



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 08:44 PM BST

PDB ID : 5MUB
Title : ACC1 Fab fragment in complex with citrullinated C1 epitope of CII (CG05)
Authors : Dobritsch, D.; Holmdahl, R.; Ge, C.
Deposited on : 2017-01-13
Resolution : 3.10 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 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 : 2.13.1
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) : 2.13.1

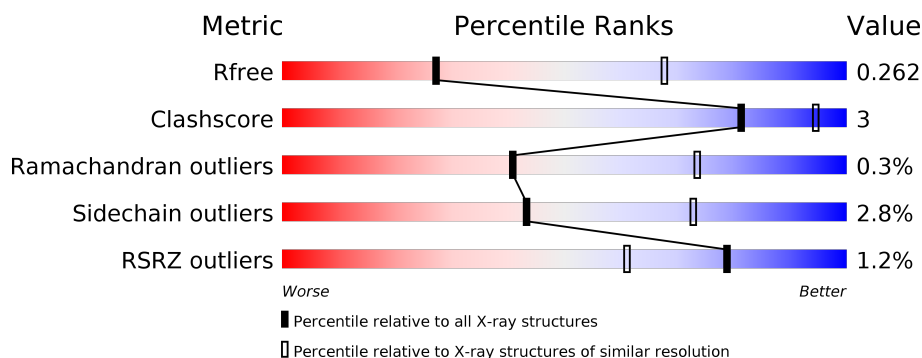
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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 $\leq 5\%$. 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	218	<div><div></div><div>91%8%</div></div>
1	C	218	<div><div></div><div>89%9%</div></div>
1	I	218	<div><div></div><div>90%9%</div></div>
1	L	218	<div><div>%</div><div>91%8%</div></div>
1	O	218	<div><div>4%</div><div>92%5%</div></div>
1	U	218	<div><div>%</div><div>89%10%</div></div>

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Mol	Chain	Length	Quality of chain
2	B	218	 91% 8%
2	D	218	 89% 11%
2	G	218	 92% 7%
2	J	218	 94% 6%
2	M	218	 90% 9%
2	P	218	 88% 11%
2	S	218	 89% 10%
2	V	218	 90% 9%
3	E	33	 24% 6% 73%
3	H	33	 21% 6% 73%
3	K	33	 24% 6% 70%
3	N	33	 18% 9% 73%
3	Q	33	 18% 6% 76%
3	T	33	 24% 12% 64%
3	W	33	 21% 6% 73%
3	X	33	 24% 6% 67%
4	F	220	 89% 10%
4	R	220	 90% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26877 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 ACC1 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1633	1030	272	323	8			
1	C	216	Total	C	N	O	S	0	0	0
			1629	1028	271	322	8			
1	I	217	Total	C	N	O	S	0	0	0
			1636	1032	272	324	8			
1	L	216	Total	C	N	O	S	0	0	0
			1626	1026	271	321	8			
1	O	212	Total	C	N	O	S	0	0	0
			1608	1017	267	317	7			
1	U	218	Total	C	N	O	S	0	0	0
			1640	1034	273	325	8			

- Molecule 2 is a protein called ACC1 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	D	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	G	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	J	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	M	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	P	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	S	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	V	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			

- Molecule 3 is a protein called triple-helical peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, triple-helical peptide containing the citrullinated C1 epitope of collagen type II.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	X	11	Total	C	N	O	0	0	0
			77	46	16	15			
3	E	9	Total	C	N	O	0	0	0
			62	36	14	12			
3	H	9	Total	C	N	O	0	0	0
			62	36	14	12			
3	K	10	Total	C	N	O	0	0	0
			66	38	15	13			
3	N	9	Total	C	N	O	0	0	0
			62	36	14	12			
3	Q	8	Total	C	N	O	0	0	0
			58	34	13	11			
3	T	12	Total	C	N	O	0	0	0
			81	48	17	16			
3	W	9	Total	C	N	O	0	0	0
			62	36	14	12			

- Molecule 4 is a protein called ACC1 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	217	Total	C	N	O	S	0	0	0
			1640	1036	272	324	8			
4	R	220	Total	C	N	O	S	0	0	0
			1655	1044	275	328	8			

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.

