



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2017 – 11:05 PM EDT

PDB ID : 5MU0  
Title : ACC1 Fab fragment in complex with citrullinated C1 epitope of CII (IA03)  
Authors : Dobritsch, D.; Holmdahl, R.; Ge, C.  
Deposited on : unknown  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

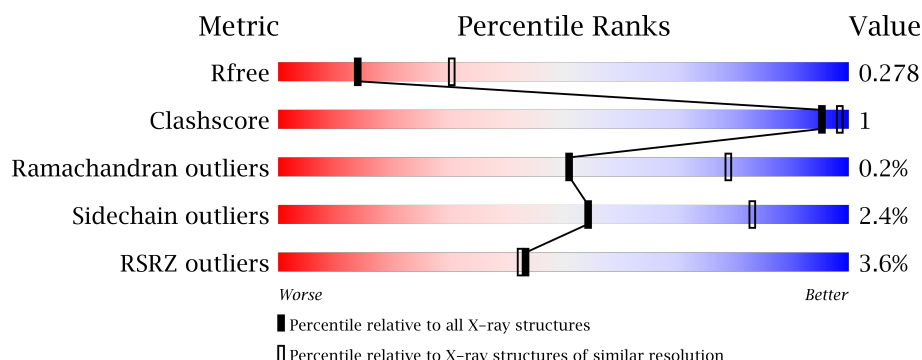
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div> <div></div> <div>94%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	C	218	<div> <div> <div></div> <div>91%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> <div>6%</div> </div> </div>
1	E	218	<div> <div> <div></div> <div>99%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	G	218	<div> <div> <div></div> <div>96%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> </div> </div>
1	I	218	<div> <div> <div></div> <div>95%</div> <div></div> </div> <div> <div></div> <div></div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	218	
1	M	218	
1	O	218	
2	B	218	
2	D	218	
2	F	218	
2	H	218	
2	J	218	
2	L	218	
2	N	218	
2	P	218	
3	Q	18	
3	R	18	
3	S	18	
3	T	18	
3	U	18	
3	V	18	
3	W	18	
3	X	18	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26780 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 heavy chain of ACC1 antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1618	1021	269	320	8			
1	C	212	Total	C	N	O	S	0	0	0
			1600	1011	264	317	8			
1	E	218	Total	C	N	O	S	0	0	0
			1640	1034	273	325	8			
1	G	215	Total	C	N	O	S	0	0	0
			1622	1023	270	321	8			
1	I	216	Total	C	N	O	S	0	0	0
			1629	1028	271	322	8			
1	K	215	Total	C	N	O	S	0	0	0
			1625	1026	270	321	8			
1	M	212	Total	C	N	O	S	0	0	0
			1600	1011	264	317	8			
1	O	211	Total	C	N	O	S	0	0	0
			1589	1005	262	314	8			

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

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	F	216	Total	C	N	O	S	0	0	0
			1651	1030	280	335	6			
2	H	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	L	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	215	Total	C	N	O	S	0	0	0
			1643	1026	278	333	6			
2	P	216	Total	C	N	O	S	0	0	0
			1651	1030	280	335	6			

- Molecule 3 is a protein called IA03 peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, IA03 peptide containing the citrullinated C1 epitope of collagen type II.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	11	Total	C	N	O	0	0	0
			74	43	16	15			
3	R	10	Total	C	N	O	0	0	0
			66	38	15	13			
3	S	10	Total	C	N	O	0	0	0
			66	38	15	13			
3	T	10	Total	C	N	O	0	0	0
			66	38	15	13			
3	U	10	Total	C	N	O	0	0	0
			66	38	15	13			
3	V	10	Total	C	N	O	0	0	0
			66	38	15	13			
3	W	9	Total	C	N	O	0	0	0
			62	36	14	12			
3	X	10	Total	C	N	O	0	0	0
			66	38	15	13			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	6	Total	O	0	0
			6	6		
4	C	9	Total	O	0	0
			9	9		
4	D	20	Total	O	0	0
			20	20		
4	E	5	Total	O	0	0
			5	5		
4	F	3	Total	O	0	0
			3	3		

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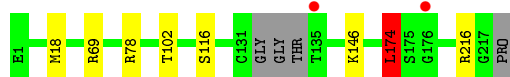
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	5	Total 5	O 5	0	0
4	H	7	Total 7	O 7	0	0
4	I	4	Total 4	O 4	0	0
4	J	6	Total 6	O 6	0	0
4	K	1	Total 1	O 1	0	0
4	L	2	Total 2	O 2	0	0
4	M	2	Total 2	O 2	0	0
4	N	1	Total 1	O 1	0	0
4	T	1	Total 1	O 1	0	0
4	V	1	Total 1	O 1	0	0

