Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:20 PM GMT

PDB ID	:	1JQY
Title	:	HEAT-LABILE ENTEROTOXIN B-PENTAMER WITH LIGAND BMSC-0010
Authors	:	Merritt, E.A.; Hol, W.G.J.
Deposited on	:	2001-08-09
Resolution	:	2.14 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

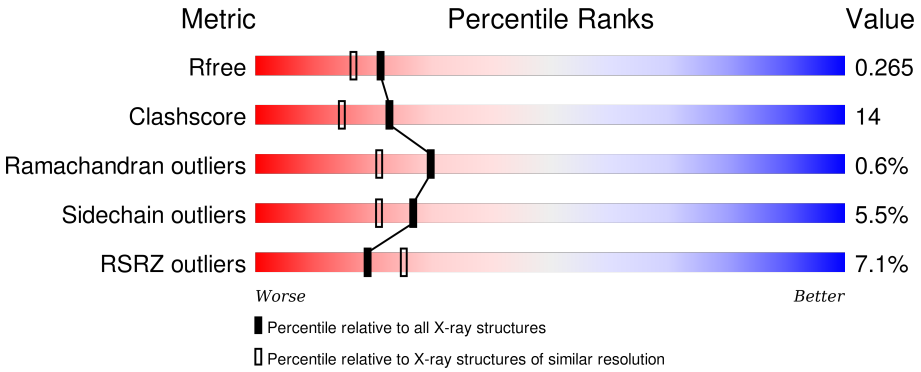
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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}	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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. 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	D	103	71% 24%
1	E	103	71% 27%
1	F	103	73% 22% 5%
1	G	103	76% 21%
1	H	103	77% 19%

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Mol	Chain	Length	Quality of chain
1	L	103	4% 58% 39%
1	M	103	5% 62% 32% 5%
1	N	103	4% 69% 27%
1	O	103	3% 75% 20% 5%
1	P	103	2% 70% 23% 6%
1	V	103	39% 54% 38% 6%
1	W	103	20% 49% 43% 9%
1	X	103	8% 61% 34%
1	Y	103	8% 50% 46%
1	Z	103	9% 50% 37% 12%

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
2	A32	D	104	-	-	-	X
2	A32	E	104	-	-	-	X
2	A32	H	104	-	-	-	X
2	A32	O	104	-	-	-	X
2	A32	P	104	-	-	-	X
2	A32	V	104	X	-	-	-
2	A32	W	104	-	-	-	X
2	A32	X	104	-	-	-	X
2	A32	Y	104	-	-	-	X

2 Entry composition

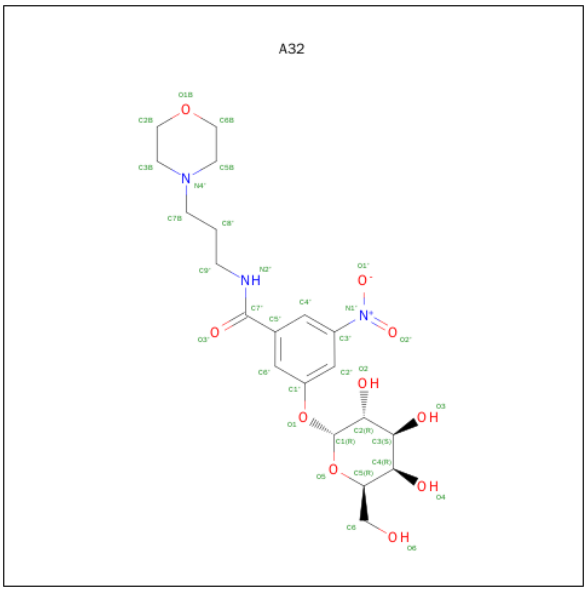
There are 3 unique types of molecules in this entry. The entry contains 13904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEAT-LABILE ENTEROTOXIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	E	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	F	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	G	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	H	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	L	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	M	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	N	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	O	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	P	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	V	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	W	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	X	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	Y	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	Z	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			

- Molecule 2 is (3-NITRO-5-(3-MORPHOLIN-4-YL-PROPYLAMINOCARBONYL)PHENYL)-GALACTOPYRANOSIDE (three-letter code: A32) (formula: $C_{20}H_{29}N_3O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			33	20	3	10		
2	E	1	Total	C	N	O	0	0
			33	20	3	10		
2	F	1	Total	C	N	O	0	0
			33	20	3	10		
2	G	1	Total	C	N	O	0	0
			33	20	3	10		
2	H	1	Total	C	N	O	0	0
			33	20	3	10		
2	L	1	Total	C	N	O	0	0
			33	20	3	10		
2	M	1	Total	C	N	O	0	0
			33	20	3	10		
2	O	1	Total	C	N	O	0	0
			33	20	3	10		
2	P	1	Total	C	N	O	0	0
			33	20	3	10		
2	V	1	Total	C	N	O	0	0
			33	20	3	10		
2	W	1	Total	C	N	O	0	0
			33	20	3	10		
2	X	1	Total	C	N	O	0	0
			33	20	3	10		
2	Y	1	Total	C	N	O	0	0
			33	20	3	10		
2	Z	1	Total	C	N	O	0	0
			33	20	3	10		

- Molecule 3 is water.

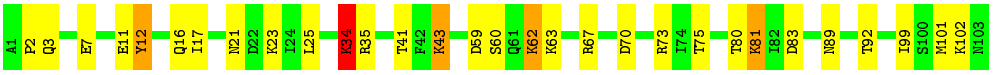
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	89	Total O 89 89	0	0
3	E	87	Total O 87 87	0	0
3	F	113	Total O 113 113	0	0
3	G	78	Total O 78 78	0	0
3	H	100	Total O 100 100	0	0
3	L	51	Total O 51 51	0	0
3	M	49	Total O 49 49	0	0
3	N	65	Total O 65 65	0	0
3	O	75	Total O 75 75	0	0
3	P	80	Total O 80 80	0	0
3	V	41	Total O 41 41	0	0
3	W	49	Total O 49 49	0	0
3	X	81	Total O 81 81	0	0
3	Y	63	Total O 63 63	0	0
3	Z	61	Total O 61 61	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 errors 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: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain D:

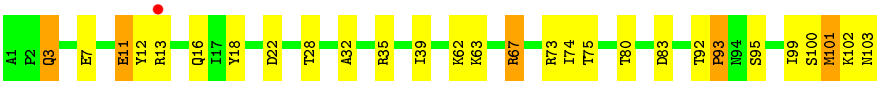


- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain E:

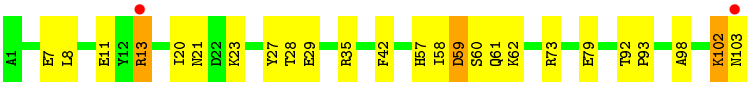
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain F:



- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain G:

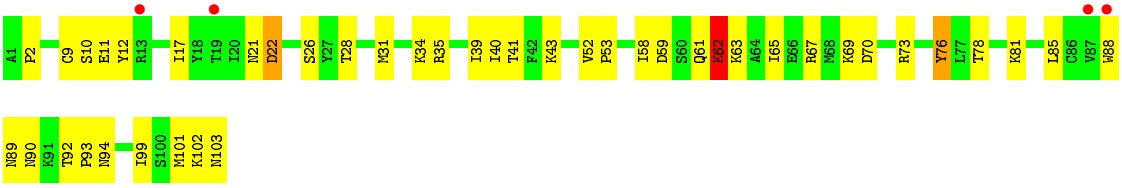


- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain H:

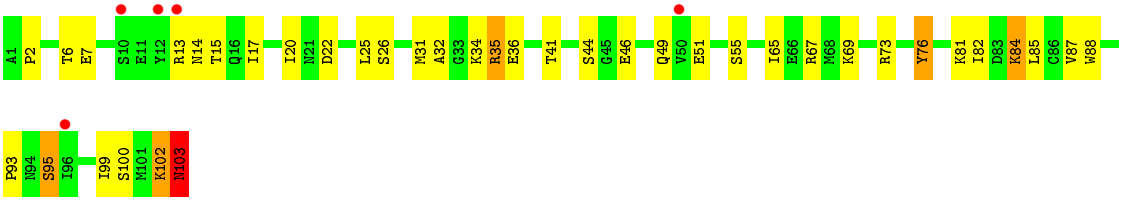
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain L:



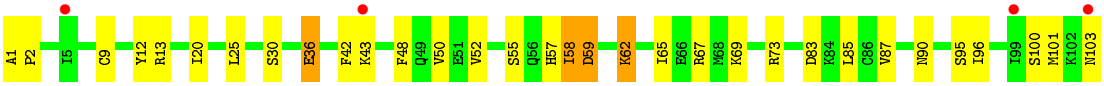
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain M:



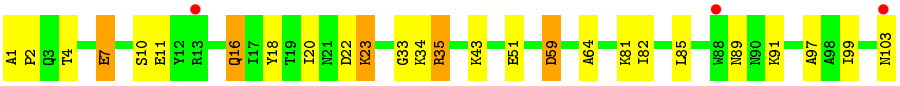
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain N:



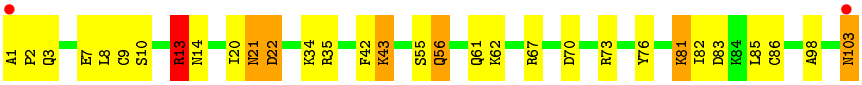
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain O:



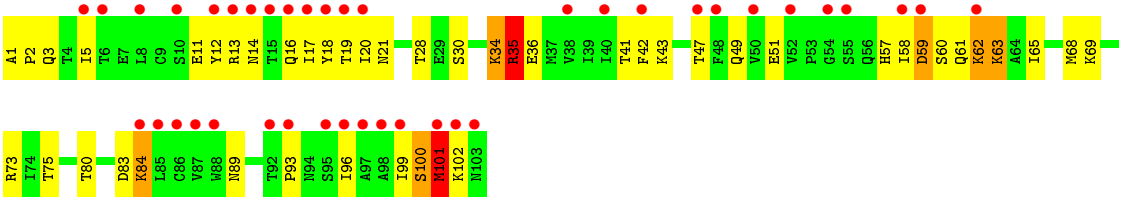
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain P:



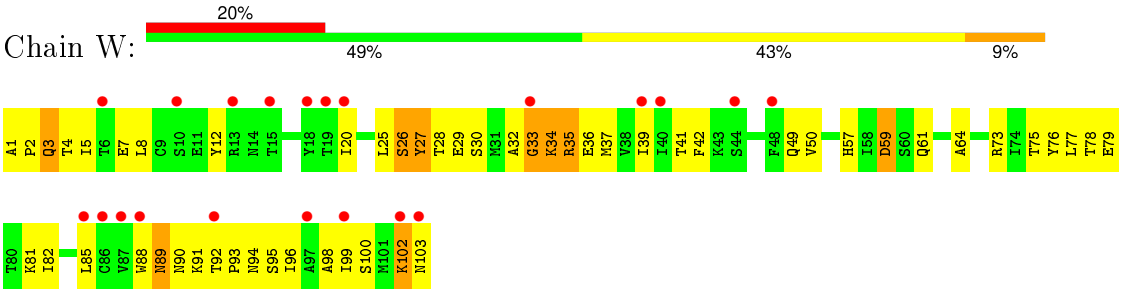
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain V:



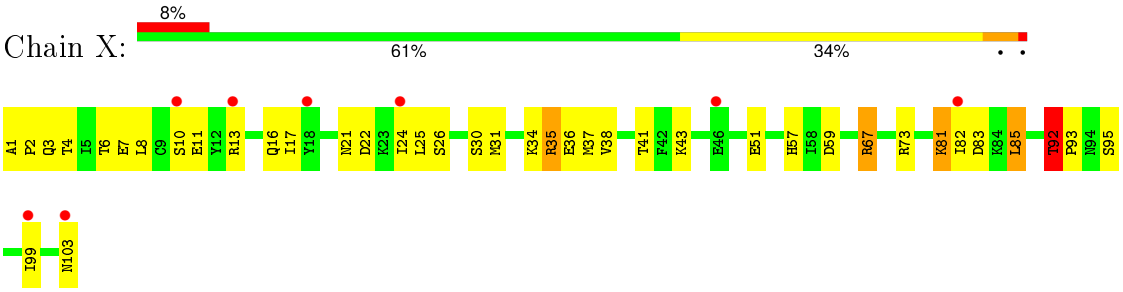
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain W:



