



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:08 pm BST

PDB ID : 6BWY
Title : DNA substrate selection by APOBEC3G
Authors : Ziegler, S.J.; Buzovetsky, O.
Deposited on : 2017-12-15
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

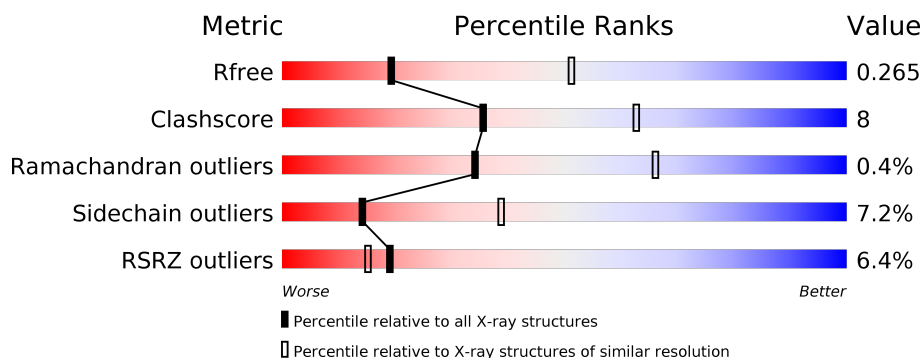
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	30	<div> <div style="width: 17%; background-color: red;"></div> <div style="width: 77%; background-color: grey;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 77%; background-color: green;"></div> </div>
1	D	30	<div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 77%; background-color: grey;"></div> <div style="width: 20%; background-color: green;"></div> </div>
1	F	30	<div> <div style="width: 17%; background-color: green;"></div> <div style="width: 77%; background-color: grey;"></div> <div style="width: 7%; background-color: yellow;"></div> </div>
1	I	30	<div> <div style="width: 7%; background-color: red;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 77%; background-color: grey;"></div> <div style="width: 7%; background-color: yellow;"></div> <div style="width: 77%; background-color: green;"></div> </div>
2	A	361	<div> <div style="width: 9%; background-color: red;"></div> <div style="width: 70%; background-color: green;"></div> <div style="width: 23%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> </div>
2	B	361	<div> <div style="width: 3%; background-color: red;"></div> <div style="width: 73%; background-color: green;"></div> <div style="width: 19%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	E	361	
2	G	361	

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
3	PO4	E	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11882 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	7	Total	C	N	O	P	0	0	0
			145	69	27	42	7			
1	C	7	Total	C	N	O	P	0	0	0
			142	69	27	40	6			
1	D	7	Total	C	N	O	P	0	0	0
			145	69	27	42	7			
1	F	7	Total	C	N	O	P	0	0	0
			145	69	27	42	7			

- Molecule 2 is a protein called Protection of telomeres protein 1, DNA dC->dU-editing enzyme APOBEC-3G fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	344	Total	C	N	O	S	0	0	0
			2781	1766	484	516	15			
2	B	346	Total	C	N	O	S	0	0	0
			2794	1773	486	520	15			
2	E	346	Total	C	N	O	S	0	0	0
			2794	1773	486	520	15			
2	G	346	Total	C	N	O	S	0	0	0
			2800	1776	489	520	15			

There are 24 discrepancies between the modelled and reference sequences:

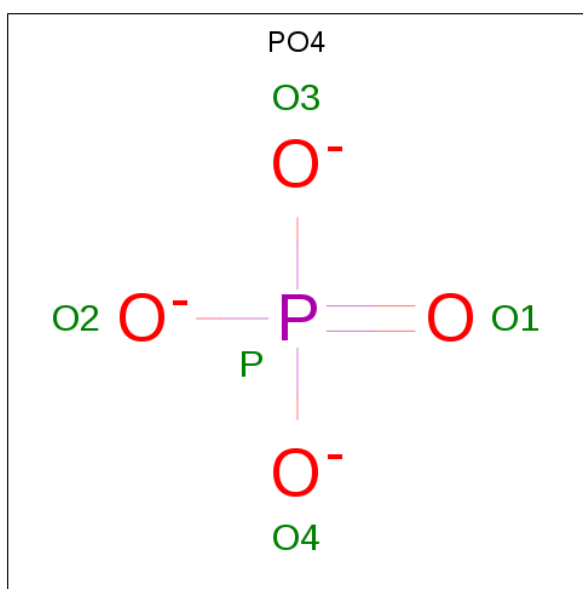
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP O13988
A	234	LYS	LEU	engineered mutation	UNP Q9HC16
A	243	ALA	CYS	engineered mutation	UNP Q9HC16
A	310	LYS	PHE	engineered mutation	UNP Q9HC16
A	321	ALA	CYS	engineered mutation	UNP Q9HC16
A	356	ALA	CYS	engineered mutation	UNP Q9HC16
B	24	MET	-	initiating methionine	UNP O13988

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Chain	Residue	Modelled	Actual	Comment	Reference
B	234	LYS	LEU	engineered mutation	UNP Q9HC16
B	243	ALA	CYS	engineered mutation	UNP Q9HC16
B	310	LYS	PHE	engineered mutation	UNP Q9HC16
B	321	ALA	CYS	engineered mutation	UNP Q9HC16
B	356	ALA	CYS	engineered mutation	UNP Q9HC16
E	24	MET	-	initiating methionine	UNP O13988
E	234	LYS	LEU	engineered mutation	UNP Q9HC16
E	243	ALA	CYS	engineered mutation	UNP Q9HC16
E	310	LYS	PHE	engineered mutation	UNP Q9HC16
E	321	ALA	CYS	engineered mutation	UNP Q9HC16
E	356	ALA	CYS	engineered mutation	UNP Q9HC16
G	24	MET	-	initiating methionine	UNP O13988
G	234	LYS	LEU	engineered mutation	UNP Q9HC16
G	243	ALA	CYS	engineered mutation	UNP Q9HC16
G	310	LYS	PHE	engineered mutation	UNP Q9HC16
G	321	ALA	CYS	engineered mutation	UNP Q9HC16
G	356	ALA	CYS	engineered mutation	UNP Q9HC16

