Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 12:23 AM EST

PDB ID	:	2OM0
Title	:	Structure of human insulin in presence of urea at pH 6.5
Authors	:	Norrman, M.; Schluckebier, G.
Deposited on	:	2007-01-20
Resolution	:	2.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

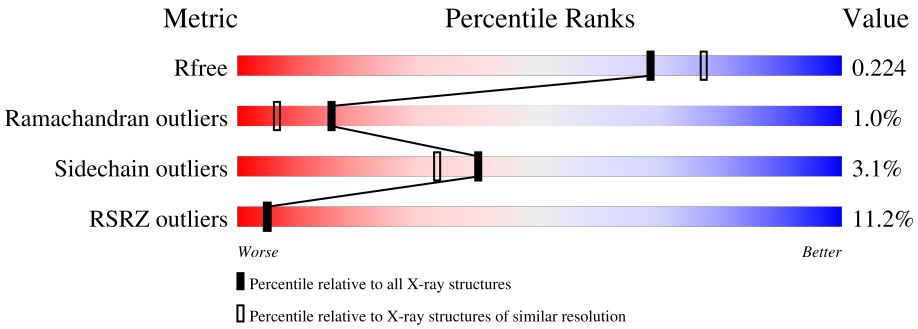
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	1	21	5% 100%
1	3	21	5% 100%
1	A	21	5% 100%
1	C	21	5% 100%
1	E	21	100%
1	G	21	5% 95% 5%
1	I	21	86% 14%

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Mol	Chain	Length	Quality of chain
1	K	21	5% 95% 5%
1	Q	21	95% 5%
1	S	21	100%
1	U	21	100%
1	X	21	100%
1	a	21	10% 90% 10%
1	c	21	10% 100%
1	e	21	19% 100%
1	g	21	10% 100%
1	i	21	24% 95% 5%
1	k	21	19% 100%
2	2	30	23% 93%
2	4	30	23% 93%
2	B	30	10% 93%
2	D	30	10% 90% 7%
2	F	30	10% 93%
2	H	30	10% 93%
2	J	30	10% 90% 7%
2	L	30	13% 90% 7%
2	R	30	13% 87% 10%
2	T	30	10% 93%
2	V	30	7% 93%
2	Y	30	13% 90% 7%
2	b	30	13% 87% 10%
2	d	30	23% 93%

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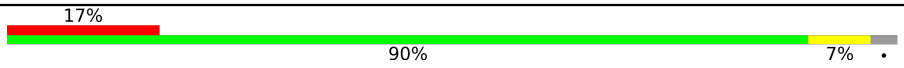
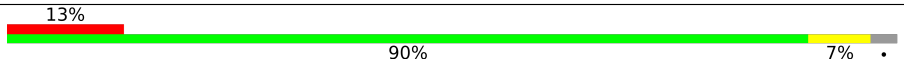
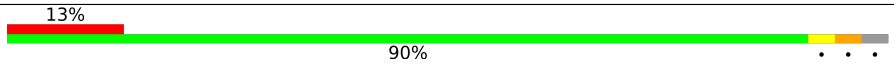
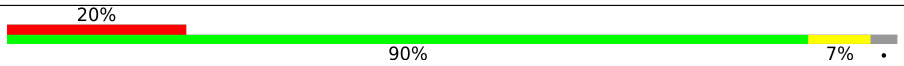
Mol	Chain	Length	Quality of chain
2	f	30	
2	h	30	
2	j	30	
2	l	30	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7978 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 Insulin A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	E	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	G	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	I	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	K	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	Q	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	S	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	U	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	X	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	1	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	3	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	a	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	c	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	e	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	g	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	i	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	k	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	29	Total	C	N	O	S	0	1	0
			234	155	38	39	2			
2	D	29	Total	C	N	O	S	0	0	0
			231	152	38	39	2			
2	F	29	Total	C	N	O	S	0	0	0
			232	153	38	39	2			
2	H	29	Total	C	N	O	S	0	1	0
			241	157	42	40	2			
2	J	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			
2	L	29	Total	C	N	O	S	0	1	0
			237	156	39	40	2			
2	R	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			
2	T	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			
2	V	29	Total	C	N	O	S	0	0	0
			230	151	38	39	2			
2	Y	29	Total	C	N	O	S	0	1	0
			234	155	38	39	2			
2	2	29	Total	C	N	O	S	0	0	0
			231	152	38	39	2			
2	4	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			
2	b	29	Total	C	N	O	S	0	1	0
			239	157	40	40	2			
2	d	29	Total	C	N	O	S	0	0	0
			231	152	38	39	2			
2	f	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			
2	h	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			
2	j	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			

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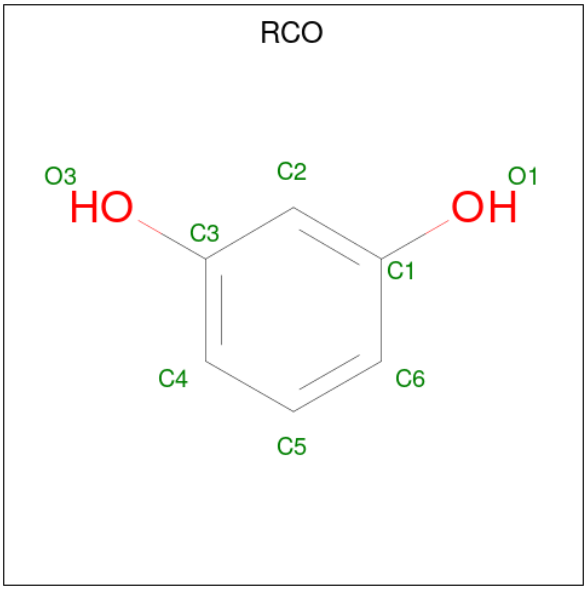
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	l	29	Total	C	N	O	S	0	0	0
			234	154	39	39	2			