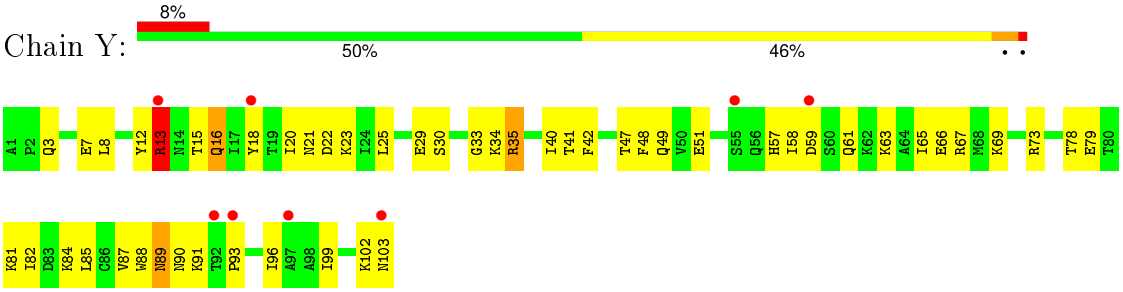
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain X:



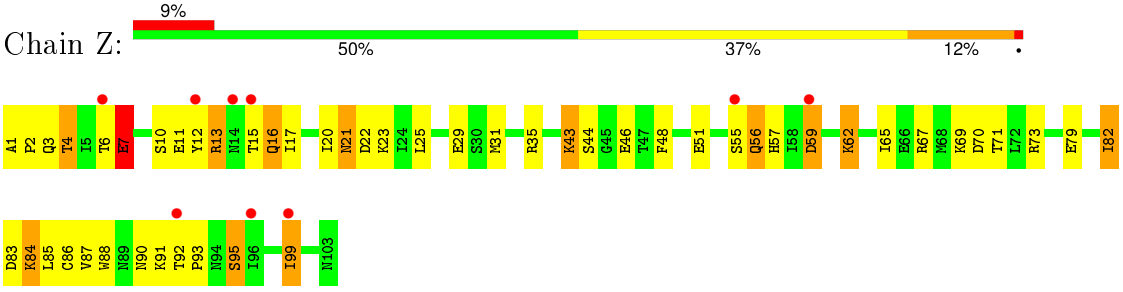
• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain Y:



• Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.99Å 166.01Å 74.42Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	25.00 – 2.14 19.99 – 2.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.14) 97.4 (19.99-2.14)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 2.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.284 0.200 , 0.265	Depositor DCC
R_{free} test set	4235 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.5	EDS
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 84172 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13904	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: A32

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	D	0.86	0/835	1.89	14/1124 (1.2%)
1	E	0.88	0/835	1.83	18/1124 (1.6%)
1	F	0.89	0/835	1.89	19/1124 (1.7%)
1	G	0.81	0/835	1.84	12/1124 (1.1%)
1	H	0.86	0/835	1.97	20/1124 (1.8%)
1	L	0.66	0/835	1.60	10/1124 (0.9%)
1	M	0.62	0/835	1.73	11/1124 (1.0%)
1	N	0.73	0/835	1.74	16/1124 (1.4%)
1	O	0.68	0/835	1.57	9/1124 (0.8%)
1	P	0.80	0/835	2.14	17/1124 (1.5%)
1	V	0.55	0/835	1.50	10/1124 (0.9%)
1	W	0.61	0/835	1.67	13/1124 (1.2%)
1	X	0.76	0/835	1.85	17/1124 (1.5%)
1	Y	0.72	0/835	1.78	14/1124 (1.2%)
1	Z	0.68	0/835	1.78	15/1124 (1.3%)
All	All	0.75	0/12525	1.79	215/16860 (1.3%)

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	N	0	1

There are no bond length outliers.

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	73	ARG	NE-CZ-NH1	24.32	132.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	13	ARG	CD-NE-CZ	21.60	153.84	123.60
1	P	73	ARG	NE-CZ-NH2	-20.18	110.21	120.30
1	Z	35	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	F	35	ARG	CD-NE-CZ	16.48	146.68	123.60
1	E	35	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	D	67	ARG	NE-CZ-NH2	-15.28	112.66	120.30
1	M	35	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	H	73	ARG	NE-CZ-NH2	-14.35	113.12	120.30
1	M	35	ARG	NE-CZ-NH2	-14.21	113.20	120.30
1	D	73	ARG	NE-CZ-NH1	13.69	127.15	120.30
1	Y	67	ARG	NE-CZ-NH1	13.67	127.13	120.30
1	F	67	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	X	67	ARG	NE-CZ-NH2	-13.40	113.60	120.30
1	H	13	ARG	CD-NE-CZ	13.37	142.32	123.60
1	D	43	LYS	CA-CB-CG	13.15	142.32	113.40
1	P	13	ARG	CG-CD-NE	12.84	138.77	111.80
1	G	73	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	F	35	ARG	NE-CZ-NH1	12.45	126.53	120.30
1	D	59	ASP	CB-CG-OD1	11.85	128.96	118.30
1	E	35	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	D	35	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	E	73	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	H	13	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	P	67	ARG	CD-NE-CZ	11.48	139.67	123.60
1	G	73	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	G	35	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	N	73	ARG	NE-CZ-NH2	-10.97	114.81	120.30
1	P	76	TYR	CB-CG-CD1	-10.63	114.62	121.00
1	E	73	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	H	35	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	W	73	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	P	76	TYR	CB-CG-CD2	10.19	127.12	121.00
1	F	83	ASP	CB-CG-OD2	10.04	127.34	118.30
1	X	13	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	P	70	ASP	CB-CG-OD2	-9.41	109.83	118.30
1	Z	73	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	P	73	ARG	CD-NE-CZ	9.20	136.47	123.60
1	W	59	ASP	CB-CG-OD1	9.18	126.56	118.30
1	E	11	GLU	OE1-CD-OE2	-9.16	112.30	123.30
1	V	73	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	M	35	ARG	CD-NE-CZ	8.97	136.16	123.60
1	L	59	ASP	CB-CG-OD1	8.91	126.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	59	ASP	CB-CG-OD2	-8.88	110.30	118.30
1	Z	67	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	E	81	LYS	CA-CB-CG	8.53	132.17	113.40
1	F	35	ARG	NH1-CZ-NH2	-8.49	110.06	119.40
1	Y	59	ASP	CB-CG-OD1	8.28	125.75	118.30
1	H	102	LYS	CA-C-O	8.27	137.46	120.10
1	M	73	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	Z	73	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	H	67	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	X	92	THR	CA-CB-CG2	-8.17	100.96	112.40
1	H	59	ASP	CB-CG-OD1	8.15	125.64	118.30
1	Y	22	ASP	CB-CG-OD1	8.06	125.56	118.30
1	H	29	GLU	OE1-CD-OE2	-8.05	113.63	123.30
1	P	7	GLU	CA-CB-CG	8.04	131.10	113.40
1	G	102	LYS	CA-CB-CG	7.92	130.83	113.40
1	Z	67	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	N	96	ILE	C-N-CA	7.71	140.99	121.70
1	Y	13	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	Y	66	GLU	OE1-CD-OE2	-7.69	114.07	123.30
1	F	73	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	Y	35	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	N	59	ASP	CB-CG-OD1	7.56	125.10	118.30
1	G	59	ASP	CB-CG-OD1	7.50	125.05	118.30
1	G	7	GLU	OE1-CD-OE2	7.43	132.22	123.30
1	M	76	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	V	35	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	Y	7	GLU	OE1-CD-OE2	7.37	132.14	123.30
1	E	103	ASN	CA-CB-CG	7.35	129.58	113.40
1	H	13	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	H	18	TYR	CB-CG-CD1	-7.34	116.60	121.00
1	M	22	ASP	CB-CG-OD1	-7.33	111.71	118.30
1	X	22	ASP	CB-CG-OD2	7.28	124.85	118.30
1	N	83	ASP	CB-CG-OD2	7.23	124.81	118.30
1	M	73	ARG	CD-NE-CZ	7.23	133.72	123.60
1	Z	35	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	M	36	GLU	OE1-CD-OE2	-7.03	114.86	123.30
1	D	70	ASP	CB-CG-OD1	7.00	124.59	118.30
1	Z	13	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	34	LYS	CD-CE-NZ	6.93	127.64	111.70
1	E	18	TYR	CB-CG-CD2	-6.91	116.86	121.00
1	W	59	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	W	3	GLN	CA-CB-CG	6.86	128.48	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	86	CYS	CA-CB-SG	-6.83	101.71	114.00
1	X	73	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	12	TYR	CB-CG-CD1	-6.77	116.94	121.00
1	G	35	ARG	CD-NE-CZ	6.74	133.04	123.60
1	V	59	ASP	CB-CG-OD1	6.74	124.36	118.30
1	G	13	ARG	CD-NE-CZ	6.74	133.03	123.60
1	Z	13	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	O	11	GLU	CA-CB-CG	6.70	128.15	113.40
1	W	50	VAL	N-CA-C	-6.70	92.91	111.00
1	O	10	SER	CB-CA-C	6.67	122.78	110.10
1	V	18	TYR	CA-CB-CG	6.59	125.92	113.40
1	Y	13	ARG	CD-NE-CZ	6.58	132.81	123.60
1	V	101	MET	CA-CB-CG	6.55	124.44	113.30
1	Z	7	GLU	OE1-CD-OE2	6.52	131.13	123.30
1	O	35	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	N	67	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	H	33	GLY	O-C-N	-6.43	112.41	122.70
1	N	59	ASP	OD1-CG-OD2	-6.41	111.12	123.30
1	O	7	GLU	CA-CB-CG	6.41	127.50	113.40
1	N	73	ARG	NH1-CZ-NH2	6.37	126.41	119.40
1	F	13	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	P	21	ASN	CB-CG-OD1	-6.35	108.89	121.60
1	N	85	LEU	CA-CB-CG	6.35	129.90	115.30
1	V	68	MET	CG-SD-CE	6.33	110.33	100.20
1	W	27	TYR	CB-CG-CD2	6.29	124.78	121.00
1	X	35	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	L	76	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	P	70	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	11	GLU	OE1-CD-OE2	-6.18	115.88	123.30
1	N	13	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	F	35	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	W	73	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	F	67	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	N	59	ASP	CB-CG-OD2	6.09	123.78	118.30
1	L	70	ASP	CB-CG-OD1	6.08	123.77	118.30
1	P	83	ASP	CB-CG-OD2	6.07	123.76	118.30
1	W	35	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	H	33	GLY	CA-C-O	6.03	131.46	120.60
1	E	35	ARG	CD-NE-CZ	6.02	132.03	123.60
1	Z	70	ASP	CB-CG-OD1	6.01	123.71	118.30
1	F	18	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	E	70	ASP	CB-CG-OD2	5.98	123.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	22	ASP	CB-CG-OD1	5.98	123.68	118.30
1	Y	63	LYS	N-CA-CB	5.97	121.34	110.60
1	M	67	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	D	60	SER	N-CA-CB	-5.96	101.56	110.50
1	L	62	LYS	CA-CB-CG	5.87	126.31	113.40
1	Z	4	THR	N-CA-CB	5.85	121.42	110.30
1	L	73	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	Y	63	LYS	CB-CA-C	-5.82	98.76	110.40
1	X	59	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	83	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	W	26	SER	N-CA-CB	-5.79	101.81	110.50
1	E	28	THR	CA-CB-CG2	5.78	120.49	112.40
1	V	35	ARG	CG-CD-NE	5.77	123.91	111.80
1	L	22	ASP	CB-CG-OD1	5.75	123.48	118.30
1	P	62	LYS	CA-CB-CG	5.75	126.05	113.40
1	H	102	LYS	C-N-CA	5.74	136.05	121.70
1	X	4	THR	N-CA-CB	5.73	121.18	110.30
1	N	36	GLU	OE1-CD-OE2	-5.71	116.44	123.30
1	M	73	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
1	E	63	LYS	CA-CB-CG	-5.70	100.86	113.40
1	V	35	ARG	CD-NE-CZ	5.69	131.56	123.60
1	Y	35	ARG	CD-NE-CZ	5.69	131.56	123.60
1	E	59	ASP	CB-CG-OD1	5.67	123.40	118.30
1	O	11	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	F	11	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	F	35	ARG	CG-CD-NE	5.66	123.69	111.80
1	L	41	THR	N-CA-CB	5.66	121.06	110.30
1	W	75	THR	O-C-N	-5.64	113.68	122.70
1	X	13	ARG	CA-CB-CG	5.64	125.80	113.40
1	O	64	ALA	CB-CA-C	5.63	118.55	110.10
1	X	7	GLU	CA-CB-CG	5.62	125.77	113.40
1	Z	84	LYS	CA-CB-CG	5.62	125.77	113.40
1	H	26	SER	N-CA-CB	5.62	118.93	110.50
1	L	22	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	F	7	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	M	103	ASN	CA-CB-CG	5.58	125.68	113.40
1	O	35	ARG	CA-CB-CG	5.58	125.67	113.40
1	D	67	ARG	NH1-CZ-NH2	5.57	125.53	119.40
1	F	62	LYS	CB-CG-CD	5.57	126.08	111.60
1	F	7	GLU	CG-CD-OE2	-5.55	107.19	118.30
1	X	67	ARG	NH1-CZ-NH2	5.54	125.49	119.40
1	F	95	SER	N-CA-CB	-5.54	102.20	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	73	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	92	THR	CB-CA-C	-5.50	96.75	111.60
1	X	22	ASP	OD1-CG-OD2	-5.48	112.89	123.30
1	G	28	THR	CA-CB-CG2	-5.47	104.74	112.40
1	L	67	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	E	44	SER	CB-CA-C	-5.45	99.75	110.10
1	W	27	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	Z	48	PHE	N-CA-CB	5.42	120.35	110.60
1	P	62	LYS	N-CA-CB	5.41	120.34	110.60
1	V	41	THR	N-CA-CB	5.41	120.58	110.30
1	N	58	ILE	O-C-N	-5.41	114.05	122.70
1	G	98	ALA	N-CA-CB	5.38	117.64	110.10
1	H	13	ARG	CG-CD-NE	5.37	123.08	111.80
1	E	71	THR	CA-CB-CG2	-5.35	104.90	112.40
1	H	68	MET	N-CA-CB	5.35	120.23	110.60
1	O	22	ASP	CB-CG-OD2	5.33	123.10	118.30
1	F	100	SER	N-CA-CB	5.29	118.43	110.50
1	Y	73	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	X	92	THR	CA-CB-OG1	5.27	120.07	109.00
1	W	98	ALA	N-CA-CB	5.26	117.46	110.10
1	H	48	PHE	O-C-N	5.25	131.10	122.70
1	V	68	MET	CA-CB-CG	5.24	122.21	113.30
1	W	89	ASN	CA-C-N	5.24	128.73	117.20
1	X	16	GLN	CB-CG-CD	5.23	125.20	111.60
1	D	41	THR	N-CA-CB	5.22	120.21	110.30
1	F	93	PRO	CB-CA-C	-5.19	99.03	112.00
1	N	50	VAL	CA-CB-CG1	-5.18	103.12	110.90
1	P	35	ARG	CD-NE-CZ	5.16	130.83	123.60
1	H	35	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	N	100	SER	C-N-CA	5.14	134.54	121.70
1	G	11	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	E	83	ASP	CB-CG-OD1	5.13	122.91	118.30
1	F	22	ASP	CB-CG-OD1	5.13	122.91	118.30
1	N	58	ILE	C-N-CA	5.12	134.49	121.70
1	H	48	PHE	N-CA-CB	5.06	119.70	110.60
1	Y	63	LYS	CA-CB-CG	5.06	124.53	113.40
1	E	18	TYR	CB-CG-CD1	5.03	124.02	121.00
1	N	101	MET	CA-CB-CG	5.02	121.83	113.30
1	Z	71	THR	CA-CB-OG1	-5.02	98.46	109.00
1	G	35	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	H	102	LYS	CA-C-N	-5.01	106.17	117.20
1	X	81	LYS	CA-CB-CG	5.01	124.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	78	THR	CA-CB-CG2	-5.01	105.39	112.40
1	X	57	HIS	CA-CB-CG	-5.01	105.09	113.60
1	X	85	LEU	CB-CA-C	-5.00	100.69	110.20
1	E	79	GLU	OE1-CD-OE2	-5.00	117.30	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	52	VAL	Mainchain

