.70
2	C	428	DA	O4'-C1'-N9	5.25	111.67	108.00
3	F	501	DC	N1-C1'-C2'	5.25	122.56	112.60
2	E	403	DG	N3-C2-N2	5.24	123.57	119.90
2	C	409	DG	C8-N9-C4	-5.23	104.31	106.40
2	E	425	DG	N9-C1'-C2'	5.22	122.51	112.60
2	C	425	DG	C8-N9-C4	-5.20	104.32	106.40
3	D	521	DT	O4'-C4'-C3'	-5.20	102.42	104.50
3	D	523	DA	N1-C2-N3	-5.18	126.71	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	512	DG	C1'-O4'-C4'	-5.18	104.92	110.10
3	F	519	DC	N3-C4-C5	5.18	123.97	121.90
3	D	511	DA	C3'-C2'-C1'	-5.17	96.29	102.50
3	D	515	DA	O4'-C4'-C3'	5.17	109.10	106.00
3	D	501	DC	C4'-C3'-C2'	-5.15	98.47	103.10
2	E	411	DG	P-O3'-C3'	5.14	125.87	119.70
2	E	412	DG	N1-C6-O6	-5.14	116.81	119.90
3	D	527	DC	O4'-C1'-C2'	5.11	109.99	105.90
1	B	158	LEU	CA-CB-CG	5.10	127.03	115.30
3	D	517	DC	P-O3'-C3'	5.09	125.81	119.70
2	C	410	DA	O4'-C1'-N9	-5.08	104.44	108.00
3	F	517	DC	P-O5'-C5'	-5.08	112.77	120.90
3	D	525	DC	N3-C4-C5	5.06	123.92	121.90
2	E	421	DT	N3-C4-O4	5.06	122.93	119.90
3	F	516	DC	P-O3'-C3'	5.04	125.75	119.70
2	E	417	DT	N3-C4-O4	5.04	122.92	119.90
2	E	417	DT	C5-C4-O4	-5.02	121.38	124.90
2	C	422	DT	OP2-P-O3'	5.01	116.23	105.20
2	C	412	DG	O4'-C1'-C2'	-5.01	101.89	105.90
3	F	503	DC	O4'-C1'-N1	5.00	111.50	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2099	0	2161	96	0
1	B	2091	0	2148	145	0
2	C	577	0	318	20	0
2	E	577	0	318	35	0
3	D	565	0	315	18	0
3	F	565	0	315	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	E	2	0	0	0	0
5	A	7	0	10	0	0
5	B	7	0	10	4	0
5	E	7	0	10	0	0
5	F	7	0	10	0	0
6	B	5	0	0	0	0
7	B	1	0	0	0	0
8	A	43	0	0	5	0
8	B	44	0	0	11	0
8	C	26	0	0	1	0
8	D	9	0	0	1	0
8	E	26	0	0	5	0
8	F	26	0	0	6	0
All	All	6688	0	5615	314	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 26.

All (314) 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:D:526:DG:H4'	3:D:527:DC:OP1	1.37	1.15
1:B:80:LYS:HD2	5:B:302:PEG:H22	1.14	1.09
1:A:97:GLN:HA	1:A:97:GLN:HE21	1.15	1.05
1:B:36:ILE:CG2	1:B:38:LEU:HG	1.89	1.02
1:B:17:GLY:O	1:B:150:GLU:OE2	1.80	1.00
1:B:80:LYS:CD	5:B:302:PEG:H22	1.92	0.98
1:B:80:LYS:HD2	5:B:302:PEG:C2	1.93	0.97
1:B:36:ILE:HG22	1:B:38:LEU:HG	1.46	0.95
3:D:508:DC:OP2	8:D:604:HOH:O	1.83	0.95
1:A:97:GLN:HA	1:A:97:GLN:NE2	1.84	0.91
1:B:98:TYR:HB3	1:B:120:TYR:OH	1.72	0.89
1:B:26:LYS:NZ	2:E:406:DG:O6	2.04	0.89
1:B:76:LYS:CB	8:E:626:HOH:O	2.22	0.88
1:B:174:LYS:NZ	1:B:198:THR:O	2.08	0.87
1:B:57:LYS:HE3	2:E:407:DA:OP1	1.75	0.86