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	O	0	0
			1	1		

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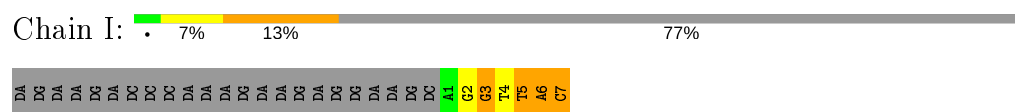
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	O 1	0	0
5	D	1	Total 1	O 1	0	0
5	A	11	Total 11	O 11	0	0
5	B	13	Total 13	O 13	0	0
5	E	14	Total 14	O 14	0	0
5	G	16	Total 16	O 16	0	0

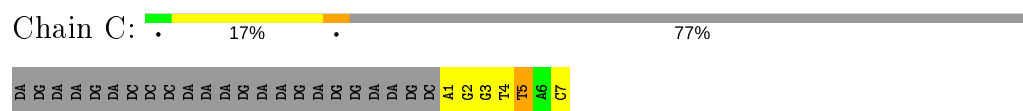
3 Residue-property plots [i](#)

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

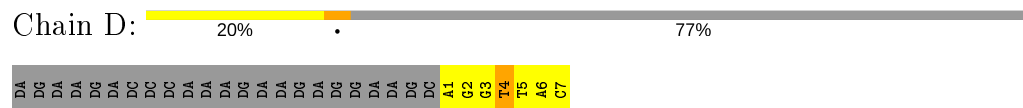
- Molecule 1: DNA (30-MER)



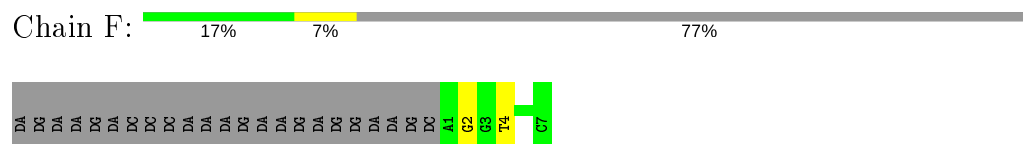
- Molecule 1: DNA (30-MER)



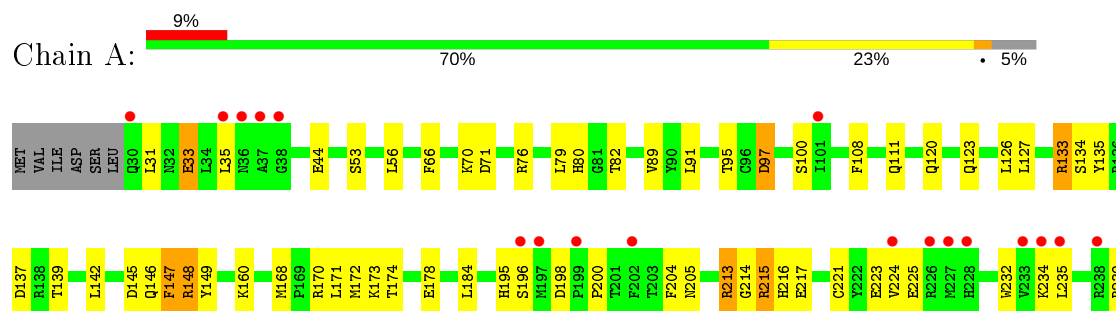
- Molecule 1: DNA (30-MER)

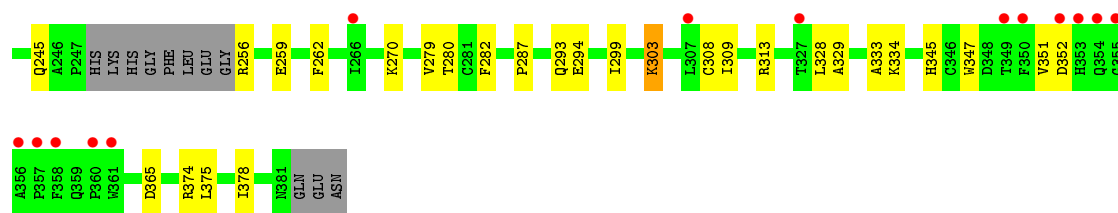


- Molecule 1: DNA (30-MER)

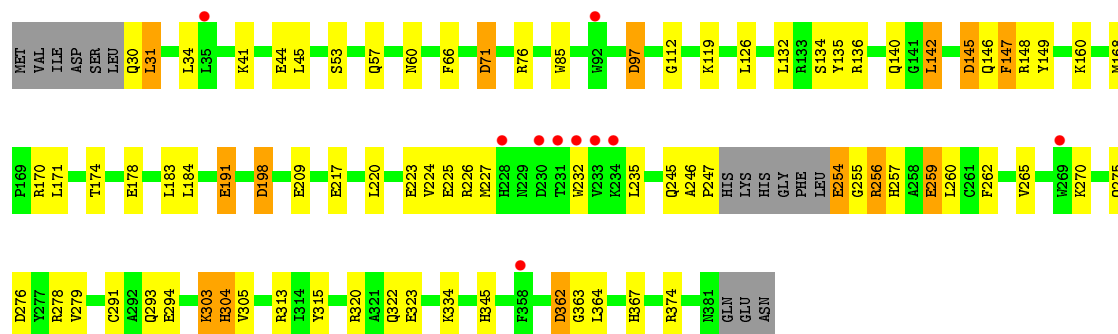
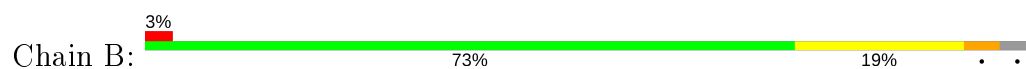


- Molecule 2: Protection of telomeres protein 1, DNA dC->dU-editing enzyme APOBEC-3G fusion

