WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 07:37 AM EDT

PDB ID	:	6Z7W
Title	:	Human insulin in complex with the analytical antibody HUI-018 Fab
Authors	:	Johansson, E.
Deposited on	:	2020-06-02
Resolution	:	2.42 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 (i) 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 (i)) were used in the production of this report:

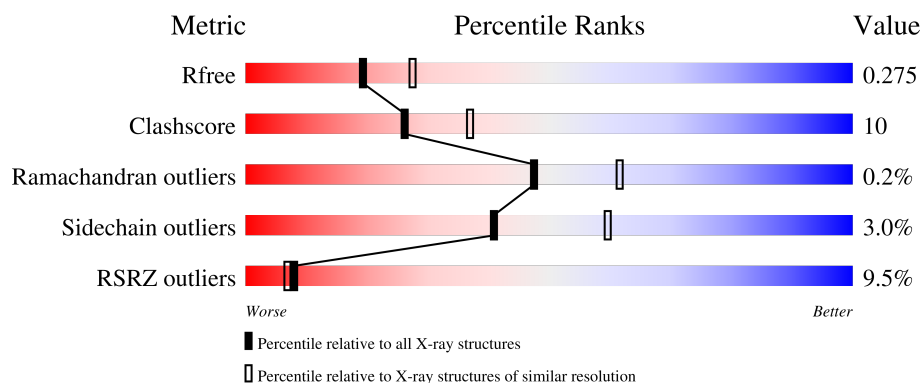|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.42 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		3.0%
RSRZ outliers		9.5%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	A	214	5% / 82% / 18%
1	C	214	6% / 78% / 22%
1	E	214	14% / 73% / 25% / •
1	G	214	% / 81% / 18% / •
2	B	224	12% / 75% / 22% / • •

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Mol	Chain	Length	Quality of chain
2	D	224	11% 78% 16% 5%
2	F	224	15% 68% 25%
2	H	224	2% 79% 17%
3	I	21	10% 52% 24% 24%
3	K	21	24% 86% 14%
3	M	21	24% 52% 48%
3	O	21	29% 67% 29% 5%
4	J	30	10% 63% 13% 20%
4	L	30	10% 70% 10% 20%
4	N	30	27% 50% 27% 7% 13%
4	P	30	7% 63% 23% 13%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15292 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 MAb 6H10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1672	1038	288	338	8			
1	C	213	Total	C	N	O	S	0	0	0
			1665	1035	287	336	7			
1	E	214	Total	C	N	O	S	0	0	0
			1672	1038	288	338	8			
1	G	214	Total	C	N	O	S	0	0	0
			1672	1038	288	338	8			

- Molecule 2 is a protein called HUI-018 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1641	1032	274	328	7			
2	D	213	Total	C	N	O	S	0	0	0
			1593	1008	263	316	6			
2	F	216	Total	C	N	O	S	0	0	0
			1618	1021	269	321	7			
2	H	219	Total	C	N	O	S	0	0	0
			1636	1030	273	326	7			

- Molecule 3 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	16	Total	C	N	O	S	0	0	0
			126	76	19	27	4			
3	K	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
3	M	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
3	O	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

• Molecule 4 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	24	Total 190	C 125	N 31	O 32	S 2	0	0	0
4	L	24	Total 190	C 125	N 31	O 32	S 2	0	0	0
4	N	26	Total 207	C 135	N 34	O 36	S 2	0	0	0
4	P	26	Total 208	C 136	N 35	O 35	S 2	0	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total 107	O 107	0	0
5	B	78	Total 78	O 78	0	0
5	C	80	Total 80	O 80	0	0
5	D	84	Total 84	O 84	0	0
5	E	34	Total 34	O 34	0	0
5	F	49	Total 49	O 49	0	0
5	G	110	Total 110	O 110	0	0
5	H	115	Total 115	O 115	0	0
5	I	15	Total 15	O 15	0	0
5	J	3	Total 3	O 3	0	0
5	K	5	Total 5	O 5	0	0
5	L	6	Total 6	O 6	0	0
5	M	3	Total 3	O 3	0	0
5	N	7	Total 7	O 7	0	0
5	O	6	Total 6	O 6	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	11	Total O 11 11		0	0