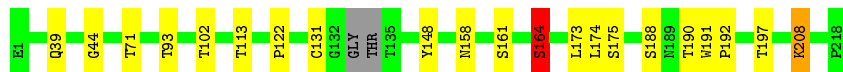
- Molecule 1: ACC1 Fab fragment heavy chain

Chain A: 



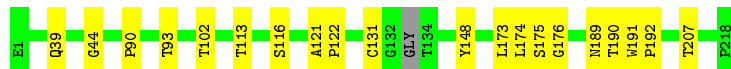
- Molecule 1: ACC1 Fab fragment heavy chain

Chain C: 




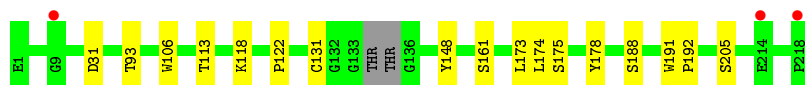
- Molecule 1: ACC1 Fab fragment heavy chain

Chain I: 



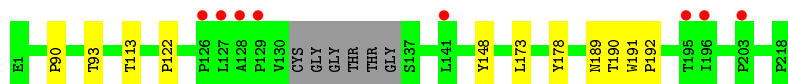
- Molecule 1: ACC1 Fab fragment heavy chain

Chain L: 

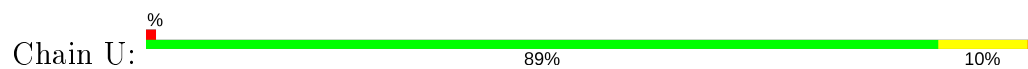


- Molecule 1: ACC1 Fab fragment heavy chain

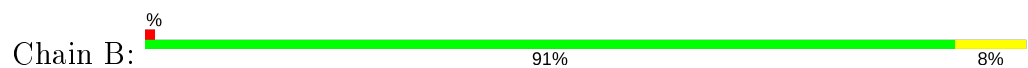
Chain O: 



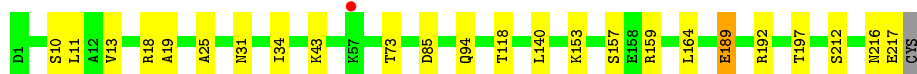
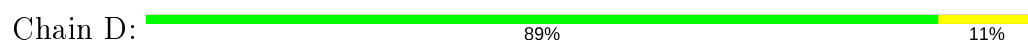
- Molecule 1: ACC1 Fab fragment heavy chain



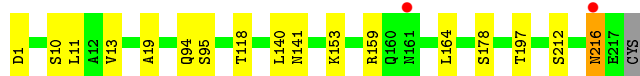
- Molecule 2: ACC1 Fab fragment light chain



- Molecule 2: ACC1 Fab fragment light chain



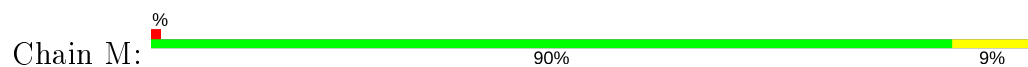
- Molecule 2: ACC1 Fab fragment light chain



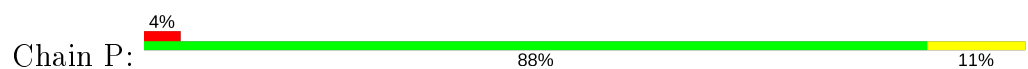
- Molecule 2: ACC1 Fab fragment light chain



- Molecule 2: ACC1 Fab fragment light chain

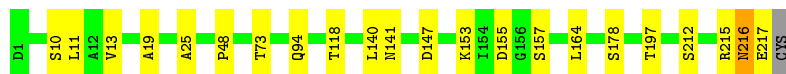


- Molecule 2: ACC1 Fab fragment light chain



- Molecule 2: ACC1 Fab fragment light chain

Chain S: 



- Molecule 2: ACC1 Fab fragment light chain

Chain V: 



- Molecule 3: triple-helical peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, triple-helical peptide containing the citrullinated C1 epitope of collagen type II

Chain X: 



