



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:30 am BST

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 : 2017-01-11
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

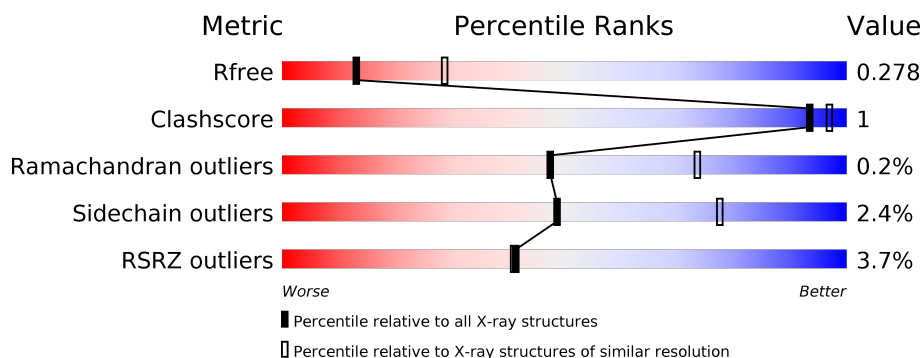
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 ≥ 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 style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 94% 6% 2% </div> </div>
1	C	218	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 91% 6% 2% </div> </div>
1	E	218	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 99%; height: 10px; background-color: green;"></div> <div style="width: 1%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 99% </div> </div>
1	G	218	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 96%; height: 10px; background-color: green;"></div> <div style="width: 4%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 96% </div> </div>
1	I	218	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 95%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 95% </div> </div>
1	K	218	<div> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 93%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 93% 6% </div> </div>

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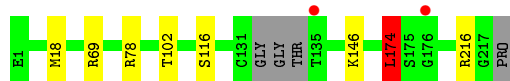
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	5	Total 5	O 5	0	0
4	H	7	Total 7	O 7	0	0
4	I	4	Total 4	O 4	0	0
4	J	6	Total 6	O 6	0	0
4	K	1	Total 1	O 1	0	0
4	L	2	Total 2	O 2	0	0
4	M	2	Total 2	O 2	0	0
4	N	1	Total 1	O 1	0	0
4	T	1	Total 1	O 1	0	0
4	V	1	Total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

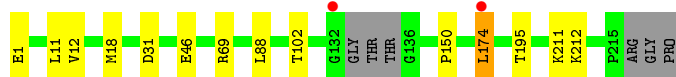
3 Residue-property plots [i](#)

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



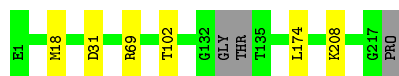
- Molecule 1: heavy chain of ACC1 antibody Fab fragment



- Molecule 1: heavy chain of ACC1 antibody Fab fragment



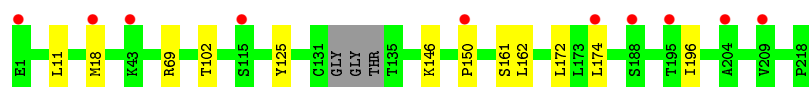
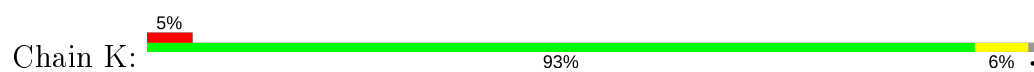
- Molecule 1: heavy chain of ACC1 antibody Fab fragment



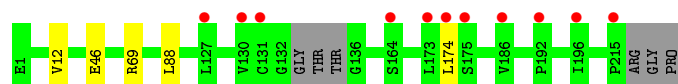
- Molecule 1: heavy chain of ACC1 antibody Fab fragment