3 Residue-property plots ⓘ

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.
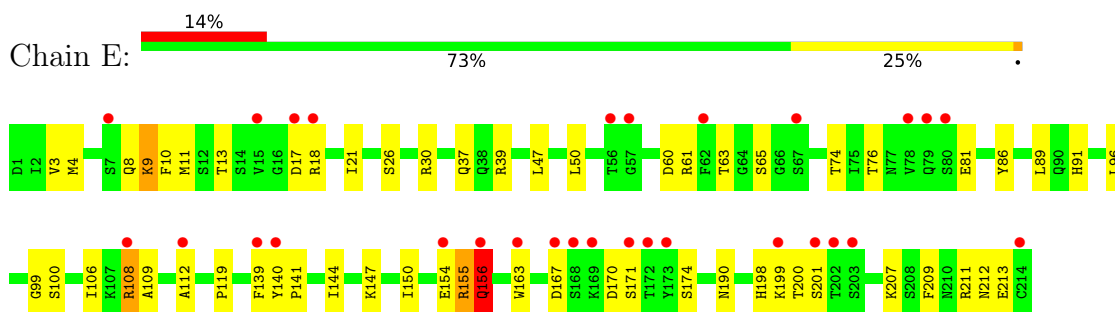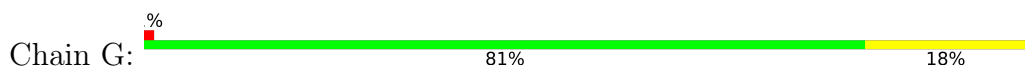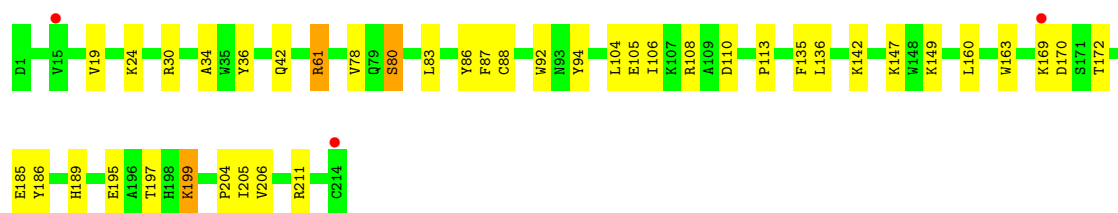
- Molecule 1: MAb 6H10 light chain
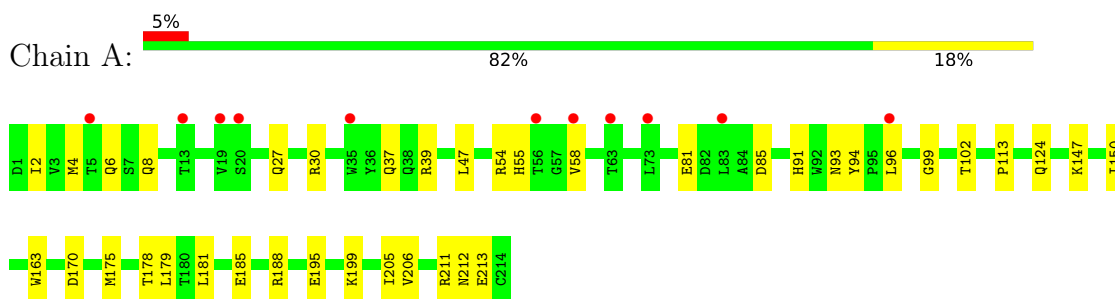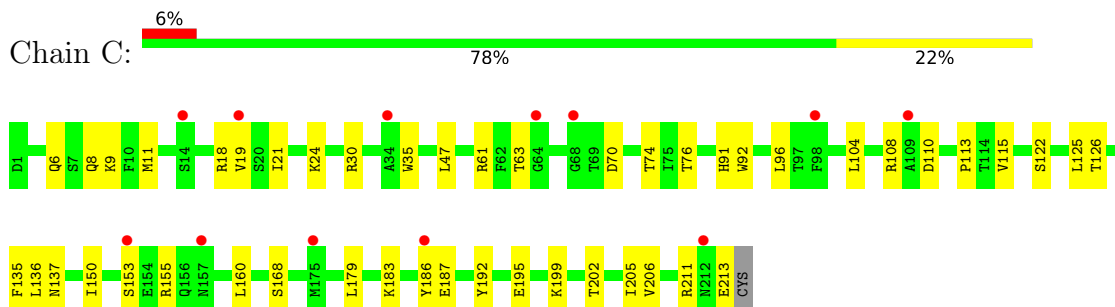
- Molecule 1: MAb 6H10 light chain