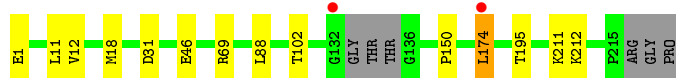
### 3 Residue-property plots [i](#)

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

- Molecule 1: heavy chain of ACC1 antibody Fab fragment



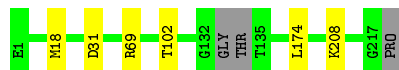
- Molecule 1: heavy chain of ACC1 antibody Fab fragment



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- Molecule 1: heavy chain of ACC1 antibody Fab fragment

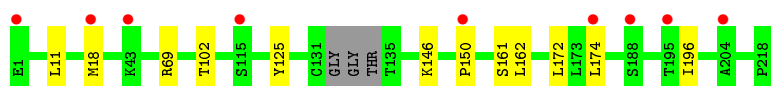


- Molecule 1: heavy chain of ACC1 antibody Fab fragment

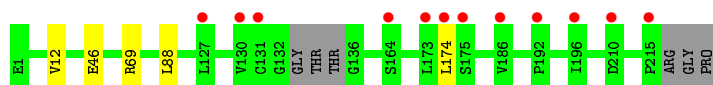


- Molecule 1: heavy chain of ACC1 antibody Fab fragment

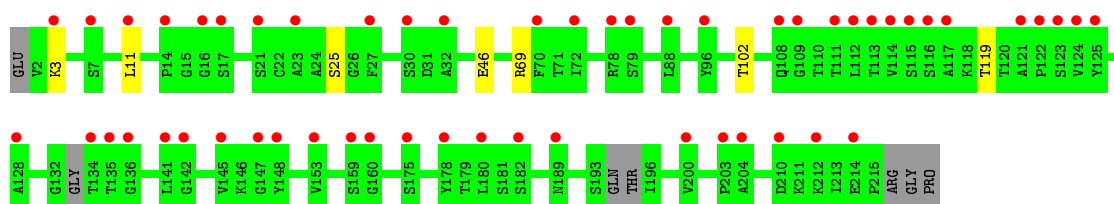




- Molecule 1: heavy chain of ACC1 antibody Fab fragment



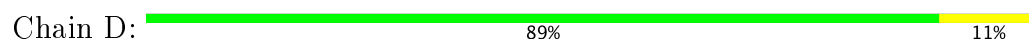
- Molecule 1: heavy chain of ACC1 antibody Fab fragment



- Molecule 2: light chain of ACC1 antibody Fab fragment



- Molecule 2: light chain of ACC1 antibody Fab fragment




- Molecule 2: light chain of ACC1 antibody Fab fragment



- Molecule 2: light chain of ACC1 antibody Fab fragment

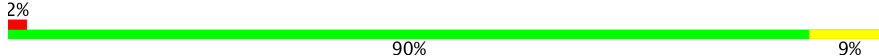


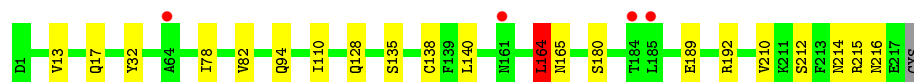
- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain J: 



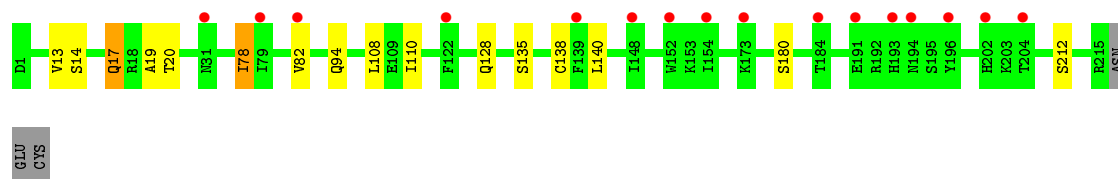
- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain L: 