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	D	824	0	841	17	0
1	E	824	0	841	18	0
1	F	824	0	841	17	0
1	G	824	0	841	17	0
1	H	824	0	841	14	0
1	L	824	0	841	26	0
1	M	824	0	841	25	0
1	N	824	0	840	23	0
1	O	824	0	841	16	0
1	P	824	0	841	23	0
1	V	824	0	841	55	0
1	W	824	0	841	39	0
1	X	824	0	841	22	0
1	Y	824	0	841	41	0
1	Z	824	0	841	40	0
2	D	33	0	28	9	0
2	E	33	0	29	2	0
2	F	33	0	29	5	0
2	G	33	0	29	2	0
2	H	33	0	28	1	0
2	L	33	0	28	3	0
2	M	33	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	33	0	28	8	0
2	P	33	0	29	0	0
2	V	33	0	28	6	0
2	W	33	0	28	4	0
2	X	33	0	29	1	0
2	Y	33	0	28	5	0
2	Z	33	0	28	9	0
3	D	89	0	0	1	0
3	E	87	0	0	4	0
3	F	113	0	0	3	0
3	G	78	0	0	1	0
3	H	100	0	0	3	0
3	L	51	0	0	1	0
3	M	49	0	0	1	0
3	N	65	0	0	4	0
3	O	75	0	0	1	0
3	P	80	0	0	1	0
3	V	41	0	0	1	0
3	W	49	0	0	3	0
3	X	81	0	0	1	0
3	Y	63	0	0	1	0
3	Z	61	0	0	2	0
All	All	13904	0	13011	351	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 14.