1:A:45:LEU:HD22	1:A:227:GLY:HA3	1.60	0.84
2:E:406:DG:H2"	2:E:407:DA:O5'	1.79	0.83
1:B:122:ARG:HG2	8:B:422:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:HG3	3:F:520:DC:C5	2.14	0.82
1:B:30:LEU:CD1	1:B:111:ILE:HG22	2.09	0.82
1:B:78:HIS:CE1	8:B:401:HOH:O	2.30	0.81
1:B:78:HIS:HE1	8:B:401:HOH:O	1.63	0.80
2:E:415:DT:H2"	2:E:416:DC:O4'	1.83	0.79
1:B:76:LYS:HB3	8:E:626:HOH:O	1.79	0.79
1:A:74:ARG:NH2	2:C:408:DG:N7	2.29	0.79
3:F:506:DA:H2"	8:F:706:HOH:O	1.81	0.78
1:B:36:ILE:HG21	1:B:38:LEU:HG	1.64	0.78
1:B:30:LEU:HD21	1:B:114:SER:HA	1.64	0.78
3:D:522:DC:H2"	3:D:523:DA:C8	2.18	0.77
1:B:225:LEU:O	1:B:230:LYS:HB2	1.85	0.77
1:A:40:ILE:O	1:A:43:VAL:HG22	1.84	0.77
3:F:525:DC:H2"	3:F:526:DG:C8	2.20	0.76
3:D:515:DA:H2"	3:D:516:DC:O5'	1.84	0.75
1:B:19:GLY:O	1:B:96:LYS:NZ	2.19	0.75
1:B:26:LYS:HD2	3:F:521:DT:O4	1.88	0.74
2:E:423:DA:H2"	2:E:424:DA:O5'	1.86	0.74
1:B:170:ASP:HB2	8:B:415:HOH:O	1.86	0.73
1:B:76:LYS:HB2	8:E:626:HOH:O	1.87	0.73
2:E:411:DG:H2"	2:E:412:DG:OP2	1.89	0.72
1:A:2:SER:HA	1:A:5:ASP:HB2	1.71	0.72
1:A:239:GLN:HA	1:A:239:GLN:OE1	1.88	0.72
2:E:401:DG:H2"	2:E:402:DC:O5'	1.90	0.72
1:A:234:LYS:HE3	1:A:256:TYR:HB3	1.71	0.71
3:D:517:DC:H2"	3:D:518:DT:O5'	1.89	0.71
2:C:420:DG:H2"	2:C:421:DT:H5'	1.72	0.71
1:A:251:GLN:NE2	2:E:414:DT:OP1	2.23	0.71
1:B:210:SER:O	1:B:214:VAL:HG23	1.91	0.70
1:B:15:PHE:CZ	1:B:34:LEU:HD12	2.29	0.68
1:A:99:ASP:OD2	1:A:122:ARG:NH2	2.18	0.67
1:A:65:GLU:OE2	1:A:65:GLU:HA	1.93	0.67
3:D:526:DG:C4'	3:D:527:DC:OP1	2.27	0.65
1:B:40:ILE:O	1:B:43:VAL:HG23	1.95	0.65
1:B:96:LYS:HB2	8:B:406:HOH:O	1.95	0.65
2:E:401:DG:H2"	2:E:402:DC:C6	2.32	0.65
1:B:38:LEU:HD12	1:B:46:ILE:CD1	2.25	0.65
2:E:428:DA:N7	8:E:614:HOH:O	2.29	0.65
1:A:150:GLU:OE1	2:C:416:DC:OP1	2.15	0.64
2:E:401:DG:H2'	2:E:402:DC:C5	2.33	0.64
1:B:15:PHE:CE2	1:B:34:LEU:HD12	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD12	1:A:118:PRO:HD2	1.80	0.63
1:B:202:ARG:HG2	2:E:417:DT:H73	1.80	0.63
1:A:192:LYS:HD2	3:D:507:DA:H3'	1.79	0.63
1:B:80:LYS:CD	5:B:302:PEG:C2	2.64	0.63
2:E:403:DG:H1	3:F:525:DC:H42	1.46	0.63
1:B:15:PHE:CE2	1:B:34:LEU:CD1	2.82	0.63
2:C:420:DG:C2'	2:C:421:DT:H5'	2.29	0.62
1:A:120:TYR:HA	8:A:434:HOH:O	1.99	0.62
1:B:35:GLY:HA3	1:B:71:LEU:O	2.00	0.62
1:B:164:TYR:HH	3:F:504:DT:H6	1.47	0.62
1:A:175:ASP:OD1	1:A:199:ASN:ND2	2.27	0.61
1:B:29:TYR:HB3	8:E:602:HOH:O	1.99	0.61