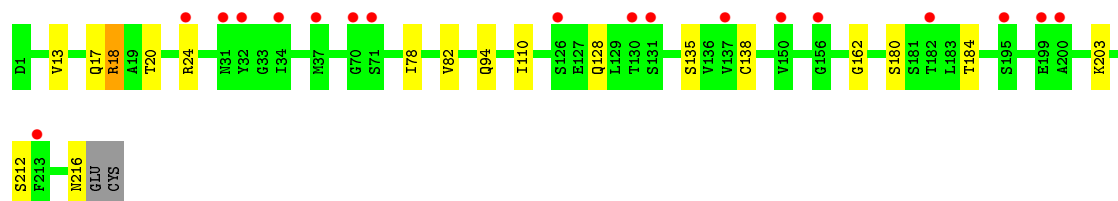
- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain N: 



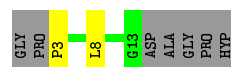
- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain P: 



- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain Q: 



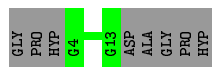
- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain R: 

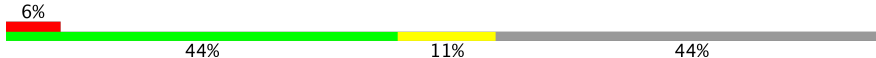


- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain S: 



- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain T: 



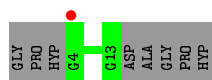
- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain U: 



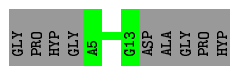
- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain V: 



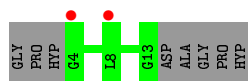
- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain W: 



- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain X: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.15Å 93.05Å 121.75Å 92.75° 106.45° 104.37°	Depositor
Resolution (Å)	78.15 – 2.70 78.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.2 (78.15-2.70) 85.4 (78.15-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.61 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.252 , 0.279 0.253 , 0.278	Depositor DCC
$R_{free}$ test set	4339 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	26780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	0/1657	0.75	5/2260 (0.2%)
1	C	0.52	0/1639	0.74	3/2236 (0.1%)
1	E	0.51	0/1681	0.72	2/2295 (0.1%)
1	G	0.51	0/1661	0.71	2/2265 (0.1%)
1	I	0.49	0/1669	0.74	5/2277 (0.2%)
1	K	0.47	0/1665	0.71	1/2272 (0.0%)
1	M	0.46	0/1639	0.70	2/2236 (0.1%)
1	O	0.48	0/1627	1.04	4/2219 (0.2%)
2	B	0.51	0/1697	0.73	1/2302 (0.0%)
2	D	0.54	0/1697	0.74	2/2302 (0.1%)
2	F	0.46	0/1688	0.69	1/2290 (0.0%)
2	H	0.58	0/1697	0.75	1/2302 (0.0%)
2	J	0.55	0/1697	0.73	0/2302
2	L	0.51	0/1697	0.74	2/2302 (0.1%)
2	N	0.47	0/1680	0.70	1/2279 (0.0%)
2	P	0.49	0/1688	0.70	1/2290 (0.0%)
3	Q	0.76	0/45	0.97	0/56
3	R	0.80	0/45	0.84	0/56
3	S	0.65	0/45	0.83	0/56
3	T	0.81	0/45	1.67	2/56 (3.6%)
3	U	0.91	0/45	1.00	0/56
3	V	0.89	0/45	1.12	0/56
3	W	0.71	0/41	1.15	0/51
3	X	0.85	0/45	0.96	0/56
All	All	0.51	0/27135	0.75	35/36872 (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
3	Q	0	1

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	69	ARG	NE-CZ-NH2	-24.90	107.85	120.30
1	O	69	ARG	NE-CZ-NH1	24.67	132.63	120.30
1	O	69	ARG	CD-NE-CZ	8.96	136.15	123.60
3	T	6	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	174	LEU	CA-CB-CG	8.10	133.93	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Q	3	HYP	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	1618	0	1580	1	2
1	C	1600	0	1560	8	0
1	E	1640	0	1601	0	0
1	G	1622	0	1583	1	0
1	I	1629	0	1590	0	1
1	K	1625	0	1587	6	1
1	M	1600	0	1560	2	0
1	O	1589	0	1549	4	0
2	B	1660	0	1593	6	0
2	D	1660	0	1593	9	0
2	F	1651	0	1587	5	1
2	H	1660	0	1593	5	1
2	J	1660	0	1593	7	1
2	L	1660	0	1593	12	2
2	N	1643	0	1581	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1651	0	1587	7	1
3	Q	74	0	72	1	0
3	R	66	0	64	2	0
3	S	66	0	64	0	0
3	T	66	0	64	1	0
3	U	66	0	64	0	0
3	V	66	0	63	0	0
3	W	62	0	60	0	0
3	X	66	0	63	0	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
4	C	9	0	0	0	0
4	D	20	0	0	0	0
4	E	5	0	0	0	0
4	F	3	0	0	0	0
4	G	5	0	0	0	0
4	H	7	0	0	0	0
4	I	4	0	0	0	0
4	J	6	0	0	0	0
4	K	1	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	T	1	0	0	0	0
4	V	1	0	0	0	0
All	All	26780	0	25844	75	5

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 1.

