Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 12:05 AM EDT

PDB ID	:	5MU2
Title	:	ACC1 Fab fragment in complex with CII583-591 (CG10)
Authors	:	Dobritzsch, D.; Holmdahl, R.; Ge, C.
Deposited on	:	2017-01-12
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

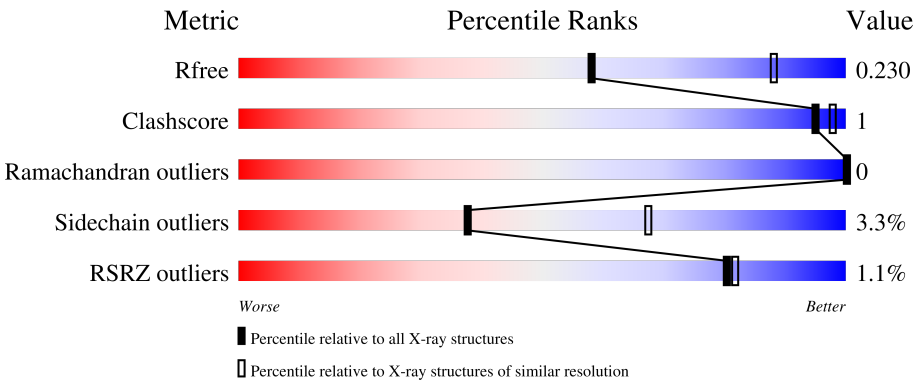
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

Mol	Chain	Length	Quality of chain
1	A	218	95% • •
1	C	218	93% 6%
1	E	218	95% • •
1	G	218	3% 92% 5% •
1	I	218	94% 6%

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Mol	Chain	Length	Quality of chain
1	K	218	95%
1	M	218	96%
1	O	218	.% 94%
2	B	218	2% 93% 7%
2	D	218	93% 6%
2	F	218	.% 93% 6%
2	H	218	4% 92% 7%
2	J	218	2% 94% 6%
2	L	218	94% 6%
2	N	218	93% 7%
2	P	218	.% 92% 7%
3	Q	30	40% 10% 50%
3	R	30	40% 10% 50%
3	S	30	40% 10% 50%
3	T	30	40% 57%
3	U	30	47% 50%
3	V	30	7% 37% 60%
3	W	30	27% 70%
3	X	30	43% 7% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27447 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
			Total	C	N	O	S			
1	A	216	1629	1028	271	322	8	0	0	0
1	C	218	1640	1034	273	325	8	0	0	0
1	E	215	1622	1024	270	320	8	0	0	0
1	G	211	1601	1011	266	317	7	0	0	0
1	I	218	1640	1034	273	325	8	0	0	0
1	K	216	1629	1028	271	322	8	0	0	0
1	M	216	1629	1028	271	322	8	0	0	0
1	O	214	1615	1019	269	319	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	1666	1038	282	339	7	0	0	0
2	D	218	1666	1038	282	339	7	0	0	0
2	F	217	1660	1035	281	338	6	0	0	0
2	H	217	1660	1035	281	338	6	0	0	0
2	J	218	1666	1038	282	339	7	0	0	0
2	L	218	1666	1038	282	339	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	218	1666	1038	282	339	7	0	0	0
			Total	C	N	O	S			
2	P	217	1660	1035	281	338	6	0	0	0

- Molecule 3 is a protein called synthetic peptide containing the CII583-591 epitope of collagen type II.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	X	15	95	59	18	18	0	0	0
			Total	C	N	O			
3	Q	15	95	59	18	18	0	0	0
			Total	C	N	O			
3	R	15	95	59	18	18	0	0	0
			Total	C	N	O			
3	S	15	95	59	18	18	0	0	0
			Total	C	N	O			
3	T	13	83	52	16	15	0	0	0
			Total	C	N	O			
3	U	15	95	59	18	18	0	0	0
			Total	C	N	O			
3	V	12	76	47	15	14	0	0	0
			Total	C	N	O			
3	W	9	57	35	12	10	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	37	37	37	0	0
			Total	O		
4	B	38	38	38	0	0
			Total	O		
4	C	18	18	18	0	0
			Total	O		
4	D	64	64	64	0	0
			Total	O		
4	E	42	42	42	0	0
			Total	O		
4	F	24	24	24	0	0
			Total	O		
4	G	21	21	21	0	0

