



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2023 – 07:10 AM EDT

PDB ID : 3IR0
Title : Crystal Structure of Human Insulin complexed with Cu⁺² metal ion
Authors : Raghavendra, N.; Pattabhi, V.; Rajan, S.S.
Deposited on : 2009-08-21
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

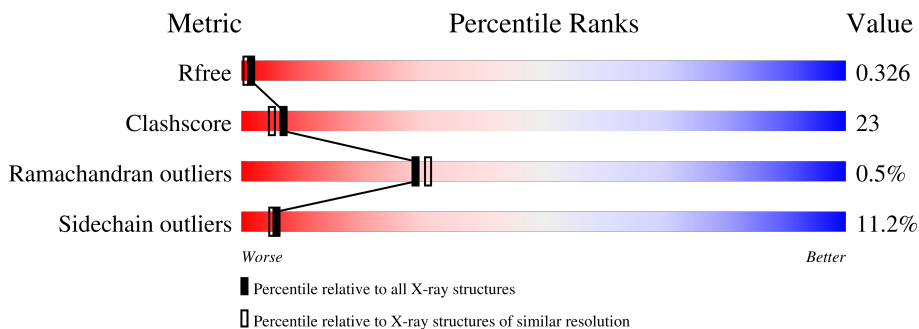
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	21	67% (green), 29% (yellow), 5% (orange)
1	C	21	33% (green), 52% (yellow), 14% (orange)
1	E	21	38% (green), 52% (yellow), 10% (orange)
1	G	21	52% (green), 38% (yellow), 10% (orange)
1	I	21	81% (green), 10% (yellow), 5% (orange), 5% (red)
1	K	21	48% (green), 52% (yellow)
1	M	21	81% (green), 14% (yellow), 5% (red)

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Mol	Chain	Length	Quality of chain
1	O	21	 52% 43% 5%
1	R	21	 38% 52% 10%
1	T	21	 57% 33% 5% 5%
1	V	21	 67% 29% 5%
1	X	21	 48% 48% 5%
2	B	30	 70% 23% 7%
2	D	30	 63% 30% 7%
2	F	30	 53% 43% 4%
2	H	30	 63% 30% 7%
2	J	30	 83% 10% 7%
2	L	30	 60% 27% 7% 7%
2	N	30	 77% 23%
2	P	30	 50% 40% 7% 3%
2	S	30	 43% 53% 4%
2	U	30	 63% 27% 10%
2	W	30	 67% 30% 3%
2	Y	30	 50% 50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5143 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
			Total	C	N	O	S			
1	A	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	C	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	E	21	Total 162	C 99	N 24	O 35	S 4	0	0	0
1	G	21	Total 162	C 99	N 25	O 34	S 4	0	0	0
1	I	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	K	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	M	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	O	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	R	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	T	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	V	21	Total 163	C 99	N 25	O 35	S 4	0	0	0
1	X	21	Total 163	C 99	N 25	O 35	S 4	0	0	0

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	30	Total 242	C 158	N 40	O 42	S 2	0	0	0
2	D	30	Total 236	C 152	N 40	O 42	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	H	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	J	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	L	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	N	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	P	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	S	30	Total	C	N	O	S	0	0	0
			242	158	40	42	2			
2	U	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			
2	W	30	Total	C	N	O	S	0	0	0
			241	158	39	42	2			
2	Y	30	Total	C	N	O	S	0	0	0
			236	152	40	42	2			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cu	0	0
			1	1		
3	D	1	Total	Cu	0	0
			1	1		
3	F	1	Total	Cu	0	0
			1	1		
3	H	1	Total	Cu	0	0
			1	1		
3	J	1	Total	Cu	0	0
			1	1		
3	L	1	Total	Cu	0	0
			1	1		
3	N	1	Total	Cu	0	0
			1	1		
3	P	1	Total	Cu	0	0
			1	1		
3	S	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	U	1	Total Cu 1 1	0	0
3	W	1	Total Cu 1 1	0	0
3	Y	1	Total Cu 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	12	Total O 12 12	0	0
4	C	9	Total O 9 9	0	0
4	D	22	Total O 22 22	0	0
4	E	8	Total O 8 8	0	0
4	F	13	Total O 13 13	0	0
4	G	8	Total O 8 8	0	0
4	H	12	Total O 12 12	0	0
4	I	12	Total O 12 12	0	0
4	J	17	Total O 17 17	0	0
4	K	5	Total O 5 5	0	0
4	L	19	Total O 19 19	0	0
4	M	7	Total O 7 7	0	0
4	N	16	Total O 16 16	0	0
4	O	11	Total O 11 11	0	0
4	P	24	Total O 24 24	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	4	Total O 4 4	0	0
4	S	15	Total O 15 15	0	0
4	T	13	Total O 13 13	0	0
4	U	10	Total O 10 10	0	0
4	V	15	Total O 15 15	0	0
4	W	20	Total O 20 20	0	0
4	X	9	Total O 9 9	0	0
4	Y	20	Total O 20 20	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. 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. 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.