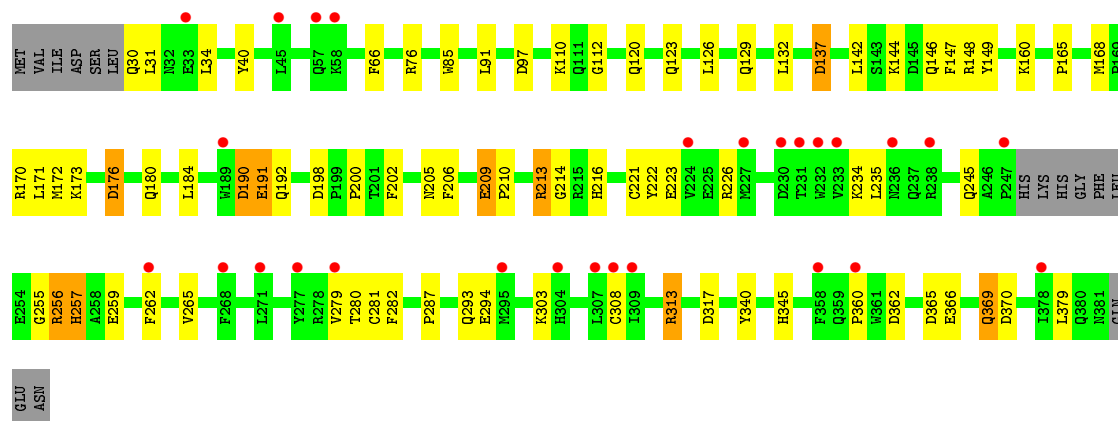
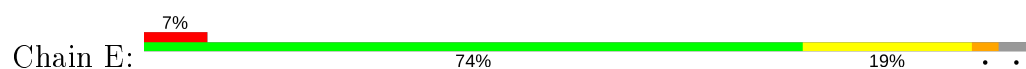




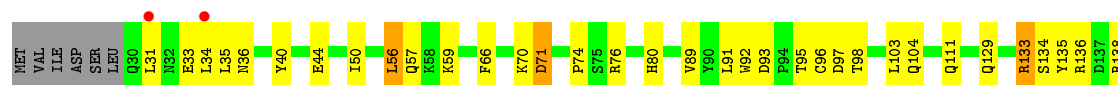
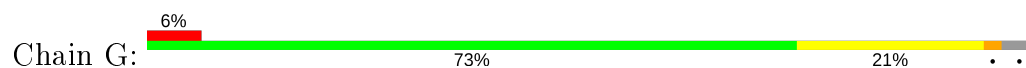
- Molecule 2: Protection of telomeres protein 1, DNA dC->dU-editing enzyme APOBEC-3G fusion

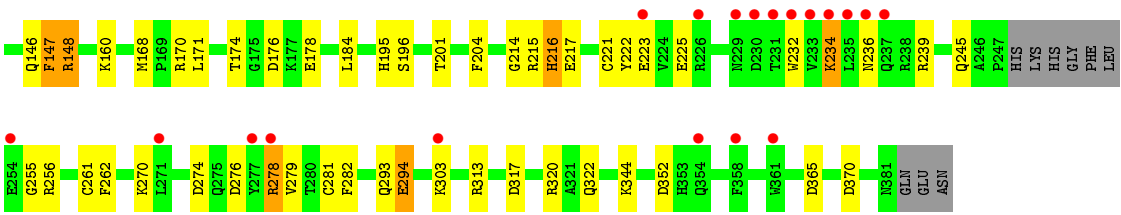


- Molecule 2: Protection of telomeres protein 1, DNA dC->dU-editing enzyme APOBEC-3G fusion



- Molecule 2: Protection of telomeres protein 1, DNA dC->dU-editing enzyme APOBEC-3G fusion





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	79.07 Å 79.07 Å 266.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.19 – 2.90 44.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (44.19-2.90) 99.3 (44.19-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.234 , 0.287 0.221 , 0.265	Depositor DCC
R_{free} test set	1786 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	72.8	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
Reported twinning fraction	0.501 for H, K, L 0.499 for -H, K, -L	Depositor
Outliers	1 of 35772 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11882	wwPDB-VP
Average B, all atoms (Å ²)	89.0	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 40.88 % 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 2.5639e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, PO4

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	0.92	0/159	1.37	4/244 (1.6%)
1	D	1.23	1/162 (0.6%)	1.67	2/248 (0.8%)
1	F	0.91	0/162	1.49	2/248 (0.8%)
1	I	1.14	1/162 (0.6%)	1.45	4/248 (1.6%)
2	A	0.95	1/2854 (0.0%)	1.00	12/3873 (0.3%)
2	B	1.05	4/2867 (0.1%)	1.05	16/3890 (0.4%)
2	E	0.96	1/2867 (0.0%)	1.00	8/3890 (0.2%)
2	G	0.99	5/2873 (0.2%)	1.03	13/3897 (0.3%)
All	All	0.99	13/12106 (0.1%)	1.05	61/16538 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	313	ARG	CZ-NH1	6.54	1.41	1.33
2	A	137	ASP	CB-CG	6.40	1.65	1.51
2	G	313	ARG	CZ-NH1	6.35	1.41	1.33
1	I	6	DA	O3'-P	-6.03	1.53	1.61
1	D	4	DT	O3'-P	-5.91	1.54	1.61
2	G	294	GLU	CD-OE1	5.86	1.32	1.25
2	B	315	TYR	CE2-CZ	-5.83	1.30	1.38
2	G	370	ASP	CB-CG	5.67	1.63	1.51
2	G	322	GLN	C-O	5.57	1.33	1.23
2	B	362	ASP	CB-CG	5.33	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	323	GLU	CG-CD	5.23	1.59	1.51
2	G	317	ASP	C-O	5.20	1.33	1.23
2	B	140	GLN	CG-CD	-5.19	1.39	1.51