1:B:84:LEU:O	1:B:88:ASP:HB2	2.00	0.61
2:E:403:DG:H2"	2:E:404:DC:OP2	2.00	0.61
2:C:423:DA:H2"	2:C:424:DA:OP2	1.98	0.61
1:A:16:GLU:OE1	1:A:94:SER:N	2.32	0.61
3:F:507:DA:O3'	8:F:707:HOH:O	2.16	0.61
1:B:11:LEU:HD22	1:B:49:ILE:HG23	1.84	0.60
2:E:401:DG:C2'	2:E:402:DC:C5	2.84	0.60
1:A:174:LYS:O	1:A:175:ASP:C	2.40	0.60
1:B:15:PHE:CZ	1:B:34:LEU:CD1	2.85	0.60
1:B:82:PHE:HE2	8:B:442:HOH:O	1.83	0.60
1:B:13:GLY:HA2	1:B:142:TRP:NE1	2.17	0.59
1:B:147:ILE:O	1:B:229:LYS:HE3	2.02	0.59
1:A:173:GLN:HA	1:A:173:GLN:HE21	1.68	0.59
1:A:4:MET:HG3	1:A:89:LYS:HD3	1.84	0.59
1:B:158:LEU:HD13	1:B:166:ILE:HD11	1.85	0.59
3:F:511:DA:H2"	3:F:512:DG:C8	2.38	0.58
1:B:24:THR:OG1	3:F:519:DC:OP2	2.22	0.58
1:B:36:ILE:O	1:B:70:SER:HA	2.02	0.58
1:B:95:ASN:C	1:B:97:GLN:H	2.07	0.57
1:B:61:ARG:N	1:B:68:MET:O	2.36	0.57
1:B:83:ILE:HG22	1:B:84:LEU:N	2.18	0.57
1:B:219:GLN:OE1	1:B:219:GLN:HA	2.03	0.57
2:E:423:DA:C2	2:E:424:DA:C2	2.92	0.57
3:F:525:DC:H2"	3:F:526:DG:N7	2.20	0.57
1:A:45:LEU:HD22	1:A:227:GLY:CA	2.34	0.56
1:A:134:ILE:HD12	1:A:134:ILE:H	1.69	0.56
1:B:56:GLY:HA3	1:B:71:LEU:CD1	2.36	0.56
1:B:215:VAL:O	1:B:219:GLN:HG2	2.06	0.56
1:A:164:TYR:CZ	1:A:245:ARG:NH2	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD11	1:B:111:ILE:HG22	1.87	0.56
1:B:93:LEU:HD13	1:B:133:ILE:HG23	1.87	0.56
1:B:158:LEU:HD23	1:B:159:ASN:HD22	1.71	0.56
1:B:26:LYS:CE	2:E:406:DG:O6	2.54	0.56
1:B:84:LEU:HD11	1:B:107:LEU:HD23	1.85	0.56
2:E:424:DA:H2"	2:E:425:DG:H8	1.70	0.56
1:B:8:TYR:HA	1:B:11:LEU:HD12	1.88	0.56
2:C:402:DC:H1'	2:C:403:DG:H5'	1.87	0.55
1:B:14:LEU:HA	1:B:145:GLY:O	2.06	0.55
1:B:80:LYS:NZ	1:B:108:LEU:HA	2.22	0.55
1:B:176:GLY:O	1:B:180:ILE:HB	2.04	0.55
3:D:523:DA:H2"	3:D:524:DG:O5'	2.06	0.55
1:A:2:SER:HB2	2:E:422:DT:H4'	1.89	0.55
1:A:165:LEU:HB2	1:A:243:ILE:HG12	1.89	0.55
1:A:240:LEU:HB3	1:A:252:LEU:HD21	1.87	0.55
1:B:75:ASP:O	1:B:76:LYS:C	2.45	0.55
1:B:245:ARG:HD3	8:F:711:HOH:O	2.07	0.55
1:A:45:LEU:CB	8:A:404:HOH:O	2.55	0.54
1:B:34:LEU:HD21	1:B:83:ILE:HG12	1.88	0.54
1:A:60:PHE:CD2	1:A:69:VAL:CG1	2.90	0.54
1:A:42:ASP:OD1	1:A:228:ASN:HB2	2.07	0.54
2:E:406:DG:H2"	2:E:407:DA:C5'	2.38	0.54
1:B:57:LYS:HE2	8:B:420:HOH:O	2.06	0.54
1:A:143:LEU:O	1:A:147:ILE:HG13	2.08	0.53
1:B:5:ASP:HB3	1:B:8:TYR:CD2	2.43	0.53
1:B:30:LEU:HD12	1:B:111:ILE:HG22	1.89	0.53
1:B:184:HIS:HB2	1:B:203:LEU:HD12	1.89	0.53
1:B:110:ASN:O	1:B:112:ILE:HG23	2.08	0.53