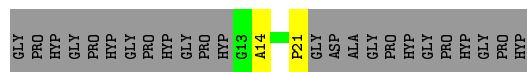
- Molecule 3: triple-helical peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, triple-helical peptide containing the citrullinated C1 epitope of collagen type II

Chain E: 



- Molecule 3: triple-helical peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, triple-helical peptide containing the citrullinated C1 epitope of collagen type II

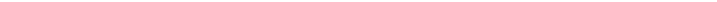
Chain H: 

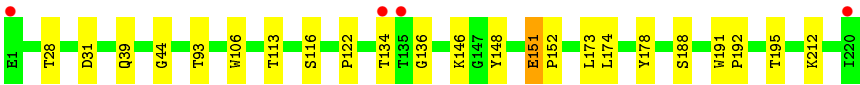


- Molecule 3: triple-helical peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, triple-helical peptide containing the citrullinated C1 epitope of collagen type II

Chain K: 



- Chain R:  2% 90% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.29Å 155.10Å 156.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.14 – 3.10 78.13 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.14-3.10) 99.9 (78.13-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.231 , 0.264 0.233 , 0.262	Depositor DCC
R_{free} test set	3245 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26877	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/1673	0.68	0/2282
1	C	0.49	0/1669	0.70	2/2277 (0.1%)
1	I	0.52	0/1676	0.67	0/2287
1	L	0.45	0/1666	0.65	0/2272
1	O	0.48	0/1648	0.65	0/2249
1	U	0.50	0/1681	0.70	1/2295 (0.0%)
2	B	0.46	0/1697	0.66	0/2302
2	D	0.54	0/1697	0.73	2/2302 (0.1%)
2	G	0.48	0/1697	0.70	0/2302
2	J	0.45	0/1697	0.65	0/2302
2	M	0.48	0/1697	0.70	1/2302 (0.0%)
2	P	0.51	0/1697	0.70	2/2302 (0.1%)
2	S	0.47	0/1697	0.68	0/2302
2	V	0.45	0/1697	0.66	1/2302 (0.0%)
3	E	0.64	0/42	0.94	0/54
3	H	0.82	0/42	0.87	0/54
3	K	0.87	0/45	1.27	0/56
3	N	0.72	0/42	0.91	0/54
3	Q	0.65	0/38	1.05	0/49
3	T	0.59	0/53	1.01	0/68
3	W	0.81	0/42	0.93	0/54
3	X	0.82	0/49	1.36	1/62 (1.6%)
4	F	0.50	0/1680	0.67	0/2293
4	R	0.51	0/1696	0.70	0/2316
All	All	0.49	0/27318	0.69	10/37138 (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	S	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	15	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	M	217	GLU	CA-CB-CG	6.77	128.30	113.40
1	C	164	SER	N-CA-C	6.53	128.63	111.00
2	P	217	GLU	N-CA-CB	5.86	121.14	110.60
2	D	217	GLU	N-CA-C	5.42	125.63	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S	216	ASN	Peptide

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	1633	0	1593	10	0
1	C	1629	0	1590	6	0
1	I	1636	0	1597	16	0
1	L	1626	0	1586	7	0
1	O	1608	0	1572	5	0
1	U	1640	0	1601	16	0
2	B	1660	0	1593	10	0
2	D	1660	0	1593	16	0
2	G	1660	0	1593	7	0
2	J	1660	0	1593	6	0
2	M	1660	0	1593	9	2
2	P	1660	0	1593	11	2
2	S	1660	0	1593	12	0
2	V	1660	0	1593	13	0
3	E	62	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	62	0	60	1	0
3	K	66	0	64	0	0
3	N	62	0	60	1	0
3	Q	58	0	57	0	0
3	T	81	0	77	2	0
3	W	62	0	61	4	0
3	X	77	0	75	3	0
4	F	1640	0	1605	13	0
4	R	1655	0	1619	13	0
All	All	26877	0	26022	139	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 3.

