



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:24 pm GMT

PDB ID : 1FD7
Title : HEAT-LABILE ENTEROTOXIN B-PENTAMER WITH BOUND LIGAND
BMSC001
Authors : Fan, E.; Merritt, E.A.; Pickens, J.; Ahn, M.; Hol, W.G.J.
Deposited on : 2000-07-19
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

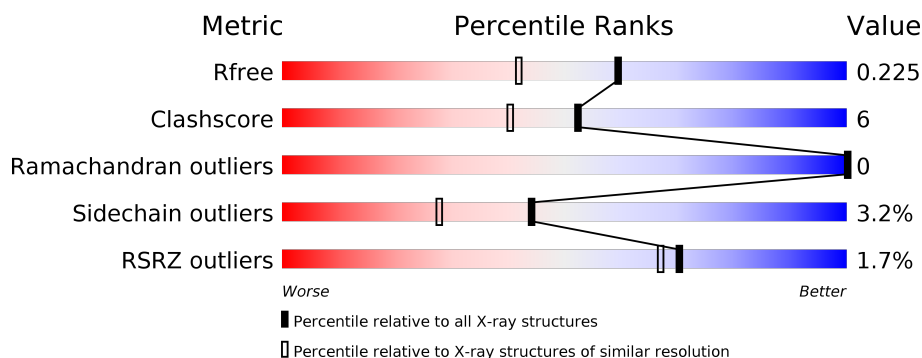
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	D	103	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
1	E	103	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
1	F	103	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	G	103	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	H	103	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>.</div> </div> </div>
1	L	103	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	103	
1	N	103	
1	O	103	
1	P	103	

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	AI1	D	104	-	-	-	X
2	AI1	E	104	-	-	-	X
2	AI1	N	104[A]	-	-	-	X
2	AI1	N	104[B]	-	-	-	X

2 Entry composition

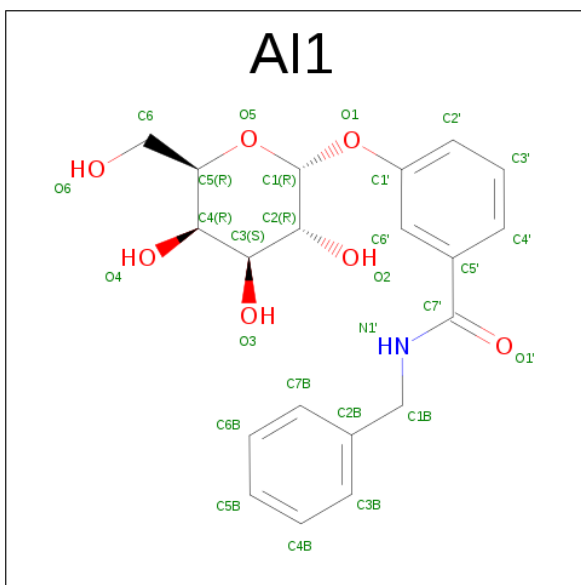
There are 3 unique types of molecules in this entry. The entry contains 9393 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

- Molecule 2 is N-BENZYL-3-(ALPHA-D-GALACTOS-1-YL)-BENZAMIDE (three-letter code: AI1) (formula: C₂₀H₂₃NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			28	20	1	7		
2	E	1	Total	C	N	O	0	0
			28	20	1	7		
2	F	1	Total	C	N	O	0	0
			28	20	1	7		
2	G	1	Total	C	N	O	0	0
			28	20	1	7		
2	H	1	Total	C	N	O	0	0
			28	20	1	7		
2	L	1	Total	C	N	O	0	0
			28	20	1	7		
2	M	1	Total	C	N	O	0	0
			28	20	1	7		
2	N	1	Total	C	N	O	0	1
			45	34	2	9		
2	O	1	Total	C	N	O	0	0
			28	20	1	7		
2	P	1	Total	C	N	O	0	0
			28	20	1	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	74	Total	O	0	0
			74	74		
3	E	83	Total	O	0	0
			83	83		

Continued on next page...

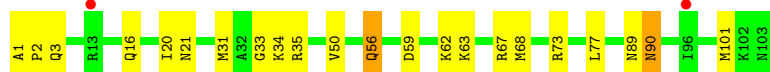
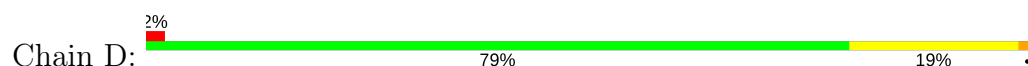
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	90	Total 90	O 90	0	0
3	G	113	Total 113	O 113	0	0
3	H	75	Total 75	O 75	0	0
3	L	89	Total 89	O 89	0	0
3	M	78	Total 78	O 78	0	0
3	N	88	Total 88	O 88	0	0
3	O	81	Total 81	O 81	0	0
3	P	85	Total 85	O 85	0	0

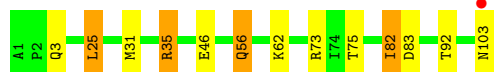
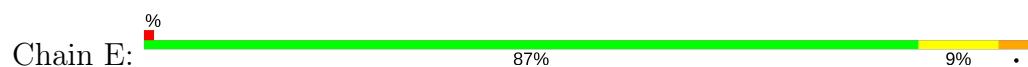
3 Residue-property plots [i](#)

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.

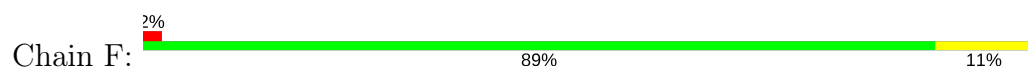
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



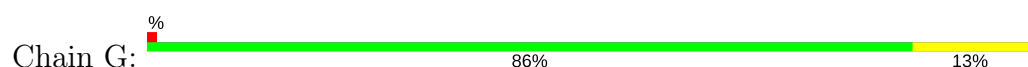
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



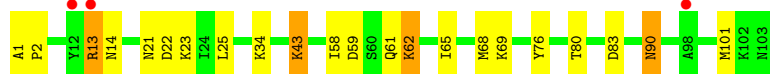
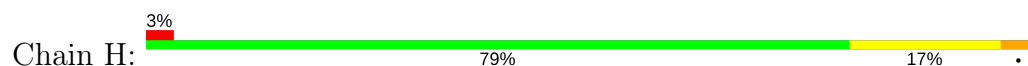
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