- Molecule 3 is RESORCINOL (three-letter code: RCO) (formula: $C_6H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	I	1	Total	C	O	0	0
			8	6	2		
3	K	1	Total	C	O	0	0
			8	6	2		
3	Q	1	Total	C	O	0	0
			8	6	2		
3	S	1	Total	C	O	0	0
			8	6	2		
3	U	1	Total	C	O	0	0
			8	6	2		
3	X	1	Total	C	O	0	0
			8	6	2		

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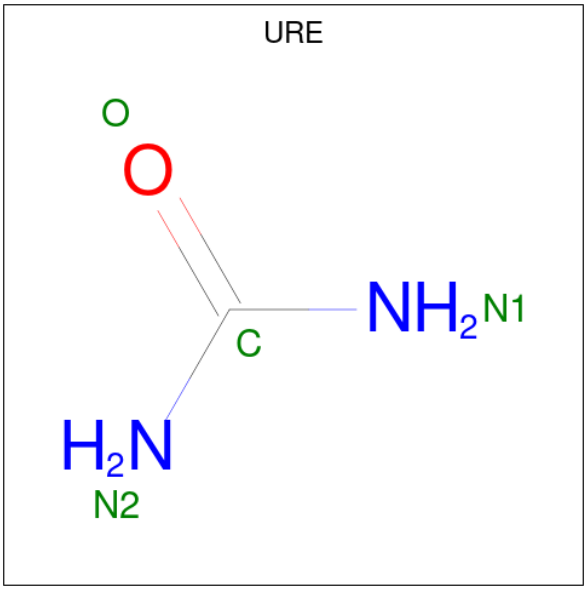
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	1	Total C O 8 6 2	0	0
3	3	1	Total C O 8 6 2	0	0
3	a	1	Total C O 8 6 2	0	0
3	c	1	Total C O 8 6 2	0	0
3	e	1	Total C O 8 6 2	0	0
3	g	1	Total C O 8 6 2	0	0
3	i	1	Total C O 8 6 2	0	0
3	k	1	Total C O 8 6 2	0	0

- Molecule 4 is UREA (three-letter code: URE) (formula: CH_4N_2O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 4 1 2 1	0	0
4	C	1	Total C N O 4 1 2 1	0	0
4	D	1	Total C N O 4 1 2 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N O 4 1 2 1	0	0
4	G	1	Total C N O 4 1 2 1	0	0
4	I	1	Total C N O 4 1 2 1	0	0
4	Q	1	Total C N O 4 1 2 1	0	0
4	S	1	Total C N O 4 1 2 1	0	0
4	U	1	Total C N O 4 1 2 1	0	0
4	1	1	Total C N O 4 1 2 1	0	0
4	d	1	Total C N O 4 1 2 1	0	0
4	g	1	Total C N O 4 1 2 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0
5	R	1	Total Zn 1 1	0	0
5	Y	1	Total Zn 1 1	0	0
5	b	1	Total Zn 1 1	0	0
5	h	1	Total Zn 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	R	1	Total Cl 1 1	0	0
6	Y	1	Total Cl 1 1	0	0
6	b	1	Total Cl 1 1	0	0
6	h	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	21	Total O 21 21	0	0
7	B	17	Total O 17 17	0	0
7	C	26	Total O 26 26	0	0
7	D	32	Total O 32 32	0	0
7	E	17	Total O 17 17	0	0
7	F	17	Total O 17 17	0	0
7	G	18	Total O 18 18	0	0
7	H	18	Total O 18 18	0	0
7	I	16	Total O 16 16	0	0
7	J	17	Total O 17 17	0	0
7	K	15	Total O 15 15	0	0
7	L	18	Total O 18 18	0	0
7	Q	14	Total O 14 14	0	0
7	R	22	Total O 22 22	0	0
7	S	20	Total O 20 20	0	0

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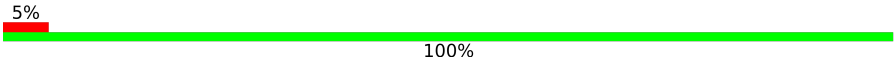
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	24	Total O 24 24	0	0
7	U	18	Total O 18 18	0	0
7	V	23	Total O 23 23	0	0
7	X	25	Total O 25 25	0	0
7	Y	14	Total O 14 14	0	0
7	1	20	Total O 20 20	0	0
7	2	22	Total O 22 22	0	0
7	3	12	Total O 12 12	0	0
7	4	19	Total O 19 19	0	0
7	a	19	Total O 19 19	0	0
7	b	16	Total O 16 16	0	0
7	c	11	Total O 11 11	0	0
7	d	8	Total O 8 8	0	0
7	e	8	Total O 8 8	0	0
7	f	19	Total O 19 19	0	0
7	g	18	Total O 18 18	0	0
7	h	21	Total O 21 21	0	0
7	i	13	Total O 13 13	0	0
7	j	14	Total O 14 14	0	0
7	k	3	Total O 3 3	0	0
7	l	13	Total O 13 13	0	0

3 Residue-property plots (i)

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

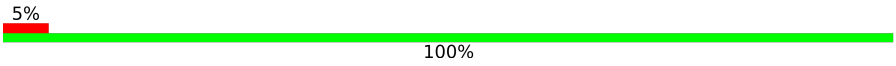
• Molecule 1: Insulin A chain

Chain A:



• Molecule 1: Insulin A chain

Chain C:



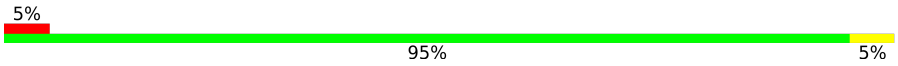
• Molecule 1: Insulin A chain

Chain E:

There are no outlier residues recorded for this chain.