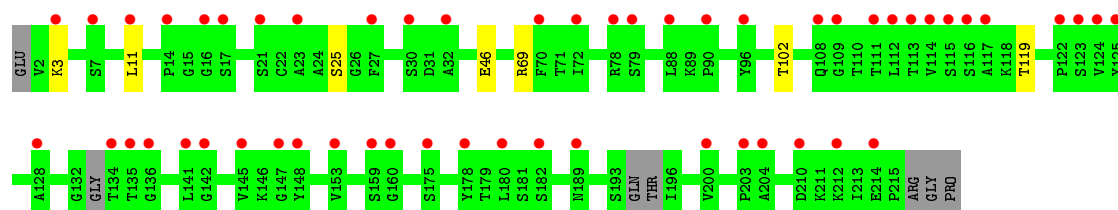
- Molecule 1: heavy chain of ACC1 antibody Fab fragment



- Molecule 1: heavy chain of ACC1 antibody Fab fragment



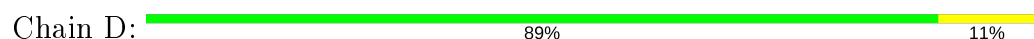
- Molecule 1: heavy chain of ACC1 antibody Fab fragment



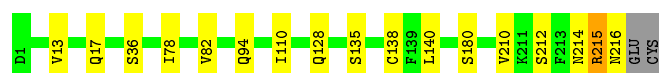
- Molecule 2: light chain of ACC1 antibody Fab fragment



- 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





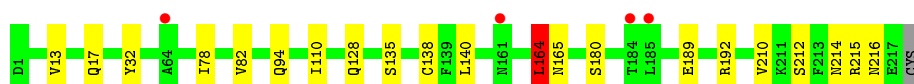
- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain J: 91% 9%



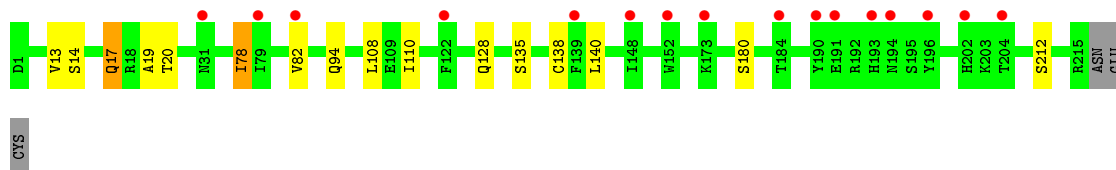
- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain L: 2% 90% 9%



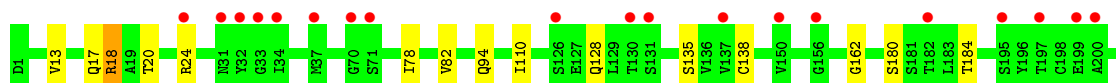
- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain N: 7% 91% 6% ..



- Molecule 2: light chain of ACC1 antibody Fab fragment

Chain P: 9% 91% 8% ..



- 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: 50% 11% 39%



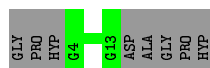
- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II, Collagen alpha-1(II) chain, IA03 peptide containing the citrullinated C1 epitope of collagen type II

Chain R: 

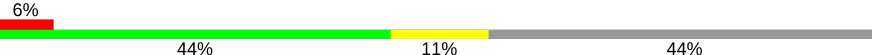


- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

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: 



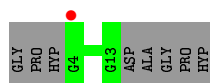
- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

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: 

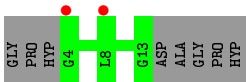


- Molecule 3: IA03 peptide containing the citrullinated C1 epitope of collagen type II,Collagen alpha-1(II) chain,IA03 peptide containing the citrullinated C1 epitope of collagen type II

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 89.2 (78.15-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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

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.