All (351) 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:O:104:A32:H5'1	1:P:34:LYS:HB2	1.33	1.06
2:D:104:A32:H5'2	1:E:34:LYS:HB2	1.47	0.97
1:N:57:HIS:HB3	1:N:62:LYS:HZ2	1.29	0.96
1:V:34:LYS:HB3	2:Z:104:A32:H2'2	1.52	0.89
1:W:1:ALA:HB1	1:W:2:PRO:HD2	1.53	0.89
1:V:47:THR:HG21	1:Z:3:GLN:HB3	1.55	0.89
2:O:104:A32:H9'1	2:O:104:A32:H4'1	1.55	0.89
1:H:56:GLN:HE21	1:H:56:GLN:H	1.20	0.88
1:Y:58:ILE:HG21	2:Y:104:A32:H7'2	1.58	0.85
1:E:16:GLN:HE21	1:E:89:ASN:HD22	1.25	0.84
1:V:1:ALA:HB1	1:V:2:PRO:HD2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:56:GLN:HE21	1:P:56:GLN:H	1.25	0.82
1:Z:11:GLU:HB3	2:Z:104:A32:H5'1	1.63	0.81
1:N:1:ALA:HB1	1:N:2:PRO:HD2	1.61	0.81
1:Y:3:GLN:HG2	1:Z:93:PRO:HG3	1.64	0.78
1:Z:56:GLN:HE21	1:Z:56:GLN:H	1.28	0.78
1:Z:6:THR:HA	1:Z:17:ILE:HD11	1.66	0.78
1:N:57:HIS:CB	1:N:62:LYS:HZ2	1.97	0.77
1:O:4:THR:OG1	1:O:7:GLU:HG2	1.85	0.77
1:M:103:ASN:HB2	3:M:133:HOH:O	1.85	0.76
1:N:57:HIS:HB3	1:N:62:LYS:NZ	2.00	0.76
1:W:82:ILE:HG12	1:W:99:ILE:HD11	1.68	0.76
1:N:103:ASN:HD22	1:O:23:LYS:HE2	1.51	0.76
1:W:1:ALA:HB1	1:W:2:PRO:CD	2.16	0.75
1:V:3:GLN:HG2	1:W:93:PRO:HG3	1.69	0.75
2:O:104:A32:C9'	2:O:104:A32:H4'1	2.18	0.74
1:X:26:SER:HB3	1:X:41:THR:OG1	1.88	0.73
1:N:62:LYS:HD2	3:N:142:HOH:O	1.88	0.73
2:O:104:A32:H5'1	1:P:34:LYS:CB	2.15	0.72
1:M:65:ILE:HG22	1:M:69:LYS:HE2	1.72	0.72
2:O:104:A32:C5B	1:P:34:LYS:HB2	2.15	0.72
1:O:16:GLN:HE21	1:O:89:ASN:HD22	1.37	0.70
1:V:19:THR:HA	1:V:84:LYS:HG3	1.72	0.70
1:F:99:ILE:HG12	1:F:101:MET:HE2	1.74	0.69
1:P:20:ILE:HG13	1:P:85:LEU:HD12	1.74	0.69
1:E:16:GLN:NE2	1:E:89:ASN:HD22	1.91	0.69
1:Y:65:ILE:HG22	1:Y:69:LYS:HE2	1.75	0.69
1:M:26:SER:HB3	1:M:41:THR:OG1	1.94	0.68
1:V:1:ALA:HB1	1:V:2:PRO:CD	2.25	0.67
1:V:2:PRO:HG3	1:V:11:GLU:OE2	1.94	0.67
1:X:92:THR:HG22	1:X:93:PRO:HA	1.77	0.66
1:D:25:LEU:O	1:H:103:ASN:HB2	1.95	0.66
1:M:82:ILE:HG12	1:M:99:ILE:HD11	1.75	0.66
1:N:9:CYS:HB3	3:N:159:HOH:O	1.94	0.66
1:O:82:ILE:HG12	1:O:99:ILE:HD11	1.77	0.66
1:V:34:LYS:CB	2:Z:104:A32:H2'2	2.26	0.66
2:D:104:A32:H4'1	2:D:104:A32:H9'1	1.79	0.65
1:Y:48:PHE:CD2	1:Y:87:VAL:HG11	2.33	0.64
2:D:104:A32:H5'2	1:E:34:LYS:CB	2.27	0.64
1:V:102:LYS:HE3	1:W:25:LEU:HD11	1.80	0.63
1:N:58:ILE:O	1:N:62:LYS:NZ	2.30	0.63
1:L:9:CYS:HB2	1:L:17:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:104:A32:H6'1	3:L:154:HOH:O	1.96	0.63
1:F:99:ILE:HG12	1:F:101:MET:CE	2.28	0.62
2:O:104:A32:C4'	2:O:104:A32:H9'1	2.29	0.62
2:D:104:A32:N2'	1:E:33:GLY:HA3	2.14	0.62
1:Z:59:ASP:O	1:Z:62:LYS:HG2	2.00	0.61
1:V:65:ILE:HG22	1:V:69:LYS:HE2	1.83	0.61
2:D:104:A32:C5B	1:E:34:LYS:HB2	2.27	0.60
1:V:93:PRO:HG3	1:Z:3:GLN:HG2	1.83	0.60
1:Y:65:ILE:HG12	1:Z:31:MET:HE3	1.84	0.60
1:P:56:GLN:N	1:P:56:GLN:HE21	1.99	0.60
1:Y:51:GLU:OE1	1:Y:91:LYS:HE2	2.02	0.60
1:P:13:ARG:HG3	1:P:14:ASN:N	2.16	0.60
1:Z:82:ILE:HD13	1:Z:99:ILE:HD12	1.83	0.60
1:Z:88:TRP:CH2	2:Z:104:A32:H62	2.37	0.60
1:Y:58:ILE:HD13	2:Y:104:A32:H7'2	1.84	0.59
1:Y:48:PHE:CE2	1:Y:87:VAL:HG11	2.38	0.59
1:W:27:TYR:OH	1:W:29:GLU:OE1	2.18	0.59
1:M:2:PRO:HB3	1:M:7:GLU:HG2	1.84	0.58
1:V:83:ASP:OD2	1:V:84:LYS:HD2	2.03	0.58
1:X:92:THR:HA	1:X:93:PRO:C	2.22	0.58
1:V:12:TYR:CE2	2:V:104:A32:H6'2	2.39	0.58
1:M:44:SER:OG	1:M:46:GLU:HG3	2.04	0.58
1:Y:89:ASN:HD22	1:Y:89:ASN:C	2.05	0.58
1:X:1:ALA:HB1	1:X:2:PRO:HD2	1.86	0.57
1:P:2:PRO:HG3	1:P:8:LEU:HD12	1.85	0.57
1:Z:85:LEU:HD23	1:Z:99:ILE:HG22	1.87	0.57
1:Z:51:GLU:HG3	1:Z:95:SER:HB2	1.87	0.57
1:Y:13:ARG:O	1:Y:15:THR:HG23	2.04	0.57
1:V:35:ARG:NH1	2:Z:104:A32:O1B	2.38	0.57
1:Z:65:ILE:HG22	1:Z:69:LYS:HE2	1.86	0.57
1:G:61:GLN:HG2	1:H:31:MET:O	2.05	0.56
1:Z:11:GLU:O	2:Z:104:A32:H7'2	2.06	0.56
1:V:12:TYR:CZ	2:V:104:A32:H6'2	2.40	0.56
1:M:102:LYS:NZ	1:N:25:LEU:HD11	2.20	0.56
1:P:20:ILE:HG13	1:P:85:LEU:CD1	2.35	0.56
1:V:60:SER:O	1:W:36:GLU:HG2	2.06	0.55
1:L:11:GLU:O	2:L:104:A32:H7'1	2.06	0.55
1:X:11:GLU:OE2	1:Y:35:ARG:NH2	2.34	0.55
1:X:8:LEU:HD11	1:Y:30:SER:HB2	1.88	0.55
1:Z:25:LEU:HD13	1:Z:43:LYS:HE3	1.87	0.55
1:Z:56:GLN:HG2	1:Z:57:HIS:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:ARG:O	1:M:15:THR:HG23	2.07	0.55
1:O:20:ILE:HG13	1:O:85:LEU:HD12	1.88	0.54
1:M:51:GLU:HG3	1:M:95:SER:OG	2.06	0.54
1:Z:17:ILE:HG21	1:Z:84:LYS:HD3	1.90	0.54
1:V:17:ILE:HG23	1:V:84:LYS:HG2	1.89	0.54
1:L:76:TYR:OH	1:P:103:ASN:HB2	2.08	0.54
1:O:1:ALA:HB1	1:O:2:PRO:HD2	1.89	0.54
1:M:84:LYS:HB2	1:M:100:SER:OG	2.07	0.54
1:V:35:ARG:HB2	1:Z:12:TYR:OH	2.07	0.54
1:W:88:TRP:HB2	1:W:95:SER:HB3	1.89	0.54
1:D:34:LYS:HE2	3:D:139:HOH:O	2.08	0.54
1:M:102:LYS:HZ3	1:N:25:LEU:HD11	1.72	0.54
1:L:52:VAL:HG12	1:L:53:PRO:O	2.07	0.53
1:Y:61:GLN:O	1:Y:65:ILE:HG13	2.09	0.53
1:L:58:ILE:HD13	1:M:34:LYS:HE2	1.90	0.53
1:F:3:GLN:NE2	1:G:92:THR:HG22	2.24	0.53
1:H:56:GLN:HE21	1:H:56:GLN:N	2.00	0.53
1:Y:102:LYS:O	1:Y:103:ASN:HB2	2.09	0.53
1:D:23:LYS:HE2	1:H:103:ASN:ND2	2.25	0.52
1:N:12:TYR:OH	1:O:35:ARG:HG2	2.10	0.52
1:Y:89:ASN:HD22	1:Y:90:ASN:N	2.08	0.52
1:H:43:LYS:HG3	3:H:119:HOH:O	2.08	0.52
1:L:2:PRO:HD3	1:M:35:ARG:CZ	2.40	0.52
1:V:13:ARG:O	1:V:14:ASN:HB2	2.09	0.52
1:F:75:THR:HG23	1:F:80:THR:HB	1.91	0.52
1:L:93:PRO:HG3	1:P:3:GLN:HG2	1.90	0.52
1:P:1:ALA:HB1	1:P:2:PRO:HD2	1.91	0.52
1:L:62:LYS:HZ1	1:L:63:LYS:HE2	1.75	0.52
1:F:103:ASN:HD22	1:G:23:LYS:NZ	2.07	0.52
1:N:1:ALA:HB1	1:N:2:PRO:CD	2.34	0.52
1:V:100:SER:HB2	1:W:28:THR:OG1	2.10	0.52
2:D:104:A32:C4'	2:D:104:A32:H9'1	2.40	0.51
1:Y:65:ILE:HG12	1:Z:31:MET:CE	2.40	0.51
1:E:12:TYR:CZ	1:F:32:ALA:HB1	2.45	0.51
1:X:103:ASN:O	1:Y:25:LEU:HD12	2.09	0.51
2:F:104:A32:H6'1	3:F:216:HOH:O	2.10	0.51
1:L:62:LYS:NZ	1:L:63:LYS:HG2	2.26	0.51
1:X:6:THR:HA	1:X:17:ILE:HD11	1.92	0.51
1:W:100:SER:HB2	3:W:142:HOH:O	2.09	0.51
2:W:104:A32:H2A1	1:X:34:LYS:HB2	1.93	0.51
1:L:21:ASN:HD21	1:L:81:LYS:HZ1	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:59:ASP:HB2	3:W:124:HOH:O	2.11	0.51
1:N:43:LYS:HG2	3:N:147:HOH:O	2.12	0.50
1:M:49:GLN:HB3	1:M:93:PRO:HG2	1.93	0.50
1:Z:11:GLU:HB3	2:Z:104:A32:C5B	2.38	0.50
1:P:13:ARG:O	1:P:14:ASN:HB2	2.10	0.50
1:W:93:PRO:HA	3:W:140:HOH:O	2.11	0.50
1:V:101:MET:HE2	1:W:76:TYR:HE2	1.76	0.50
1:X:51:GLU:HG3	1:X:95:SER:OG	2.12	0.50
1:D:2:PRO:HB3	1:D:7:GLU:HG2	1.93	0.50
1:X:8:LEU:HD11	1:Y:30:SER:CB	2.40	0.50
1:Y:12:TYR:HB2	1:Y:15:THR:HG21	1.93	0.49
1:Z:2:PRO:HB3	1:Z:7:GLU:HB2	1.92	0.49
1:N:30:SER:O	1:N:36:GLU:HA	2.12	0.49
1:W:102:LYS:HA	1:X:25:LEU:O	2.12	0.49
1:V:2:PRO:HD3	1:W:35:ARG:CZ	2.42	0.49
1:W:37:MET:HE1	1:W:39:ILE:HG12	1.93	0.49
1:L:9:CYS:CB	1:L:17:ILE:HD11	2.43	0.49
1:V:30:SER:HB3	1:V:35:ARG:O	2.13	0.49
1:L:35:ARG:HB3	1:P:8:LEU:HD11	1.94	0.49
1:E:82:ILE:HG12	1:E:99:ILE:HD11	1.95	0.49
1:V:20:ILE:HG21	1:V:42:PHE:CE1	2.47	0.49
1:Z:88:TRP:CZ3	2:Z:104:A32:H62	2.48	0.48
1:W:78:THR:O	1:W:79:GLU:C	2.52	0.48
2:O:104:A32:C4'	2:O:104:A32:C9'	2.86	0.48
2:F:104:A32:H4'1	3:F:217:HOH:O	2.12	0.48
1:V:49:GLN:O	1:V:96:ILE:HG13	2.13	0.48
1:Y:81:LYS:HB2	1:Y:81:LYS:NZ	2.28	0.48
1:W:37:MET:CE	1:W:39:ILE:HG12	2.42	0.48
1:N:62:LYS:N	1:N:62:LYS:NZ	2.61	0.48
1:X:30:SER:O	1:X:36:GLU:HA	2.14	0.48
1:H:81:LYS:HE2	3:H:141:HOH:O	2.13	0.48
1:V:75:THR:HG23	1:V:80:THR:HB	1.96	0.48
1:L:61:GLN:HG2	1:M:31:MET:O	2.14	0.48
1:N:65:ILE:HG22	1:N:69:LYS:HE2	1.95	0.47
1:W:20:ILE:HD12	1:W:85:LEU:HG	1.95	0.47
1:P:43:LYS:HB2	3:P:139:HOH:O	2.13	0.47
1:E:44:SER:HB2	3:E:156:HOH:O	2.14	0.47
1:V:16:GLN:HB2	1:V:89:ASN:ND2	2.29	0.47
1:F:103:ASN:HB3	1:G:23:LYS:HZ1	1.79	0.47
1:D:3:GLN:HG2	1:E:93:PRO:HD3	1.96	0.47
1:X:21:ASN:OD1	1:X:81:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:80:THR:HG21	1:V:101:MET:CE	2.43	0.47
1:X:103:ASN:ND2	1:Y:23:LYS:NZ	2.63	0.47
1:L:85:LEU:HD23	1:L:99:ILE:HG13	1.97	0.47
1:W:32:ALA:O	1:W:33:GLY:C	2.52	0.47
1:V:93:PRO:HG3	1:Z:3:GLN:CG	2.43	0.47
1:Y:88:TRP:HZ2	3:Y:167:HOH:O	1.97	0.47
1:P:56:GLN:NE2	1:P:56:GLN:H	2.03	0.47
1:L:21:ASN:HD21	1:L:81:LYS:NZ	2.13	0.47
1:V:80:THR:HG21	1:V:101:MET:HE2	1.97	0.47
2:X:104:A32:H6'1	3:X:141:HOH:O	2.14	0.47
1:D:62:LYS:HD2	1:D:62:LYS:O	2.15	0.47
1:F:28:THR:HB	1:F:39:ILE:HB	1.97	0.47
1:D:101:MET:HE3	1:E:77:LEU:HD21	1.97	0.47