The worst 5 of 75 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:O:11:LEU:O	1:O:11:LEU:HD12	1.87	0.74
1:O:3:LYS:HG2	1:O:25:SER:OG	1.88	0.73
1:O:11:LEU:HD21	1:O:119:THR:N	2.14	0.63
1:O:11:LEU:C	1:O:11:LEU:HD12	2.21	0.61
1:K:172:LEU:HD11	2:L:165:ASN:O	2.01	0.60

All (5) 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)
1:I:116:SER:OG	2:L:189:GLU:OE2[1_556]	1.60	0.60
1:A:116:SER:OG	2:L:214:ASN:ND2[1_556]	1.88	0.32
1:A:78:ARG:O	2:H:207:SER:CB[1_455]	2.00	0.20
2:F:214:ASN:ND2	1:K:161:SER:OG[1_545]	2.11	0.09
2:J:192:ARG:O	2:P:18:ARG:NH2[1_455]	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	210/218 (96%)	206 (98%)	3 (1%)	1 (0%)	32	60
1	C	208/218 (95%)	203 (98%)	4 (2%)	1 (0%)	32	60
1	E	216/218 (99%)	211 (98%)	4 (2%)	1 (0%)	32	60
1	G	211/218 (97%)	207 (98%)	3 (1%)	1 (0%)	32	60
1	I	212/218 (97%)	208 (98%)	3 (1%)	1 (0%)	32	60
1	K	211/218 (97%)	207 (98%)	3 (1%)	1 (0%)	32	60
1	M	208/218 (95%)	203 (98%)	5 (2%)	0	100	100
1	O	205/218 (94%)	200 (98%)	4 (2%)	1 (0%)	32	60
2	B	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
2	D	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
2	F	214/218 (98%)	208 (97%)	6 (3%)	0	100	100
2	H	215/218 (99%)	211 (98%)	4 (2%)	0	100	100
2	J	215/218 (99%)	210 (98%)	5 (2%)	0	100	100
2	L	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
2	N	213/218 (98%)	208 (98%)	5 (2%)	0	100	100
2	P	214/218 (98%)	209 (98%)	5 (2%)	0	100	100
3	Q	6/18 (33%)	6 (100%)	0	0	100	100
3	R	5/18 (28%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	5/18 (28%)	3 (60%)	2 (40%)	0	100	100
3	T	5/18 (28%)	5 (100%)	0	0	100	100
3	U	5/18 (28%)	5 (100%)	0	0	100	100
3	V	5/18 (28%)	5 (100%)	0	0	100	100
3	W	4/18 (22%)	4 (100%)	0	0	100	100
3	X	5/18 (28%)	5 (100%)	0	0	100	100
All	All	3437/3632 (95%)	3356 (98%)	74 (2%)	7 (0%)	51	79

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	102	THR
1	A	102	THR
1	E	102	THR
1	G	102	THR
1	I	102	THR

### 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	183/185 (99%)	181 (99%)	2 (1%)	78	93
1	C	181/185 (98%)	178 (98%)	3 (2%)	66	88
1	E	185/185 (100%)	185 (100%)	0	100	100
1	G	183/185 (99%)	180 (98%)	3 (2%)	68	89
1	I	184/185 (100%)	179 (97%)	5 (3%)	50	80
1	K	184/185 (100%)	183 (100%)	1 (0%)	91	97
1	M	181/185 (98%)	179 (99%)	2 (1%)	78	93
1	O	180/185 (97%)	179 (99%)	1 (1%)	89	97
2	B	187/188 (100%)	180 (96%)	7 (4%)	39	70
2	D	187/188 (100%)	179 (96%)	8 (4%)	33	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	186/188 (99%)	178 (96%)	8 (4%)	33	64
2	H	187/188 (100%)	183 (98%)	4 (2%)	59	85
2	J	187/188 (100%)	180 (96%)	7 (4%)	39	70
2	L	187/188 (100%)	179 (96%)	8 (4%)	33	64
2	N	185/188 (98%)	180 (97%)	5 (3%)	50	80
2	P	186/188 (99%)	180 (97%)	6 (3%)	44	75
3	Q	3/6 (50%)	3 (100%)	0	100	100
3	R	3/6 (50%)	3 (100%)	0	100	100
3	S	3/6 (50%)	3 (100%)	0	100	100
3	T	3/6 (50%)	3 (100%)	0	100	100
3	U	3/6 (50%)	2 (67%)	1 (33%)	0	0
3	V	3/6 (50%)	3 (100%)	0	100	100
3	W	3/6 (50%)	3 (100%)	0	100	100
3	X	3/6 (50%)	3 (100%)	0	100	100
All	All	2977/3032 (98%)	2906 (98%)	71 (2%)	54	83