All (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
1	C	174	LEU	CB-CG-CD2	7.51	123.76	111.00
1	K	69	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	G	69	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	I	69	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	E	69	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	A	69	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	I	69	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	M	69	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	M	69	ARG	NE-CZ-NH2	6.87	123.74	120.30
1	G	69	ARG	NE-CZ-NH2	6.82	123.71	120.30
2	B	215	ARG	NE-CZ-NH1	-6.77	116.92	120.30
2	L	164	LEU	CA-CB-CG	6.77	130.87	115.30
1	C	69	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	C	69	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	69	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	E	69	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	I	174	LEU	CA-CB-CG	5.62	128.22	115.30
3	T	6	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	I	91	GLU	CA-CB-CG	5.59	125.70	113.40
2	L	215	ARG	CA-CB-CG	5.53	125.56	113.40
1	I	173	LEU	CB-CG-CD2	5.48	120.32	111.00
2	N	78	ILE	CB-CG1-CD1	5.42	129.09	113.90
1	O	69	ARG	CG-CD-NE	-5.20	100.88	111.80
2	F	215	ARG	NE-CZ-NH1	-5.14	117.73	120.30
2	D	18	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	216	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	P	18	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	D	159	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	174	LEU	CB-CG-CD2	-5.03	102.45	111.00
2	H	112	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:M:12:VAL:HG11	1:M:88:LEU:CD1	2.34	0.58
1:C:12:VAL:HG11	1:C:88:LEU:CD1	2.35	0.57
2:N:20:THR:HG23	2:N:78:ILE:CD1	2.36	0.56
1:M:12:VAL:HG11	1:M:88:LEU:HD13	1.87	0.56
2:N:20:THR:HG23	2:N:78:ILE:HD12	1.88	0.54
2:B:53:TYR:CE1	3:Q:8:LEU:HD13	2.44	0.53
1:C:12:VAL:HG11	1:C:88:LEU:HD13	1.90	0.52
2:J:98:VAL:O	2:P:24:ARG:NH1	2.41	0.52
2:J:82:VAL:CG1	2:J:110:ILE:HD12	2.40	0.52
2:B:18:ARG:HH21	2:L:32:TYR:HB3	1.75	0.51
2:N:13:VAL:HG22	2:N:108:LEU:HD11	1.93	0.49
1:C:31:ASP:O	3:R:5:ALA:HB1	2.13	0.48
2:D:82:VAL:CG1	2:D:110:ILE:HD12	2.43	0.48
2:N:13:VAL:HG21	2:N:82:VAL:HG21	1.96	0.48
1:K:162:LEU:CD2	1:K:196:ILE:HD12	2.43	0.47
2:B:18:ARG:NH2	2:L:32:TYR:HB3	2.28	0.47