1:Y:91:LYS:NZ	2:Y:104:A32:O3	2.41	0.47
1:V:61:GLN:NE2	1:W:33:GLY:H	2.12	0.47
1:W:57:HIS:HA	1:W:61:GLN:OE1	2.15	0.47
2:D:104:A32:H4'1	2:D:104:A32:C9'	2.45	0.47
2:W:104:A32:H8'1	2:W:104:A32:H3'1	1.75	0.47
1:O:20:ILE:CG1	1:O:85:LEU:HD12	2.45	0.47
1:W:91:LYS:O	1:W:94:ASN:ND2	2.47	0.46
1:F:12:TYR:CE1	2:F:104:A32:H7'2	2.50	0.46
1:O:33:GLY:O	1:O:34:LYS:HB2	2.16	0.46
1:F:103:ASN:HD22	1:G:23:LYS:HZ3	1.63	0.46
2:G:104:A32:H2'1	2:G:104:A32:H51	1.97	0.46
1:X:35:ARG:O	1:X:37:MET:HG2	2.15	0.46
1:D:16:GLN:OE1	1:D:89:ASN:HB3	2.15	0.46
1:H:43:LYS:O	1:Z:13:ARG:HD3	2.15	0.46
1:V:57:HIS:HA	1:V:61:GLN:OE1	2.16	0.46
1:V:101:MET:HE1	1:W:77:LEU:HD21	1.98	0.46
1:Y:18:TYR:O	1:Y:84:LYS:HA	2.16	0.46
1:Y:88:TRP:CE2	2:Y:104:A32:H51	2.51	0.46
1:V:99:ILE:HG12	1:V:100:SER:H	1.79	0.46
1:V:12:TYR:CZ	2:V:104:A32:H2A1	2.51	0.46
1:O:16:GLN:HG2	1:O:18:TYR:CE1	2.51	0.46
1:L:89:ASN:HA	1:L:94:ASN:ND2	2.30	0.46
1:Z:20:ILE:O	1:Z:21:ASN:C	2.54	0.46
1:Y:13:ARG:HG3	1:Y:13:ARG:HH11	1.80	0.45
1:F:103:ASN:ND2	1:G:79:GLU:OE2	2.34	0.45
1:W:7:GLU:O	1:W:8:LEU:C	2.55	0.45
1:M:88:TRP:HE3	1:M:95:SER:HB3	1.82	0.45
1:G:57:HIS:O	1:G:62:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:75:THR:HG23	1:V:80:THR:CG2	2.46	0.45
1:D:80:THR:HG21	1:D:101:MET:CE	2.46	0.45
1:H:9:CYS:HB2	1:H:17:ILE:HD11	1.98	0.45
1:N:90:ASN:HB3	3:N:154:HOH:O	2.17	0.45
1:Z:10:SER:HB2	3:Z:146:HOH:O	2.16	0.45
1:V:20:ILE:O	1:V:21:ASN:C	2.54	0.45
1:Z:23:LYS:HE3	3:Z:152:HOH:O	2.16	0.45
1:N:48:PHE:CD2	1:N:87:VAL:HG11	2.51	0.45
1:W:64:ALA:HB1	1:X:31:MET:HA	1.98	0.45
1:E:44:SER:HA	3:E:146:HOH:O	2.17	0.45
1:X:24:ILE:HD11	1:X:82:ILE:HD11	1.99	0.45
1:X:8:LEU:CD1	1:Y:30:SER:HB2	2.46	0.45
1:N:20:ILE:HG21	1:N:42:PHE:CE1	2.52	0.45
2:O:104:A32:H5'1	1:P:34:LYS:CG	2.47	0.45
1:P:9:CYS:O	1:P:10:SER:C	2.55	0.45
1:D:102:LYS:HE3	1:E:25:LEU:HD11	1.98	0.45
1:O:97:ALA:HB1	3:O:158:HOH:O	2.17	0.45
1:V:11:GLU:C	2:V:104:A32:H6A1	2.37	0.44
1:F:11:GLU:OE1	2:F:104:A32:H3'1	2.18	0.44
1:W:20:ILE:HD13	1:W:42:PHE:CE2	2.51	0.44
1:L:101:MET:HE2	1:M:76:TYR:HE2	1.82	0.44
1:G:20:ILE:HG21	1:G:42:PHE:CE1	2.52	0.44
1:V:17:ILE:CG2	1:V:84:LYS:HG2	2.47	0.44
1:L:21:ASN:O	1:L:22:ASP:HB2	2.17	0.44
1:W:33:GLY:O	1:W:34:LYS:HB2	2.18	0.44
1:P:86:CYS:HB3	1:P:98:ALA:HB3	1.98	0.44
2:L:104:A32:H6A1	1:M:34:LYS:HD2	2.00	0.44
2:M:104:A32:H2'1	2:M:104:A32:O5	2.16	0.44
1:W:88:TRP:CH2	2:W:104:A32:H62	2.52	0.44
3:H:164:HOH:O	1:Z:13:ARG:HD2	2.18	0.44
1:G:20:ILE:O	1:G:21:ASN:C	2.55	0.44
1:Z:44:SER:OG	1:Z:46:GLU:OE1	2.36	0.44
1:V:75:THR:HG23	1:V:80:THR:HG22	2.00	0.44
1:Y:85:LEU:HD13	1:Y:96:ILE:HG12	2.00	0.44
1:V:58:ILE:HD11	1:W:33:GLY:HA2	2.00	0.44
1:G:20:ILE:HD12	3:G:156:HOH:O	2.17	0.44
1:L:65:ILE:HG22	1:L:69:LYS:HE2	1.99	0.44
1:Y:57:HIS:NE2	2:Y:104:A32:H61	2.33	0.43
1:G:58:ILE:CD1	1:G:60:SER:OG	2.66	0.43
1:X:85:LEU:HD23	1:X:99:ILE:HG13	2.00	0.43
1:V:35:ARG:HA	1:V:35:ARG:HD3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2:PRO:CB	1:O:7:GLU:HG3	2.48	0.43
1:V:19:THR:HG23	1:V:84:LYS:HE2	1.99	0.43
1:D:75:THR:HG23	1:D:80:THR:HB	2.00	0.43
1:Y:49:GLN:HB3	1:Y:93:PRO:HG2	2.00	0.43
2:E:104:A32:H3'1	2:E:104:A32:H8'1	1.46	0.43
1:Z:91:LYS:NZ	2:Z:104:A32:O4	2.51	0.43
1:V:30:SER:O	1:V:36:GLU:HA	2.18	0.43
2:F:104:A32:H5'1	2:F:104:A32:H8'1	1.50	0.43
2:V:104:A32:H2'1	2:V:104:A32:H11	1.78	0.43
1:M:85:LEU:HD23	1:M:99:ILE:HG13	2.00	0.43
1:G:92:THR:HA	1:G:93:PRO:C	2.38	0.43
1:W:26:SER:HB3	1:W:41:THR:OG1	2.18	0.43
1:V:35:ARG:HH11	1:V:35:ARG:HG2	1.84	0.43
1:G:59:ASP:HA	1:G:62:LYS:HG2	2.01	0.43
1:F:67:ARG:HG2	1:G:29:GLU:OE2	2.19	0.43
1:Y:21:ASN:OD1	1:Y:81:LYS:HD3	2.17	0.43
1:G:8:LEU:C	1:G:8:LEU:HD23	2.39	0.43
1:Z:6:THR:HG23	1:Z:17:ILE:HD12	2.01	0.43
1:P:20:ILE:HG21	1:P:42:PHE:CE2	2.54	0.43
2:E:104:A32:H6'1	3:E:191:HOH:O	2.19	0.43
1:X:67:ARG:HG2	1:Y:29:GLU:OE2	2.19	0.43
1:Y:78:THR:O	1:Y:79:GLU:HB2	2.19	0.43
1:Z:31:MET:HE3	1:Z:31:MET:HB2	1.83	0.42
1:V:62:LYS:HE3	1:V:63:LYS:HG2	2.01	0.42
1:L:102:LYS:HE3	1:M:25:LEU:HD11	2.00	0.42
1:H:9:CYS:CB	1:H:17:ILE:HD11	2.49	0.42
1:W:1:ALA:CB	1:W:2:PRO:CD	2.87	0.42
1:V:58:ILE:HG13	1:V:61:GLN:HG3	2.02	0.42
1:M:6:THR:HG23	1:M:17:ILE:HG13	2.01	0.42
1:Y:20:ILE:HG21	1:Y:42:PHE:CZ	2.54	0.42
1:H:62:LYS:HA	1:H:62:LYS:HD2	1.77	0.42
1:Z:85:LEU:CD2	1:Z:99:ILE:HG22	2.49	0.42
1:M:87:VAL:HA	1:M:95:SER:O	2.20	0.42
1:F:63:LYS:HE3	3:F:209:HOH:O	2.19	0.42
1:E:9:CYS:HB3	3:E:122:HOH:O	2.20	0.42
1:P:22:ASP:HA	1:P:81:LYS:HG3	2.02	0.42
2:D:104:A32:H8'1	1:E:34:LYS:HE2	2.02	0.42
1:Z:21:ASN:O	1:Z:22:ASP:HB2	2.20	0.42
1:F:102:LYS:HE3	1:F:102:LYS:HB2	1.82	0.42
1:Y:99:ILE:HG22	1:Z:29:GLU:HB3	2.01	0.42
1:Z:15:THR:O	1:Z:16:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:21:ASN:HA	1:P:82:ILE:O	2.20	0.42
1:Y:15:THR:O	1:Y:16:GLN:HB3	2.19	0.41
1:W:30:SER:O	1:W:36:GLU:HA	2.20	0.41
1:V:49:GLN:OE1	1:V:51:GLU:HA	2.19	0.41
1:V:58:ILE:HD11	1:W:33:GLY:CA	2.49	0.41
2:G:104:A32:H8'1	2:G:104:A32:H5'1	1.51	0.41
1:W:49:GLN:O	1:W:96:ILE:HG13	2.19	0.41
1:V:93:PRO:HD3	1:Z:1:ALA:O	2.21	0.41
1:Z:92:THR:HA	1:Z:93:PRO:C	2.40	0.41
1:O:16:GLN:NE2	1:O:89:ASN:HD22	2.11	0.41
1:Y:40:ILE:HG13	1:Y:40:ILE:O	2.20	0.41
1:V:5:ILE:HG22	3:V:110:HOH:O	2.19	0.41
1:W:4:THR:O	1:W:5:ILE:C	2.58	0.41
1:E:43:LYS:HB3	1:E:43:LYS:HE2	1.84	0.41
1:Y:33:GLY:O	1:Y:34:LYS:HB2	2.20	0.41
1:V:20:ILE:HG21	1:V:42:PHE:CD1	2.54	0.41
1:W:89:ASN:O	1:W:91:LYS:N	2.52	0.41
1:F:92:THR:HA	1:F:93:PRO:C	2.40	0.41
1:W:12:TYR:CE2	2:W:104:A32:H7'2	2.55	0.41
1:Y:41:THR:HG22	1:Y:47:THR:HG23	2.02	0.41
1:D:12:TYR:OH	2:D:104:A32:H6A1	2.20	0.41
1:X:25:LEU:HD22	1:X:43:LYS:HA	2.01	0.41
1:N:57:HIS:O	1:N:62:LYS:HE3	2.21	0.41
1:V:99:ILE:HG12	1:V:100:SER:N	2.36	0.41
1:H:30:SER:O	1:H:36:GLU:HA	2.21	0.41
1:Z:90:ASN:OD1	1:Z:90:ASN:N	2.50	0.41
1:D:17:ILE:HD13	1:D:17:ILE:HA	1.89	0.41
1:L:92:THR:HA	1:L:93:PRO:HA	1.85	0.41
1:L:31:MET:O	1:P:61:GLN:HG2	2.21	0.41
1:D:99:ILE:HG21	1:D:99:ILE:HD13	1.88	0.41
1:N:103:ASN:HD22	1:O:23:LYS:CE	2.28	0.41
1:D:23:LYS:CE	1:H:103:ASN:ND2	2.84	0.41
1:D:34:LYS:HB2	2:H:104:A32:H7'2	2.03	0.41
1:Y:82:ILE:HG12	1:Y:99:ILE:HD11	2.03	0.41
1:Y:8:LEU:HD23	1:Y:8:LEU:C	2.41	0.41
1:O:51:GLU:OE2	1:O:91:LYS:HE2	2.21	0.41
1:M:20:ILE:CD1	1:M:85:LEU:HG	2.51	0.40
1:N:25:LEU:CD2	1:N:43:LYS:HA	2.51	0.40
1:M:88:TRP:CE2	2:M:104:A32:H51	2.55	0.40
1:F:103:ASN:ND2	1:G:23:LYS:NZ	2.69	0.40
1:V:58:ILE:HD13	1:W:34:LYS:HE2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:88:TRP:HB3	1:L:90:ASN:OD1	2.21	0.40
1:D:21:ASN:ND2	1:D:81:LYS:HD3	2.36	0.40
1:H:21:ASN:HA	1:H:82:ILE:O	2.21	0.40
1:L:26:SER:O	1:L:40:ILE:HA	2.21	0.40
1:Z:87:VAL:HB	1:Z:95:SER:O	2.21	0.40
1:N:58:ILE:CD1	1:O:34:LYS:HE3	2.52	0.40
1:V:12:TYR:CD2	2:V:104:A32:H6'2	2.55	0.40
1:E:20:ILE:O	1:E:21:ASN:C	2.60	0.40
1:L:28:THR:HB	1:L:39:ILE:HB	2.03	0.40
1:L:12:TYR:CZ	1:M:32:ALA:HB1	2.57	0.40
1:E:92:THR:HA	1:E:93:PRO:C	2.41	0.40
1:G:58:ILE:H	1:G:58:ILE:HG13	1.75	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	D	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	E	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	F	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	G	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	H	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
1	L	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	19	10
1	M	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	19	10
1	N	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
1	O	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
1	P	101/103 (98%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	V	101/103 (98%)	88 (87%)	12 (12%)	1 (1%)	19 10
1	W	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	9 3
1	X	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	19 10
1	Y	101/103 (98%)	98 (97%)	3 (3%)	0	100 100
1	Z	101/103 (98%)	94 (93%)	4 (4%)	3 (3%)	5 1
All	All	1515/1545 (98%)	1442 (95%)	64 (4%)	9 (1%)	30 21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	14	ASN
1	V	59	ASP
1	X	83	ASP
1	W	90	ASN
1	Z	16	GLN
1	L	10	SER
1	Z	21	ASN
1	Z	83	ASP
1	W	33	GLY