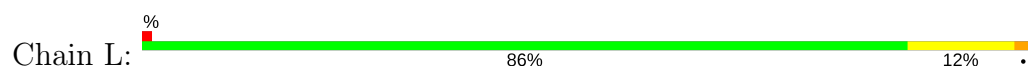
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

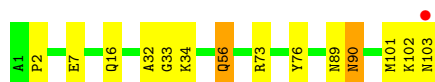


- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

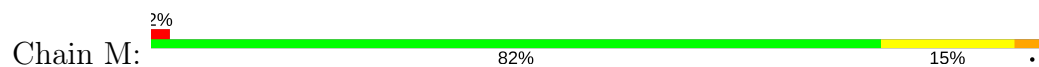


- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN

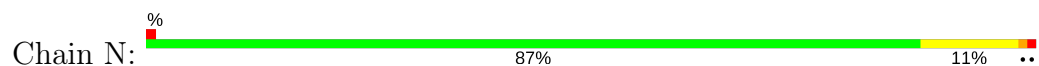




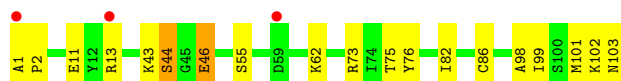
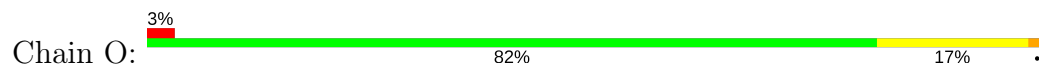
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



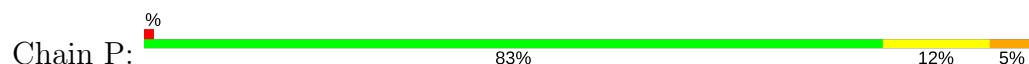
- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



- Molecule 1: HEAT-LABILE ENTEROTOXIN B CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.76Å 157.54Å 63.15Å 90.00° 116.53° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.80) 81.4 (19.86-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.234 0.180 , 0.225	Depositor DCC
R_{free} test set	3960 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9393	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AI1

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	0.56	0/835	1.34	7/1124 (0.6%)
1	E	0.61	0/835	1.31	6/1124 (0.5%)
1	F	0.62	0/835	1.31	8/1124 (0.7%)
1	G	0.61	0/835	1.44	6/1124 (0.5%)
1	H	0.57	0/835	1.31	5/1124 (0.4%)
1	L	0.60	0/835	1.24	2/1124 (0.2%)
1	M	0.67	0/835	1.50	15/1124 (1.3%)
1	N	0.58	0/835	1.37	7/1124 (0.6%)
1	O	0.57	0/835	1.24	5/1124 (0.4%)
1	P	0.57	0/835	1.43	14/1124 (1.2%)
All	All	0.60	0/8350	1.35	75/11240 (0.7%)

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	M	0	2
1	O	0	1
All	All	0	3

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	13	ARG	NE-CZ-NH2	-17.63	111.49	120.30
1	M	103	ASN	CA-C-O	13.47	148.39	120.10
1	D	101	MET	CA-CB-CG	10.78	131.62	113.30
1	P	35	ARG	CD-NE-CZ	10.36	138.10	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	13	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	M	55	SER	CB-CA-C	10.04	129.18	110.10
1	P	73	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	F	35	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	G	73	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	P	35	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	N	35	ARG	NE-CZ-NH2	8.87	124.73	120.30
1	D	73	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	F	11	GLU	OE1-CD-OE2	-7.99	113.71	123.30
1	N	73	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	E	73	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	O	73	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	P	35	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	P	103	ASN	CA-CB-CG	7.51	129.93	113.40
1	D	67	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	L	76	TYR	CB-CG-CD1	-7.35	116.59	121.00
1	E	35	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	N	67	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	F	35	ARG	CD-NE-CZ	7.07	133.50	123.60
1	N	13	ARG	CD-NE-CZ	6.95	133.32	123.60
1	H	76	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	H	83	ASP	CB-CG-OD1	6.67	124.30	118.30
1	L	73	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	P	83	ASP	CB-CG-OD2	6.53	124.17	118.30
1	F	73	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	M	103	ASN	N-CA-CB	6.46	122.22	110.60
1	M	34	LYS	CG-CD-CE	6.40	131.09	111.90
1	P	11	GLU	OE1-CD-OE2	-6.35	115.68	123.30
1	D	35	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	M	62	LYS	CA-CB-CG	6.29	127.24	113.40
1	M	103	ASN	CB-CA-C	6.29	122.97	110.40
1	E	83	ASP	CB-CG-OD1	6.17	123.86	118.30
1	E	46	GLU	OE1-CD-OE2	-6.14	115.94	123.30
1	M	43	LYS	CD-CE-NZ	6.11	125.75	111.70
1	O	46	GLU	OE1-CD-OE2	6.01	130.52	123.30
1	O	103	ASN	CA-CB-CG	-6.01	100.18	113.40
1	M	56	GLN	CG-CD-OE1	5.99	133.58	121.60
1	P	67	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	M	70	ASP	CB-CG-OD1	5.96	123.67	118.30
1	H	83	ASP	CA-CB-CG	5.91	126.41	113.40
1	N	35	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	M	35	ARG	NE-CZ-NH1	5.83	123.22	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	13	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	P	70	ASP	CB-CG-OD1	5.75	123.48	118.30
1	G	12	TYR	CB-CG-CD1	5.74	124.44	121.00
1	O	103	ASN	CB-CG-OD1	-5.70	110.19	121.60
1	F	100	SER	N-CA-CB	5.70	119.05	110.50
1	P	7	GLU	OE1-CD-OE2	5.66	130.09	123.30
1	M	67	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	G	55	SER	CA-CB-OG	-5.63	96.00	111.20
1	P	103	ASN	CB-CA-C	5.63	121.65	110.40
1	M	102	LYS	N-CA-CB	5.59	120.66	110.60
1	F	73	ARG	CD-NE-CZ	5.54	131.35	123.60
1	P	83	ASP	OD1-CG-OD2	-5.54	112.78	123.30
1	F	13	ARG	CD-NE-CZ	5.50	131.29	123.60
1	H	13	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	O	43	LYS	CA-CB-CG	5.38	125.23	113.40
1	F	11	GLU	CG-CD-OE1	5.37	129.04	118.30
1	M	100	SER	N-CA-CB	5.32	118.48	110.50
1	D	67	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	N	1	ALA	N-CA-CB	5.31	117.54	110.10
1	P	83	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	50	VAL	N-CA-C	-5.23	96.89	111.00
1	M	11	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	E	35	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	P	102	LYS	C-N-CA	-5.17	108.76	121.70
1	E	25	LEU	CA-CB-CG	5.16	127.17	115.30
1	G	18	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	D	35	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	H	83	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	M	92	THR	CA-CB-CG2	-5.00	105.40	112.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	102	LYS	Mainchain,Peptide
1	O	44	SER	Mainchain