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4	DT	O5'-P-OP2	-13.66	93.41	105.70
1	D	1	DA	O5'-P-OP1	13.09	126.40	110.70
2	G	133	ARG	NE-CZ-NH2	10.17	125.39	120.30
2	A	89	VAL	CG1-CB-CG2	-8.79	96.83	110.90
2	E	213	ARG	NE-CZ-NH2	-7.93	116.33	120.30
2	A	148	ARG	NE-CZ-NH2	-7.90	116.35	120.30
2	B	374	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	I	5	DT	O5'-P-OP2	-7.38	99.06	105.70
1	C	5	DT	O5'-P-OP2	-7.34	99.09	105.70
2	G	176	ASP	CB-CG-OD1	7.26	124.84	118.30
2	B	217	GLU	OE1-CD-OE2	6.83	131.49	123.30
1	F	4	DT	OP1-P-OP2	6.75	129.72	119.60
2	A	127	LEU	CB-CG-CD2	-6.72	99.57	111.00
1	D	1	DA	O5'-P-OP2	-6.72	99.65	105.70
2	E	170	ARG	NE-CZ-NH1	-6.63	116.98	120.30
2	B	119	LYS	CD-CE-NZ	6.61	126.89	111.70
1	I	5	DT	C1'-O4'-C4'	-6.57	103.53	110.10
2	G	71	ASP	CB-CG-OD2	6.51	124.16	118.30
2	B	315	TYR	CB-CG-CD1	6.43	124.86	121.00
2	E	172	MET	CG-SD-CE	-6.43	89.92	100.20
2	A	71	ASP	CB-CG-OD2	6.33	123.99	118.30
1	I	3	DG	O5'-P-OP1	-6.26	100.06	105.70
2	G	91	LEU	CB-CG-CD1	-6.20	100.45	111.00
1	C	5	DT	C1'-O4'-C4'	-6.20	103.90	110.10
2	E	190	ASP	CB-CG-OD2	-6.17	112.74	118.30
2	G	133	ARG	NH1-CZ-NH2	-6.17	112.61	119.40
2	E	91	LEU	CB-CG-CD1	-6.15	100.55	111.00
2	A	213	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	B	71	ASP	CB-CG-OD2	6.09	123.78	118.30
2	B	97	ASP	CB-CG-OD1	-6.08	112.83	118.30
2	G	276	ASP	CB-CG-OD1	5.97	123.68	118.30
2	B	315	TYR	OH-CZ-CE2	-5.88	104.22	120.10
2	B	259	GLU	OE1-CD-OE2	-5.87	116.26	123.30
2	E	137	ASP	CB-CG-OD2	5.83	123.55	118.30
2	B	313	ARG	NE-CZ-NH1	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	133	ARG	CG-CD-NE	5.79	123.96	111.80
1	C	1	DA	P-O3'-C3'	5.77	126.62	119.70
2	B	183	LEU	CB-CG-CD2	5.71	120.70	111.00
2	G	148	ARG	NE-CZ-NH2	-5.67	117.46	120.30
2	B	45	LEU	CB-CG-CD1	5.67	120.63	111.00
2	G	294	GLU	OE1-CD-OE2	5.67	130.10	123.30
2	B	220	LEU	CB-CG-CD1	-5.63	101.43	111.00
2	B	191	GLU	OE1-CD-OE2	-5.57	116.61	123.30
1	C	1	DA	C5'-C4'-C3'	5.56	124.11	114.10
2	A	133	ARG	CG-CD-NE	5.49	123.33	111.80
2	G	103	LEU	CB-CG-CD2	-5.47	101.71	111.00
2	A	215	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	A	214	GLY	N-CA-C	-5.38	99.65	113.10
2	B	315	TYR	CE1-CZ-OH	5.37	134.61	120.10
2	E	191	GLU	OE1-CD-OE2	-5.36	116.86	123.30
2	A	375	LEU	CB-CG-CD1	5.36	120.10	111.00
2	B	323	GLU	OE1-CD-OE2	-5.33	116.91	123.30
2	B	256	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	G	313	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	A	172	MET	CG-SD-CE	5.30	108.68	100.20
2	G	89	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	I	7	DC	C1'-O4'-C4'	-5.21	104.89	110.10
2	A	91	LEU	CB-CG-CD1	-5.18	102.20	111.00
2	A	145	ASP	CB-CG-OD1	5.09	122.89	118.30
2	E	317	ASP	CB-CG-OD2	5.04	122.84	118.30
2	G	278	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	56	LEU	Peptide

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	142	0	81	7	0
1	D	145	0	80	5	1
1	F	145	0	80	1	0
1	I	145	0	80	17	0
2	A	2781	0	2654	60	1
2	B	2794	0	2665	58	1
2	E	2794	0	2664	32	1
2	G	2800	0	2674	41	2
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	15	0	0	2	0
3	F	5	0	0	1	0
3	G	15	0	0	1	0
3	I	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	11	0	0	2	0
5	B	13	0	0	3	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	14	0	0	1	0
5	G	16	0	0	1	0
5	I	1	0	0	0	0
All	All	11882	0	10978	184	3