The worst 5 of 139 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:D:157:SER:HB2	1:I:176:GLY:HA3	1.25	1.09
1:A:206:SER:O	1:I:121:ALA:HB2	1.57	1.04
4:R:31:ASP:O	3:T:14:ALA:HB1	1.77	0.84
2:V:116:ALA:HB2	2:V:204:THR:HG21	1.64	0.80
2:D:157:SER:HB2	1:I:176:GLY:CA	2.11	0.78

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)
2:M:67:SER:OG	2:P:192:ARG:NE[2_454]	1.80	0.40
2:M:80:HIS:O	2:P:188:ASP:OD1[2_454]	2.09	0.11

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	213/218 (98%)	207 (97%)	5 (2%)	1 (0%)	29	64
1	C	212/218 (97%)	205 (97%)	4 (2%)	3 (1%)	11	40
1	I	213/218 (98%)	206 (97%)	5 (2%)	2 (1%)	17	52
1	L	212/218 (97%)	206 (97%)	5 (2%)	1 (0%)	29	64
1	O	208/218 (95%)	203 (98%)	5 (2%)	0	100	100
1	U	216/218 (99%)	210 (97%)	4 (2%)	2 (1%)	17	52
2	B	215/218 (99%)	206 (96%)	9 (4%)	0	100	100
2	D	215/218 (99%)	206 (96%)	9 (4%)	0	100	100
2	G	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
2	J	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
2	M	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
2	P	215/218 (99%)	206 (96%)	9 (4%)	0	100	100
2	S	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
2	V	215/218 (99%)	206 (96%)	9 (4%)	0	100	100
3	E	5/33 (15%)	5 (100%)	0	0	100	100
3	H	5/33 (15%)	5 (100%)	0	0	100	100
3	K	5/33 (15%)	5 (100%)	0	0	100	100
3	N	5/33 (15%)	5 (100%)	0	0	100	100
3	Q	4/33 (12%)	4 (100%)	0	0	100	100
3	T	7/33 (21%)	7 (100%)	0	0	100	100
3	W	5/33 (15%)	5 (100%)	0	0	100	100
3	X	6/33 (18%)	6 (100%)	0	0	100	100
4	F	213/220 (97%)	207 (97%)	5 (2%)	1 (0%)	29	64
4	R	218/220 (99%)	210 (96%)	7 (3%)	1 (0%)	29	64
All	All	3467/3756 (92%)	3340 (96%)	116 (3%)	11 (0%)	41	73

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	131	CYS
1	C	164	SER
4	F	28	THR
1	I	131	CYS
1	L	131	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	184/185 (100%)	179 (97%)	5 (3%)	44	74
1	C	184/185 (100%)	176 (96%)	8 (4%)	29	62
1	I	185/185 (100%)	181 (98%)	4 (2%)	52	78
1	L	183/185 (99%)	178 (97%)	5 (3%)	44	74
1	O	182/185 (98%)	180 (99%)	2 (1%)	73	89
1	U	185/185 (100%)	179 (97%)	6 (3%)	39	69
2	B	187/188 (100%)	181 (97%)	6 (3%)	39	69
2	D	187/188 (100%)	182 (97%)	5 (3%)	44	74
2	G	187/188 (100%)	179 (96%)	8 (4%)	29	62
2	J	187/188 (100%)	181 (97%)	6 (3%)	39	69
2	M	187/188 (100%)	181 (97%)	6 (3%)	39	69
2	P	187/188 (100%)	183 (98%)	4 (2%)	53	79
2	S	187/188 (100%)	182 (97%)	5 (3%)	44	74
2	V	187/188 (100%)	182 (97%)	5 (3%)	44	74
3	E	3/11 (27%)	3 (100%)	0	100	100
3	H	3/11 (27%)	3 (100%)	0	100	100
3	K	3/11 (27%)	2 (67%)	1 (33%)	0	0
3	N	3/11 (27%)	3 (100%)	0	100	100
3	Q	3/11 (27%)	3 (100%)	0	100	100
3	T	4/11 (36%)	4 (100%)	0	100	100
3	W	3/11 (27%)	3 (100%)	0	100	100
3	X	4/11 (36%)	4 (100%)	0	100	100
4	F	186/187 (100%)	183 (98%)	3 (2%)	62	84
4	R	187/187 (100%)	183 (98%)	4 (2%)	53	79
All	All	2998/3076 (98%)	2915 (97%)	83 (3%)	43	73