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	D	824	0	841	32	0
1	E	824	0	841	15	0
1	F	824	0	841	4	0
1	G	824	0	841	7	0
1	H	824	0	841	20	0
1	L	824	0	841	12	0
1	M	824	0	841	6	0
1	N	824	0	841	9	0
1	O	824	0	841	10	0
1	P	824	0	841	5	0
2	D	28	0	22	1	0
2	E	28	0	23	1	0
2	F	28	0	22	1	0
2	G	28	0	23	1	0
2	H	28	0	22	2	0
2	L	28	0	23	1	0
2	M	28	0	22	0	0
2	N	45	0	24	6	0
2	O	28	0	22	1	0
2	P	28	0	22	1	0
3	D	74	0	0	1	0
3	E	83	0	0	1	0
3	F	90	0	0	2	0
3	G	113	0	0	1	0
3	H	75	0	0	2	0
3	L	89	0	0	1	0
3	M	78	0	0	1	0
3	N	88	0	0	1	0
3	O	81	0	0	0	0
3	P	85	0	0	1	0
All	All	9393	0	8635	108	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 6.

All (108) 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)
1:D:31:MET:HE1	1:H:65:ILE:HA	1.19	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:GLN:H	1:D:56:GLN:HE21	1.03	1.03
1:D:31:MET:CE	1:H:65:ILE:HA	1.93	0.98
1:L:56:GLN:H	1:L:56:GLN:HE21	1.00	0.95
1:O:75:THR:HG21	1:O:82:ILE:HD11	1.50	0.94
1:N:13:ARG:HG3	1:N:13:ARG:HH11	1.39	0.86
1:O:82:ILE:HD12	1:O:99:ILE:HD11	1.60	0.83
1:L:16:GLN:HE21	1:L:89:ASN:HD22	1.28	0.79
1:N:16:GLN:HE21	1:N:89:ASN:HD22	1.30	0.77
2:N:104[A]:AI1:H6'	3:N:2803:HOH:O	1.85	0.76
2:D:104:AI1:H6'	3:D:2103:HOH:O	1.87	0.75
1:N:13:ARG:NH1	2:N:104[A]:AI1:H4B	2.00	0.75
1:E:75:THR:HG21	1:E:82:ILE:HD11	1.69	0.74
1:F:101:MET:HG3	1:G:76:TYR:CE2	2.26	0.71
1:L:56:GLN:N	1:L:56:GLN:HE21	1.82	0.71
1:F:16:GLN:HE21	1:F:89:ASN:HD22	1.39	0.69
2:F:104:AI1:H6'	3:F:2303:HOH:O	1.92	0.69
1:D:16:GLN:HE21	1:D:89:ASN:HD22	1.42	0.67
1:O:82:ILE:CD1	1:O:99:ILE:HD11	2.24	0.67
1:D:1:ALA:HB1	1:E:92:THR:O	1.94	0.67
1:N:101:MET:HG3	1:O:76:TYR:CE2	2.30	0.67
1:P:90:ASN:HD22	1:P:90:ASN:H	1.43	0.67
1:D:1:ALA:N	1:D:2:PRO:HD3	2.10	0.66
1:D:56:GLN:N	1:D:56:GLN:HE21	1.86	0.66
1:N:13:ARG:HH12	2:N:104[A]:AI1:H4B	1.59	0.65
1:D:1:ALA:N	1:D:2:PRO:CD	2.61	0.63
1:H:58:ILE:H	1:H:61:GLN:HE21	1.46	0.62
2:L:104:AI1:H6'	3:L:2603:HOH:O	1.99	0.62
2:E:104:AI1:H6'	3:E:2203:HOH:O	1.99	0.62
1:L:90:ASN:H	1:L:90:ASN:HD22	1.48	0.62
1:M:1:ALA:HB1	1:M:2:PRO:HD2	1.85	0.59
2:P:104:AI1:H6'	3:P:2003:HOH:O	2.02	0.59
2:N:104[B]:AI1:C7'	2:N:104[B]:AI1:H3B	2.32	0.59
1:H:1:ALA:HB1	1:H:2:PRO:HD2	1.86	0.57
2:N:104[B]:AI1:H3B	2:N:104[B]:AI1:O1'	2.04	0.57
1:D:90:ASN:HD22	1:D:90:ASN:H	1.53	0.57
1:G:1:ALA:HB1	1:G:2:PRO:HD2	1.87	0.57
1:P:58:ILE:H	1:P:61:GLN:HE21	1.52	0.56
1:H:90:ASN:H	1:H:90:ASN:HD22	1.53	0.56
1:H:80:THR:HG21	1:H:101:MET:CE	2.36	0.55
1:D:31:MET:CE	1:H:68:MET:HB3	2.36	0.55
1:H:13:ARG:HG3	1:H:14:ASN:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:LYS:HG2	1:G:103:ASN:ND2	2.24	0.53
1:N:1:ALA:N	1:N:2:PRO:CD	2.72	0.53
1:E:75:THR:CG2	1:E:82:ILE:HD11	2.36	0.52
1:D:68:MET:HG2	1:E:31:MET:CE	2.39	0.52
1:H:80:THR:HG21	1:H:101:MET:HE3	1.91	0.52
1:M:43:LYS:HE2	3:M:1739:HOH:O	2.09	0.52
1:P:83:ASP:OD2	1:P:102:LYS:HE3	2.09	0.52
1:D:1:ALA:H2	1:E:35:ARG:NH1	2.07	0.52
1:P:22:ASP:OD2	1:P:43:LYS:HD3	2.09	0.52
1:D:1:ALA:H3	1:D:2:PRO:HD3	1.75	0.51
1:D:3:GLN:HE21	1:E:92:THR:HG22	1.75	0.51
1:H:59:ASP:HA	1:H:62:LYS:HD3	1.92	0.51
1:G:78:THR:O	1:G:79:GLU:HB2	2.10	0.51
1:D:77:LEU:HD21	1:H:101:MET:HE3	1.93	0.50
1:D:31:MET:HE1	1:H:65:ILE:CA	2.14	0.50
1:G:102:LYS:HG2	1:G:103:ASN:HD22	1.77	0.50