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 8.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:329:ALA:HB1	2:B:303:LYS:HG3	1.22	1.17
2:A:329:ALA:HB1	2:B:303:LYS:CG	1.80	1.08
2:A:329:ALA:O	2:B:303:LYS:HD3	1.54	1.06
2:B:320:ARG:NH2	2:G:71:ASP:OD2	2.03	0.91
5:A:502:HOH:O	2:B:278:ARG:HD3	1.76	0.85
2:G:214:GLY:O	2:G:216:HIS:CD2	2.29	0.85
2:E:129:GLN:HE22	3:E:403:PO4:P	2.04	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:PRO:HG3	2:G:201:THR:HA	1.63	0.79
2:G:171:LEU:HB2	5:G:501:HOH:O	1.84	0.78
2:G:214:GLY:O	2:G:216:HIS:HD2	1.65	0.77
2:A:329:ALA:C	2:B:303:LYS:HD3	2.04	0.76
1:I:5:DT:H4'	2:A:80:HIS:C	2.06	0.74
2:G:234:LYS:HB2	2:G:239:ARG:HH22	1.53	0.74
1:I:5:DT:H4'	2:A:80:HIS:HB2	1.72	0.71
2:B:303:LYS:O	2:B:304:HIS:ND1	2.26	0.69
2:A:329:ALA:O	2:B:303:LYS:CD	2.39	0.66
2:G:204:PHE:O	2:G:215:ARG:NH2	2.28	0.66
2:A:215:ARG:O	2:A:217:GLU:N	2.24	0.65
2:A:262:PHE:HZ	2:A:279:VAL:HG11	1.60	0.65
2:B:227:MET:O	2:B:275:GLN:NE2	2.25	0.64
2:G:262:PHE:HZ	2:G:279:VAL:HG11	1.63	0.64
2:B:291:CYS:SG	4:B:401:ZN:ZN	1.87	0.64
1:I:6:DA:OP1	2:A:79:LEU:N	2.31	0.62
1:I:5:DT:C4'	2:A:80:HIS:HB2	2.29	0.62
2:G:215:ARG:O	2:G:217:GLU:N	2.33	0.62
2:G:195:HIS:ND1	2:G:239:ARG:O	2.29	0.62
1:I:3:DG:H2'	2:A:133:ARG:NH1	2.15	0.61
2:E:262:PHE:HZ	2:E:279:VAL:HG11	1.66	0.61
2:B:364:LEU:HA	5:B:503:HOH:O	1.99	0.60
2:B:246:ALA:HB2	2:B:255:GLY:N	2.16	0.60
2:A:329:ALA:CA	2:B:303:LYS:HD3	2.31	0.60
2:G:234:LYS:HB2	2:G:239:ARG:NH2	2.17	0.59
1:I:5:DT:O3'	2:A:80:HIS:HB2	2.01	0.59
2:A:329:ALA:HB1	2:B:303:LYS:CD	2.32	0.59
2:E:245:GLN:HB2	2:E:255:GLY:O	2.03	0.59
2:B:31:LEU:HD23	2:B:34:LEU:HD12	1.84	0.58
2:B:303:LYS:HZ2	2:B:304:HIS:H	1.50	0.58
2:B:262:PHE:HZ	2:B:279:VAL:HG11	1.68	0.58
1:C:7:DC:H5'	2:B:322:GLN:OE1	2.04	0.58
1:I:5:DT:H3'	1:I:6:DA:N7	2.18	0.58
2:E:34:LEU:HD22	2:E:40:TYR:HB2	1.86	0.57
2:G:196:SER:OG	2:G:352:ASP:HB2	2.05	0.57
2:E:223:GLU:OE2	2:E:345:HIS:NE2	2.37	0.56
2:B:303:LYS:NZ	2:B:304:HIS:H	2.04	0.55
2:G:70:LYS:NZ	2:G:98:THR:O	2.38	0.55
2:A:196:SER:OG	2:A:352:ASP:HB2	2.07	0.55
2:B:226:ARG:HB2	2:B:235:LEU:HD11	1.88	0.55
2:B:60:ASN:HA	5:B:502:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:236:ASN:HA	2:G:239:ARG:HD2	1.88	0.55
1:I:7:DC:C5	2:A:135:TYR:CZ	2.94	0.55
1:I:7:DC:C6	2:A:135:TYR:CZ	2.96	0.54
2:E:365:ASP:O	2:E:369:GLN:NE2	2.39	0.54
2:A:259:GLU:HG2	2:A:287:PRO:HB3	1.89	0.53
2:G:34:LEU:HD22	2:G:40:TYR:HB2	1.89	0.53
2:G:204:PHE:O	2:G:215:ARG:NE	2.42	0.53
2:A:223:GLU:OE2	2:A:345:HIS:NE2	2.34	0.53
1:D:5:DT:H3'	1:D:6:DA:C8	2.43	0.53
2:G:147:PHE:O	2:G:170:ARG:NH1	2.41	0.52
2:A:53:SER:O	2:A:139:THR:HG21	2.10	0.52
1:I:5:DT:H5''	2:A:80:HIS:CB	2.39	0.52
1:I:5:DT:H4'	2:A:80:HIS:CB	2.37	0.52
2:B:126:LEU:O	2:B:149:TYR:HA	2.10	0.52
2:B:225:GLU:HB3	2:B:232:TRP:HB3	1.92	0.52
2:G:129:GLN:HE22	3:G:403:PO4:P	2.33	0.51
2:G:95:THR:O	2:G:270:LYS:HE2	2.11	0.51
2:G:225:GLU:HB3	2:G:232:TRP:HB3	1.91	0.51
2:A:224:VAL:O	2:A:235:LEU:HB2	2.11	0.51
2:E:120:GLN:O	2:E:123:GLN:HG3	2.11	0.51
2:G:56:LEU:HD13	2:G:134:SER:OG	2.11	0.51
2:E:202:PHE:O	2:E:206:PHE:HB2	2.10	0.50
1:C:3:DG:H2'	2:G:133:ARG:NH1	2.25	0.50
2:B:303:LYS:HZ2	2:B:304:HIS:N	2.10	0.50
2:G:135:TYR:O	2:G:138:ARG:HG2	2.11	0.50
2:B:174:THR:HB	2:B:178:GLU:HG3	1.93	0.50
2:A:232:TRP:HE1	2:B:232:TRP:HD1	1.57	0.50
2:E:256:ARG:H	2:E:256:ARG:HD3	1.76	0.50
2:A:56:LEU:HD13	2:A:134:SER:OG	2.11	0.50
1:C:5:DT:H4'	2:G:80:HIS:O	2.12	0.50
2:B:226:ARG:HG2	2:B:275:GLN:HE21	1.77	0.49
2:A:329:ALA:CB	2:B:303:LYS:CG	2.71	0.49
2:B:303:LYS:HB3	2:B:303:LYS:HZ2	1.78	0.49
2:E:226:ARG:HB2	2:E:235:LEU:HD11	1.94	0.49
2:B:304:HIS:ND1	2:B:305:VAL:HG23	2.27	0.49
2:A:347:TRP:O	2:A:351:VAL:HG22	2.13	0.49
1:I:4:DT:H3	2:A:82:THR:CG2	2.25	0.49
1:D:2:DG:O6	2:B:145:ASP:OD1	2.31	0.49
2:B:191:GLU:OE1	2:B:265:VAL:HG11	2.12	0.49
2:A:303:LYS:O	2:B:334:LYS:HG2	2.13	0.48
2:A:198:ASP:OD1	2:A:200:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:245:GLN:HB2	2:G:256:ARG:N	2.29	0.48
2:A:221:CYS:O	2:A:282:PHE:N	2.38	0.48
2:E:257:HIS:ND1	2:E:259:GLU:OE1	2.46	0.47
1:I:6:DA:OP1	2:A:80:HIS:N	2.45	0.47
2:A:147:PHE:O	2:A:170:ARG:NH1	2.48	0.47
2:E:126:LEU:O	2:E:149:TYR:HA	2.15	0.47
2:E:259:GLU:HG2	2:E:287:PRO:HB3	1.96	0.47
2:A:204:PHE:O	2:A:215:ARG:NE	2.36	0.47
2:A:126:LEU:O	2:A:149:TYR:HA	2.15	0.47
2:A:35:LEU:HB3	2:A:95:THR:HG23	1.96	0.47
2:B:320:ARG:HH22	2:G:71:ASP:CG	2.15	0.46
1:I:5:DT:H5"	2:A:80:HIS:HB3	1.97	0.46