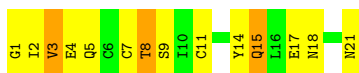
- Molecule 1: Insulin A chain

Chain A: 

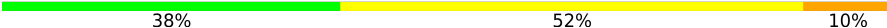


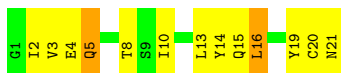
- Molecule 1: Insulin A chain

Chain C: 



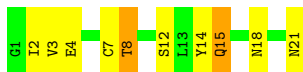
- Molecule 1: Insulin A chain

Chain E: 




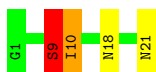
- Molecule 1: Insulin A chain

Chain G: 



- Molecule 1: Insulin A chain

Chain I: 

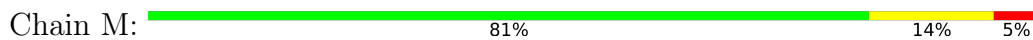


- Molecule 1: Insulin A chain

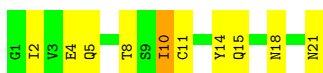
Chain K: 



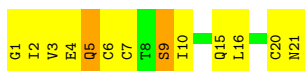
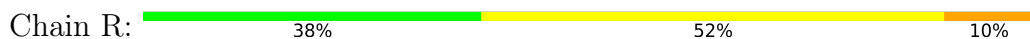
- Molecule 1: Insulin A chain