- Molecule 1: MAb 6H10 light chain
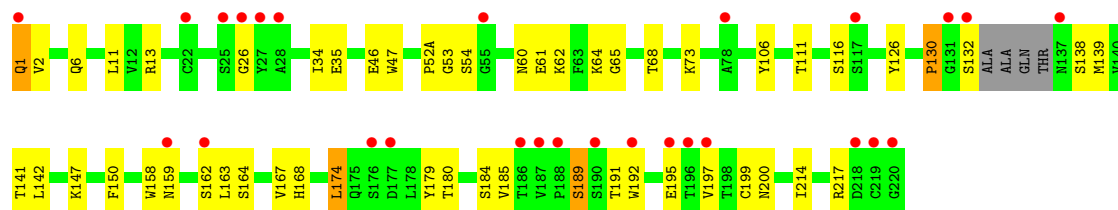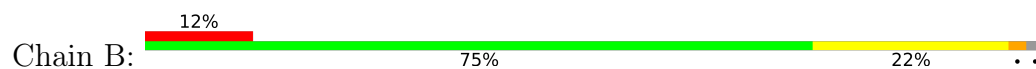

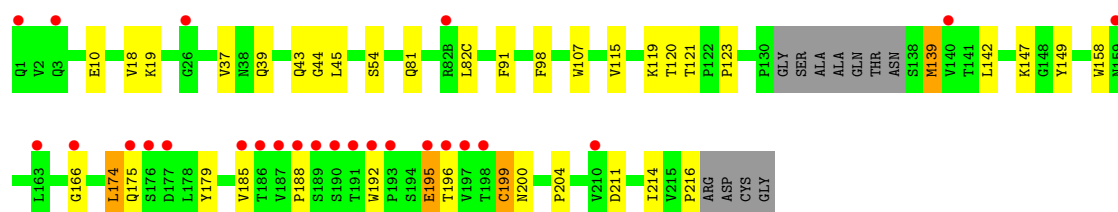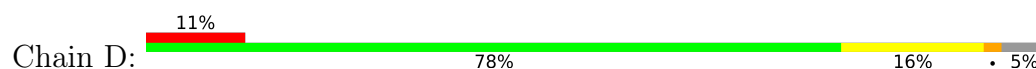- Molecule 1: MAb 6H10 light chain

• Molecule 2: HUI-018 Fab Heavy Chain

• Molecule 2: HUI-018 Fab Heavy Chain

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• Molecule 2: HUI-018 Fab Heavy Chain

W158 N159 S160 V173 S176 L181 T191 E195 T196 V197 H203 S206 I214 R217 D218 C219 GLY

• Molecule 3: Insulin

Chain I:

• Molecule 3: Insulin

GLY ILE VAL GLN C6 C7 L13 Y14 E17 C20 N21

• Molecule 3: Insulin

Chain K:

G1 E4 Q5 C6 C7 T8 Y14 N21

• Molecule 3: Insulin

Chain M:

G1 I2 V3 E4 Q5 C6 C7 T8 S9 I10 C11 S12 Q15 L16 E17 N18 Y19 C20 N21

• Molecule 3: Insulin

Chain O:

G1 I2 V3 E4 C7 L13 Y14 Q15 L16 N21

• Molecule 4: Insulin

Chain J:

PHE VAL ASN GLN H5 L6 C7 G8 S9 V18 T27 P28 LYS THR

• Molecule 4: Insulin

Chain L:

PHE VAL ASN GLN H5 E21 R22 G23 F24 F25 Y26 T27 P28 LYS THR
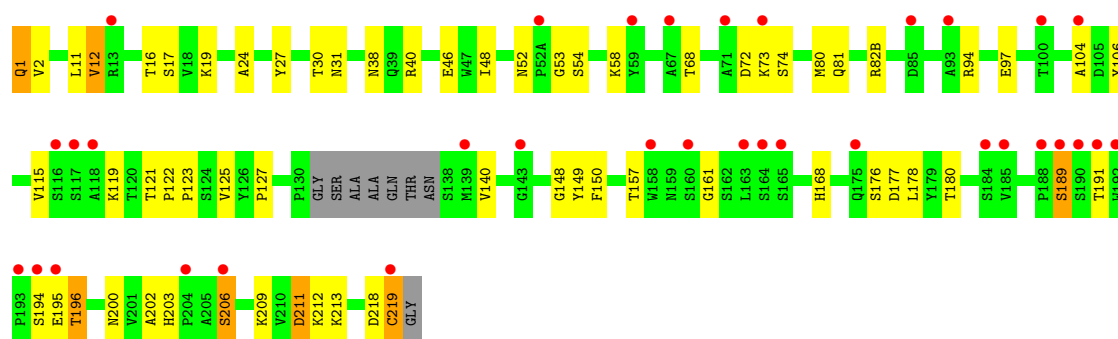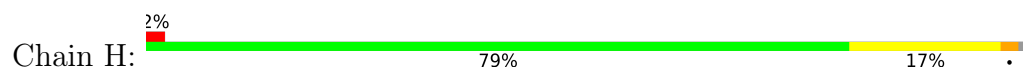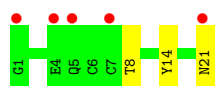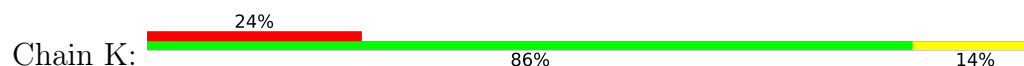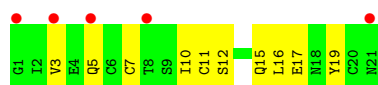
• Molecule 4: Insulin

Chain N:

• Molecule 4: Insulin

Chain P:
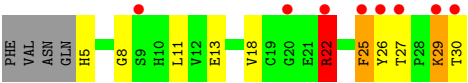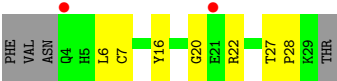
4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.23Å　216.61Å　101.09Å 90.00°　103.84°　90.00°	Depositor
Resolution (Å)	29.87　–　2.42 29.87　–　2.42	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.87-2.42) 89.3 (29.87-2.42)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.69 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.209　,　0.275 0.209　,　0.275	Depositor DCC
R_{free} test set	1784 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.9	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15292	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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	0.50	0/1709	0.67	1/2320 (0.0%)
1	C	0.50	1/1702 (0.1%)	0.70	4/2312 (0.2%)
1	E	0.47	0/1709	0.77	5/2320 (0.2%)
1	G	0.52	0/1709	0.64	0/2320
2	B	0.46	0/1680	0.76	2/2293 (0.1%)
2	D	0.54	0/1632	0.74	3/2231 (0.1%)
2	F	0.48	1/1657 (0.1%)	0.75	3/2264 (0.1%)
2	H	0.58	0/1675	0.68	1/2288 (0.0%)
3	I	0.58	0/127	0.70	0/170
3	K	0.63	0/164	0.65	0/220
3	M	0.48	0/164	0.73	0/220
3	O	0.68	0/164	0.94	1/220 (0.5%)
4	J	0.46	0/196	0.84	1/265 (0.4%)
4	L	0.83	1/196 (0.5%)	1.17	4/265 (1.5%)
4	N	0.68	0/213	1.29	4/286 (1.4%)
4	P	0.53	0/214	0.65	0/288
All	All	0.52	3/14911 (0.0%)	0.74	29/20282 (0.1%)