1:L:102:LYS:O	1:L:103:ASN:HB2	2.11	0.50
1:M:25:LEU:HD13	1:M:25:LEU:C	2.32	0.50
1:F:1:ALA:HB1	1:F:2:PRO:HD2	1.93	0.49
1:D:34:LYS:HB2	2:H:104:AI1:C5B	2.43	0.49
1:D:1:ALA:N	1:E:35:ARG:NH1	2.60	0.49
1:D:68:MET:HG2	1:E:31:MET:HE1	1.94	0.49
1:E:75:THR:HG21	1:E:82:ILE:CD1	2.42	0.49
1:L:16:GLN:NE2	1:L:89:ASN:HD22	2.04	0.49
1:L:33:GLY:O	1:L:34:LYS:HB2	2.13	0.49
1:L:2:PRO:HB3	1:L:7:GLU:HG2	1.94	0.48
1:N:16:GLN:NE2	1:N:89:ASN:HD22	2.05	0.48
1:E:3:GLN:OE1	1:F:92:THR:HG22	2.14	0.47
1:H:23:LYS:HE2	3:H:1214:HOH:O	2.15	0.47
1:D:63:LYS:HE3	1:E:62:LYS:NZ	2.30	0.47
1:D:31:MET:HE2	1:H:68:MET:CB	2.46	0.46
1:O:75:THR:HG21	1:O:82:ILE:CD1	2.33	0.46
1:D:1:ALA:H2	1:D:2:PRO:CD	2.28	0.46
1:E:56:GLN:H	1:E:56:GLN:NE2	2.14	0.46
1:D:31:MET:HE2	1:H:68:MET:HB3	1.96	0.46
1:N:65:ILE:HG22	1:N:69:LYS:HE2	1.97	0.46
1:L:56:GLN:H	1:L:56:GLN:NE2	1.85	0.46
1:D:90:ASN:N	1:D:90:ASN:HD22	2.13	0.45
1:D:31:MET:HE3	1:H:68:MET:HB3	1.98	0.45
1:N:13:ARG:HG3	1:N:13:ARG:NH1	2.16	0.45
3:F:1472:HOH:O	1:G:23:LYS:HE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:104:AI1:H1'2	3:H:1859:HOH:O	2.16	0.45
1:O:44:SER:OG	1:O:46:GLU:HB2	2.18	0.44
1:O:1:ALA:HB1	1:O:2:PRO:HD2	1.99	0.43
1:D:33:GLY:O	1:D:34:LYS:HB2	2.18	0.43
2:N:104[B]:AI1:C7'	2:N:104[B]:AI1:C3B	2.95	0.43
1:D:20:ILE:O	1:D:21:ASN:C	2.56	0.43
1:O:86:CYS:HB3	1:O:98:ALA:HB3	2.01	0.43
1:L:102:LYS:NZ	1:M:25:LEU:HD11	2.33	0.42
1:H:1:ALA:HB1	1:H:2:PRO:CD	2.48	0.42
1:D:3:GLN:NE2	1:E:92:THR:CG2	2.82	0.42
1:O:11:GLU:OE1	2:O:104:AI1:H6B	2.19	0.42
1:H:65:ILE:HG22	1:H:69:LYS:HE2	2.01	0.42
1:D:3:GLN:NE2	1:E:92:THR:HG22	2.34	0.42
1:H:22:ASP:OD2	1:H:43:LYS:HD3	2.20	0.42
1:H:90:ASN:H	1:H:90:ASN:ND2	2.18	0.41
1:D:62:LYS:HA	1:D:62:LYS:HD3	1.69	0.41
1:M:21:ASN:OD1	1:M:81:LYS:HD3	2.20	0.41
1:E:82:ILE:HD13	1:E:82:ILE:N	2.36	0.41
2:G:104:AI1:H6'	3:G:2403:HOH:O	2.21	0.41
1:L:101:MET:HG3	1:M:76:TYR:CE2	2.56	0.41
1:D:90:ASN:H	1:D:90:ASN:ND2	2.18	0.41
1:D:56:GLN:NE2	1:D:56:GLN:H	1.88	0.41
1:L:32:ALA:HB1	1:P:12:TYR:CZ	2.56	0.40
1:G:8:LEU:HD23	1:G:8:LEU:C	2.42	0.40
1:O:62:LYS:HD3	1:O:62:LYS:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	101/103 (98%)	97 (96%)	4 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	F	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	G	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	H	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	L	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	M	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	N	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	O	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	P	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
All	All	1010/1030 (98%)	995 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	D	95/95 (100%)	92 (97%)	3 (3%)	44	28
1	E	95/95 (100%)	91 (96%)	4 (4%)	34	17
1	F	95/95 (100%)	95 (100%)	0	100	100
1	G	95/95 (100%)	94 (99%)	1 (1%)	78	72
1	H	95/95 (100%)	89 (94%)	6 (6%)	21	7
1	L	95/95 (100%)	93 (98%)	2 (2%)	59	46
1	M	95/95 (100%)	93 (98%)	2 (2%)	59	46
1	N	95/95 (100%)	92 (97%)	3 (3%)	44	28
1	O	95/95 (100%)	91 (96%)	4 (4%)	34	17
1	P	95/95 (100%)	90 (95%)	5 (5%)	26	11
All	All	950/950 (100%)	920 (97%)	30 (3%)	44	28