- Molecule 1: Insulin A chain



- Molecule 1: Insulin A chain



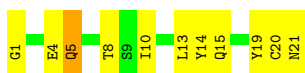
- Molecule 1: Insulin A chain



- Molecule 1: Insulin A chain

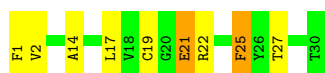


- Molecule 1: Insulin A chain

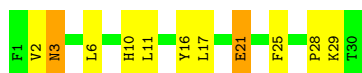


- Molecule 2: Insulin B chain





- Molecule 2: Insulin B chain



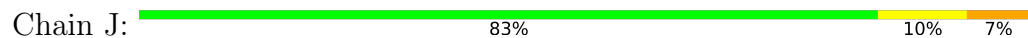
- Molecule 2: Insulin B chain



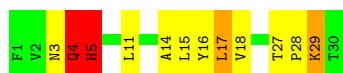
- Molecule 2: Insulin B chain



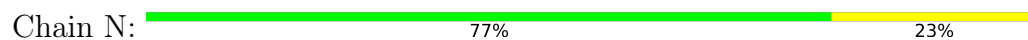
- Molecule 2: Insulin B chain



- Molecule 2: Insulin B chain



- Molecule 2: Insulin B chain



- Molecule 2: Insulin B chain

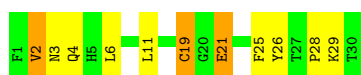




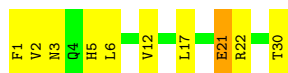
- Molecule 2: Insulin B chain



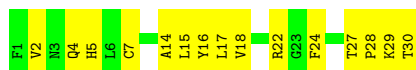
- Molecule 2: Insulin B chain



- Molecule 2: Insulin B chain



- Molecule 2: Insulin B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	81.56Å 81.56Å 68.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.70 – 2.20 26.70 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.70-2.20) 99.9 (26.70-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.04Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.299 0.300 , 0.326	Depositor DCC
R_{free} test set	1645 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.047 for h,-h-k,-l 0.000 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5143	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9868e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	0/164	1.06	1/220 (0.5%)
1	C	0.95	0/164	1.03	0/220
1	E	0.83	0/163	1.30	2/219 (0.9%)
1	G	0.84	0/163	0.86	0/220
1	I	0.95	0/164	1.02	1/220 (0.5%)
1	K	0.97	1/164 (0.6%)	0.85	0/220
1	M	0.93	0/164	1.06	1/220 (0.5%)
1	O	0.98	0/164	0.95	0/220
1	R	0.94	0/164	0.84	0/220
1	T	0.80	0/164	1.12	1/220 (0.5%)
1	V	0.94	0/164	0.95	0/220
1	X	1.05	0/164	1.02	0/220
2	B	0.89	0/249	0.86	0/335
2	D	1.03	0/242	1.01	0/326
2	F	0.85	0/249	0.85	0/335
2	H	0.90	0/242	1.42	4/326 (1.2%)
2	J	0.99	0/249	0.81	0/335
2	L	1.01	0/242	1.11	3/326 (0.9%)
2	N	0.97	1/249 (0.4%)	0.80	0/335
2	P	1.06	0/242	1.26	5/326 (1.5%)
2	S	0.85	1/249 (0.4%)	0.78	0/335
2	U	0.84	0/242	1.35	4/326 (1.2%)
2	W	0.96	0/248	0.78	0/333
2	Y	0.88	0/242	0.91	0/326
All	All	0.94	3/4911 (0.1%)	1.02	22/6603 (0.3%)

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
2	D	0	1
2	L	0	2
2	P	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	20	CYS	CB-SG	-5.93	1.72	1.81
2	S	7	CYS	CB-SG	-5.73	1.72	1.81
2	N	25	PHE	CE2-CZ	5.10	1.47	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	ASN	N-CA-CB	-14.07	85.27	110.60
2	U	3	ASN	N-CA-CB	-12.06	88.89	110.60
1	E	5	GLN	CB-CA-C	-10.92	88.56	110.40
2	H	2	VAL	CB-CA-C	-10.91	90.67	111.40
1	E	5	GLN	N-CA-C	9.59	136.90	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	ASN	Peptide
2	L	4	GLN	Peptide
2	L	5	HIS	Peptide
2	P	4	GLN	Peptide
2	P	5	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	163	0	149	7	0
1	C	163	0	149	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	162	0	144	16	0
1	G	162	0	149	8	0
1	I	163	0	149	5	1
1	K	163	0	149	12	0
1	M	163	0	149	6	0
1	O	163	0	149	14	0
1	R	163	0	149	15	0
1	T	163	0	149	8	0
1	V	163	0	149	4	2
1	X	163	0	149	22	0
2	B	242	0	232	10	0
2	D	236	0	225	9	0
2	F	242	0	232	16	0
2	H	236	0	225	9	0
2	J	242	0	232	6	0
2	L	236	0	225	12	1
2	N	242	0	232	3	0
2	P	236	0	225	16	1
2	S	242	0	232	20	1
2	U	236	0	225	13	0
2	W	241	0	228	8	0
2	Y	236	0	225	14	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	U	1	0	0	0	0
3	W	1	0	0	0	0
3	Y	1	0	0	0	0
4	A	9	0	0	2	0
4	B	12	0	0	3	0
4	C	9	0	0	5	0
4	D	22	0	0	5	0
4	E	8	0	0	1	0
4	F	13	0	0	4	0
4	G	8	0	0	2	0
4	H	12	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	12	0	0	0	0
4	J	17	0	0	4	0
4	K	5	0	0	7	1
4	L	19	0	0	3	0
4	M	7	0	0	1	0
4	N	16	0	0	0	0
4	O	11	0	0	7	0
4	P	24	0	0	7	0
4	R	4	0	0	0	0
4	S	15	0	0	6	0
4	T	13	0	0	1	0
4	U	10	0	0	4	1
4	V	15	0	0	1	0
4	W	20	0	0	6	0
4	X	9	0	0	8	0
4	Y	20	0	0	4	0
All	All	5143	0	4521	215	4

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 23.