1:B:25:LYS:NZ	8:B:421:HOH:O	2.41	0.53
1:A:136:THR:HB	1:A:139:PHE:HB2	1.90	0.53
1:A:208:VAL:HG23	3:D:505:DT:OP1	2.09	0.53
3:F:521:DT:C2'	3:F:522:DC:C6	2.91	0.53
1:B:38:LEU:HD12	1:B:46:ILE:HG12	1.89	0.53
3:D:504:DT:H2"	3:D:505:DT:O5'	2.08	0.53
3:D:522:DC:C2'	3:D:523:DA:C8	2.91	0.53
1:A:16:GLU:HG3	1:A:96:LYS:HD3	1.91	0.53
1:A:132:SER:O	1:A:136:THR:OG1	2.25	0.53
1:B:89:LYS:O	1:B:91:PRO:HD3	2.09	0.53
1:B:95:ASN:C	1:B:97:GLN:N	2.63	0.53
1:A:158:LEU:HD21	2:C:422:DT:H72	1.91	0.52
1:B:97:GLN:OE1	1:B:100:TYR:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:504:DT:C2'	3:F:505:DT:H71	2.40	0.52
3:F:521:DT:H2'	3:F:522:DC:C6	2.44	0.52
1:A:29:TYR:OH	2:C:403:DG:H2"	2.09	0.52
1:B:39:SER:OG	3:F:514:DA:H3'	2.10	0.52
1:A:96:LYS:O	1:A:99:ASP:N	2.43	0.52
2:C:405:DT:H2'	2:C:406:DG:C8	2.45	0.52
1:B:38:LEU:HD12	1:B:46:ILE:HD11	1.90	0.52
2:E:401:DG:H2"	2:E:402:DC:C5	2.45	0.52
2:E:408:DG:H2'	2:E:409:DG:H8	1.75	0.52
1:B:44:GLN:HA	1:B:44:GLN:OE1	2.09	0.51
1:A:60:PHE:CD2	1:A:69:VAL:HG12	2.45	0.51
1:B:61:ARG:NH1	2:E:410:DA:C5	2.78	0.51
1:A:158:LEU:HD21	2:C:422:DT:C7	2.40	0.51
1:A:45:LEU:HB3	8:A:404:HOH:O	2.10	0.51
1:B:136:THR:O	1:B:139:PHE:HB3	2.11	0.51
1:B:34:LEU:CD2	1:B:83:ILE:HG21	2.40	0.51
1:A:76:LYS:O	1:A:80:LYS:HG3	2.11	0.51
1:B:196:ASP:C	1:B:196:ASP:OD1	2.49	0.51
1:A:15:PHE:O	1:A:19:GLY:N	2.43	0.50
1:B:163:ASP:O	1:B:165:LEU:HD23	2.10	0.50
1:A:15:PHE:CE2	1:A:36:ILE:HB	2.46	0.50
1:B:85:PRO:HA	1:B:88:ASP:CB	2.41	0.50
1:A:2:SER:C	2:E:422:DT:H5"	2.31	0.50
1:A:158:LEU:CD2	2:C:422:DT:H73	2.41	0.50
1:A:250:ILE:HB	1:A:252:LEU:HD13	1.94	0.50
1:B:93:LEU:HD22	1:B:133:ILE:HG12	1.94	0.50
1:B:26:LYS:HG3	3:F:520:DC:H5	1.75	0.50
1:B:104:LYS:O	1:B:108:LEU:HD12	2.12	0.49
3:F:512:DG:N2	3:F:513:DA:C2	2.80	0.49
1:B:40:ILE:C	1:B:42:ASP:H	2.16	0.49
1:A:7:THR:O	1:A:10:TYR:HB3	2.13	0.49
1:A:74:ARG:HD3	8:C:503:HOH:O	2.12	0.49
1:A:157:LYS:HD2	1:A:162:ASP:O	2.12	0.49
1:B:83:ILE:CG2	1:B:84:LEU:N	2.75	0.49
1:B:96:LYS:O	1:B:99:ASP:HB2	2.12	0.49
1:B:158:LEU:CD1	1:B:166:ILE:HD11	2.43	0.49
3:F:508:DC:P	8:F:707:HOH:O	2.70	0.49
1:B:33:GLU:O	1:B:103:PHE:CE1	2.66	0.49
1:A:10:TYR:CE2	1:A:226:LEU:HD12	2.48	0.48
2:E:425:DG:H2'	2:E:426:DC:C6	2.49	0.48
1:A:173:GLN:HA	1:A:173:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TYR:CE1	3:F:517:DC:H5	2.31	0.48
1:B:212:LYS:NZ	1:B:249:LYS:O	2.40	0.48
1:A:4:MET:CG	1:A:89:LYS:HD3	2.44	0.48