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	189	ASN
1	L	118	LYS
1	U	188	SER
1	I	190	THR
2	J	118	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	161	ASN
2	M	161	ASN
2	V	58	GLN
2	M	58	GLN
2	M	202	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	CIR	N	20	3	9,10,11	0.77	0	6,11,13	1.27	2 (33%)
3	CIR	K	20	3	9,10,11	0.58	0	6,11,13	1.51	2 (33%)
3	HYP	K	21	3	6,8,9	0.64	0	5,10,12	1.47	0
3	HYP	H	21	3	6,8,9	0.60	0	5,10,12	1.75	1 (20%)
3	CIR	W	20	3	9,10,11	0.76	0	6,11,13	1.31	0
3	CIR	H	20	3	9,10,11	0.64	0	6,11,13	0.89	0
3	HYP	W	21	3	6,8,9	1.19	1 (16%)	5,10,12	1.74	2 (40%)
3	HYP	T	21	3	6,8,9	0.74	0	5,10,12	1.64	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CIR	T	20	3	9,10,11	0.72	0	6,11,13	2.10	2 (33%)
3	CIR	Q	20	3	9,10,11	0.70	0	6,11,13	4.55	4 (66%)
3	HYP	Q	21	3	6,8,9	0.73	0	5,10,12	2.10	1 (20%)
3	HYP	X	21	3	6,8,9	1.19	1 (16%)	5,10,12	1.65	2 (40%)
3	CIR	X	20	3	9,10,11	0.89	0	6,11,13	1.13	0
3	CIR	E	20	3	9,10,11	0.90	0	6,11,13	1.07	0
3	HYP	X	12	3	6,8,9	0.73	0	5,10,12	1.87	1 (20%)
3	HYP	E	21	3	6,8,9	1.10	0	5,10,12	1.29	1 (20%)
3	HYP	T	12	3	6,8,9	1.21	1 (16%)	5,10,12	1.55	1 (20%)
3	HYP	N	21	3	6,8,9	0.54	0	5,10,12	1.63	1 (20%)