2:F:82:VAL:CG1	2:F:110:ILE:HD12	2.43	0.47
2:P:162:GLY:O	2:P:184:THR:HG22	2.14	0.47
2:D:162:GLY:O	2:D:184:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:82:VAL:CG1	2:L:110:ILE:HD12	2.45	0.47
1:K:11:LEU:HB2	1:K:150:PRO:HG3	1.96	0.47
2:N:82:VAL:CG1	2:N:110:ILE:HD12	2.45	0.47
2:L:164:LEU:HD23	2:L:164:LEU:C	2.35	0.47
2:B:78:ILE:N	2:B:78:ILE:HD12	2.31	0.46
2:N:13:VAL:HG23	2:N:13:VAL:O	2.15	0.46
2:H:78:ILE:HD12	2:H:78:ILE:N	2.31	0.46
2:D:78:ILE:HD12	2:D:78:ILE:N	2.32	0.45
2:J:78:ILE:HD12	2:J:78:ILE:N	2.31	0.45
2:J:34:ILE:HD11	2:J:54:ALA:HB1	1.99	0.45
2:F:78:ILE:HD12	2:F:78:ILE:N	2.31	0.45
1:C:11:LEU:HB2	1:C:150:PRO:HG3	1.99	0.44
2:N:13:VAL:HG11	2:N:19:ALA:HB2	2.00	0.44
2:H:82:VAL:CG1	2:H:110:ILE:HD12	2.48	0.44
2:L:78:ILE:HD12	2:L:78:ILE:N	2.32	0.44
2:P:13:VAL:CG1	2:P:17:GLN:HB2	2.48	0.43
2:P:78:ILE:HD12	2:P:78:ILE:N	2.32	0.43
2:N:13:VAL:CG2	2:N:108:LEU:HD11	2.48	0.43
1:A:146:LYS:NZ	1:A:174:LEU:HD21	2.34	0.43
2:H:140:LEU:HD12	2:H:140:LEU:N	2.34	0.43
2:L:13:VAL:CG1	2:L:17:GLN:HB2	2.48	0.42
2:F:13:VAL:CG1	2:F:17:GLN:HB2	2.49	0.42
2:H:13:VAL:CG1	2:H:17:GLN:HB2	2.49	0.42
2:P:82:VAL:CG1	2:P:110:ILE:HD12	2.49	0.42
2:F:128:GLN:HE22	2:F:135:SER:CB	2.33	0.42
2:H:128:GLN:HE22	2:H:135:SER:CB	2.33	0.42
2:D:13:VAL:CG1	2:D:17:GLN:HB2	2.50	0.42
2:J:13:VAL:CG1	2:J:17:GLN:HB2	2.49	0.42
2:B:13:VAL:CG1	2:B:17:GLN:HB2	2.50	0.41
2:D:128:GLN:HE22	2:D:135:SER:CB	2.33	0.41
1:C:195:THR:HG22	1:C:212:LYS:HE3	2.02	0.41
1:C:211:LYS:HE3	2:D:127:GLU:OE1	2.19	0.41
2:D:140:LEU:HD12	2:D:140:LEU:N	2.36	0.41
2:N:140:LEU:N	2:N:140:LEU:HD12	2.36	0.41
1:C:174:LEU:HD12	2:D:164:LEU:HD13	2.03	0.41
1:G:31:ASP:O	3:T:5:ALA:HB1	2.20	0.41
2:J:128:GLN:HE22	2:J:135:SER:CB	2.34	0.41
1:K:174:LEU:HB2	2:L:164:LEU:HD12	2.02	0.41
2:L:128:GLN:HE22	2:L:135:SER:CB	2.33	0.41
2:N:14:SER:HB2	2:N:17:GLN:HG3	2.03	0.41
2:J:140:LEU:N	2:J:140:LEU:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:140:LEU:HD12	2:L:140:LEU:N	2.35	0.41
2:P:128:GLN:HE22	2:P:135:SER:CB	2.33	0.41
1:K:146:LYS:HE2	2:L:135:SER:OG	2.21	0.41
2:B:128:GLN:HE22	2:B:135:SER:CB	2.33	0.41
2:N:128:GLN:HE22	2:N:135:SER:CB	2.33	0.40
1:C:12:VAL:HG11	1:C:88:LEU:HD12	2.03	0.40
2:D:53:TYR:CZ	3:R:8:LEU:HD22	2.56	0.40
1:K:125:TYR:CZ	2:L:128:GLN:HG3	2.56	0.40
2:F:140:LEU:HD12	2:F:140:LEU:N	2.35	0.40
2:P:20:THR:O	2:P:20:THR:HG23	2.21	0.40