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	56	GLN
1	D	59	ASP
1	D	90	ASN
1	E	25	LEU
1	E	56	GLN
1	E	82	ILE
1	E	103	ASN
1	G	55	SER
1	H	21	ASN
1	H	25	LEU
1	H	34	LYS
1	H	43	LYS
1	H	62	LYS
1	H	90	ASN
1	L	56	GLN
1	L	90	ASN
1	M	55	SER
1	M	103	ASN
1	N	13	ARG
1	N	81	LYS
1	N	91	LYS
1	O	13	ARG
1	O	55	SER
1	O	101	MET
1	O	102	LYS
1	P	43	LYS
1	P	59	ASP
1	P	90	ASN
1	P	101	MET
1	P	103	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	D	16	GLN
1	D	56	GLN
1	D	90	ASN
1	E	56	GLN
1	F	16	GLN
1	F	21	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	94	ASN
1	G	94	ASN
1	G	103	ASN
1	H	61	GLN
1	H	90	ASN
1	H	103	ASN
1	L	16	GLN
1	L	56	GLN
1	L	90	ASN
1	M	3	GLN
1	M	103	ASN
1	N	16	GLN
1	N	21	ASN
1	N	94	ASN
1	O	94	ASN
1	P	3	GLN
1	P	21	ASN
1	P	61	GLN
1	P	90	ASN
1	P	94	ASN
1	P	103	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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	AI1	D	104	-	30,30,30	1.68	6 (20%)	41,41,41	2.16	13 (31%)
2	AI1	E	104	-	30,30,30	1.64	7 (23%)	41,41,41	2.35	12 (29%)
2	AI1	F	104	-	30,30,30	1.79	9 (30%)	41,41,41	1.86	12 (29%)
2	AI1	G	104	-	30,30,30	1.93	9 (30%)	41,41,41	2.40	16 (39%)
2	AI1	H	104	-	30,30,30	1.90	8 (26%)	41,41,41	2.79	19 (46%)
2	AI1	L	104	-	30,30,30	1.80	9 (30%)	41,41,41	2.09	14 (34%)
2	AI1	M	104	-	30,30,30	1.71	7 (23%)	41,41,41	2.10	13 (31%)
2	AI1	N	104[A]	-	30,30,30	1.77	8 (26%)	41,41,41	1.89	11 (26%)
2	AI1	N	104[B]	-	30,30,30	1.80	8 (26%)	41,41,41	2.36	13 (31%)
2	AI1	O	104	-	30,30,30	1.75	8 (26%)	41,41,41	2.17	13 (31%)
2	AI1	P	104	-	30,30,30	1.69	7 (23%)	41,41,41	1.99	13 (31%)

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	AI1	D	104	-	-	0/15/35/35	0/3/3/3
2	AI1	E	104	-	-	0/15/35/35	0/3/3/3
2	AI1	F	104	-	-	0/15/35/35	0/3/3/3
2	AI1	G	104	-	-	0/15/35/35	0/3/3/3
2	AI1	H	104	-	-	0/15/35/35	0/3/3/3
2	AI1	L	104	-	-	0/15/35/35	0/3/3/3
2	AI1	M	104	-	-	0/15/35/35	0/3/3/3
2	AI1	N	104[A]	-	-	0/15/35/35	0/3/3/3
2	AI1	N	104[B]	-	-	0/15/35/35	0/3/3/3
2	AI1	O	104	-	-	0/15/35/35	0/3/3/3
2	AI1	P	104	-	-	0/15/35/35	0/3/3/3