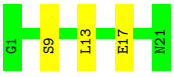
• Molecule 1: Insulin A chain

Chain G:



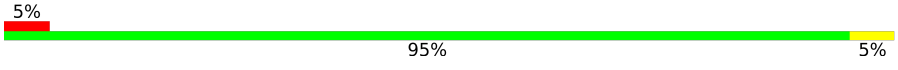
• Molecule 1: Insulin A chain

Chain I:



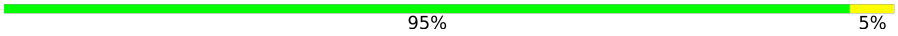
• Molecule 1: Insulin A chain

Chain K:



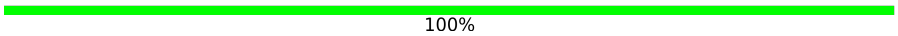
• Molecule 1: Insulin A chain

Chain Q:



• Molecule 1: Insulin A chain

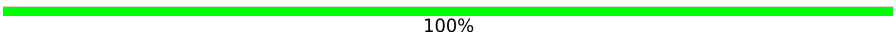
Chain S:



There are no outlier residues recorded for this chain.

• Molecule 1: Insulin A chain

Chain U:



There are no outlier residues recorded for this chain.

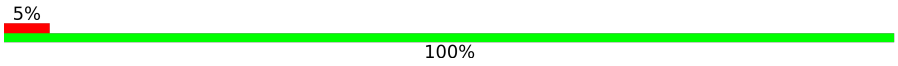
• Molecule 1: Insulin A chain

Chain X:

There are no outlier residues recorded for this chain.

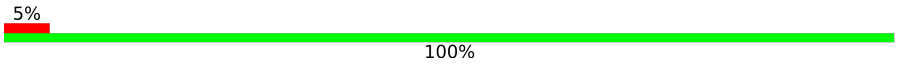
• Molecule 1: Insulin A chain

Chain 1:



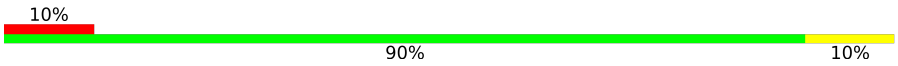
• Molecule 1: Insulin A chain

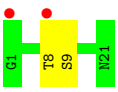
Chain 3:



• Molecule 1: Insulin A chain

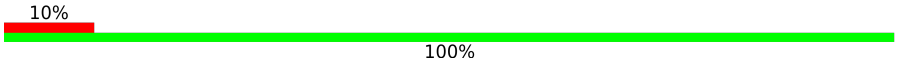
Chain a:

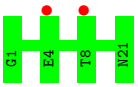




• Molecule 1: Insulin A chain

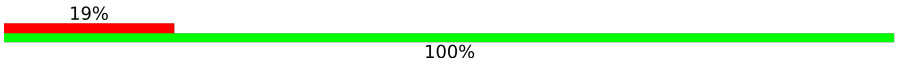
Chain c:

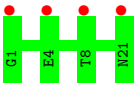




• Molecule 1: Insulin A chain

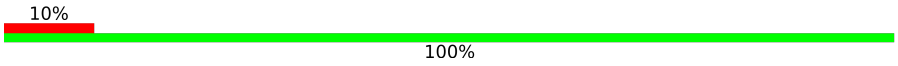
Chain e:





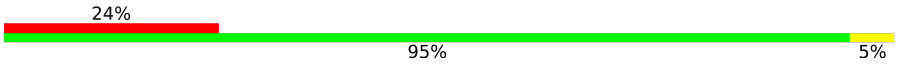
• Molecule 1: Insulin A chain

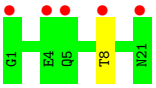
Chain g:



• Molecule 1: Insulin A chain

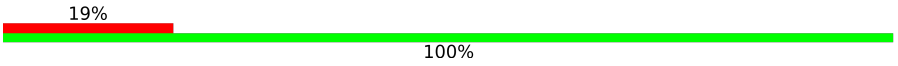
Chain i:

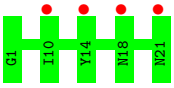




• Molecule 1: Insulin A chain

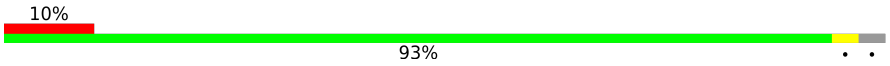
Chain k:

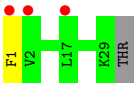




• Molecule 2: Insulin B chain

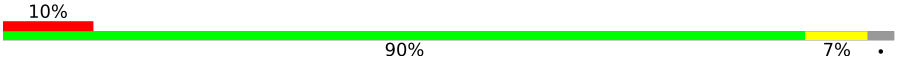
Chain B:

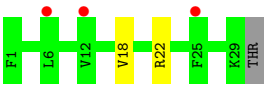




• Molecule 2: Insulin B chain

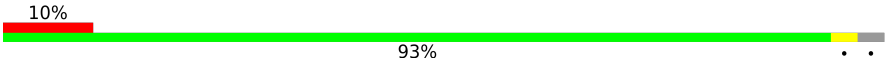
Chain D:

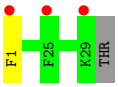




• Molecule 2: Insulin B chain

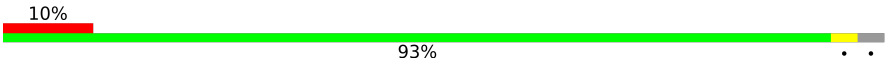
Chain F:

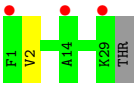




• Molecule 2: Insulin B chain

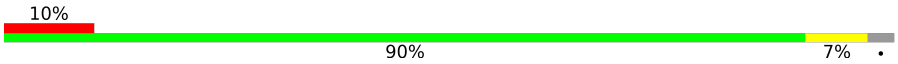
Chain H:

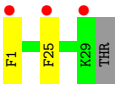




• Molecule 2: Insulin B chain

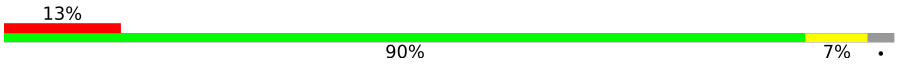
Chain J:

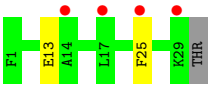




• Molecule 2: Insulin B chain

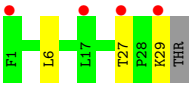
Chain L:





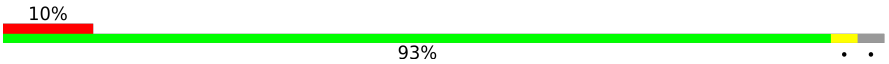
• Molecule 2: Insulin B chain

Chain R:



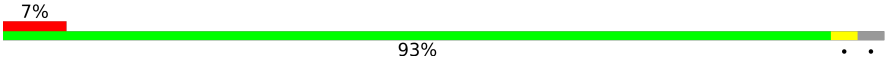
• Molecule 2: Insulin B chain

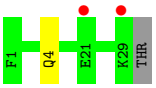
Chain T:



• Molecule 2: Insulin B chain

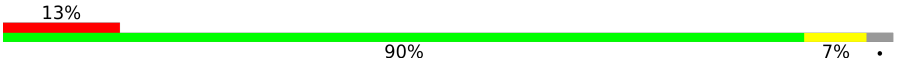
Chain V:

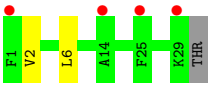




• Molecule 2: Insulin B chain

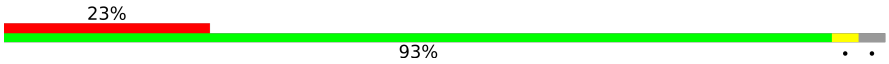
Chain Y:

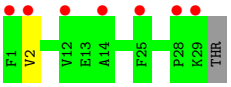




• Molecule 2: Insulin B chain

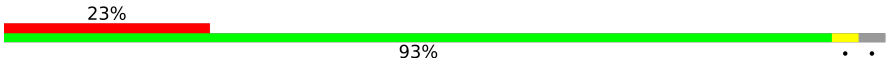
Chain 2:

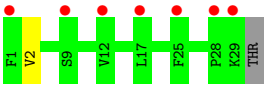




• Molecule 2: Insulin B chain

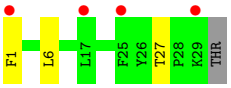
Chain 4:





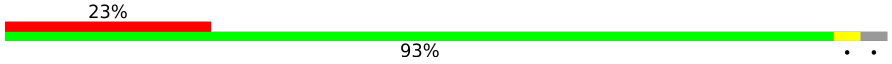
• Molecule 2: Insulin B chain

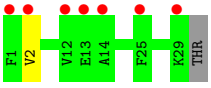
Chain b:



• Molecule 2: Insulin B chain

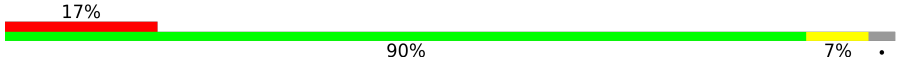
Chain d:

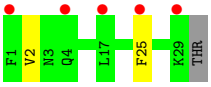




• Molecule 2: Insulin B chain

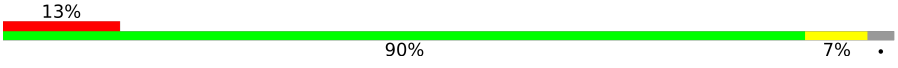
Chain f:





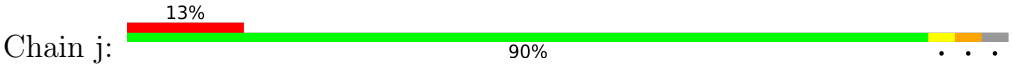
• Molecule 2: Insulin B chain

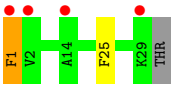
Chain h:



• Molecule 2: Insulin B chain

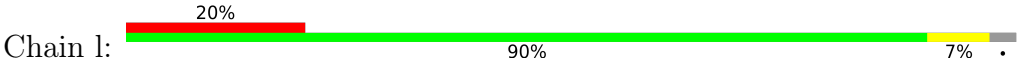
Chain j:

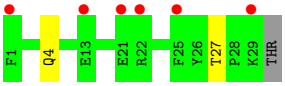




• Molecule 2: Insulin B chain

Chain l:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	58.94Å 219.32Å 223.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.31 – 2.05 28.31 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.31-2.05) 100.0 (28.31-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.227 0.182 , 0.224	Depositor DCC
R_{free} test set	4536 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7978	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.333 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: CL, URE, RCO, ZN