1:B:95:ASN:O	1:B:97:GLN:N	2.47	0.48
1:A:61:ARG:NH1	2:C:411:DG:N7	2.59	0.47
2:E:406:DG:C2'	2:E:407:DA:O5'	2.56	0.47
1:B:8:TYR:HB3	1:B:86:ILE:HG21	1.96	0.47
1:B:38:LEU:HD12	1:B:46:ILE:CG1	2.45	0.47
1:B:40:ILE:O	1:B:42:ASP:N	2.47	0.47
1:B:61:ARG:O	1:B:67:GLU:HA	2.15	0.47
1:B:121:ALA:O	1:B:122:ARG:C	2.53	0.47
1:B:203:LEU:O	8:B:415:HOH:O	2.20	0.47
1:A:2:SER:O	1:A:3:HIS:HB3	2.15	0.47
1:A:55:VAL:HB	8:A:417:HOH:O	2.15	0.47
1:A:120:TYR:CG	1:A:121:ALA:N	2.82	0.47
1:B:194:TYR:CE2	1:B:202:ARG:NH1	2.83	0.47
1:A:136:THR:O	1:A:139:PHE:N	2.43	0.47
1:A:46:ILE:HG23	1:A:71:LEU:HB2	1.96	0.46
1:B:15:PHE:HZ	1:B:34:LEU:HD12	1.79	0.46
1:B:202:ARG:NE	8:B:414:HOH:O	2.47	0.46
1:B:97:GLN:O	1:B:100:TYR:N	2.49	0.46
1:A:134:ILE:HD12	1:A:134:ILE:N	2.30	0.46
1:B:10:TYR:C	1:B:10:TYR:CD2	2.89	0.46
1:B:191:THR:HG22	8:F:708:HOH:O	2.16	0.46
1:B:195:LEU:HD11	1:B:199:ASN:OD1	2.16	0.46
1:A:96:LYS:O	1:A:97:GLN:C	2.54	0.46
2:C:416:DC:H2"	2:C:417:DT:O4'	2.16	0.46
2:E:403:DG:C5	2:E:404:DC:C4	3.04	0.46
3:D:507:DA:H2"	3:D:508:DC:O5'	2.15	0.46
1:A:75:ASP:OD1	1:A:78:HIS:N	2.48	0.45
1:B:8:TYR:O	1:B:12:VAL:HG13	2.16	0.45
1:B:15:PHE:CE2	1:B:34:LEU:HD11	2.52	0.45
3:D:514:DA:C2	3:D:515:DA:C4	3.04	0.45
1:B:40:ILE:C	1:B:42:ASP:N	2.69	0.45
2:C:416:DC:N4	3:D:511:DA:N6	2.65	0.45
2:E:424:DA:H2"	2:E:425:DG:C8	2.51	0.45
2:E:402:DC:H1'	2:E:403:DG:C8	2.51	0.45
1:A:2:SER:HA	1:A:5:ASP:CB	2.44	0.45
1:A:92:MET:O	1:A:93:LEU:HD23	2.15	0.45
1:B:56:GLY:O	1:B:57:LYS:HG2	2.16	0.45
1:B:136:THR:O	1:B:139:PHE:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:DG:H2'	2:C:421:DT:C6	2.51	0.45
1:B:117:LEU:HA	1:B:118:PRO:HD2	1.45	0.45
1:A:97:GLN:HE21	1:A:97:GLN:CA	1.94	0.45
1:B:20:TYR:HE1	3:F:517:DC:H5	1.65	0.45
3:F:501:DC:H2"	3:F:502:DG:C8	2.52	0.45
3:F:517:DC:H2"	3:F:518:DT:H6	1.82	0.45
1:A:26:LYS:HD3	1:A:31:THR:OG1	2.17	0.44
1:B:36:ILE:HG21	1:B:38:LEU:CG	2.42	0.44
1:B:189:PHE:CG	1:B:205:VAL:HG11	2.52	0.44
1:A:192:LYS:NZ	3:D:507:DA:H5"	2.32	0.44
1:B:102:ARG:HA	1:B:102:ARG:HD3	1.68	0.44
1:A:227:GLY:C	1:A:229:LYS:N	2.71	0.44
1:B:85:PRO:HA	1:B:88:ASP:HB3	1.99	0.44
1:A:203:LEU:HD23	1:A:204:LYS:N	2.32	0.44
2:C:404:DC:H2"	2:C:405:DT:O5'	2.18	0.44
1:B:9:ALA:HA	1:B:12:VAL:HG22	1.99	0.44
1:A:2:SER:O	1:A:3:HIS:CB	2.66	0.44
1:A:237:ILE:O	1:A:238:LYS:C	2.56	0.44
1:A:134:ILE:HG23	1:A:186:TYR:HD1	1.83	0.44
1:A:147:ILE:HG23	1:A:151:GLY:HA3	1.99	0.44