2:B:303:LYS:HA	2:B:303:LYS:HD2	1.73	0.46
2:E:198:ASP:OD1	2:E:200:PRO:HD2	2.16	0.46
2:G:35:LEU:HB3	2:G:95:THR:HG23	1.97	0.46
2:A:225:GLU:HB3	2:A:232:TRP:HB3	1.97	0.46
5:A:502:HOH:O	2:B:278:ARG:CD	2.47	0.46
2:E:148:ARG:NH2	2:E:171:LEU:O	2.48	0.46
2:B:198:ASP:N	2:B:198:ASP:OD1	2.46	0.46
1:I:6:DA:N3	2:A:108:PHE:HZ	2.13	0.45
2:A:70:LYS:HD3	2:A:100:SER:O	2.16	0.45
2:B:223:GLU:OE2	2:B:345:HIS:NE2	2.42	0.45
2:E:255:GLY:HA3	2:E:256:ARG:HA	1.69	0.45
2:G:104:GLN:OE1	2:G:138:ARG:NH1	2.49	0.45
1:I:5:DT:H5"	2:A:80:HIS:HB2	1.99	0.45
2:B:209:GLU:HG3	2:B:367:HIS:CE1	2.52	0.45
2:B:246:ALA:HB2	2:B:254:GLU:C	2.38	0.45
2:B:53:SER:HB3	2:B:132:LEU:HD21	1.99	0.45
2:E:256:ARG:N	2:E:256:ARG:HD3	2.31	0.44
2:G:225:GLU:OE2	2:G:278:ARG:NH1	2.50	0.44
2:E:205:ASN:O	2:E:313:ARG:NH1	2.49	0.44
2:A:120:GLN:O	2:A:123:GLN:HG3	2.18	0.44
1:C:2:DG:H21	1:C:4:DT:H71	1.83	0.44
2:A:245:GLN:HB2	2:A:256:ARG:N	2.33	0.44
2:A:280:THR:HA	2:A:308:CYS:O	2.17	0.44
2:B:363:GLY:HA3	5:B:503:HOH:O	2.17	0.44
1:I:2:DG:H21	1:I:4:DT:H71	1.83	0.44
2:A:148:ARG:NH2	2:A:171:LEU:O	2.51	0.43
2:A:174:THR:HB	2:A:178:GLU:HG3	2.00	0.43
2:A:33:GLU:H	2:A:33:GLU:CD	2.22	0.43
2:B:256:ARG:HH21	2:B:260:LEU:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:HIS:HB3	2:B:259:GLU:OE2	2.18	0.43
2:A:374:ARG:O	2:A:378:ILE:HG13	2.18	0.43
2:B:364:LEU:O	2:B:364:LEU:HD23	2.19	0.43
1:D:2:DG:H21	1:D:4:DT:H71	1.83	0.43
2:G:256:ARG:HD3	2:G:261:CYS:SG	2.59	0.43
1:C:2:DG:N2	1:C:4:DT:H71	2.33	0.43
2:A:35:LEU:HB3	2:A:95:THR:CG2	2.49	0.43
1:D:7:DC:H2'	1:D:7:DC:H6	1.61	0.43
2:G:221:CYS:O	2:G:282:PHE:N	2.43	0.43
2:G:50:ILE:HG12	2:G:93:ASP:OD2	2.19	0.43
2:B:147:PHE:O	2:B:170:ARG:NH1	2.52	0.42
2:B:85:TRP:CG	2:B:112:GLY:HA3	2.54	0.42
2:A:232:TRP:NE1	2:B:232:TRP:HD1	2.17	0.42
2:G:255:GLY:HA2	2:G:256:ARG:HA	1.73	0.42
1:F:2:DG:H8	3:F:101:PO4:O1	2.02	0.42
2:B:364:LEU:HD23	2:B:364:LEU:C	2.40	0.42
2:E:221:CYS:O	2:E:282:PHE:N	2.38	0.42
2:G:223:GLU:HA	2:G:239:ARG:HG2	2.02	0.42
2:G:222:TYR:HA	2:G:281:CYS:HA	2.00	0.42
2:E:176:ASP:O	2:E:180:GLN:HG2	2.20	0.42
2:E:85:TRP:CG	2:E:112:GLY:HA3	2.54	0.42
2:G:33:GLU:HA	2:G:36:ASN:OD1	2.19	0.42
2:A:97:ASP:HB3	2:A:270:LYS:HD2	2.01	0.42
2:B:224:VAL:O	2:B:235:LEU:HB2	2.20	0.42
2:A:205:ASN:O	2:A:313:ARG:NH1	2.50	0.42
2:A:334:LYS:HG2	2:B:276:ASP:HB3	2.02	0.42
2:E:144:LYS:HE3	2:E:144:LYS:HB3	1.86	0.42
2:A:299:ILE:HD11	2:A:333:ALA:HB2	2.02	0.42
2:E:213:ARG:HA	2:E:214:GLY:HA2	1.82	0.42
2:G:204:PHE:CE1	2:G:215:ARG:HD2	2.55	0.42
2:A:195:HIS:NE2	2:A:239:ARG:O	2.52	0.41
1:C:5:DT:H4'	2:G:80:HIS:C	2.41	0.41
2:A:347:TRP:CD2	2:A:351:VAL:HG21	2.56	0.41
2:B:41:LYS:HE2	2:B:44:GLU:HA	2.01	0.41
2:B:246:ALA:HA	2:B:247:PRO:HD3	1.83	0.41
2:E:129:GLN:NE2	3:E:403:PO4:O1	2.53	0.41
2:G:148:ARG:NH2	2:G:171:LEU:O	2.53	0.41
2:B:303:LYS:O	2:B:305:VAL:N	2.54	0.41
2:A:333:ALA:O	2:B:303:LYS:HE2	2.21	0.41
2:E:191:GLU:OE1	2:E:265:VAL:HG11	2.21	0.41
2:E:370:ASP:CG	5:E:501:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:TRP:CD1	2:G:96:CYS:HB2	2.55	0.41
2:A:309:ILE:HD12	2:A:328:LEU:HD21	2.03	0.41
2:E:280:THR:HA	2:E:308:CYS:O	2.21	0.41
2:B:148:ARG:NH2	2:B:171:LEU:O	2.54	0.40
2:E:190:ASP:C	2:E:192:GLN:H	2.25	0.40
2:E:222:TYR:HA	2:E:281:CYS:HA	2.03	0.40
2:E:340:TYR:HE1	2:E:360:PRO:HG3	1.86	0.40
1:C:4:DT:H2''	1:C:5:DT:O5'	2.21	0.40
2:G:174:THR:HB	2:G:178:GLU:HG3	2.04	0.40
2:A:213:ARG:O	2:A:215:ARG:NH1	2.51	0.40
2:B:135:TYR:CZ	2:B:136:ARG:HD2	2.56	0.40
1:D:3:DG:C4	2:B:142:LEU:HD23	2.55	0.40
2:E:209:GLU:HA	2:E:210:PRO:HD3	2.00	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:SER:OG	2:E:137:ASP:OD2[3_844]	2.01	0.19
1:D:4:DT:OP1	2:G:136:ARG:NH1[4_575]	2.15	0.05
2:B:71:ASP:OD2	2:G:320:ARG:NH2[1_545]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	340/361 (94%)	324 (95%)	15 (4%)	1 (0%)	41 71
2	B	342/361 (95%)	322 (94%)	19 (6%)	1 (0%)	41 71
2	E	342/361 (95%)	322 (94%)	19 (6%)	1 (0%)	41 71
2	G	342/361 (95%)	321 (94%)	19 (6%)	2 (1%)	25 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1366/1444 (95%)	1289 (94%)	72 (5%)	5 (0%)	34 66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	245	GLN
2	A	216	HIS
2	G	216	HIS
2	E	216	HIS
2	G	74	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
2	A	302/327 (92%)	283 (94%)	19 (6%)	18 46
2	B	303/327 (93%)	281 (93%)	22 (7%)	14 38
2	E	303/327 (93%)	277 (91%)	26 (9%)	10 30
2	G	304/327 (93%)	284 (93%)	20 (7%)	16 44
All	All	1212/1308 (93%)	1125 (93%)	87 (7%)	14 39