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	1	0.81	0/164	0.67	0/220
1	3	0.81	0/164	0.60	0/220
1	A	0.98	0/164	0.85	0/220
1	C	0.80	0/164	0.78	0/220
1	E	0.74	0/164	0.70	0/220
1	G	1.25	1/164 (0.6%)	0.84	0/220
1	I	0.93	0/164	0.81	0/220
1	K	1.14	1/164 (0.6%)	0.64	0/220
1	Q	0.71	0/164	0.68	0/220
1	S	0.73	0/164	0.67	0/220
1	U	0.81	0/164	0.73	0/220
1	X	0.71	0/164	0.67	0/220
1	a	0.73	0/164	0.61	0/220
1	c	0.62	0/164	0.63	0/220
1	e	0.65	0/164	0.60	0/220
1	g	0.76	0/164	0.70	0/220
1	i	0.54	0/164	0.61	0/220
1	k	0.61	0/164	0.55	0/220
2	2	0.97	0/238	0.75	0/322
2	4	0.95	0/241	0.70	0/325
2	B	1.00	0/244	0.83	0/330
2	D	1.01	0/238	0.81	1/322 (0.3%)
2	F	1.01	0/239	0.74	0/323
2	H	0.91	0/248	0.77	0/335
2	J	0.94	0/241	0.72	0/325
2	L	0.99	0/247	0.67	0/334
2	R	0.94	0/241	0.67	0/325
2	T	0.85	0/241	0.74	0/325
2	V	0.88	0/237	0.67	0/321
2	Y	0.94	0/244	0.79	0/331
2	b	0.76	0/249	0.64	0/336
2	d	0.85	0/238	0.76	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	f	0.85	0/241	0.79	0/325
2	h	0.78	0/241	0.75	0/325
2	j	0.87	0/241	0.70	0/325
2	l	0.78	0/241	0.63	0/325
All	All	0.87	2/7302 (0.0%)	0.72	1/9836 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
2	R	0	1
2	j	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	21	ASN	C-OXT	-11.47	1.01	1.23
1	K	21	ASN	C-OXT	-10.11	1.04	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	22	ARG	NE-CZ-NH1	-5.41	117.60	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	PHE	Peptide
2	F	1	PHE	Peptide
2	R	27	THR	Peptide
2	j	1	PHE	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1	19/21 (90%)	19 (100%)	0	0	100	100
1	3	19/21 (90%)	19 (100%)	0	0	100	100
1	A	19/21 (90%)	19 (100%)	0	0	100	100
1	C	19/21 (90%)	19 (100%)	0	0	100	100
1	E	19/21 (90%)	19 (100%)	0	0	100	100
1	G	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	I	19/21 (90%)	19 (100%)	0	0	100	100
1	K	19/21 (90%)	19 (100%)	0	0	100	100
1	Q	19/21 (90%)	19 (100%)	0	0	100	100
1	S	19/21 (90%)	19 (100%)	0	0	100	100
1	U	19/21 (90%)	19 (100%)	0	0	100	100
1	X	19/21 (90%)	19 (100%)	0	0	100	100
1	a	19/21 (90%)	19 (100%)	0	0	100	100
1	c	19/21 (90%)	19 (100%)	0	0	100	100
1	e	19/21 (90%)	19 (100%)	0	0	100	100
1	g	19/21 (90%)	19 (100%)	0	0	100	100
1	i	19/21 (90%)	19 (100%)	0	0	100	100
1	k	19/21 (90%)	19 (100%)	0	0	100	100
2	2	27/30 (90%)	26 (96%)	0	1 (4%)	3	0
2	4	27/30 (90%)	26 (96%)	0	1 (4%)	3	0
2	B	28/30 (93%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	27/30 (90%)	27 (100%)	0	0	100 100
2	F	27/30 (90%)	27 (100%)	0	0	100 100
2	H	28/30 (93%)	27 (96%)	0	1 (4%)	3 0
2	J	27/30 (90%)	27 (100%)	0	0	100 100
2	L	28/30 (93%)	28 (100%)	0	0	100 100
2	R	27/30 (90%)	27 (100%)	0	0	100 100
2	T	27/30 (90%)	26 (96%)	0	1 (4%)	3 0
2	V	27/30 (90%)	26 (96%)	1 (4%)	0	100 100
2	Y	28/30 (93%)	27 (96%)	0	1 (4%)	3 0
2	b	28/30 (93%)	28 (100%)	0	0	100 100
2	d	27/30 (90%)	26 (96%)	0	1 (4%)	3 0
2	f	27/30 (90%)	26 (96%)	0	1 (4%)	3 0
2	h	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	3 0
2	j	27/30 (90%)	26 (96%)	1 (4%)	0	100 100
2	l	27/30 (90%)	27 (100%)	0	0	100 100
All	All	833/918 (91%)	820 (98%)	5 (1%)	8 (1%)	15 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	2	VAL
2	4	2	VAL
2	f	2	VAL
2	d	2	VAL
2	h	2	VAL
2	T	2	VAL
2	Y	2	VAL
2	H	2	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	20/20 (100%)	20 (100%)	0	100 100
1	3	20/20 (100%)	20 (100%)	0	100 100
1	A	20/20 (100%)	20 (100%)	0	100 100
1	C	20/20 (100%)	20 (100%)	0	100 100
1	E	20/20 (100%)	20 (100%)	0	100 100
1	G	20/20 (100%)	20 (100%)	0	100 100
1	I	20/20 (100%)	17 (85%)	3 (15%)	3 0
1	K	20/20 (100%)	20 (100%)	0	100 100
1	Q	20/20 (100%)	19 (95%)	1 (5%)	24 16
1	S	20/20 (100%)	20 (100%)	0	100 100
1	U	20/20 (100%)	20 (100%)	0	100 100
1	X	20/20 (100%)	20 (100%)	0	100 100
1	a	20/20 (100%)	18 (90%)	2 (10%)	7 2
1	c	20/20 (100%)	20 (100%)	0	100 100
1	e	20/20 (100%)	20 (100%)	0	100 100
1	g	20/20 (100%)	20 (100%)	0	100 100
1	i	20/20 (100%)	19 (95%)	1 (5%)	24 16
1	k	20/20 (100%)	20 (100%)	0	100 100
2	2	24/26 (92%)	24 (100%)	0	100 100
2	4	25/26 (96%)	25 (100%)	0	100 100
2	B	25/26 (96%)	25 (100%)	0	100 100
2	D	24/26 (92%)	23 (96%)	1 (4%)	30 22
2	F	24/26 (92%)	24 (100%)	0	100 100
2	H	25/26 (96%)	25 (100%)	0	100 100
2	J	25/26 (96%)	23 (92%)	2 (8%)	12 5
2	L	25/26 (96%)	23 (92%)	2 (8%)	12 5
2	R	25/26 (96%)	23 (92%)	2 (8%)	12 5
2	T	25/26 (96%)	25 (100%)	0	100 100
2	V	24/26 (92%)	23 (96%)	1 (4%)	30 22
2	Y	25/26 (96%)	24 (96%)	1 (4%)	31 24
2	b	26/26 (100%)	23 (88%)	3 (12%)	5 1
2	d	24/26 (92%)	24 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	f	25/26 (96%)	24 (96%)	1 (4%)	31 24
2	h	25/26 (96%)	24 (96%)	1 (4%)	31 24
2	j	25/26 (96%)	23 (92%)	2 (8%)	12 5
2	l	25/26 (96%)	23 (92%)	2 (8%)	12 5
All	All	806/828 (97%)	781 (97%)	25 (3%)	40 33