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	CIR	N	20	3	-	1/8/9/11	-
3	CIR	K	20	3	-	1/8/9/11	-
3	HYP	K	21	3	-	0/0/11/13	0/1/1/1
3	HYP	H	21	3	-	0/0/11/13	0/1/1/1
3	CIR	W	20	3	-	2/8/9/11	-
3	CIR	H	20	3	-	0/8/9/11	-
3	HYP	W	21	3	-	0/0/11/13	0/1/1/1
3	HYP	T	21	3	-	0/0/11/13	0/1/1/1
3	CIR	T	20	3	-	2/8/9/11	-
3	CIR	Q	20	3	-	4/8/9/11	-
3	HYP	Q	21	3	-	0/0/11/13	0/1/1/1
3	HYP	X	21	3	-	0/0/11/13	0/1/1/1
3	CIR	X	20	3	-	0/8/9/11	-
3	CIR	E	20	3	-	4/8/9/11	-
3	HYP	X	12	3	-	0/0/11/13	0/1/1/1
3	HYP	E	21	3	-	0/0/11/13	0/1/1/1
3	HYP	T	12	3	-	0/0/11/13	0/1/1/1
3	HYP	N	21	3	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	12	HYP	CD-N	2.30	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	21	HYP	CD-N	2.21	1.55	1.47
3	X	21	HYP	CD-N	2.07	1.54	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	20	CIR	N8-C7-N6	8.10	125.40	116.85
3	Q	20	CIR	O7-C7-N6	-5.53	117.64	121.74
3	Q	21	HYP	CB-CG-CD	4.06	108.25	103.27
3	Q	20	CIR	C5-N6-C7	3.76	127.20	122.73
3	Q	20	CIR	O7-C7-N8	-3.65	116.96	123.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	W	20	CIR	C1-C2-C3-C4
3	W	20	CIR	N2-C2-C3-C4
3	T	20	CIR	C1-C2-C3-C4
3	T	20	CIR	N2-C2-C3-C4
3	Q	20	CIR	C3-C4-C5-N6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	21	HYP	3	0
3	X	21	HYP	3	0
3	E	21	HYP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	A	217/218 (99%)	-0.09	1 (0%) 91 81	35, 57, 93, 108	0
1	C	216/218 (99%)	-0.04	0 100 100	50, 74, 91, 101	0
1	I	217/218 (99%)	-0.12	0 100 100	41, 56, 88, 108	0
1	L	216/218 (99%)	0.38	3 (1%) 75 56	60, 95, 119, 131	0
1	O	212/218 (97%)	0.25	8 (3%) 40 20	45, 75, 130, 157	0
1	U	218/218 (100%)	0.25	3 (1%) 75 56	46, 78, 114, 129	0
2	B	217/218 (99%)	0.04	2 (0%) 84 69	40, 68, 103, 125	0
2	D	217/218 (99%)	-0.04	1 (0%) 91 81	44, 67, 94, 109	0
2	G	217/218 (99%)	0.01	2 (0%) 84 69	43, 66, 103, 115	0
2	J	217/218 (99%)	0.03	0 100 100	43, 68, 108, 119	0
2	M	217/218 (99%)	0.23	3 (1%) 75 56	59, 82, 109, 120	0
2	P	217/218 (99%)	0.34	8 (3%) 41 21	45, 77, 139, 166	0
2	S	217/218 (99%)	0.09	0 100 100	46, 72, 107, 118	0
2	V	217/218 (99%)	0.39	5 (2%) 60 39	51, 88, 114, 127	0
3	E	7/33 (21%)	0.13	0 100 100	63, 71, 81, 81	0
3	H	7/33 (21%)	0.53	0 100 100	77, 79, 82, 84	0
3	K	8/33 (24%)	0.49	1 (12%) 3 1	74, 76, 87, 97	0
3	N	7/33 (21%)	0.02	0 100 100	78, 85, 91, 92	0
3	Q	6/33 (18%)	0.46	0 100 100	73, 77, 79, 81	0
3	T	9/33 (27%)	0.18	0 100 100	63, 71, 103, 111	0
3	W	7/33 (21%)	0.71	1 (14%) 2 1	81, 86, 95, 102	0
3	X	8/33 (24%)	0.29	0 100 100	62, 66, 86, 111	0
4	F	217/220 (98%)	-0.02	2 (0%) 84 69	49, 67, 87, 103	0
4	R	220/220 (100%)	0.09	4 (1%) 68 47	44, 68, 103, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3528/3756 (93%)	0.12	44 (1%) 79 61	35, 73, 110, 166	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	1	GLU	4.0
2	P	188	ASP	3.8
1	O	195	THR	3.8
1	O	128	ALA	3.8
1	L	218	PRO	3.6

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

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, 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	B-factors(Å ²)	Q<0.9
3	HYP	T	12	8/9	0.75	0.33	96,100,103,104	0
3	CIR	N	20	11/12	0.80	0.25	97,105,117,122	0
3	HYP	W	21	8/9	0.81	0.41	87,89,91,91	0
3	HYP	E	21	8/9	0.82	0.30	75,78,80,80	0
3	HYP	X	12	8/9	0.82	0.38	95,98,104,105	0
3	HYP	N	21	8/9	0.84	0.30	102,108,111,112	0
3	HYP	H	21	8/9	0.85	0.23	90,93,96,96	0
3	CIR	T	20	11/12	0.85	0.28	64,68,76,76	0
3	CIR	W	20	11/12	0.85	0.40	89,92,97,98	0
3	CIR	H	20	11/12	0.87	0.30	84,87,92,95	0
3	CIR	Q	20	11/12	0.87	0.23	79,82,85,85	0
3	HYP	K	21	8/9	0.90	0.26	81,85,88,89	0
3	HYP	Q	21	8/9	0.90	0.28	87,88,96,100	0
3	CIR	K	20	11/12	0.91	0.21	76,80,91,91	0
3	CIR	X	20	11/12	0.91	0.25	64,67,73,77	0
3	HYP	T	21	8/9	0.91	0.21	65,67,71,73	0
3	HYP	X	21	8/9	0.92	0.18	70,72,74,74	0
3	CIR	E	20	11/12	0.93	0.30	65,70,84,84	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.