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	31	LEU
2	A	33	GLU
2	A	44	GLU
2	A	66	PHE
2	A	76	ARG
2	A	97	ASP
2	A	111	GLN
2	A	142	LEU
2	A	146	GLN
2	A	147	PHE

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Mol	Chain	Res	Type
2	A	160	LYS
2	A	168	MET
2	A	173	LYS
2	A	184	LEU
2	A	234	LYS
2	A	293	GLN
2	A	294	GLU
2	A	303	LYS
2	A	365	ASP
2	B	30	GLN
2	B	31	LEU
2	B	57	GLN
2	B	66	PHE
2	B	76	ARG
2	B	97	ASP
2	B	134	SER
2	B	142	LEU
2	B	145	ASP
2	B	146	GLN
2	B	147	PHE
2	B	160	LYS
2	B	168	MET
2	B	184	LEU
2	B	198	ASP
2	B	254	GLU
2	B	270	LYS
2	B	293	GLN
2	B	294	GLU
2	B	303	LYS
2	B	304	HIS
2	B	362	ASP
2	E	30	GLN
2	E	31	LEU
2	E	66	PHE
2	E	76	ARG
2	E	97	ASP
2	E	110	LYS
2	E	132	LEU
2	E	142	LEU
2	E	146	GLN
2	E	147	PHE
2	E	160	LYS

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Mol	Chain	Res	Type
2	E	168	MET
2	E	173	LYS
2	E	176	ASP
2	E	184	LEU
2	E	209	GLU
2	E	234	LYS
2	E	256	ARG
2	E	257	HIS
2	E	293	GLN
2	E	294	GLU
2	E	303	LYS
2	E	362	ASP
2	E	366	GLU
2	E	369	GLN
2	E	379	LEU
2	G	31	LEU
2	G	44	GLU
2	G	57	GLN
2	G	59	LYS
2	G	66	PHE
2	G	76	ARG
2	G	97	ASP
2	G	111	GLN
2	G	146	GLN
2	G	147	PHE
2	G	160	LYS
2	G	168	MET
2	G	184	LEU
2	G	234	LYS
2	G	274	ASP
2	G	293	GLN
2	G	294	GLU
2	G	303	LYS
2	G	344	LYS
2	G	365	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	129	GLN
2	E	245	GLN
2	G	129	GLN

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Mol	Chain	Res	Type
2	G	216	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	$\# Z > 2$
3	PO4	E	404	-	4,4,4	0.62	0	6,6,6	0.89	0
3	PO4	G	404	-	4,4,4	0.63	0	6,6,6	1.34	1 (16%)
3	PO4	E	403	-	4,4,4	1.18	0	6,6,6	1.36	2 (33%)
3	PO4	A	403	-	4,4,4	0.88	0	6,6,6	0.72	0
3	PO4	B	403	-	4,4,4	0.91	0	6,6,6	0.64	0
3	PO4	G	403	-	4,4,4	0.80	0	6,6,6	0.81	0
3	PO4	G	402	-	4,4,4	0.92	0	6,6,6	0.55	0
3	PO4	D	101	-	4,4,4	0.78	0	6,6,6	1.07	0
3	PO4	E	402	-	4,4,4	0.78	0	6,6,6	1.10	1 (16%)
3	PO4	A	402	-	4,4,4	0.77	0	6,6,6	0.86	0
3	PO4	B	402	-	4,4,4	0.82	0	6,6,6	0.98	0
3	PO4	C	101	-	4,4,4	1.05	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	F	101	-	4,4,4	0.76	0	6,6,6	0.81	0
3	PO4	A	404	-	4,4,4	0.88	0	6,6,6	0.71	0
3	PO4	I	101	-	4,4,4	0.70	0	6,6,6	1.02	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	PO4	O3-P-O1	-2.12	103.14	110.89
3	G	404	PO4	O3-P-O1	-2.11	103.17	110.89
3	E	403	PO4	O4-P-O2	2.08	114.63	107.97
3	E	403	PO4	O2-P-O1	-2.01	103.53	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	403	PO4	2	0
3	G	403	PO4	1	0
3	F	101	PO4	1	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 ⓘ