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	94	GLN
1	I	193	SER
2	P	138	CYS
2	H	138	CYS
1	I	46	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	128	GLN
2	B	216	ASN
2	H	58	GLN
2	H	128	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

17 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	Q	11	3	10,10,11	0.68	0	8,11,13	2.67	4 (50%)
3	HYP	Q	12	3	7,8,9	1.16	1 (14%)	5,10,12	1.98	2 (40%)
3	HYP	Q	3	3	7,8,9	1.01	1 (14%)	5,10,12	1.32	0
3	CIR	R	11	3	10,10,11	1.48	1 (10%)	8,11,13	1.43	2 (25%)
3	HYP	R	12	3	7,8,9	0.80	0	5,10,12	1.40	0
3	CIR	S	11	3	10,10,11	0.58	0	8,11,13	3.95	6 (75%)
3	HYP	S	12	3	7,8,9	0.62	0	5,10,12	1.63	2 (40%)
3	CIR	T	11	3	10,10,11	1.33	2 (20%)	8,11,13	1.91	1 (12%)
3	HYP	T	12	3	7,8,9	1.05	0	5,10,12	0.87	0
3	CIR	U	11	3	10,10,11	0.99	1 (10%)	8,11,13	2.97	6 (75%)
3	HYP	U	12	3	7,8,9	1.03	1 (14%)	5,10,12	1.61	2 (40%)
3	CIR	V	11	3	10,10,11	0.90	1 (10%)	8,11,13	1.49	1 (12%)
3	HYP	V	12	3	7,8,9	1.16	1 (14%)	5,10,12	1.88	2 (40%)
3	CIR	W	11	3	10,10,11	1.28	2 (20%)	8,11,13	2.00	3 (37%)
3	HYP	W	12	3	7,8,9	0.73	0	5,10,12	1.45	1 (20%)
3	CIR	X	11	3	10,10,11	1.26	1 (10%)	8,11,13	1.76	4 (50%)
3	HYP	X	12	3	7,8,9	1.30	1 (14%)	5,10,12	1.78	2 (40%)

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	Q	11	3	-	0/7/9/11	0/0/0/0
3	HYP	Q	12	3	-	0/0/11/13	0/1/1/1
3	HYP	Q	3	3	-	0/0/11/13	0/1/1/1
3	CIR	R	11	3	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HYP	R	12	3	-	0/0/11/13	0/1/1/1
3	CIR	S	11	3	-	0/7/9/11	0/0/0/0
3	HYP	S	12	3	-	0/0/11/13	0/1/1/1
3	CIR	T	11	3	-	0/7/9/11	0/0/0/0
3	HYP	T	12	3	-	0/0/11/13	0/1/1/1
3	CIR	U	11	3	-	0/7/9/11	0/0/0/0
3	HYP	U	12	3	-	0/0/11/13	0/1/1/1
3	CIR	V	11	3	-	0/7/9/11	0/0/0/0
3	HYP	V	12	3	-	0/0/11/13	0/1/1/1
3	CIR	W	11	3	-	0/7/9/11	0/0/0/0
3	HYP	W	12	3	-	0/0/11/13	0/1/1/1
3	CIR	X	11	3	-	0/7/9/11	0/0/0/0
3	HYP	X	12	3	-	0/0/11/13	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	12	HYP	CB-CA	-2.82	1.48	1.54
3	T	11	CIR	O7-C7	-2.26	1.20	1.24
3	T	11	CIR	C7-N6	-2.17	1.31	1.34
3	W	11	CIR	C3-C2	2.16	1.56	1.53
3	Q	3	HYP	CA-C	2.26	1.53	1.50