3:D:501:DC:H1'	3:D:502:DG:H5'	2.00	0.43
2:E:405:DT:C2'	2:E:406:DG:H5'	2.48	0.43
1:A:62:LYS:HA	1:A:66:ILE:O	2.18	0.43
1:B:28:LYS:O	1:B:113:TYR:HA	2.18	0.43
1:B:40:ILE:HG21	1:B:67:GLU:HB2	2.01	0.43
1:B:65:GLU:C	1:B:66:ILE:HG13	2.38	0.43
1:B:143:LEU:O	1:B:147:ILE:HG13	2.19	0.43
1:B:170:ASP:HB2	1:B:203:LEU:O	2.18	0.43
1:B:20:TYR:N	1:B:20:TYR:CD2	2.86	0.43
3:F:527:DC:H1'	3:F:528:DT:H5'	2.00	0.43
3:F:504:DT:H2'	3:F:505:DT:H71	2.00	0.43
1:A:12:VAL:HB	1:A:87:PHE:CE2	2.53	0.43
1:A:14:LEU:HD13	1:A:148:GLU:HG2	2.01	0.43
1:A:23:ILE:HD11	1:A:103:PHE:HA	2.01	0.43
1:A:4:MET:HB2	1:A:90:TYR:HE1	1.84	0.43
2:E:408:DG:H2'	2:E:409:DG:C8	2.54	0.43
2:E:408:DG:C2'	2:E:409:DG:C8	3.02	0.43
1:A:33:GLU:CD	1:A:72[B]:ARG:HE	2.23	0.43
1:B:85:PRO:HA	1:B:88:ASP:HB2	2.01	0.43
3:F:521:DT:H2"	3:F:522:DC:C6	2.53	0.43
1:A:42:ASP:O	1:A:43:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:GLY:O	1:A:55:VAL:HG13	2.19	0.42
1:A:84:LEU:N	1:A:85:PRO:CD	2.82	0.42
1:A:127:ILE:HG23	1:A:128:ASN:HB2	2.00	0.42
3:F:516:DC:H1'	3:F:517:DC:H5"	2.00	0.42
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.68	0.42
1:B:26:LYS:HB3	1:B:26:LYS:HE2	1.80	0.42
1:B:80:LYS:HZ1	1:B:108:LEU:HA	1.84	0.42
2:C:419:DT:H2'	2:C:419:DT:O5'	2.18	0.42
3:F:523:DA:H2'	8:F:717:HOH:O	2.20	0.42
1:A:203:LEU:HD23	1:A:203:LEU:C	2.40	0.42
3:D:507:DA:C2	3:D:508:DC:C2	3.08	0.42
1:B:158:LEU:CD2	1:B:159:ASN:ND2	2.83	0.42
1:B:173:GLN:O	1:B:176:GLY:N	2.45	0.42
1:B:205:VAL:HA	8:B:416:HOH:O	2.19	0.42
1:B:79:LEU:O	1:B:80:LYS:C	2.57	0.42
1:B:20:TYR:HE1	3:F:517:DC:C5	2.38	0.42
3:F:505:DT:H2"	3:F:506:DA:OP2	2.19	0.42
2:E:409:DG:H2'	2:E:409:DG:OP2	2.20	0.42
3:F:513:DA:H1'	3:F:514:DA:C8	2.55	0.42
1:A:84:LEU:HD13	1:A:104:LYS:HG3	2.01	0.42
1:B:82:PHE:O	1:B:85:PRO:HD2	2.20	0.42
1:B:7:THR:O	1:B:10:TYR:HB3	2.20	0.41
3:F:525:DC:OP2	3:F:525:DC:H6	2.02	0.41
1:B:121:ALA:O	1:B:122:ARG:O	2.38	0.41
1:B:165:LEU:HD12	1:B:243:ILE:HD11	2.02	0.41
1:B:194:TYR:HE2	1:B:202:ARG:NH1	2.18	0.41
1:A:45:LEU:HB2	8:A:404:HOH:O	2.19	0.41
1:A:239:GLN:OE1	1:A:239:GLN:CA	2.59	0.41
1:A:21:PHE:CZ	1:A:34:LEU:HD13	2.56	0.41
1:A:76:LYS:HB2	1:A:76:LYS:HE3	1.89	0.41
1:A:234:LYS:O	1:A:238:LYS:HG2	2.20	0.41
1:B:100:TYR:O	1:B:104:LYS:HB2	2.21	0.41
1:A:91:PRO:HD2	1:A:138:TYR:OH	2.20	0.41
2:C:416:DC:H2'	2:C:417:DT:C6	2.56	0.41
3:D:518:DT:H2'	3:D:519:DC:C6	2.55	0.41
2:E:408:DG:C2'	2:E:409:DG:H8	2.34	0.41