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	D	95/95 (100%)	90 (95%)	5 (5%)	28 23
1	E	95/95 (100%)	92 (97%)	3 (3%)	46 44
1	F	95/95 (100%)	91 (96%)	4 (4%)	36 32
1	G	95/95 (100%)	91 (96%)	4 (4%)	36 32
1	H	95/95 (100%)	91 (96%)	4 (4%)	36 32
1	L	95/95 (100%)	91 (96%)	4 (4%)	36 32
1	M	95/95 (100%)	89 (94%)	6 (6%)	22 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	95/95 (100%)	91 (96%)	4 (4%)	36 32
1	O	95/95 (100%)	89 (94%)	6 (6%)	22 16
1	P	95/95 (100%)	89 (94%)	6 (6%)	22 16
1	V	95/95 (100%)	86 (90%)	9 (10%)	11 5
1	W	95/95 (100%)	89 (94%)	6 (6%)	22 16
1	X	95/95 (100%)	91 (96%)	4 (4%)	36 32
1	Y	95/95 (100%)	92 (97%)	3 (3%)	46 44
1	Z	95/95 (100%)	84 (88%)	11 (12%)	7 3
All	All	1425/1425 (100%)	1346 (94%)	79 (6%)	27 21

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	34	LYS
1	D	43	LYS
1	D	62	LYS
1	D	63	LYS
1	D	81	LYS
1	E	44	SER
1	E	101	MET
1	E	103	ASN
1	F	3	GLN
1	F	16	GLN
1	F	74	ILE
1	F	101	MET
1	G	13	ARG
1	G	27	TYR
1	G	102	LYS
1	G	103	ASN
1	H	13	ARG
1	H	56	GLN
1	H	59	ASP
1	H	103	ASN
1	L	34	LYS
1	L	43	LYS
1	L	62	LYS
1	L	103	ASN
1	M	55	SER
1	M	81	LYS

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Mol	Chain	Res	Type
1	M	84	LYS
1	M	95	SER
1	M	102	LYS
1	M	103	ASN
1	N	55	SER
1	N	59	ASP
1	N	62	LYS
1	N	95	SER
1	O	16	GLN
1	O	23	LYS
1	O	43	LYS
1	O	59	ASP
1	O	81	LYS
1	O	103	ASN
1	P	13	ARG
1	P	43	LYS
1	P	55	SER
1	P	56	GLN
1	P	81	LYS
1	P	103	ASN
1	V	28	THR
1	V	34	LYS
1	V	35	ARG
1	V	43	LYS
1	V	62	LYS
1	V	63	LYS
1	V	84	LYS
1	V	100	SER
1	V	101	MET
1	W	3	GLN
1	W	34	LYS
1	W	81	LYS
1	W	92	THR
1	W	102	LYS
1	W	103	ASN
1	X	3	GLN
1	X	10	SER
1	X	38	VAL
1	X	92	THR
1	Y	13	ARG
1	Y	16	GLN
1	Y	89	ASN

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Mol	Chain	Res	Type
1	Z	4	THR
1	Z	7	GLU
1	Z	43	LYS
1	Z	55	SER
1	Z	56	GLN
1	Z	59	ASP
1	Z	62	LYS
1	Z	79	GLU
1	Z	82	ILE
1	Z	95	SER
1	Z	99	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	21	ASN
1	D	103	ASN
1	E	16	GLN
1	E	94	ASN
1	F	3	GLN
1	F	103	ASN
1	G	3	GLN
1	H	56	GLN
1	H	103	ASN
1	L	21	ASN
1	L	103	ASN
1	N	3	GLN
1	N	94	ASN
1	N	103	ASN
1	O	89	ASN
1	P	56	GLN
1	P	103	ASN
1	V	21	ASN
1	V	94	ASN
1	V	103	ASN
1	W	3	GLN
1	X	94	ASN
1	X	103	ASN
1	Y	3	GLN
1	Y	14	ASN
1	Y	16	GLN
1	Y	89	ASN

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Mol	Chain	Res	Type
1	Z	3	GLN
1	Z	56	GLN

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

14 ligands 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	$\#\|Z\| > 2$
2	A32	D	104	-	33,35,35	1.75	7 (21%)	46,48,48	2.91	22 (47%)
2	A32	E	104	-	33,35,35	1.81	9 (27%)	46,48,48	3.14	17 (36%)
2	A32	F	104	-	33,35,35	1.67	7 (21%)	46,48,48	2.80	19 (41%)
2	A32	G	104	-	33,35,35	1.57	6 (18%)	46,48,48	1.41	7 (15%)
2	A32	H	104	-	33,35,35	2.04	13 (39%)	46,48,48	3.24	18 (39%)
2	A32	L	104	-	33,35,35	1.70	9 (27%)	46,48,48	1.85	15 (32%)
2	A32	M	104	-	33,35,35	1.63	7 (21%)	46,48,48	1.91	13 (28%)
2	A32	O	104	-	33,35,35	1.68	7 (21%)	46,48,48	2.08	8 (17%)
2	A32	P	104	-	33,35,35	1.72	7 (21%)	46,48,48	2.14	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A32	V	104	-	33,35,35	1.75	5 (15%)	46,48,48	1.99	15 (32%)
2	A32	W	104	-	33,35,35	1.78	11 (33%)	46,48,48	2.51	12 (26%)
2	A32	X	104	-	33,35,35	1.66	8 (24%)	46,48,48	2.59	12 (26%)
2	A32	Y	104	-	33,35,35	1.77	6 (18%)	46,48,48	1.59	10 (21%)
2	A32	Z	104	-	33,35,35	1.80	9 (27%)	46,48,48	2.04	14 (30%)

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
2	A32	D	104	-	-	0/21/49/49	0/3/3/3
2	A32	E	104	-	-	0/21/49/49	0/3/3/3
2	A32	F	104	-	-	0/21/49/49	0/3/3/3
2	A32	G	104	-	-	0/21/49/49	0/3/3/3
2	A32	H	104	-	-	0/21/49/49	0/3/3/3
2	A32	L	104	-	-	0/21/49/49	0/3/3/3
2	A32	M	104	-	-	0/21/49/49	0/3/3/3
2	A32	O	104	-	-	0/21/49/49	0/3/3/3
2	A32	P	104	-	-	0/21/49/49	0/3/3/3
2	A32	V	104	-	1/1/8/9	0/21/49/49	0/3/3/3
2	A32	W	104	-	-	0/21/49/49	0/3/3/3
2	A32	X	104	-	-	0/21/49/49	0/3/3/3
2	A32	Y	104	-	-	0/21/49/49	0/3/3/3
2	A32	Z	104	-	-	0/21/49/49	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	104	A32	C7'-N2'	-4.44	1.24	1.33
2	V	104	A32	C7'-N2'	-4.26	1.24	1.33
2	H	104	A32	C7'-N2'	-4.24	1.24	1.33
2	P	104	A32	C5'-C7'	-4.23	1.41	1.50
2	Z	104	A32	C7'-N2'	-4.14	1.24	1.33
2	O	104	A32	C7'-N2'	-3.96	1.25	1.33
2	L	104	A32	C7'-N2'	-3.94	1.25	1.33
2	Z	104	A32	C5'-C7'	-3.86	1.42	1.50
2	Y	104	A32	C7'-N2'	-3.83	1.25	1.33
2	Y	104	A32	C5'-C7'	-3.81	1.42	1.50
2	M	104	A32	C7'-N2'	-3.76	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	104	A32	C5'-C7'	-3.74	1.42	1.50
2	V	104	A32	C5'-C7'	-3.72	1.42	1.50
2	O	104	A32	C5'-C7'	-3.68	1.42	1.50
2	H	104	A32	C5'-C7'	-3.62	1.42	1.50
2	D	104	A32	C5'-C7'	-3.57	1.42	1.50
2	G	104	A32	C5'-C7'	-3.56	1.42	1.50
2	M	104	A32	C5'-C7'	-3.55	1.42	1.50
2	W	104	A32	C5'-C7'	-3.55	1.42	1.50
2	L	104	A32	C5'-C7'	-3.44	1.42	1.50
2	E	104	A32	C5'-C7'	-3.32	1.43	1.50
2	G	104	A32	C7'-N2'	-3.26	1.26	1.33
2	X	104	A32	C7'-N2'	-3.23	1.26	1.33
2	W	104	A32	C7'-N2'	-3.21	1.26	1.33
2	F	104	A32	C5'-C7'	-3.00	1.43	1.50
2	E	104	A32	C7'-N2'	-2.94	1.27	1.33
2	P	104	A32	C7'-N2'	-2.68	1.28	1.33
2	F	104	A32	C7'-N2'	-2.64	1.28	1.33
2	L	104	A32	C9'-N2'	-2.49	1.40	1.46
2	H	104	A32	C9'-N2'	-2.40	1.40	1.46
2	Z	104	A32	O3-C3	-2.21	1.37	1.43
2	M	104	A32	C9'-N2'	-2.04	1.41	1.46
2	M	104	A32	O3'-C7'	2.01	1.27	1.23
2	G	104	A32	C5B-N4'	2.01	1.52	1.46
2	W	104	A32	C4'-C3'	2.01	1.42	1.39
2	G	104	A32	C4'-C5'	2.02	1.42	1.39
2	Z	104	A32	C2'-C3'	2.02	1.42	1.39
2	H	104	A32	C7B-N4'	2.04	1.52	1.47
2	O	104	A32	O3'-C7'	2.04	1.27	1.23
2	L	104	A32	O2'-N1'	2.04	1.26	1.22
2	H	104	A32	C3B-N4'	2.05	1.52	1.46
2	O	104	A32	C3B-N4'	2.06	1.52	1.46
2	Z	104	A32	C3B-N4'	2.06	1.52	1.46
2	M	104	A32	C4'-C5'	2.06	1.42	1.39
2	P	104	A32	C3B-N4'	2.09	1.52	1.46
2	L	104	A32	C2'-C3'	2.12	1.43	1.39
2	P	104	A32	C5B-N4'	2.12	1.52	1.46
2	V	104	A32	C4'-C3'	2.12	1.43	1.39
2	O	104	A32	C4'-C5'	2.13	1.42	1.39
2	W	104	A32	O5-C1	2.14	1.47	1.41
2	W	104	A32	C2'-C3'	2.21	1.43	1.39
2	Y	104	A32	C7B-N4'	2.22	1.52	1.47
2	W	104	A32	O3'-C7'	2.22	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	104	A32	C7B-N4'	2.23	1.52	1.47
2	Z	104	A32	O2'-N1'	2.24	1.27	1.22
2	L	104	A32	C5B-N4'	2.26	1.53	1.46
2	Y	104	A32	O3'-C7'	2.30	1.27	1.23
2	L	104	A32	C4'-C5'	2.31	1.42	1.39
2	E	104	A32	C7B-N4'	2.37	1.53	1.47
2	M	104	A32	O1-C1	2.38	1.45	1.41
2	X	104	A32	C2'-C3'	2.38	1.43	1.39
2	W	104	A32	O2'-N1'	2.38	1.27	1.22
2	W	104	A32	C6'-C5'	2.40	1.43	1.39
2	D	104	A32	C6'-C5'	2.40	1.43	1.39
2	H	104	A32	C4-C3	2.41	1.58	1.52
2	X	104	A32	C4-C3	2.46	1.58	1.52
2	H	104	A32	C4'-C5'	2.46	1.43	1.39
2	X	104	A32	C4'-C3'	2.47	1.43	1.39
2	H	104	A32	C6'-C5'	2.47	1.43	1.39
2	D	104	A32	C4'-C3'	2.51	1.43	1.39
2	E	104	A32	O1-C1'	2.53	1.43	1.38
2	F	104	A32	C2'-C3'	2.54	1.43	1.39
2	E	104	A32	C4'-C5'	2.57	1.43	1.39
2	O	104	A32	O1-C1	2.58	1.45	1.41
2	Z	104	A32	O1-C1	2.59	1.45	1.41
2	E	104	A32	C4'-C3'	2.61	1.44	1.39
2	F	104	A32	O2'-N1'	2.67	1.28	1.22
2	X	104	A32	C4'-C5'	2.69	1.43	1.39
2	H	104	A32	C2'-C3'	2.69	1.44	1.39
2	H	104	A32	O1-C1'	2.70	1.44	1.38
2	Z	104	A32	O1-C1'	2.73	1.44	1.38
2	Z	104	A32	C5B-N4'	2.73	1.54	1.46
2	L	104	A32	O1-C1	2.76	1.45	1.41
2	G	104	A32	O1-C1	2.81	1.45	1.41
2	V	104	A32	O1-C1'	2.86	1.44	1.38
2	D	104	A32	O3'-C7'	2.89	1.29	1.23
2	X	104	A32	O2'-N1'	2.95	1.28	1.22
2	W	104	A32	O1-C1	2.97	1.46	1.41
2	P	104	A32	O1-C1	2.98	1.46	1.41
2	G	104	A32	O1-C1'	3.01	1.44	1.38
2	E	104	A32	C6'-C5'	3.03	1.43	1.39
2	W	104	A32	C4'-C5'	3.04	1.43	1.39
2	F	104	A32	C4'-C5'	3.04	1.43	1.39
2	W	104	A32	O1-C1'	3.05	1.44	1.38
2	L	104	A32	O1-C1'	3.08	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	104	A32	C2'-C3'	3.09	1.45	1.39
2	H	104	A32	O2'-N1'	3.17	1.29	1.22
2	D	104	A32	O1-C1'	3.23	1.45	1.38
2	P	104	A32	O1-C1'	3.23	1.45	1.38
2	M	104	A32	O1-C1'	3.24	1.45	1.38
2	O	104	A32	O1-C1'	3.26	1.45	1.38
2	P	104	A32	C4'-C5'	3.27	1.44	1.39
2	Y	104	A32	O1-C1'	3.33	1.45	1.38
2	H	104	A32	O3'-C7'	3.41	1.30	1.23
2	F	104	A32	O1-C1'	3.51	1.45	1.38
2	D	104	A32	O1-C1	3.64	1.47	1.41
2	F	104	A32	O3'-C7'	3.75	1.30	1.23
2	Y	104	A32	O1-C1	3.79	1.47	1.41
2	E	104	A32	O2'-N1'	3.89	1.30	1.22
2	V	104	A32	O1-C1	3.99	1.47	1.41
2	H	104	A32	O1-C1	4.14	1.48	1.41