The worst 5 of 215 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:X:4:GLU:HA	1:X:8:THR:OG1	1.40	1.21
2:D:21:GLU:HG2	4:D:199:HOH:O	1.43	1.15
2:S:15:LEU:HA	4:S:192:HOH:O	1.56	1.05
1:K:14:TYR:CD1	4:K:181:HOH:O	2.15	0.98
1:I:9:SER:O	1:I:10:ILE:HG23	1.64	0.98

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:21:GLU:OE1	4:U:324:HOH:O[2_655]	2.14	0.06
2:L:27:THR:CG2	1:V:18:ASN:OD1[2_655]	2.15	0.05
1:V:15:GLN:NE2	4:K:114:HOH:O[3_665]	2.18	0.02
1:I:18:ASN:OD1	2:P:27:THR:CG2[3_675]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
1	C	19/21 (90%)	14 (74%)	4 (21%)	1 (5%)	2	0
1	E	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	G	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	I	19/21 (90%)	17 (90%)	1 (5%)	1 (5%)	2	0
1	K	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	M	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	O	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
1	R	19/21 (90%)	16 (84%)	2 (10%)	1 (5%)	2	0
1	T	19/21 (90%)	15 (79%)	4 (21%)	0	100	100
1	V	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	X	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
2	B	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	D	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	F	28/30 (93%)	28 (100%)	0	0	100	100
2	H	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	J	28/30 (93%)	28 (100%)	0	0	100	100
2	L	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	N	28/30 (93%)	28 (100%)	0	0	100	100
2	P	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
2	S	28/30 (93%)	28 (100%)	0	0	100	100
2	U	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
2	W	28/30 (93%)	28 (100%)	0	0	100	100
2	Y	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
All	All	564/612 (92%)	520 (92%)	41 (7%)	3 (0%)	29	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	5	GLN
1	C	3	VAL
1	I	10	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	20/20 (100%)	20 (100%)	0	100	100
1	C	20/20 (100%)	17 (85%)	3 (15%)	3	2
1	E	20/20 (100%)	19 (95%)	1 (5%)	24	30
1	G	20/20 (100%)	17 (85%)	3 (15%)	3	2
1	I	20/20 (100%)	19 (95%)	1 (5%)	24	30
1	K	20/20 (100%)	18 (90%)	2 (10%)	7	7
1	M	20/20 (100%)	19 (95%)	1 (5%)	24	30
1	O	20/20 (100%)	18 (90%)	2 (10%)	7	7
1	R	20/20 (100%)	19 (95%)	1 (5%)	24	30
1	T	20/20 (100%)	18 (90%)	2 (10%)	7	7
1	V	20/20 (100%)	19 (95%)	1 (5%)	24	30
1	X	20/20 (100%)	17 (85%)	3 (15%)	3	2
2	B	26/26 (100%)	23 (88%)	3 (12%)	5	5
2	D	25/26 (96%)	20 (80%)	5 (20%)	1	1
2	F	26/26 (100%)	20 (77%)	6 (23%)	1	0
2	H	25/26 (96%)	23 (92%)	2 (8%)	12	12
2	J	26/26 (100%)	24 (92%)	2 (8%)	13	13
2	L	25/26 (96%)	21 (84%)	4 (16%)	2	2
2	N	26/26 (100%)	23 (88%)	3 (12%)	5	5
2	P	25/26 (96%)	22 (88%)	3 (12%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	26/26 (100%)	21 (81%)	5 (19%)	1	1
2	U	25/26 (96%)	22 (88%)	3 (12%)	5	4
2	W	25/26 (96%)	23 (92%)	2 (8%)	12	12
2	Y	25/26 (96%)	22 (88%)	3 (12%)	5	4
All	All	545/552 (99%)	484 (89%)	61 (11%)	6	5

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	4	GLN
1	X	5	GLN
2	N	29	LYS
2	W	30	THR
2	Y	4	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	4	GLN
1	R	5	GLN
1	X	18	ASN
2	P	5	HIS
2	S	3	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.