1:A:158:LEU:HG	1:A:159:ASN:HA	2.02	0.41
1:A:196:ASP:C	1:A:196:ASP:OD1	2.59	0.41
1:B:5:ASP:HB3	1:B:8:TYR:HD2	1.84	0.41
1:B:56:GLY:C	1:B:57:LYS:HG2	2.41	0.41
1:A:204:LYS:NZ	2:C:420:DG:N7	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:408:DG:H2"	2:E:409:DG:O5'	2.20	0.41
1:A:211:VAL:O	1:A:215:VAL:HG23	2.20	0.40
2:C:427:DG:C5	2:C:428:DA:C2	3.09	0.40
1:A:97:GLN:NE2	1:A:97:GLN:CA	2.59	0.40
1:B:46:ILE:HA	1:B:49:ILE:HD12	2.03	0.40
1:B:8:TYR:HB3	1:B:86:ILE:CG2	2.51	0.40
1:B:189:PHE:HD1	1:B:203:LEU:HD11	1.86	0.40
1:B:12:VAL:O	1:B:16:GLU:HB2	2.22	0.40
1:B:18:ASP:OD1	1:B:149:ALA:HB1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	254/255 (100%)	230 (91%)	20 (8%)	4 (2%)	9 40
1	B	253/255 (99%)	200 (79%)	42 (17%)	11 (4%)	2 15
All	All	507/510 (99%)	430 (85%)	62 (12%)	15 (3%)	4 24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	B	122	ARG
1	B	40	ILE
1	B	41	LYS
1	B	45	LEU
1	B	76	LYS
1	B	110	ASN
1	A	228	ASN
1	B	137	SER

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Mol	Chain	Res	Type
1	A	64	ASN
1	B	79	LEU
1	B	115	ASP
1	A	130	VAL
1	B	46	ILE
1	B	130	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/233 (100%)	216 (92%)	18 (8%)	13	42
1	B	233/233 (100%)	218 (94%)	15 (6%)	17	51
All	All	467/466 (100%)	434 (93%)	33 (7%)	15	46

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	39	SER
1	A	43	VAL
1	A	44	GLN
1	A	65	GLU
1	A	69	VAL
1	A	72[A]	ARG
1	A	72[B]	ARG
1	A	105	ASP
1	A	123	SER
1	A	168	SER
1	A	170	ASP
1	A	196	ASP
1	A	200	CYS
1	A	218	ILE
1	A	244	SER
1	A	245	ARG

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Mol	Chain	Res	Type
1	A	252	LEU
1	B	4	MET
1	B	7	THR
1	B	20	TYR
1	B	33	GLU
1	B	52	ILE
1	B	74	ARG
1	B	75	ASP
1	B	83	ILE
1	B	105	ASP
1	B	117	LEU
1	B	124	ASN
1	B	125	GLU
1	B	130	VAL
1	B	140	SER
1	B	252	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	173	GLN
1	A	213	ASN
1	B	77	ASN
1	B	135	ASN
1	B	159	ASN
1	B	213	ASN
1	B	251	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
6	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.34	0
5	PEG	B	302	-	6,6,6	0.41	0	5,5,5	0.49	0
5	PEG	F	601	-	6,6,6	0.56	0	5,5,5	0.36	0
5	PEG	A	304	-	6,6,6	0.49	0	5,5,5	0.22	0
5	PEG	E	503	-	6,6,6	0.46	0	5,5,5	0.22	0

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
5	PEG	A	304	-	-	2/4/4/4	-
5	PEG	B	302	-	-	4/4/4/4	-
5	PEG	E	503	-	-	2/4/4/4	-