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%)	29 54
1	C	208/218 (95%)	203 (98%)	4 (2%)	1 (0%)	29 54
1	E	216/218 (99%)	211 (98%)	4 (2%)	1 (0%)	29 54
1	G	211/218 (97%)	207 (98%)	3 (1%)	1 (0%)	29 54
1	I	212/218 (97%)	208 (98%)	3 (1%)	1 (0%)	29 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	211/218 (97%)	207 (98%)	3 (1%)	1 (0%)	29	54
1	M	208/218 (95%)	203 (98%)	5 (2%)	0	100	100
1	O	205/218 (94%)	200 (98%)	4 (2%)	1 (0%)	29	54
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
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%)	47	73

All (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
1	K	102	THR
1	O	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%)	73	90
1	C	181/185 (98%)	178 (98%)	3 (2%)	60	84
1	E	185/185 (100%)	185 (100%)	0	100	100
1	G	183/185 (99%)	180 (98%)	3 (2%)	62	85
1	I	184/185 (100%)	179 (97%)	5 (3%)	44	74
1	K	184/185 (100%)	183 (100%)	1 (0%)	88	96
1	M	181/185 (98%)	179 (99%)	2 (1%)	73	90
1	O	180/185 (97%)	179 (99%)	1 (1%)	86	95
2	B	187/188 (100%)	180 (96%)	7 (4%)	34	63
2	D	187/188 (100%)	179 (96%)	8 (4%)	29	57
2	F	186/188 (99%)	178 (96%)	8 (4%)	29	57
2	H	187/188 (100%)	183 (98%)	4 (2%)	53	80
2	J	187/188 (100%)	180 (96%)	7 (4%)	34	63
2	L	187/188 (100%)	179 (96%)	8 (4%)	29	57
2	N	185/188 (98%)	180 (97%)	5 (3%)	44	74
2	P	186/188 (99%)	180 (97%)	6 (3%)	39	68
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%)	49	77

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	174	LEU
2	B	36	SER
2	B	94	GLN
2	B	138	CYS
2	B	180	SER
2	B	210	VAL
2	B	212	SER
2	B	215	ARG
1	C	1	GLU
1	C	18	MET
1	C	46	GLU
2	D	36	SER
2	D	94	GLN
2	D	138	CYS
2	D	180	SER
2	D	210	VAL
2	D	211	LYS
2	D	212	SER
2	D	216	ASN
2	F	36	SER
2	F	94	GLN
2	F	138	CYS
2	F	180	SER
2	F	210	VAL
2	F	212	SER
2	F	215	ARG
2	F	216	ASN
1	G	18	MET
1	G	174	LEU
1	G	208	LYS
2	H	36	SER
2	H	94	GLN
2	H	138	CYS
2	H	180	SER
1	I	18	MET
1	I	46	GLU
1	I	91	GLU
1	I	173	LEU
1	I	193	SER
2	J	36	SER
2	J	94	GLN
2	J	138	CYS

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Mol	Chain	Res	Type
2	J	180	SER
2	J	206	THR
2	J	210	VAL
2	J	212	SER
1	K	18	MET
2	L	94	GLN
2	L	138	CYS
2	L	164	LEU
2	L	180	SER
2	L	192	ARG
2	L	210	VAL
2	L	212	SER
2	L	216	ASN
1	M	46	GLU
1	M	174	LEU
2	N	17	GLN
2	N	94	GLN
2	N	138	CYS
2	N	180	SER
2	N	212	SER
1	O	46	GLU
2	P	94	GLN
2	P	138	CYS
2	P	180	SER
2	P	203	LYS
2	P	212	SER
2	P	216	ASN
3	U	6	ARG