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	18	VAL
1	I	9	SER
1	I	13	LEU
1	I	17	GLU
2	J	1	PHE
2	J	25	PHE
2	L	13	GLU
2	L	25	PHE
1	Q	21	ASN
2	R	6	LEU
2	R	29	LYS
2	V	4	GLN
2	Y	6	LEU
1	a	8	THR
1	a	9	SER
2	b	1	PHE
2	b	6	LEU
2	b	27	THR
2	f	25	PHE
2	h	25	PHE
1	i	8	THR
2	j	1	PHE
2	j	25	PHE
2	l	4	GLN
2	l	27	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	4	GLN
1	E	21	ASN

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Mol	Chain	Res	Type
1	G	21	ASN
2	H	3	ASN
1	Q	21	ASN
2	T	4	GLN
2	V	5	HIS
1	X	21	ASN
2	Y	5	HIS
1	1	21	ASN
2	4	3	ASN
1	a	21	ASN
1	c	21	ASN
1	g	21	ASN
1	k	21	ASN
2	l	4	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	RCO	C	701	-	8,8,8	0.84	0	10,10,10	0.95	0
3	RCO	1	713	-	8,8,8	0.74	0	10,10,10	0.86	0
3	RCO	i	717	-	8,8,8	0.79	0	10,10,10	0.43	0
3	RCO	g	709	-	8,8,8	0.79	0	10,10,10	0.87	1 (10%)
4	URE	C	1002	-	3,3,3	0.40	0	3,3,3	0.52	0
3	RCO	c	715	-	8,8,8	0.60	0	10,10,10	0.44	0
3	RCO	I	702	-	8,8,8	0.65	0	10,10,10	0.89	0
4	URE	1	1008	-	3,3,3	0.57	0	3,3,3	0.51	0
4	URE	S	1007	-	3,3,3	0.52	0	3,3,3	0.77	0
4	URE	U	1012	-	3,3,3	0.38	0	3,3,3	0.06	0
4	URE	Q	1006	-	3,3,3	0.44	0	3,3,3	0.35	0
4	URE	d	1011	-	3,3,3	0.41	0	3,3,3	0.27	0
3	RCO	A	714	-	8,8,8	0.82	0	10,10,10	0.82	0
4	URE	E	1003	-	3,3,3	0.39	0	3,3,3	0.42	0
3	RCO	X	718	-	8,8,8	0.74	0	10,10,10	1.03	0
3	RCO	S	711	-	8,8,8	1.05	0	10,10,10	0.91	0
3	RCO	K	703	-	8,8,8	0.81	0	10,10,10	0.90	0
4	URE	I	1005	-	3,3,3	0.59	0	3,3,3	0.44	0
4	URE	D	1010	-	3,3,3	0.66	0	3,3,3	0.72	0
3	RCO	Q	710	-	8,8,8	0.68	0	10,10,10	0.56	0
3	RCO	E	712	-	8,8,8	0.93	0	10,10,10	0.73	0
3	RCO	3	706	-	8,8,8	0.85	0	10,10,10	0.46	0
4	URE	g	1009	-	3,3,3	0.38	0	3,3,3	0.58	0
4	URE	A	1001	-	3,3,3	0.56	0	3,3,3	0.54	0
3	RCO	a	716	-	8,8,8	0.90	0	10,10,10	0.69	0
3	RCO	k	708	-	8,8,8	0.83	0	10,10,10	0.54	0
3	RCO	e	707	-	8,8,8	0.63	0	10,10,10	0.35	0
4	URE	G	1004	-	3,3,3	0.50	0	3,3,3	0.43	0
3	RCO	G	705	-	8,8,8	1.02	1 (12%)	10,10,10	0.27	0
3	RCO	U	704	-	8,8,8	1.15	1 (12%)	10,10,10	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RCO	C	701	-	-	-	0/1/1/1
3	RCO	1	713	-	-	-	0/1/1/1
3	RCO	3	706	-	-	-	0/1/1/1
3	RCO	e	707	-	-	-	0/1/1/1
3	RCO	i	717	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RCO	A	714	-	-	-	0/1/1/1
3	RCO	g	709	-	-	-	0/1/1/1
3	RCO	a	716	-	-	-	0/1/1/1
3	RCO	X	718	-	-	-	0/1/1/1
3	RCO	c	715	-	-	-	0/1/1/1
3	RCO	I	702	-	-	-	0/1/1/1
3	RCO	S	711	-	-	-	0/1/1/1
3	RCO	K	703	-	-	-	0/1/1/1
3	RCO	k	708	-	-	-	0/1/1/1
3	RCO	G	705	-	-	-	0/1/1/1
3	RCO	U	704	-	-	-	0/1/1/1
3	RCO	Q	710	-	-	-	0/1/1/1
3	RCO	E	712	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	705	RCO	C2-C1	2.28	1.42	1.39
3	U	704	RCO	C2-C1	2.22	1.42	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	g	709	RCO	C3-C2-C1	2.01	121.62	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1	21/21 (100%)	0.34	1 (4%) 30 33	21, 27, 36, 38	0