5	PEG	F	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	PEG	O2-C3-C4-O4
5	A	304	PEG	O2-C3-C4-O4
5	E	503	PEG	O1-C1-C2-O2
5	B	302	PEG	C1-C2-O2-C3
5	B	302	PEG	C4-C3-O2-C2
5	E	503	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	B	302	PEG	O1-C1-C2-O2
5	A	304	PEG	C4-C3-O2-C2
5	F	601	PEG	O2-C3-C4-O4
5	F	601	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	302	PEG	4	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	255/255 (100%)	-0.14	2 (0%) 86 65	38, 50, 71, 94	0
1	B	255/255 (100%)	1.05	35 (13%) 3 1	66, 76, 88, 105	0
2	C	28/28 (100%)	0.43	0 100 100	47, 57, 90, 103	0
2	E	28/28 (100%)	1.94	10 (35%) 0 0	72, 84, 97, 100	0
3	D	28/28 (100%)	0.35	0 100 100	43, 64, 89, 103	0
3	F	28/28 (100%)	1.80	10 (35%) 0 0	78, 86, 90, 95	0
All	All	622/622 (100%)	0.58	57 (9%) 9 3	38, 70, 89, 105	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	501	DC	5.3
1	B	116	ASP	3.9
3	F	525	DC	3.9
1	B	31	THR	3.7
1	B	166	ILE	3.6
2	E	402	DC	3.5
1	B	22	SER	3.4
1	B	255	ASN	3.4
3	F	527	DC	3.3
2	E	423	DA	3.3
1	B	114	SER	3.1
1	B	4	MET	3.1
1	B	198	THR	3.1
2	E	404	DC	3.0
3	F	524	DG	3.0
3	F	528	DT	3.0
1	B	131	ASP	2.9
1	B	117	LEU	2.8
1	B	64	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	401	DG	2.8
1	B	170	ASP	2.8
1	B	163	ASP	2.7
1	B	20	TYR	2.7
2	E	405	DT	2.7
1	B	106	ALA	2.6
1	B	161	ASP	2.6
1	B	88	ASP	2.6
3	F	526	DG	2.6
1	A	2	SER	2.5
1	B	169	PHE	2.5
1	B	98	TYR	2.5
2	E	424	DA	2.5
1	B	118	PRO	2.5
1	B	175	ASP	2.5
1	B	80	LYS	2.4
1	B	102	ARG	2.4
1	A	123	SER	2.4
3	F	521	DT	2.3
3	F	502	DG	2.3
2	E	428	DA	2.3
1	B	3	HIS	2.3
1	B	52	ILE	2.3
1	B	253	PRO	2.2
2	E	420	DG	2.2
2	E	403	DG	2.2
1	B	235	LEU	2.2
3	F	507	DA	2.2
1	B	192	LYS	2.2
1	B	152	CYS	2.2
1	B	105	ASP	2.1
2	E	421	DT	2.1
3	F	518	DT	2.1
1	B	126	SER	2.1
1	B	53	LEU	2.1
1	B	179	LEU	2.1
1	B	32	TYR	2.1
1	B	168	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	F	601	7/7	0.60	0.31	99,103,113,118	0
4	CA	B	301	1/1	0.72	0.42	67,67,67,67	0
5	PEG	A	304	7/7	0.74	0.47	99,103,107,109	0
5	PEG	E	503	7/7	0.75	0.46	89,96,105,114	7
5	PEG	B	302	7/7	0.75	0.26	93,97,107,108	0
6	SO4	B	303	5/5	0.81	0.23	104,113,117,120	0
4	CA	A	302	1/1	0.83	0.20	42,42,42,42	0
7	NA	B	304	1/1	0.83	0.38	71,71,71,71	0
4	CA	A	301	1/1	0.90	0.13	42,42,42,42	0
4	CA	E	501	1/1	0.93	0.08	67,67,67,67	0
4	CA	E	502	1/1	0.93	0.14	93,93,93,93	0
4	CA	A	303	1/1	0.95	0.30	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.