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	HYP	S	12	3	6,8,9	0.58	0	5,10,12	1.58	2 (40%)
3	HYP	Q	12	3	6,8,9	1.30	1 (16%)	5,10,12	1.99	2 (40%)
3	HYP	V	12	3	6,8,9	0.68	0	5,10,12	1.93	1 (20%)
3	HYP	W	12	3	6,8,9	0.55	0	5,10,12	1.38	0
3	HYP	T	12	3	6,8,9	1.15	0	5,10,12	0.80	0
3	HYP	U	12	3	6,8,9	0.58	0	5,10,12	1.52	2 (40%)
3	CIR	X	11	3	9,10,11	0.92	0	6,11,13	1.60	2 (33%)
3	CIR	Q	11	3	9,10,11	0.73	0	6,11,13	3.06	4 (66%)
3	CIR	S	11	3	9,10,11	0.63	0	6,11,13	3.73	4 (66%)
3	CIR	U	11	3	9,10,11	0.61	0	6,11,13	2.92	4 (66%)
3	CIR	R	11	3	9,10,11	1.01	1 (11%)	6,11,13	1.11	0
3	CIR	W	11	3	9,10,11	1.04	1 (11%)	6,11,13	2.15	2 (33%)
3	CIR	T	11	3	9,10,11	1.44	2 (22%)	6,11,13	1.07	0
3	CIR	V	11	3	9,10,11	0.48	0	6,11,13	1.66	1 (16%)
3	HYP	Q	3	3	6,8,9	0.61	0	5,10,12	1.24	1 (20%)
3	HYP	X	12	3	6,8,9	0.48	0	5,10,12	1.77	2 (40%)
3	HYP	R	12	3	6,8,9	0.57	0	5,10,12	1.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HYP	S	12	3	-	0/0/11/13	0/1/1/1
3	HYP	Q	12	3	-	0/0/11/13	0/1/1/1
3	HYP	V	12	3	-	0/0/11/13	0/1/1/1
3	HYP	W	12	3	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HYP	T	12	3	-	0/0/11/13	0/1/1/1
3	HYP	U	12	3	-	0/0/11/13	0/1/1/1
3	CIR	X	11	3	-	1/8/9/11	-
3	CIR	Q	11	3	-	4/8/9/11	-
3	CIR	S	11	3	-	2/8/9/11	-
3	CIR	U	11	3	-	4/8/9/11	-
3	CIR	R	11	3	-	2/8/9/11	-
3	CIR	W	11	3	-	2/8/9/11	-
3	CIR	T	11	3	-	5/8/9/11	-
3	CIR	V	11	3	-	1/8/9/11	-
3	HYP	Q	3	3	-	0/0/11/13	0/1/1/1
3	HYP	X	12	3	-	0/0/11/13	0/1/1/1
3	HYP	R	12	3	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	12	HYP	CB-CA	-2.92	1.48	1.54
3	T	11	CIR	C7-N6	-2.44	1.31	1.34
3	T	11	CIR	O7-C7	-2.27	1.20	1.24
3	R	11	CIR	C7-N6	-2.22	1.32	1.34
3	W	11	CIR	C3-C2	2.18	1.56	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	11	CIR	N8-C7-N6	6.54	123.75	116.85
3	U	11	CIR	N8-C7-N6	4.95	122.08	116.85
3	Q	11	CIR	N8-C7-N6	4.73	121.84	116.85
3	Q	11	CIR	O7-C7-N6	-4.44	118.44	121.74
3	S	11	CIR	O7-C7-N6	-3.77	118.95	121.74
3	V	12	HYP	CB-CG-CD	3.74	107.85	103.27
3	Q	12	HYP	CB-CG-CD	3.72	107.82	103.27
3	S	11	CIR	C5-N6-C7	3.67	127.10	122.73
3	W	11	CIR	O7-C7-N8	-3.45	117.30	123.22
3	S	11	CIR	O7-C7-N8	-3.45	117.30	123.22
3	V	11	CIR	O7-C7-N6	3.27	124.16	121.74
3	U	11	CIR	C5-N6-C7	3.17	126.50	122.73
3	X	12	HYP	CB-CG-CD	3.08	107.04	103.27
3	W	11	CIR	N8-C7-N6	2.96	119.97	116.85
3	U	11	CIR	O7-C7-N8	-2.88	118.27	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	11	CIR	C5-N6-C7	2.84	126.10	122.73