1	3	21/21 (100%)	0.44	1 (4%) 30 33	23, 32, 37, 40	0
1	A	21/21 (100%)	0.10	1 (4%) 30 33	18, 26, 33, 36	0
1	C	21/21 (100%)	-0.15	1 (4%) 30 33	20, 23, 28, 33	0
1	E	21/21 (100%)	0.21	0 100 100	25, 31, 38, 40	0
1	G	21/21 (100%)	0.04	1 (4%) 30 33	23, 29, 35, 36	0
1	I	21/21 (100%)	0.31	0 100 100	24, 32, 37, 39	0
1	K	21/21 (100%)	0.28	1 (4%) 30 33	22, 30, 36, 38	0
1	Q	21/21 (100%)	0.19	0 100 100	22, 30, 33, 33	0
1	S	21/21 (100%)	-0.05	0 100 100	22, 28, 31, 35	0
1	U	21/21 (100%)	0.22	0 100 100	20, 30, 36, 39	0
1	X	21/21 (100%)	0.09	0 100 100	23, 29, 37, 39	0
1	a	21/21 (100%)	0.32	2 (9%) 8 9	25, 33, 40, 42	0
1	c	21/21 (100%)	0.68	2 (9%) 8 9	28, 34, 44, 45	0
1	e	21/21 (100%)	0.53	4 (19%) 1 0	25, 36, 40, 42	0
1	g	21/21 (100%)	0.28	2 (9%) 8 9	20, 28, 35, 40	0
1	i	21/21 (100%)	0.83	5 (23%) 0 0	29, 38, 44, 46	0
1	k	21/21 (100%)	1.10	4 (19%) 1 0	39, 44, 47, 49	0
2	2	29/30 (96%)	1.15	7 (24%) 0 0	19, 25, 42, 53	0
2	4	29/30 (96%)	1.16	7 (24%) 0 0	23, 28, 43, 55	0
2	B	29/30 (96%)	1.30	3 (10%) 6 6	16, 23, 42, 50	0
2	D	29/30 (96%)	0.71	3 (10%) 6 6	18, 23, 33, 46	0
2	F	29/30 (96%)	1.00	3 (10%) 6 6	22, 28, 44, 56	0
2	H	29/30 (96%)	0.86	3 (10%) 6 6	21, 26, 39, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
2	J	29/30 (96%)	1.05	3 (10%)	6 6	19, 26, 45, 57	0
2	L	29/30 (96%)	0.72	4 (13%)	2 2	23, 26, 44, 58	0
2	R	29/30 (96%)	0.91	4 (13%)	2 2	21, 26, 46, 60	0
2	T	29/30 (96%)	0.66	3 (10%)	6 6	22, 26, 39, 52	0
2	V	29/30 (96%)	0.69	2 (6%)	16 18	21, 27, 45, 54	0
2	Y	29/30 (96%)	1.06	4 (13%)	2 2	20, 27, 42, 53	0
2	b	29/30 (96%)	1.13	4 (13%)	2 2	27, 31, 48, 61	0
2	d	29/30 (96%)	1.32	7 (24%)	0 0	25, 30, 44, 54	0
2	f	29/30 (96%)	1.24	5 (17%)	1 1	26, 32, 46, 59	0
2	h	29/30 (96%)	0.84	4 (13%)	2 2	21, 28, 43, 52	0
2	j	29/30 (96%)	1.20	4 (13%)	2 2	27, 35, 49, 60	0
2	l	29/30 (96%)	1.31	6 (20%)	1 0	27, 37, 53, 63	0
All	All	900/918 (98%)	0.72	101 (11%)	5 5	16, 30, 46, 63	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	1	PHE	9.3
2	l	1	PHE	8.6
2	B	1	PHE	7.9
2	F	1	PHE	7.7
2	2	1	PHE	7.0
2	j	1	PHE	7.0
2	d	1	PHE	6.7
2	f	1	PHE	6.3
2	h	1	PHE	6.2
2	J	1	PHE	5.7
2	Y	1	PHE	5.2
2	f	25	PHE	5.0
2	Y	25	PHE	4.9
2	J	25	PHE	4.5
2	4	1	PHE	4.4
2	d	25	PHE	4.2
1	g	8	THR	4.0
2	2	29	LYS	4.0
2	l	21	GLU	4.0
2	H	29	LYS	3.7
1	k	14	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	25	PHE	3.7
2	f	29	LYS	3.7
2	4	25	PHE	3.7
2	L	29	LYS	3.6
2	R	27	THR	3.6
2	4	29	LYS	3.4
1	k	18	ASN	3.4
2	V	21	GLU	3.4
2	T	29	LYS	3.3
2	B	17[A]	LEU	3.3
2	B	2	VAL	3.3
2	J	29	LYS	3.1
1	k	10	ILE	3.1
2	b	29	LYS	3.1
2	R	29	LYS	2.9
2	f	17	LEU	2.9
1	i	1	GLY	2.9
1	K	21	ASN	2.9
2	F	29	LYS	2.8
1	k	21	ASN	2.8
2	V	29	LYS	2.8
2	j	29	LYS	2.7
2	Y	29	LYS	2.7