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	104	AI1	C7'-N1'	-4.35	1.24	1.33
2	L	104	AI1	C5'-C7'	-4.00	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	104	AI1	C5'-C7'	-3.89	1.41	1.50
2	N	104[B]	AI1	C5'-C7'	-3.86	1.42	1.50
2	N	104[B]	AI1	C7'-N1'	-3.81	1.25	1.33
2	O	104	AI1	C5'-C7'	-3.80	1.42	1.50
2	N	104[A]	AI1	C7'-N1'	-3.63	1.25	1.33
2	F	104	AI1	C5'-C7'	-3.61	1.42	1.50
2	E	104	AI1	C5'-C7'	-3.54	1.42	1.50
2	O	104	AI1	C7'-N1'	-3.50	1.26	1.33
2	N	104[A]	AI1	C5'-C7'	-3.46	1.42	1.50
2	H	104	AI1	C5'-C7'	-3.45	1.42	1.50
2	M	104	AI1	C7'-N1'	-3.42	1.26	1.33
2	D	104	AI1	C7'-N1'	-3.38	1.26	1.33
2	G	104	AI1	C7'-N1'	-3.22	1.26	1.33
2	P	104	AI1	C5'-C7'	-3.20	1.43	1.50
2	D	104	AI1	C5'-C7'	-3.19	1.43	1.50
2	P	104	AI1	C7'-N1'	-3.10	1.26	1.33
2	F	104	AI1	C7'-N1'	-3.10	1.26	1.33
2	M	104	AI1	C5'-C7'	-3.09	1.43	1.50
2	L	104	AI1	C7'-N1'	-2.79	1.27	1.33
2	E	104	AI1	C7'-N1'	-2.48	1.28	1.33
2	F	104	AI1	C4-C3	2.01	1.57	1.52
2	N	104[B]	AI1	C6'-C5'	2.05	1.42	1.39
2	N	104[B]	AI1	C1-C2	2.09	1.58	1.52
2	N	104[A]	AI1	C1-C2	2.09	1.58	1.52
2	L	104	AI1	C4'-C5'	2.10	1.42	1.39
2	E	104	AI1	C6'-C5'	2.11	1.42	1.39
2	L	104	AI1	C4-C3	2.13	1.57	1.52
2	F	104	AI1	C4'-C5'	2.15	1.42	1.39
2	N	104[A]	AI1	C6'-C5'	2.16	1.42	1.39
2	G	104	AI1	C4-C3	2.18	1.57	1.52
2	L	104	AI1	C6'-C5'	2.18	1.42	1.39
2	O	104	AI1	C4-C3	2.28	1.58	1.52
2	H	104	AI1	C3'-C4'	2.29	1.43	1.38
2	M	104	AI1	C3'-C4'	2.30	1.43	1.38
2	E	104	AI1	C3'-C4'	2.31	1.43	1.38
2	P	104	AI1	C4'-C5'	2.31	1.43	1.39
2	E	104	AI1	C3'-C2'	2.31	1.43	1.38
2	N	104[B]	AI1	C3'-C4'	2.32	1.43	1.38
2	L	104	AI1	C3'-C4'	2.36	1.43	1.38
2	G	104	AI1	C3'-C4'	2.39	1.43	1.38
2	P	104	AI1	C3'-C4'	2.46	1.43	1.38
2	H	104	AI1	C4-C3	2.49	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	104	AI1	C4-C3	2.50	1.58	1.52
2	N	104[A]	AI1	C3'-C4'	2.50	1.43	1.38
2	O	104	AI1	O1-C1	2.51	1.45	1.41
2	O	104	AI1	C6'-C5'	2.52	1.43	1.39
2	O	104	AI1	C3'-C4'	2.53	1.43	1.38
2	F	104	AI1	C1-C2	2.55	1.59	1.52
2	F	104	AI1	C3'-C4'	2.63	1.43	1.38
2	D	104	AI1	C3'-C4'	2.67	1.44	1.38
2	G	104	AI1	O1'-C7'	2.71	1.29	1.23
2	M	104	AI1	O1'-C7'	2.74	1.29	1.23
2	M	104	AI1	O1-C1	2.80	1.45	1.41
2	D	104	AI1	O1-C1	2.87	1.45	1.41
2	F	104	AI1	O1-C1	2.93	1.45	1.41
2	H	104	AI1	O1'-C7'	2.98	1.29	1.23
2	G	104	AI1	O1-C1'	3.04	1.44	1.38
2	N	104[B]	AI1	O1'-C7'	3.04	1.29	1.23
2	P	104	AI1	O1-C1	3.07	1.46	1.41
2	G	104	AI1	O1-C1	3.10	1.46	1.41
2	L	104	AI1	O1-C1'	3.11	1.44	1.38
2	G	104	AI1	C6'-C5'	3.14	1.44	1.39
2	E	104	AI1	O1-C1'	3.17	1.44	1.38
2	N	104[A]	AI1	O1-C1	3.21	1.46	1.41
2	P	104	AI1	O1-C1'	3.21	1.45	1.38
2	N	104[A]	AI1	O1-C1'	3.22	1.45	1.38
2	F	104	AI1	O1-C1'	3.23	1.45	1.38
2	N	104[B]	AI1	O1-C1'	3.27	1.45	1.38
2	H	104	AI1	C6'-C5'	3.28	1.44	1.39
2	E	104	AI1	O1'-C7'	3.35	1.30	1.23
2	D	104	AI1	O1-C1'	3.36	1.45	1.38
2	O	104	AI1	O1'-C7'	3.41	1.30	1.23
2	O	104	AI1	O1-C1'	3.44	1.45	1.38
2	H	104	AI1	O1-C1	3.52	1.46	1.41
2	M	104	AI1	O1-C1'	3.52	1.45	1.38
2	N	104[A]	AI1	O1'-C7'	3.59	1.30	1.23
2	D	104	AI1	O1'-C7'	3.63	1.30	1.23
2	H	104	AI1	O1-C1'	3.69	1.46	1.38
2	L	104	AI1	O1-C1	3.72	1.47	1.41
2	P	104	AI1	O1'-C7'	3.73	1.31	1.23
2	F	104	AI1	O1'-C7'	3.77	1.31	1.23
2	L	104	AI1	O1'-C7'	3.78	1.31	1.23
2	N	104[B]	AI1	O1-C1	3.79	1.47	1.41
2	G	104	AI1	C4B-C3B	4.09	1.46	1.38