3	U	11	CIR	O7-C7-N6	-2.82	119.65	121.74
3	S	12	HYP	CB-CG-CD	2.47	106.29	103.27
3	X	11	CIR	O7-C7-N6	-2.28	120.05	121.74
3	Q	12	HYP	O-C-CA	-2.19	119.04	124.78
3	U	12	HYP	CG-CB-CA	2.19	106.73	103.96
3	U	12	HYP	O-C-CA	-2.19	119.04	124.78
3	S	12	HYP	O-C-CA	-2.10	119.28	124.78
3	X	11	CIR	N8-C7-N6	2.04	119.01	116.85
3	Q	11	CIR	O7-C7-N8	-2.04	119.71	123.22
3	X	12	HYP	O-C-CA	-2.03	119.47	124.78
3	Q	3	HYP	OD1-CG-CD	2.01	114.74	110.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	11	CIR	C1-C2-C3-C4
3	Q	11	CIR	N2-C2-C3-C4
3	T	11	CIR	C1-C2-C3-C4
3	T	11	CIR	N2-C2-C3-C4
3	T	11	CIR	O7-C7-N6-C5
3	T	11	CIR	N8-C7-N6-C5
3	T	11	CIR	C3-C4-C5-N6
3	X	11	CIR	C3-C4-C5-N6
3	R	11	CIR	C2-C3-C4-C5
3	Q	11	CIR	O7-C7-N6-C5
3	Q	11	CIR	N8-C7-N6-C5
3	S	11	CIR	O7-C7-N6-C5
3	S	11	CIR	N8-C7-N6-C5
3	U	11	CIR	O7-C7-N6-C5
3	U	11	CIR	N8-C7-N6-C5
3	U	11	CIR	C1-C2-C3-C4
3	V	11	CIR	C1-C2-C3-C4
3	U	11	CIR	C2-C3-C4-C5
3	W	11	CIR	C3-C4-C5-N6
3	R	11	CIR	N2-C2-C3-C4
3	W	11	CIR	N2-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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, 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	214/218 (98%)	-0.18	2 (0%) 84 85	30, 56, 88, 102	0
1	C	212/218 (97%)	-0.04	2 (0%) 84 85	32, 61, 96, 115	0
1	E	218/218 (100%)	-0.03	4 (1%) 68 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%)	0.34	10 (4%) 31 30	41, 78, 106, 124	0
1	M	212/218 (97%)	0.29	11 (5%) 27 25	40, 83, 125, 139	0
1	O	211/218 (96%)	1.26	54 (25%) 0 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%)	-0.20	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%)	-0.20	1 (0%) 91 92	33, 53, 79, 104	0
2	J	217/218 (99%)	-0.07	1 (0%) 91 92	31, 66, 111, 126	0
2	L	217/218 (99%)	0.07	4 (1%) 68 70	32, 68, 107, 127	0
2	N	215/218 (98%)	0.46	16 (7%) 14 12	52, 93, 125, 138	0
2	P	216/218 (99%)	0.72	20 (9%) 8 6	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%)	0.04	0 100 100	58, 63, 66, 79	0
3	S	8/18 (44%)	-0.11	0 100 100	67, 71, 78, 89	0
3	T	8/18 (44%)	0.55	1 (12%) 3 3	61, 66, 78, 85	0
3	U	8/18 (44%)	-0.06	0 100 100	63, 70, 73, 80	0
3	V	8/18 (44%)	0.31	1 (12%) 3 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%) 0 0	94, 101, 104, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	3508/3632 (96%)	0.12	131 (3%)	41	41	27, 69, 121, 192	0