1	A	8	THR	2.7
2	j	2	VAL	2.6
1	c	4	GLU	2.6
2	d	13	GLU	2.6
1	e	8	THR	2.6
2	T	25	PHE	2.6
2	2	2	VAL	2.5
2	h	29	LYS	2.5
2	R	1	PHE	2.5
2	2	25	PHE	2.5
1	a	1	GLY	2.5
1	a	8	THR	2.5
2	l	29	LYS	2.5
2	l	22	ARG	2.5
1	i	21	ASN	2.5
1	G	14	TYR	2.5
2	h	25	PHE	2.4
1	c	8	THR	2.4
2	b	25	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	4	12	VAL	2.4
1	i	4	GLU	2.4
2	b	17	LEU	2.4
2	2	12	VAL	2.4
1	i	8	THR	2.4
2	L	25	PHE	2.3
2	D	12	VAL	2.3
2	2	28	PRO	2.3
1	e	1	GLY	2.3
2	d	12	VAL	2.3
1	1	4	GLU	2.3
2	4	28	PRO	2.3
2	H	1	PHE	2.3
1	3	1	GLY	2.2
2	d	29	LYS	2.2
2	H	14	ALA	2.2
2	4	17	LEU	2.2
2	D	25	PHE	2.2
1	C	1	GLY	2.2
1	e	21	ASN	2.2
1	g	21	ASN	2.2
2	d	14	ALA	2.2
2	j	14	ALA	2.2
2	D	6	LEU	2.1
2	d	2	VAL	2.1
1	e	4	GLU	2.1
2	4	9	SER	2.1
2	Y	14	ALA	2.1
2	R	17	LEU	2.0
2	f	4	GLN	2.0
2	l	25	PHE	2.0
2	h	3	ASN	2.0
2	L	17	LEU	2.0
2	T	17	LEU	2.0
2	L	14	ALA	2.0
2	l	13	GLU	2.0
1	i	5	GLN	2.0
2	2	14	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
4	URE	U	1012	4/4	0.55	0.29	73,73,73,73	0
4	URE	d	1011	4/4	0.75	0.23	62,62,62,63	0
4	URE	Q	1006	4/4	0.77	0.35	63,63,63,63	0
4	URE	A	1001	4/4	0.89	0.25	44,45,46,46	0
3	RCO	k	708	8/8	0.92	0.16	32,35,37,37	0
4	URE	G	1004	4/4	0.93	0.41	51,52,52,53	0
4	URE	C	1002	4/4	0.93	0.26	49,49,49,49	0
4	URE	D	1010	4/4	0.93	0.20	32,33,33,33	0
4	URE	E	1003	4/4	0.93	0.28	52,53,53,53	0
4	URE	I	1005	4/4	0.94	0.44	65,65,65,65	0
3	RCO	A	714	8/8	0.94	0.10	25,27,28,28	0
3	RCO	c	715	8/8	0.94	0.11	31,33,35,35	0
4	URE	1	1008	4/4	0.94	0.32	44,44,44,45	0
3	RCO	i	717	8/8	0.94	0.15	30,33,34,35	0
3	RCO	E	712	8/8	0.96	0.10	27,29,30,30	0
3	RCO	1	713	8/8	0.96	0.09	20,24,25,25	0
4	URE	S	1007	4/4	0.96	0.27	43,45,45,45	0
4	URE	g	1009	4/4	0.96	0.32	40,41,42,43	0
3	RCO	e	707	8/8	0.97	0.08	28,29,31,32	0
3	RCO	I	702	8/8	0.97	0.08	23,24,26,26	0
3	RCO	3	706	8/8	0.97	0.07	20,21,23,25	0
3	RCO	a	716	8/8	0.97	0.09	26,28,29,29	0
3	RCO	Q	710	8/8	0.97	0.07	21,22,23,24	0
3	RCO	G	705	8/8	0.98	0.06	16,18,19,20	0
3	RCO	S	711	8/8	0.98	0.06	19,21,22,24	0
3	RCO	X	718	8/8	0.98	0.07	21,24,25,25	0
3	RCO	g	709	8/8	0.98	0.06	21,24,25,26	0
3	RCO	C	701	8/8	0.98	0.07	18,20,22,24	0
3	RCO	K	703	8/8	0.98	0.06	24,25,26,27	0
3	RCO	U	704	8/8	0.99	0.05	20,21,22,22	0
6	CL	B	903	1/1	0.99	0.04	23,23,23,23	0
6	CL	D	904	1/1	0.99	0.03	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	b	902	1/1	0.99	0.04	26,26,26,26	0
6	CL	h	901	1/1	0.99	0.03	26,26,26,26	0
5	ZN	b	806	1/1	1.00	0.03	23,23,23,23	0
5	ZN	h	805	1/1	1.00	0.03	26,26,26,26	0
5	ZN	B	801	1/1	1.00	0.05	22,22,22,22	0
5	ZN	D	802	1/1	1.00	0.02	18,18,18,18	0
6	CL	R	905	1/1	1.00	0.03	23,23,23,23	0
6	CL	Y	906	1/1	1.00	0.02	23,23,23,23	0
5	ZN	R	803	1/1	1.00	0.01	20,20,20,20	0
5	ZN	Y	804	1/1	1.00	0.02	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.