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	104	A32	C2'-C3'-N1'	-6.85	112.80	118.80
2	H	104	A32	C6'-C5'-C4'	-5.43	113.17	119.64
2	E	104	A32	O3'-C7'-N2'	-5.39	111.27	122.58
2	D	104	A32	O3'-C7'-C5'	-5.23	112.04	120.97
2	X	104	A32	C6'-C5'-C4'	-5.22	113.41	119.64
2	F	104	A32	C6'-C5'-C4'	-5.10	113.56	119.64
2	E	104	A32	C6'-C5'-C4'	-4.44	114.35	119.64
2	P	104	A32	O3'-C7'-N2'	-4.37	113.41	122.58
2	F	104	A32	C2'-C3'-N1'	-4.23	115.09	118.80
2	V	104	A32	O3'-C7'-C5'	-4.22	113.76	120.97
2	H	104	A32	C1'-O1-C1	-4.00	111.91	117.87
2	D	104	A32	C1'-O1-C1	-3.95	111.98	117.87
2	M	104	A32	O3'-C7'-C5'	-3.92	114.27	120.97
2	H	104	A32	O3'-C7'-N2'	-3.88	114.42	122.58
2	W	104	A32	C2'-C3'-N1'	-3.79	115.47	118.80
2	Z	104	A32	C6'-C5'-C4'	-3.68	115.25	119.64
2	X	104	A32	C4-C3-C2	-3.54	104.18	110.79
2	O	104	A32	O3'-C7'-C5'	-3.51	114.98	120.97
2	D	104	A32	C5'-C6'-C1'	-3.47	115.86	119.56
2	W	104	A32	C6'-C5'-C4'	-3.44	115.54	119.64
2	X	104	A32	O3'-C7'-N2'	-3.44	115.36	122.58
2	F	104	A32	C2B-C3B-N4'	-3.40	104.98	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	104	A32	C6'-C5'-C4'	-3.37	115.63	119.64
2	X	104	A32	O3-C3-C4	-3.36	102.77	110.34
2	G	104	A32	C8'-C7B-N4'	-3.35	105.46	113.89
2	Y	104	A32	C1'-O1-C1	-3.28	112.98	117.87
2	Z	104	A32	C2B-C3B-N4'	-3.19	105.29	110.12
2	V	104	A32	C1-O5-C5	-3.16	107.61	113.75
2	E	104	A32	C8'-C7B-N4'	-3.13	106.02	113.89
2	L	104	A32	C6B-C5B-N4'	-3.12	105.39	110.12
2	E	104	A32	C4'-C3'-C2'	-3.04	115.56	120.69
2	Y	104	A32	C6'-C5'-C4'	-3.04	116.02	119.64
2	Z	104	A32	O3'-C7'-C5'	-2.93	115.96	120.97
2	D	104	A32	C4-C3-C2	-2.93	105.32	110.79
2	Z	104	A32	C3-C4-C5	-2.84	105.25	110.20
2	P	104	A32	C2B-C3B-N4'	-2.79	105.90	110.12
2	F	104	A32	C8'-C7B-N4'	-2.72	107.06	113.89
2	G	104	A32	C6'-C5'-C4'	-2.70	116.42	119.64
2	V	104	A32	C6B-C5B-N4'	-2.68	106.07	110.12
2	H	104	A32	O3-C3-C2	-2.66	104.35	110.34
2	M	104	A32	C6'-C5'-C4'	-2.65	116.48	119.64
2	D	104	A32	C4'-C3'-C2'	-2.64	116.23	120.69
2	E	104	A32	O2-C2-C3	-2.57	104.54	110.34
2	Z	104	A32	C7B-N4'-C5B	-2.53	104.78	111.27
2	L	104	A32	C2B-C3B-N4'	-2.53	106.30	110.12
2	H	104	A32	C4'-C3'-C2'	-2.49	116.50	120.69
2	L	104	A32	C6'-C5'-C4'	-2.48	116.68	119.64
2	H	104	A32	O2'-N1'-C3'	-2.48	114.44	118.89
2	E	104	A32	C6B-C5B-N4'	-2.40	106.49	110.12
2	Y	104	A32	O3'-C7'-C5'	-2.36	116.94	120.97
2	W	104	A32	C1-O5-C5	-2.32	109.23	113.75
2	E	104	A32	O5-C1-C2	-2.28	105.59	110.28
2	O	104	A32	C4'-C3'-C2'	-2.27	116.86	120.69
2	H	104	A32	O3'-C7'-C5'	-2.23	117.16	120.97
2	G	104	A32	O2-C2-C1	-2.22	105.16	110.02
2	F	104	A32	C6B-C5B-N4'	-2.18	106.81	110.12
2	M	104	A32	O1B-C2B-C3B	-2.17	106.87	111.84
2	V	104	A32	C1'-O1-C1	-2.14	114.69	117.87
2	W	104	A32	O3'-C7'-N2'	-2.12	118.13	122.58
2	F	104	A32	C4'-C3'-C2'	-2.12	117.12	120.69
2	Z	104	A32	O5-C5-C4	-2.11	105.72	109.68
2	F	104	A32	C9'-N2'-C7'	-2.10	117.44	122.15
2	F	104	A32	O3'-C7'-N2'	-2.09	118.18	122.58
2	W	104	A32	C4'-C3'-C2'	-2.09	117.17	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	104	A32	C8'-C7B-N4'	-2.08	108.66	113.89
2	E	104	A32	O1B-C2B-C3B	-2.07	107.10	111.84
2	D	104	A32	C4'-C3'-N1'	-2.05	117.00	118.80
2	D	104	A32	O3-C3-C4	-2.04	105.75	110.34
2	G	104	A32	C3'-C2'-C1'	-2.01	116.65	119.12
2	M	104	A32	C9'-N2'-C7'	2.00	126.63	122.15
2	M	104	A32	C5'-C7'-N2'	2.00	121.62	117.12
2	D	104	A32	C8'-C7B-N4'	2.01	118.94	113.89
2	W	104	A32	C5B-N4'-C3B	2.01	113.25	108.90
2	V	104	A32	O3'-C7'-N2'	2.02	126.82	122.58
2	F	104	A32	C6B-O1B-C2B	2.02	116.69	109.89
2	G	104	A32	O5-C5-C6	2.04	111.51	106.36
2	V	104	A32	C4-C3-C2	2.05	114.62	110.79
2	P	104	A32	C6'-C1'-C2'	2.05	124.54	120.99
2	Z	104	A32	O5-C5-C6	2.06	111.56	106.36
2	L	104	A32	O3-C3-C2	2.07	115.00	110.34
2	M	104	A32	C5'-C6'-C1'	2.08	121.79	119.56
2	F	104	A32	C3'-C2'-C1'	2.09	121.68	119.12
2	V	104	A32	C5B-N4'-C3B	2.10	113.44	108.90
2	X	104	A32	C5B-N4'-C3B	2.10	113.46	108.90
2	M	104	A32	C5'-C4'-C3'	2.11	122.20	119.74
2	D	104	A32	C6B-O1B-C2B	2.20	117.29	109.89
2	L	104	A32	C6B-O1B-C2B	2.20	117.30	109.89
2	V	104	A32	O4-C4-C3	2.20	115.30	110.34
2	D	104	A32	C4'-C5'-C7'	2.24	127.50	120.49
2	L	104	A32	O2-C2-C1	2.24	114.94	110.02
2	V	104	A32	C1-C2-C3	2.27	114.44	109.97
2	Y	104	A32	C2'-C3'-N1'	2.28	120.80	118.80
2	Y	104	A32	C6'-C1'-C2'	2.32	124.99	120.99
2	D	104	A32	O2-C2-C1	2.34	115.15	110.02
2	V	104	A32	C6-C5-C4	2.34	118.79	113.02
2	Y	104	A32	C6B-C5B-N4'	2.40	113.75	110.12
2	Z	104	A32	C5'-C7'-N2'	2.40	122.51	117.12
2	W	104	A32	C1-C2-C3	2.41	114.71	109.97
2	F	104	A32	C4'-C5'-C7'	2.45	128.16	120.49
2	G	104	A32	C5B-N4'-C3B	2.48	114.28	108.90
2	Z	104	A32	C9'-N2'-C7'	2.50	127.75	122.15
2	D	104	A32	O2'-N1'-C3'	2.55	123.47	118.89
2	L	104	A32	O5-C1-O1	2.56	115.22	108.39
2	O	104	A32	C9'-N2'-C7'	2.56	127.89	122.15
2	E	104	A32	C3'-C2'-C1'	2.58	122.28	119.12
2	H	104	A32	O5-C1-O1	2.64	115.43	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	104	A32	O5-C1-O1	2.65	115.46	108.39
2	O	104	A32	C5'-C4'-C3'	2.68	122.86	119.74
2	V	104	A32	C6'-C1'-C2'	2.68	125.62	120.99
2	H	104	A32	C6B-C5B-N4'	2.69	114.20	110.12
2	D	104	A32	C7B-N4'-C3B	2.70	118.18	111.27
2	P	104	A32	O2-C2-C3	2.78	116.59	110.34
2	V	104	A32	O3-C3-C4	2.78	116.61	110.34
2	M	104	A32	O5-C1-O1	2.80	115.88	108.39
2	L	104	A32	C7B-N4'-C3B	2.84	118.54	111.27
2	L	104	A32	O2-C2-C3	2.90	116.88	110.34
2	H	104	A32	C5B-N4'-C3B	2.91	115.20	108.90
2	Y	104	A32	O3-C3-C4	2.91	116.90	110.34
2	O	104	A32	C7B-N4'-C3B	2.94	118.82	111.27
2	Z	104	A32	O1-C1-C2	2.95	111.92	107.12
2	Y	104	A32	C5'-C7'-N2'	2.96	123.77	117.12
2	P	104	A32	C6'-C5'-C7'	2.99	129.85	120.49
2	H	104	A32	C6'-C1'-C2'	3.07	126.28	120.99
2	Z	104	A32	C5'-C4'-C3'	3.13	123.39	119.74
2	L	104	A32	C5'-C6'-C1'	3.15	122.93	119.56
2	W	104	A32	C5'-C4'-C3'	3.15	123.42	119.74
2	L	104	A32	C1'-O1-C1	3.16	122.58	117.87
2	V	104	A32	C9'-N2'-C7'	3.18	129.28	122.15
2	G	104	A32	O5-C1-O1	3.19	116.90	108.39
2	Y	104	A32	C4'-C3'-N1'	3.20	121.61	118.80
2	H	104	A32	C2B-C3B-N4'	3.22	115.01	110.12
2	D	104	A32	C6B-C5B-N4'	3.25	115.05	110.12
2	D	104	A32	C5'-C7'-N2'	3.26	124.44	117.12
2	F	104	A32	C5'-C4'-C3'	3.29	123.58	119.74
2	M	104	A32	O2-C2-C1	3.32	117.31	110.02
2	P	104	A32	C5'-C4'-C3'	3.35	123.64	119.74
2	L	104	A32	C4'-C3'-N1'	3.37	121.76	118.80
2	X	104	A32	C5'-C4'-C3'	3.42	123.73	119.74
2	E	104	A32	C5B-N4'-C3B	3.46	116.39	108.90
2	M	104	A32	C4'-C3'-N1'	3.47	121.84	118.80
2	M	104	A32	C5B-N4'-C3B	3.49	116.45	108.90
2	L	104	A32	O4-C4-C3	3.50	118.21	110.34
2	Z	104	A32	C1'-O1-C1	3.54	123.16	117.87
2	M	104	A32	C1'-O1-C1	3.57	123.20	117.87
2	D	104	A32	C6'-C1'-C2'	3.61	127.23	120.99
2	Y	104	A32	C5'-C4'-C3'	3.66	124.01	119.74
2	P	104	A32	O2-C2-C1	3.67	118.06	110.02
2	H	104	A32	C4'-C5'-C7'	3.68	132.01	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	104	A32	C9'-N2'-C7'	3.75	130.55	122.15
2	X	104	A32	O5-C1-O1	3.77	118.45	108.39
2	F	104	A32	O3'-C7'-C5'	4.01	127.82	120.97
2	E	104	A32	C5'-C7'-N2'	4.12	126.38	117.12
2	E	104	A32	C5'-C6'-C1'	4.12	123.96	119.56
2	P	104	A32	O1-C1-C2	4.14	113.86	107.12
2	W	104	A32	O1-C1-C2	4.15	113.88	107.12
2	E	104	A32	C5'-C4'-C3'	4.19	124.63	119.74
2	F	104	A32	C7B-N4'-C3B	4.20	122.04	111.27
2	D	104	A32	C5'-C4'-C3'	4.26	124.71	119.74
2	D	104	A32	O1B-C2B-C3B	4.29	121.66	111.84
2	L	104	A32	O1-C1-C2	4.34	114.18	107.12
2	X	104	A32	C5'-C6'-C1'	4.35	124.21	119.56
2	P	104	A32	C4'-C3'-N1'	4.44	122.69	118.80
2	W	104	A32	C1'-O1-C1	4.55	124.66	117.87
2	F	104	A32	O1-C1-C2	4.61	114.62	107.12
2	V	104	A32	O2-C2-C1	4.86	120.67	110.02
2	E	104	A32	O5-C1-O1	4.88	121.41	108.39
2	H	104	A32	C5'-C7'-N2'	5.01	128.38	117.12
2	H	104	A32	C9'-N2'-C7'	5.06	133.49	122.15
2	X	104	A32	O1-C1-C2	5.16	115.52	107.12
2	D	104	A32	C9'-N2'-C7'	5.22	133.84	122.15
2	F	104	A32	C1'-O1-C1	5.30	125.77	117.87
2	Z	104	A32	C4'-C3'-N1'	5.53	123.65	118.80
2	V	104	A32	C2'-C3'-N1'	5.57	123.69	118.80
2	D	104	A32	O1-C1-C2	5.63	116.28	107.12
2	Z	104	A32	O3-C3-C2	5.69	123.14	110.34
2	F	104	A32	C5'-C6'-C1'	5.70	125.65	119.56
2	H	104	A32	C5'-C4'-C3'	5.87	126.59	119.74
2	O	104	A32	C2'-C3'-N1'	6.02	124.08	118.80
2	D	104	A32	C2B-C3B-N4'	6.16	119.45	110.12
2	O	104	A32	O1-C1-C2	6.36	117.47	107.12
2	O	104	A32	O2-C2-C1	6.47	124.19	110.02
2	M	104	A32	O1-C1-C2	6.64	117.93	107.12
2	E	104	A32	O1-C1-C2	6.83	118.23	107.12
2	X	104	A32	C4'-C3'-N1'	7.05	124.98	118.80
2	P	104	A32	O3'-C7'-C5'	7.14	133.19	120.97
2	W	104	A32	O2-C2-C1	8.05	127.67	110.02
2	X	104	A32	C1'-O1-C1	8.92	131.16	117.87
2	D	104	A32	C2'-C3'-N1'	9.04	126.73	118.80
2	W	104	A32	C4'-C3'-N1'	9.73	127.33	118.80
2	E	104	A32	C4'-C3'-N1'	9.74	127.34	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	104	A32	C1'-O1-C1	9.91	132.64	117.87
2	F	104	A32	C4'-C3'-N1'	10.25	127.79	118.80
2	H	104	A32	C4'-C3'-N1'	13.58	130.70	118.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	V	104	A32	C2