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	104[B]	AI1	C1'-O1-C1	-6.08	109.03	117.88
2	H	104	AI1	O1'-C7'-C5'	-5.93	110.42	120.94
2	E	104	AI1	O3-C3-C2	-5.58	98.21	110.36
2	L	104	AI1	C5B-C4B-C3B	-5.26	112.98	120.21
2	M	104	AI1	O3-C3-C4	-4.96	99.56	110.36
2	N	104[B]	AI1	C2B-C1B-N1'	-4.56	102.90	112.96
2	H	104	AI1	O2-C2-C3	-4.53	100.51	110.36
2	N	104[B]	AI1	C5'-C6'-C1'	-4.49	114.72	119.57
2	O	104	AI1	C4-C3-C2	-4.47	102.95	110.84
2	D	104	AI1	O2-C2-C3	-4.27	101.07	110.36
2	H	104	AI1	C5'-C6'-C1'	-4.09	115.15	119.57
2	O	104	AI1	O3-C3-C2	-4.08	101.49	110.36
2	G	104	AI1	C5'-C6'-C1'	-3.96	115.29	119.57
2	M	104	AI1	C4-C3-C2	-3.96	103.85	110.84
2	G	104	AI1	C1-C2-C3	-3.90	102.73	109.98
2	D	104	AI1	C4'-C5'-C6'	-3.88	114.67	119.23
2	N	104[B]	AI1	O2-C2-C3	-3.88	101.91	110.36
2	N	104[A]	AI1	O2-C2-C3	-3.88	101.91	110.36
2	M	104	AI1	O1'-C7'-C5'	-3.88	114.06	120.94
2	E	104	AI1	C4'-C5'-C6'	-3.79	114.77	119.23
2	E	104	AI1	O2-C2-C3	-3.77	102.15	110.36
2	G	104	AI1	O3-C3-C2	-3.74	102.23	110.36
2	O	104	AI1	O2-C2-C3	-3.69	102.33	110.36
2	P	104	AI1	O3-C3-C2	-3.68	102.35	110.36
2	L	104	AI1	O2-C2-C3	-3.67	102.36	110.36
2	G	104	AI1	C4B-C3B-C2B	-3.67	115.05	120.64
2	E	104	AI1	C4'-C3'-C2'	-3.62	115.16	120.24
2	F	104	AI1	O2-C2-C1	-3.59	102.52	110.03
2	H	104	AI1	C5B-C6B-C7B	-3.50	115.39	120.21
2	H	104	AI1	O3-C3-C2	-3.45	102.85	110.36
2	H	104	AI1	O3-C3-C4	-3.44	102.88	110.36
2	D	104	AI1	O3-C3-C2	-3.33	103.10	110.36
2	M	104	AI1	O3-C3-C2	-3.30	103.17	110.36
2	P	104	AI1	C1-C2-C3	-3.25	103.93	109.98
2	L	104	AI1	C4-C3-C2	-3.23	105.14	110.84
2	O	104	AI1	O3-C3-C4	-3.20	103.40	110.36
2	P	104	AI1	O2-C2-C3	-3.17	103.45	110.36
2	F	104	AI1	O3-C3-C4	-3.11	103.60	110.36
2	H	104	AI1	C1'-O1-C1	-3.10	113.37	117.88
2	L	104	AI1	O3-C3-C2	-3.06	103.71	110.36
2	N	104[B]	AI1	C5B-C4B-C3B	-3.02	116.05	120.21
2	G	104	AI1	O3-C3-C4	-2.98	103.88	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	104	AI1	C4'-C3'-C2'	-2.97	116.07	120.24
2	G	104	AI1	O1'-C7'-N1'	-2.95	116.49	122.59
2	L	104	AI1	O3-C3-C4	-2.91	104.03	110.36
2	G	104	AI1	O1'-C7'-C5'	-2.90	115.80	120.94
2	O	104	AI1	C5'-C6'-C1'	-2.86	116.48	119.57
2	L	104	AI1	O1'-C7'-C5'	-2.86	115.87	120.94
2	P	104	AI1	O1'-C7'-C5'	-2.85	115.88	120.94
2	O	104	AI1	C4'-C3'-C2'	-2.82	116.28	120.24
2	P	104	AI1	O3-C3-C4	-2.80	104.26	110.36
2	N	104[B]	AI1	C1-C2-C3	-2.79	104.79	109.98
2	N	104[A]	AI1	C1-C2-C3	-2.79	104.79	109.98
2	F	104	AI1	O2-C2-C3	-2.77	104.34	110.36
2	P	104	AI1	C4'-C5'-C6'	-2.76	115.99	119.23
2	L	104	AI1	C4'-C5'-C6'	-2.68	116.08	119.23
2	F	104	AI1	O3-C3-C2	-2.65	104.59	110.36
2	G	104	AI1	C2B-C1B-N1'	-2.65	107.12	112.96
2	N	104[B]	AI1	O3-C3-C2	-2.64	104.62	110.36
2	N	104[A]	AI1	O3-C3-C2	-2.64	104.62	110.36
2	M	104	AI1	O2-C2-C3	-2.63	104.63	110.36
2	M	104	AI1	C5B-C6B-C7B	-2.62	116.60	120.21
2	M	104	AI1	C1-C2-C3	-2.61	105.12	109.98
2	N	104[A]	AI1	O1'-C7'-C5'	-2.60	116.33	120.94
2	M	104	AI1	C5'-C6'-C1'	-2.58	116.78	119.57
2	M	104	AI1	O2-C2-C1	-2.57	104.65	110.03
2	H	104	AI1	C4-C3-C2	-2.54	106.36	110.84
2	H	104	AI1	C1-O5-C5	-2.53	108.94	113.72
2	E	104	AI1	O1'-C7'-N1'	-2.52	117.38	122.59
2	E	104	AI1	C5B-C6B-C7B	-2.51	116.76	120.21
2	N	104[B]	AI1	C4'-C3'-C2'	-2.50	116.72	120.24
2	E	104	AI1	C4-C3-C2	-2.49	106.45	110.84
2	F	104	AI1	C4-C3-C2	-2.48	106.46	110.84
2	O	104	AI1	C1-O5-C5	-2.46	109.09	113.72
2	H	104	AI1	C5B-C4B-C3B	-2.45	116.83	120.21
2	D	104	AI1	C4-C3-C2	-2.36	106.67	110.84
2	N	104[B]	AI1	C4-C3-C2	-2.30	106.78	110.84
2	N	104[A]	AI1	C4-C3-C2	-2.30	106.78	110.84
2	G	104	AI1	C1-O5-C5	-2.28	109.43	113.72
2	P	104	AI1	C4-C3-C2	-2.27	106.83	110.84
2	F	104	AI1	C3-C4-C5	-2.26	106.23	110.22
2	G	104	AI1	O2-C2-C3	-2.26	105.45	110.36
2	M	104	AI1	C1'-O1-C1	-2.25	114.60	117.88
2	H	104	AI1	O2-C2-C1	-2.19	105.44	110.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	104	AI1	O1'-C7'-N1'	-2.18	118.09	122.59
2	H	104	AI1	C1-C2-C3	-2.17	105.95	109.98
2	N	104[B]	AI1	O1'-C7'-C5'	-2.12	117.19	120.94
2	E	104	AI1	C5'-C6'-C1'	-2.11	117.28	119.57
2	D	104	AI1	O3-C3-C4	-2.07	105.86	110.36
2	F	104	AI1	C5B-C4B-C3B	-2.06	117.38	120.21
2	P	104	AI1	C5B-C4B-C3B	-2.05	117.38	120.21
2	O	104	AI1	O1'-C7'-C5'	-2.04	117.32	120.94
2	L	104	AI1	O2-C2-C1	-2.02	105.80	110.03
2	F	104	AI1	C4'-C5'-C6'	-2.02	116.86	119.23
2	G	104	AI1	C4'-C3'-C2'	-2.01	117.41	120.24