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	E	0	1
4	N	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	21	GLU	CB-CG	-7.88	1.37	1.52
1	C	24	LYS	CD-CE	5.60	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	12	VAL	C-N	-5.38	1.21	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLN	N-CA-C	-10.42	82.86	111.00
2	D	195	GLU	CA-CB-CG	9.96	135.31	113.40
4	N	22	ARG	NE-CZ-NH2	9.61	125.11	120.30
4	N	22	ARG	CG-CD-NE	-9.16	92.56	111.80
2	B	139	MET	CG-SD-CE	-8.71	86.27	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	213	GLU	Peptide
4	N	22	ARG	Sidechain

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	A	1672	0	1601	23	0
1	C	1665	0	1597	27	0
1	E	1672	0	1602	44	0
1	G	1672	0	1602	33	0
2	B	1641	0	1609	35	0
2	D	1593	0	1571	30	0
2	F	1618	0	1592	45	0
2	H	1636	0	1607	32	0
3	I	126	0	109	5	0
3	K	163	0	149	4	0
3	M	163	0	149	8	0
3	O	163	0	149	7	0
4	J	190	0	177	12	0
4	L	190	0	177	2	0
4	N	207	0	197	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	208	0	198	8	0
5	A	107	0	0	2	0
5	B	78	0	0	9	0
5	C	80	0	0	4	1
5	D	84	0	0	7	0
5	E	34	0	0	4	1
5	F	49	0	0	5	0
5	G	110	0	0	9	1
5	H	115	0	0	9	1
5	I	15	0	0	2	0
5	J	3	0	0	0	0
5	K	5	0	0	0	0
5	L	6	0	0	0	0
5	M	3	0	0	0	0
5	N	7	0	0	2	0
5	O	6	0	0	0	0
5	P	11	0	0	2	0
All	All	15292	0	14086	299	2

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 10.

The worst 5 of 299 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:82(B):ARG:NH2	5:F:301:HOH:O	1.83	1.08
1:G:24:LYS:NZ	5:G:302:HOH:O	1.89	0.98
1:G:195:GLU:OE1	5:G:301:HOH:O	1.82	0.97
1:A:54:ARG:HD2	1:A:58:VAL:HG23	1.49	0.94
3:I:6:CYS:N	5:I:101:HOH:O	2.02	0.91

All (2) 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)
5:E:333:HOH:O	5:G:408:HOH:O[1_556]	1.86	0.34
5:C:674:HOH:O	5:H:401:HOH:O[2_344]	2.15	0.05

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	A	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
1	C	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	E	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
1	G	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	216/224 (96%)	206 (95%)	9 (4%)	1 (0%)	29	40
2	D	209/224 (93%)	200 (96%)	9 (4%)	0	100	100
2	F	212/224 (95%)	204 (96%)	7 (3%)	1 (0%)	29	40
2	H	215/224 (96%)	208 (97%)	7 (3%)	0	100	100
3	I	14/21 (67%)	12 (86%)	1 (7%)	1 (7%)	1	0
3	K	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
3	M	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
3	O	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
4	J	22/30 (73%)	20 (91%)	1 (4%)	1 (4%)	2	1
4	L	22/30 (73%)	21 (96%)	1 (4%)	0	100	100
4	N	24/30 (80%)	22 (92%)	2 (8%)	0	100	100
4	P	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
All	All	1862/1956 (95%)	1781 (96%)	77 (4%)	4 (0%)	47	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	6	LEU
2	F	196	THR
2	B	130	PRO
3	I	20	CYS