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	7/30 (23%)	-0.07	0 100 100	59, 64, 70, 77	0
1	D	7/30 (23%)	-0.20	0 100 100	53, 57, 62, 73	0
1	F	7/30 (23%)	-0.31	0 100 100	59, 64, 72, 77	0
1	I	7/30 (23%)	-0.37	0 100 100	57, 63, 69, 76	0
2	A	344/361 (95%)	0.47	32 (9%) 8 6	47, 90, 154, 190	0
2	B	346/361 (95%)	0.19	10 (2%) 51 47	40, 79, 128, 222	0
2	E	346/361 (95%)	0.42	27 (7%) 13 10	49, 92, 140, 247	0
2	G	346/361 (95%)	0.36	21 (6%) 21 17	49, 83, 140, 200	0
All	All	1410/1564 (90%)	0.35	90 (6%) 19 15	40, 85, 141, 247	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	232	TRP	20.2
2	B	232	TRP	10.8
2	B	233	VAL	10.4
2	G	232	TRP	7.2
2	A	361	TRP	7.1
2	E	233	VAL	6.1
2	G	230	ASP	5.6
2	A	358	PHE	5.6
2	G	233	VAL	5.6
2	B	234	LYS	5.4
2	E	231	THR	5.3
2	G	254	GLU	4.9
2	A	228	HIS	4.5
2	A	352	ASP	4.4
2	G	358	PHE	4.4
2	A	360	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	A	238	ARG	4.3
2	A	196	SER	4.3
2	G	231	THR	4.3
2	G	234	LYS	4.2
2	A	235	LEU	4.2
2	E	238	ARG	4.2
2	B	230	ASP	4.2
2	A	357	PRO	3.9
2	E	224	VAL	3.9
2	B	231	THR	3.9
2	E	57	GLN	3.8
2	G	223	GLU	3.7
2	G	235	LEU	3.7
2	B	35	LEU	3.5
2	A	30	GLN	3.4
2	G	237	GLN	3.4
2	E	227	MET	3.3
2	A	349	THR	3.2
2	G	277	TYR	3.1
2	A	354	GLN	3.1
2	A	35	LEU	3.1
2	E	247	PRO	3.0
2	A	356	ALA	3.0
2	A	307	LEU	2.9
2	E	308	CYS	2.9
2	A	224	VAL	2.9
2	A	197	MET	2.8
2	G	31	LEU	2.8
2	G	236	ASN	2.8
2	E	58	LYS	2.8
2	E	277	TYR	2.8
2	A	353	HIS	2.7
2	A	202	PHE	2.6
2	G	271	LEU	2.6
2	A	37	ALA	2.6
2	B	228	HIS	2.5
2	E	236	ASN	2.5
2	E	271	LEU	2.5
2	E	230	ASP	2.4
2	E	268	PHE	2.4
2	A	101	ILE	2.4
2	B	358	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	307	LEU	2.3
2	E	33	GLU	2.3
2	A	350	PHE	2.3
2	A	226	ARG	2.3
2	E	45	LEU	2.3
2	A	234	LYS	2.3
2	G	34	LEU	2.3
2	B	269	TRP	2.3
2	A	199	PRO	2.3
2	E	262	PHE	2.3
2	G	229	ASN	2.3
2	A	227	MET	2.3
2	E	358	PHE	2.3
2	E	378	ILE	2.2
2	E	360	PRO	2.2
2	G	278	ARG	2.2
2	E	295	MET	2.2
2	B	92	TRP	2.1
2	E	279	VAL	2.1
2	E	304	HIS	2.1
2	E	309	ILE	2.1
2	G	354	GLN	2.1
2	E	189	TRP	2.1
2	G	361	TRP	2.1
2	A	38	GLY	2.1
2	A	355	GLY	2.1
2	A	233	VAL	2.1
2	A	36	ASN	2.1
2	A	266	ILE	2.0
2	A	327	THR	2.0
2	G	303	LYS	2.0
2	G	226	ARG	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 carbohydrates 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
3	PO4	A	404	5/5	0.82	0.19	104,112,128,138	0
3	PO4	G	403	5/5	0.88	0.20	83,85,98,107	0
3	PO4	A	403	5/5	0.90	0.25	82,88,100,103	0
3	PO4	E	404	5/5	0.92	0.18	99,102,122,122	0
3	PO4	I	101	5/5	0.92	0.19	92,99,102,104	0
3	PO4	G	404	5/5	0.93	0.18	81,81,95,97	0
3	PO4	D	101	5/5	0.93	0.22	70,82,84,100	0
3	PO4	E	402	5/5	0.94	0.18	83,91,103,107	0
3	PO4	B	402	5/5	0.94	0.15	84,86,92,95	0
3	PO4	B	403	5/5	0.95	0.17	72,87,94,95	0
3	PO4	F	101	5/5	0.95	0.16	81,92,104,107	0
4	ZN	A	401	1/1	0.95	0.16	126,126,126,126	0
3	PO4	A	402	5/5	0.95	0.22	78,87,91,101	0
3	PO4	C	101	5/5	0.96	0.20	71,84,87,97	0
3	PO4	E	403	5/5	0.96	0.16	70,71,83,84	0
4	ZN	G	401	1/1	0.97	0.20	104,104,104,104	0
3	PO4	G	402	5/5	0.97	0.19	67,80,90,91	0
4	ZN	E	401	1/1	0.98	0.19	102,102,102,102	0
4	ZN	B	401	1/1	0.99	0.26	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.