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	104	A32	9	0
2	E	104	A32	2	0
2	F	104	A32	5	0
2	G	104	A32	2	0
2	H	104	A32	1	0
2	L	104	A32	3	0
2	M	104	A32	2	0
2	O	104	A32	8	0
2	V	104	A32	6	0
2	W	104	A32	4	0
2	X	104	A32	1	0
2	Y	104	A32	5	0
2	Z	104	A32	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	D	103/103 (100%)	-0.38	0 100 100	12, 23, 36, 48	0
1	E	103/103 (100%)	-0.45	1 (0%) 84 88	12, 21, 40, 54	0
1	F	103/103 (100%)	-0.47	1 (0%) 84 88	12, 21, 33, 50	0
1	G	103/103 (100%)	-0.21	2 (1%) 70 77	13, 26, 42, 59	0
1	H	103/103 (100%)	-0.44	1 (0%) 84 88	12, 23, 34, 60	0
1	L	103/103 (100%)	0.16	4 (3%) 43 53	18, 37, 70, 84	0
1	M	103/103 (100%)	0.52	5 (4%) 33 43	22, 46, 78, 102	0
1	N	103/103 (100%)	0.22	4 (3%) 43 53	17, 36, 57, 71	0
1	O	103/103 (100%)	0.17	3 (2%) 55 64	18, 36, 60, 83	0
1	P	103/103 (100%)	-0.18	2 (1%) 70 77	17, 28, 46, 62	0
1	V	103/103 (100%)	1.62	40 (38%) 0 1	27, 68, 106, 117	0
1	W	103/103 (100%)	1.07	21 (20%) 1 2	21, 50, 77, 86	0
1	X	103/103 (100%)	0.32	8 (7%) 16 21	16, 36, 64, 77	0
1	Y	103/103 (100%)	0.41	8 (7%) 16 21	17, 37, 62, 79	0
1	Z	103/103 (100%)	0.54	9 (8%) 13 18	19, 42, 72, 93	0
All	All	1545/1545 (100%)	0.19	109 (7%) 19 25	12, 33, 73, 117	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	88	TRP	7.4
1	V	85	LEU	7.2
1	V	86	CYS	6.5
1	V	87	VAL	6.0
1	V	17	ILE	5.8
1	V	96	ILE	5.7
1	O	103	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
1	W	40	ILE	4.8
1	V	16	GLN	4.6
1	W	103	ASN	4.4
1	W	33	GLY	4.2
1	W	88	TRP	4.2
1	V	98	ALA	4.1
1	H	103	ASN	3.8
1	V	5	ILE	3.8
1	Y	103	ASN	3.8
1	V	48	PHE	3.8
1	M	10	SER	3.7
1	G	103	ASN	3.7
1	V	20	ILE	3.6
1	V	15	THR	3.5
1	V	12	TYR	3.5
1	V	18	TYR	3.5
1	V	92	THR	3.5
1	V	99	ILE	3.5
1	Z	14	ASN	3.4
1	L	13	ARG	3.4
1	W	13	ARG	3.3
1	W	6	THR	3.3
1	V	6	THR	3.3
1	V	103	ASN	3.2
1	M	96	ILE	3.2
1	W	85	LEU	3.2
1	V	97	ALA	3.2
1	M	12	TYR	3.1
1	X	10	SER	3.1
1	Z	96	ILE	2.8
1	M	50	VAL	2.8
1	W	15	THR	2.8
1	G	13	ARG	2.8
1	W	19	THR	2.7
1	V	50	VAL	2.7
1	V	93	PRO	2.7
1	V	42	PHE	2.7
1	L	88	TRP	2.7
1	V	38	VAL	2.7
1	X	103	ASN	2.7
1	Z	6	THR	2.6
1	Y	92	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	Z	15	THR	2.6
1	M	13	ARG	2.6
1	V	58	ILE	2.6
1	W	87	VAL	2.6
1	V	84	LYS	2.6
1	Y	55	SER	2.6
1	W	20	ILE	2.6
1	W	39	ILE	2.6
1	Z	99	ILE	2.6
1	V	10	SER	2.5
1	V	102	LYS	2.5
1	V	95	SER	2.5
1	W	86	CYS	2.5
1	W	10	SER	2.5
1	W	48	PHE	2.5
1	N	99	ILE	2.5
1	N	43	LYS	2.5
1	Z	12	TYR	2.4
1	L	19	THR	2.4
1	P	103	ASN	2.4
1	X	24	ILE	2.4
1	N	103	ASN	2.4
1	V	59	ASP	2.4
1	V	52	VAL	2.4
1	V	40	ILE	2.4
1	F	13	ARG	2.4
1	V	54	GLY	2.4
1	W	44	SER	2.4
1	O	13	ARG	2.3
1	X	13	ARG	2.3
1	X	46	GLU	2.3
1	V	62	LYS	2.3
1	X	82	ILE	2.3
1	V	14	ASN	2.3
1	W	92	THR	2.3
1	Y	59	ASP	2.3
1	Y	93	PRO	2.3
1	Y	13	ARG	2.2
1	O	88	TRP	2.2
1	W	18	TYR	2.2
1	V	19	THR	2.2
1	V	8	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	18	TYR	2.2
1	Y	18	TYR	2.2
1	E	44	SER	2.2
1	Z	55	SER	2.2
1	W	97	ALA	2.2
1	W	99	ILE	2.2
1	V	13	ARG	2.1
1	N	5	ILE	2.1
1	X	99	ILE	2.1
1	P	1	ALA	2.1
1	V	47	THR	2.1
1	Z	92	THR	2.1
1	Y	97	ALA	2.1
1	V	55	SER	2.1
1	L	87	VAL	2.1
1	W	102	LYS	2.0
1	V	101	MET	2.0
1	Z	59	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	A32	D	104	33/33	0.78	0.22	6.59	26,54,80,81	0
2	A32	H	104	33/33	0.82	0.22	4.27	22,58,81,81	0
2	A32	Y	104	33/33	0.58	0.37	4.05	65,84,92,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	A32	O	104	33/33	0.66	0.32	3.99	57,94,111,112	0
2	A32	P	104	33/33	0.80	0.22	3.93	34,72,94,95	0
2	A32	W	104	33/33	0.51	0.40	3.07	60,87,108,108	0
2	A32	X	104	33/33	0.77	0.23	2.29	25,58,71,72	0
2	A32	E	104	33/33	0.87	0.17	2.26	23,48,59,59	0
2	A32	F	104	33/33	0.75	0.23	1.99	24,58,77,77	0
2	A32	L	104	33/33	0.58	0.32	1.93	47,77,83,84	0
2	A32	V	104	33/33	0.47	0.36	1.60	86,97,102,103	0
2	A32	M	104	33/33	0.71	0.25	1.24	64,82,87,87	0
2	A32	Z	104	33/33	0.69	0.25	1.08	55,76,87,88	0
2	A32	G	104	33/33	0.87	0.17	0.75	31,56,78,79	0

6.5 Other polymers (i)

There are no such residues in this entry.