All (131) 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	4.6
1	O	114	VAL	4.6
1	O	113	THR	4.3
1	M	186	VAL	4.3
1	O	109	GLY	4.1
1	O	123	SER	4.0
1	O	200	VAL	4.0
1	O	160	GLY	3.9
1	K	115	SER	3.9
1	O	79	SER	3.9
2	P	137	VAL	3.8
1	M	196	ILE	3.7
2	L	184	THR	3.7
2	L	185	LEU	3.5
1	O	134	THR	3.5
2	P	199	GLU	3.5
1	O	124	VAL	3.5
2	P	31	ASN	3.3
1	O	147	GLY	3.3
1	K	43	LYS	3.3
1	O	135	THR	3.3
1	O	141	LEU	3.2
2	N	194	ASN	3.2
1	O	3	LYS	3.2
3	V	4	GLY	3.2
1	O	212	LYS	3.2
1	O	178	TYR	3.2
3	X	4	GLY	3.1
1	M	192	PRO	3.1
1	O	175	SER	3.1
2	P	131	SER	3.1
2	J	158	GLU	3.1
2	P	156	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	1	GLU	3.0
1	M	175	SER	3.0
1	O	72	ILE	3.0
2	P	70	GLY	3.0
1	M	174	LEU	3.0
1	O	88	LEU	2.9
2	N	82	VAL	2.9
1	O	128	ALA	2.9
1	A	135	THR	2.9
1	O	23	ALA	2.9
1	O	16	GLY	2.9
1	M	215	PRO	2.8
2	P	130	THR	2.8
1	O	11	LEU	2.8
2	P	213	PHE	2.7
1	O	111	THR	2.7
1	O	204	ALA	2.7
1	O	30	SER	2.7
2	N	152	TRP	2.7
1	M	164	SER	2.7
1	O	27	PHE	2.6
2	P	24	ARG	2.6
1	K	174	LEU	2.6
2	N	191	GLU	2.6
1	K	18	MET	2.6
1	O	125	TYR	2.6
1	C	174	LEU	2.6
1	E	163	SER	2.6
2	L	64	ALA	2.6
2	N	202	HIS	2.5
3	T	4	GLY	2.5
1	O	21	SER	2.5
1	M	130	VAL	2.5
1	O	17	SER	2.5
2	N	79	ILE	2.5
1	O	116	SER	2.5
1	O	115	SER	2.5
2	N	204	THR	2.5
1	O	153	VAL	2.5
1	M	173	LEU	2.4
1	O	112	LEU	2.4
2	L	161	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	212	LYS	2.4
1	O	182	SER	2.4
2	N	148	ILE	2.4
1	O	32	ALA	2.4
2	N	184	THR	2.3
1	C	132	GLY	2.3
1	O	14	PRO	2.3
2	N	173	LYS	2.3
1	K	188	SER	2.3
2	P	71	SER	2.3
1	O	145	VAL	2.3
1	O	78	ARG	2.3
2	P	195	SER	2.3
2	P	200	ALA	2.3
2	P	37	MET	2.3
3	X	8	LEU	2.3
1	O	203	PRO	2.2
1	I	208	LYS	2.2
2	N	122	PHE	2.2
1	K	150	PRO	2.2
2	P	182	THR	2.2
1	O	96	TYR	2.2
1	O	136	GLY	2.2
1	O	7	SER	2.2
1	A	176	GLY	2.2
1	O	159	SER	2.2
1	E	190	THR	2.2
1	O	108	GLN	2.2
1	O	210	ASP	2.2
1	O	189	ASN	2.2
1	O	180	LEU	2.2
1	E	134	THR	2.2
1	K	195	THR	2.2
1	I	17	SER	2.2
1	O	214	GLU	2.1
1	M	127	LEU	2.1
1	O	70	PHE	2.1
1	M	131	CYS	2.1
2	P	126	SER	2.1
1	O	142	GLY	2.1
2	N	196	TYR	2.1
2	N	31	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	117	ALA	2.1
2	H	59	GLY	2.1
2	N	193	HIS	2.0
1	O	90	PRO	2.0
2	P	197	THR	2.0
2	N	190	TYR	2.0
2	P	33	GLY	2.0
2	N	139	PHE	2.0
1	K	204	ALA	2.0
1	K	209	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CIR	V	11	11/12	0.77	0.17	70,72,76,78	0
3	CIR	X	11	11/12	0.80	0.20	92,93,95,99	0
3	HYP	Q	3	8/9	0.83	0.21	77,82,88,90	0
3	CIR	U	11	11/12	0.86	0.17	77,80,83,83	0
3	CIR	W	11	11/12	0.86	0.18	71,75,91,97	0
3	HYP	X	12	8/9	0.87	0.16	95,96,98,99	0
3	HYP	V	12	8/9	0.88	0.21	84,89,93,93	0
3	CIR	R	11	11/12	0.88	0.15	63,64,69,70	0
3	CIR	Q	11	11/12	0.88	0.18	44,47,60,65	0
3	HYP	R	12	8/9	0.88	0.14	71,73,75,75	0
3	HYP	S	12	8/9	0.89	0.20	83,86,87,87	0
3	CIR	T	11	11/12	0.89	0.18	65,69,74,77	0
3	HYP	U	12	8/9	0.90	0.20	82,83,83,83	0
3	HYP	W	12	8/9	0.91	0.16	74,76,79,80	0
3	CIR	S	11	11/12	0.93	0.20	76,80,87,88	0
3	HYP	T	12	8/9	0.93	0.12	73,76,78,79	0
3	HYP	Q	12	8/9	0.93	0.14	49,50,52,52	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.