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	11	CIR	C3-C2-C1	-6.36	101.17	111.65
3	T	11	CIR	C3-C2-C1	-4.44	104.34	111.65
3	Q	11	CIR	O7-C7-N6	-4.22	118.44	121.73
3	S	11	CIR	O7-C7-N6	-3.57	118.95	121.73
3	W	11	CIR	O7-C7-N8	-3.39	117.30	123.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	214/218 (98%)	-0.18	2 (0%) 84 85	30, 56, 88, 102	0
1	C	212/218 (97%)	-0.03	2 (0%) 84 85	32, 61, 96, 115	0
1	E	218/218 (100%)	-0.03	4 (1%) 69 70	47, 70, 104, 121	0
1	G	215/218 (98%)	-0.31	0 100 100	36, 53, 76, 91	0
1	I	216/218 (99%)	0.16	2 (0%) 84 85	45, 78, 101, 117	0
1	K	215/218 (98%)	0.33	9 (4%) 37 35	41, 78, 106, 124	0
1	M	212/218 (97%)	0.28	12 (5%) 24 23	40, 83, 125, 139	0
1	O	211/218 (96%)	1.24	54 (25%) 1 0	77, 119, 163, 192	0
2	B	217/218 (99%)	-0.20	0 100 100	33, 60, 94, 113	0
2	D	217/218 (99%)	-0.21	0 100 100	27, 51, 93, 109	0
2	F	216/218 (99%)	-0.14	0 100 100	42, 64, 103, 117	0
2	H	217/218 (99%)	-0.21	0 100 100	33, 53, 79, 104	0
2	J	217/218 (99%)	-0.07	1 (0%) 90 92	31, 66, 111, 126	0
2	L	217/218 (99%)	0.07	4 (1%) 69 70	32, 68, 107, 127	0
2	N	215/218 (98%)	0.45	16 (7%) 15 13	52, 93, 125, 138	0
2	P	216/218 (99%)	0.72	18 (8%) 12 9	55, 98, 141, 165	0
3	Q	8/18 (44%)	-0.36	0 100 100	41, 44, 59, 71	0
3	R	8/18 (44%)	0.05	0 100 100	58, 63, 66, 79	0
3	S	8/18 (44%)	-0.10	0 100 100	67, 71, 78, 89	0
3	T	8/18 (44%)	0.55	1 (12%) 4 3	61, 66, 78, 85	0
3	U	8/18 (44%)	-0.05	0 100 100	63, 70, 73, 80	0
3	V	8/18 (44%)	0.33	1 (12%) 4 3	62, 69, 76, 92	0
3	W	7/18 (38%)	-0.55	0 100 100	60, 62, 70, 75	0
3	X	8/18 (44%)	1.19	2 (25%) 1 0	94, 101, 104, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3508/3632 (96%)	0.12	128 (3%)	43	42	27, 69, 121, 192	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	34	ILE	7.9
2	P	32	TYR	6.1
1	O	122	PRO	5.6
1	O	148	TYR	4.8
2	P	150	VAL	4.7

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	HYP	S	12	8/9	0.89	0.20	-	83,86,87,87	0
3	HYP	Q	12	8/9	0.93	0.15	-	49,50,52,52	0
3	HYP	V	12	8/9	0.88	0.21	-	84,89,93,93	0
3	HYP	W	12	8/9	0.91	0.15	-	74,76,79,80	0
3	HYP	T	12	8/9	0.93	0.12	-	73,76,78,79	0
3	HYP	U	12	8/9	0.91	0.20	-	82,83,83,83	0
3	CIR	X	11	11/12	0.80	0.21	-	92,93,95,99	0
3	CIR	Q	11	11/12	0.88	0.18	-	44,47,60,65	0
3	CIR	S	11	11/12	0.92	0.20	-	76,80,87,88	0
3	CIR	U	11	11/12	0.86	0.17	-	77,80,83,83	0
3	CIR	R	11	11/12	0.89	0.14	-	63,64,69,70	0
3	CIR	W	11	11/12	0.87	0.18	-	71,75,91,97	0
3	CIR	T	11	11/12	0.89	0.18	-	65,69,74,77	0
3	CIR	V	11	11/12	0.78	0.17	-	70,72,76,78	0
3	HYP	Q	3	8/9	0.83	0.21	-	77,82,88,90	0
3	HYP	X	12	8/9	0.86	0.16	-	95,96,98,99	0
3	HYP	R	12	8/9	0.88	0.14	-	71,73,75,75	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.