2	O	104	AI1	O4-C4-C5	2.05	114.46	109.28
2	H	104	AI1	C4'-C5'-C7'	2.07	127.26	120.61
2	D	104	AI1	C2'-C1'-C6'	2.07	123.34	120.53
2	N	104[A]	AI1	C5'-C7'-N1'	2.09	121.62	117.12
2	N	104[A]	AI1	C4'-C5'-C7'	2.10	127.36	120.61
2	D	104	AI1	C4'-C5'-C7'	2.11	127.39	120.61
2	L	104	AI1	C4B-C3B-C2B	2.12	123.86	120.64
2	L	104	AI1	O1-C1-C2	2.18	110.33	107.11
2	D	104	AI1	O4-C4-C5	2.27	115.00	109.28
2	P	104	AI1	C5'-C7'-N1'	2.34	122.17	117.12
2	N	104[A]	AI1	C3'-C4'-C5'	2.45	123.23	120.35
2	G	104	AI1	O1-C1-C2	2.68	111.08	107.11
2	F	104	AI1	C3'-C4'-C5'	2.74	123.57	120.35
2	D	104	AI1	C5'-C7'-N1'	2.84	123.25	117.12
2	E	104	AI1	C1'-O1-C1	2.88	122.07	117.88
2	M	104	AI1	C5'-C7'-N1'	2.91	123.40	117.12
2	N	104[B]	AI1	C1B-N1'-C7'	2.92	129.24	121.82
2	N	104[A]	AI1	C2'-C1'-C6'	2.93	124.51	120.53
2	P	104	AI1	C3'-C4'-C5'	3.00	123.88	120.35
2	O	104	AI1	C3'-C4'-C5'	3.00	123.88	120.35
2	H	104	AI1	C6B-C5B-C4B	3.02	124.91	119.89
2	P	104	AI1	C2'-C1'-C6'	3.09	124.72	120.53
2	L	104	AI1	C3'-C4'-C5'	3.09	123.99	120.35
2	F	104	AI1	C1B-N1'-C7'	3.10	129.71	121.82
2	L	104	AI1	C6B-C5B-C4B	3.19	125.19	119.89
2	O	104	AI1	C5'-C7'-N1'	3.19	124.00	117.12
2	N	104[B]	AI1	C3'-C4'-C5'	3.20	124.12	120.35
2	D	104	AI1	C1B-N1'-C7'	3.34	130.31	121.82
2	D	104	AI1	C3'-C4'-C5'	3.36	124.30	120.35
2	F	104	AI1	C2'-C1'-C6'	3.49	125.27	120.53
2	M	104	AI1	C2'-C1'-C6'	3.55	125.35	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	104	AI1	C2'-C1'-C6'	3.56	125.36	120.53
2	L	104	AI1	C5'-C7'-N1'	3.58	124.83	117.12
2	P	104	AI1	C1B-N1'-C7'	3.81	131.51	121.82
2	H	104	AI1	C5'-C7'-N1'	3.82	125.35	117.12
2	N	104[A]	AI1	C1B-N1'-C7'	3.82	131.53	121.82
2	M	104	AI1	O1-C1-C2	3.88	112.84	107.11
2	G	104	AI1	C7B-C2B-C3B	3.90	124.34	118.16
2	G	104	AI1	C3'-C4'-C5'	3.94	124.98	120.35
2	O	104	AI1	C2'-C1'-C6'	3.95	125.89	120.53
2	H	104	AI1	C3'-C4'-C5'	4.58	125.73	120.35
2	F	104	AI1	O1-C1-C2	4.61	113.93	107.11
2	E	104	AI1	O1-C1-C2	4.74	114.12	107.11
2	P	104	AI1	O1-C1-C2	4.88	114.32	107.11
2	G	104	AI1	C5'-C7'-N1'	4.90	127.69	117.12
2	N	104[A]	AI1	O1-C1-C2	5.31	114.97	107.11
2	E	104	AI1	C2'-C1'-C6'	5.34	127.78	120.53
2	H	104	AI1	C2'-C1'-C6'	5.73	128.30	120.53
2	O	104	AI1	O1-C1-C2	5.79	115.68	107.11
2	G	104	AI1	C2'-C1'-C6'	5.92	128.56	120.53
2	N	104[B]	AI1	C2'-C1'-C6'	6.11	128.82	120.53
2	E	104	AI1	C3'-C4'-C5'	6.48	127.97	120.35
2	H	104	AI1	C1B-N1'-C7'	7.49	140.87	121.82
2	D	104	AI1	O1-C1-C2	7.77	118.60	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	104	AI1	1	0
2	E	104	AI1	1	0
2	F	104	AI1	1	0
2	G	104	AI1	1	0
2	H	104	AI1	2	0
2	L	104	AI1	1	0
2	N	104[A]	AI1	3	0
2	N	104[B]	AI1	3	0
2	O	104	AI1	1	0
2	P	104	AI1	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	D	103/103 (100%)	-0.19	2 (1%) 67 63	10, 17, 24, 29	0
1	E	103/103 (100%)	-0.34	1 (0%) 82 80	10, 14, 21, 34	0
1	F	103/103 (100%)	-0.36	2 (1%) 67 63	9, 13, 22, 29	0
1	G	103/103 (100%)	-0.43	1 (0%) 82 80	9, 13, 18, 31	0
1	H	103/103 (100%)	-0.15	3 (2%) 52 47	10, 18, 25, 32	0
1	L	103/103 (100%)	-0.31	1 (0%) 82 80	11, 15, 23, 30	0
1	M	103/103 (100%)	-0.29	2 (1%) 67 63	9, 14, 21, 26	0
1	N	103/103 (100%)	-0.42	1 (0%) 82 80	10, 14, 23, 31	0
1	O	103/103 (100%)	-0.12	3 (2%) 52 47	11, 19, 27, 38	0
1	P	103/103 (100%)	-0.20	1 (0%) 82 80	11, 16, 24, 32	0
All	All	1030/1030 (100%)	-0.28	17 (1%) 70 67	9, 15, 25, 38	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	13	ARG	3.5
1	F	13	ARG	3.0
1	P	103	ASN	3.0
1	M	55	SER	2.8
1	O	1	ALA	2.7
1	N	103	ASN	2.7
1	D	96	ILE	2.5
1	F	55	SER	2.4
1	D	13	ARG	2.4
1	H	13	ARG	2.3
1	E	103	ASN	2.3
1	G	103	ASN	2.2
1	L	103	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	98	ALA	2.2
1	H	12	TYR	2.2
1	O	59	ASP	2.2
1	M	103	ASN	2.1

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	AI1	N	104[B]	28/28	0.88	0.17	6.20	16,20,21,21	17
2	AI1	N	104[A]	28/28	0.88	0.17	6.20	16,20,22,22	17
2	AI1	D	104	28/28	0.75	0.25	2.68	25,34,43,43	0
2	AI1	E	104	28/28	0.88	0.14	2.21	13,18,26,26	0
2	AI1	P	104	28/28	0.81	0.18	1.78	19,30,38,38	0
2	AI1	L	104	28/28	0.89	0.14	1.26	16,22,32,32	0
2	AI1	O	104	28/28	0.85	0.18	0.96	25,32,39,39	0
2	AI1	G	104	28/28	0.97	0.09	0.01	12,13,14,15	0
2	AI1	F	104	28/28	0.91	0.11	-0.07	14,23,31,31	0
2	AI1	H	104	28/28	0.91	0.11	-0.21	18,24,32,32	0
2	AI1	M	104	28/28	0.96	0.08	-0.65	12,14,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.