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	A	191/191 (100%)	188 (98%)	3 (2%)	62	78
1	C	190/191 (100%)	183 (96%)	7 (4%)	34	51
1	E	191/191 (100%)	182 (95%)	9 (5%)	26	41
1	G	191/191 (100%)	186 (97%)	5 (3%)	46	64
2	B	187/189 (99%)	181 (97%)	6 (3%)	39	57
2	D	182/189 (96%)	178 (98%)	4 (2%)	52	69
2	F	185/189 (98%)	179 (97%)	6 (3%)	39	57
2	H	187/189 (99%)	182 (97%)	5 (3%)	44	63
3	I	16/20 (80%)	16 (100%)	0	100	100
3	K	20/20 (100%)	20 (100%)	0	100	100
3	M	20/20 (100%)	20 (100%)	0	100	100
3	O	20/20 (100%)	19 (95%)	1 (5%)	24	38
4	J	20/26 (77%)	20 (100%)	0	100	100
4	L	20/26 (77%)	20 (100%)	0	100	100
4	N	22/26 (85%)	18 (82%)	4 (18%)	1	1
4	P	22/26 (85%)	22 (100%)	0	100	100
All	All	1664/1704 (98%)	1614 (97%)	50 (3%)	41	59

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	201	SER
1	G	61	ARG
3	O	14	TYR
2	F	54	SER
2	F	206	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	C	8	GLN
2	F	200	ASN
2	H	175	GLN
4	J	10	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	214/214 (100%)	0.45	11 (5%)	28	26	19, 33, 49, 65	0
1	C	213/214 (99%)	0.60	12 (5%)	24	22	22, 43, 57, 70	0
1	E	214/214 (100%)	1.01	29 (13%)	3	2	28, 52, 78, 85	0
1	G	214/214 (100%)	0.15	3 (1%)	75	73	16, 29, 48, 59	0
2	B	220/224 (98%)	0.72	27 (12%)	4	3	25, 41, 65, 85	0
2	D	213/224 (95%)	0.63	25 (11%)	4	4	18, 34, 72, 86	0
2	F	216/224 (96%)	1.03	34 (15%)	2	1	34, 50, 81, 94	0
2	H	219/224 (97%)	0.24	5 (2%)	60	57	16, 30, 47, 67	0
3	I	16/21 (76%)	0.83	2 (12%)	3	3	36, 44, 55, 60	0
3	K	21/21 (100%)	1.36	5 (23%)	0	0	32, 51, 74, 79	0
3	M	21/21 (100%)	1.02	5 (23%)	0	0	45, 59, 69, 72	0
3	O	21/21 (100%)	1.07	6 (28%)	0	0	29, 45, 58, 74	0
4	J	24/30 (80%)	0.81	3 (12%)	3	3	33, 47, 63, 84	0
4	L	24/30 (80%)	0.93	3 (12%)	3	3	40, 48, 75, 81	0
4	N	26/30 (86%)	1.45	8 (30%)	0	0	43, 55, 75, 88	0
4	P	26/30 (86%)	0.62	2 (7%)	13	11	34, 45, 67, 75	0
All	All	1902/1956 (97%)	0.64	180 (9%)	8	7	16, 40, 70, 94	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	168	SER	8.9
2	D	190	SER	7.7
2	B	137	ASN	7.0
1	E	203	SER	6.8
2	D	186	THR	6.6

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

There are no ligands in this entry.

6.5   Other polymers ⓘ

There are no such residues in this entry.