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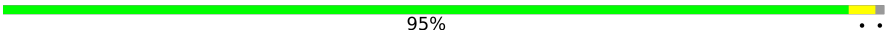
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	H	12	12	12	0	0
			Total	O		
4	I	37	37	37	0	0
			Total	O		
4	J	25	25	25	0	0
			Total	O		
4	K	17	17	17	0	0
			Total	O		
4	L	28	28	28	0	0
			Total	O		
4	M	15	15	15	0	0
			Total	O		
4	N	19	19	19	0	0
			Total	O		
4	O	10	10	10	0	0
			Total	O		
4	P	22	22	22	0	0
			Total	O		
4	X	1	1	1	0	0
			Total	O		
4	Q	3	3	3	0	0
			Total	O		
4	R	2	2	2	0	0
			Total	O		
4	S	2	2	2	0	0
			Total	O		
4	T	3	3	3	0	0
			Total	O		
4	U	1	1	1	0	0

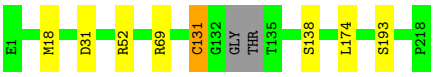
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

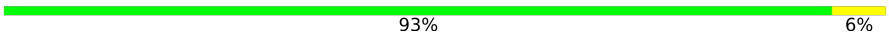
Chain A:

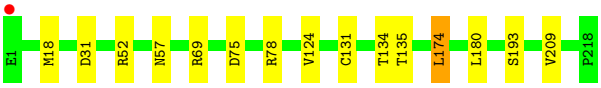




• Molecule 1: ACC1 Fab fragment heavy chain

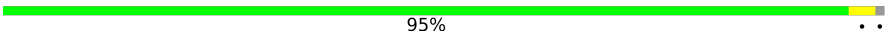
Chain C:

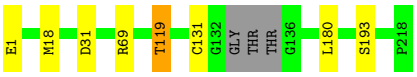




• Molecule 1: ACC1 Fab fragment heavy chain

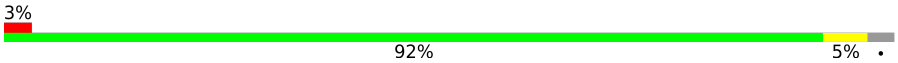
Chain E:

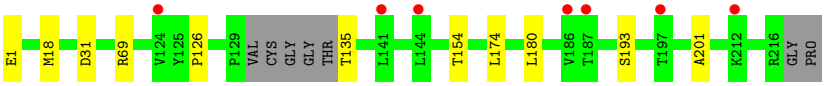




• Molecule 1: ACC1 Fab fragment heavy chain

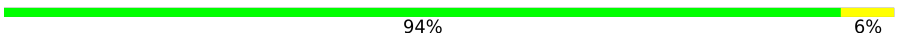
Chain G:

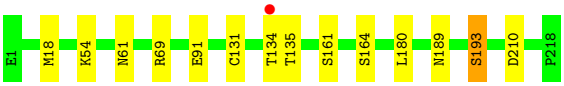




• Molecule 1: ACC1 Fab fragment heavy chain

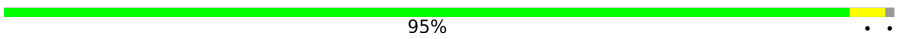
Chain I:

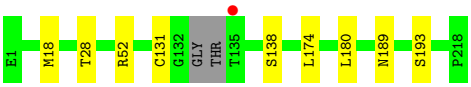




• Molecule 1: ACC1 Fab fragment heavy chain

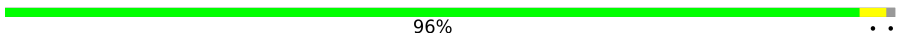
Chain K:

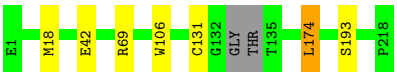




• Molecule 1: ACC1 Fab fragment heavy chain

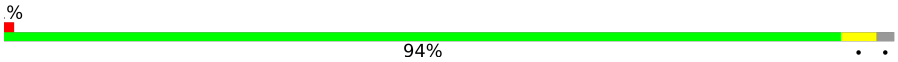
Chain M:

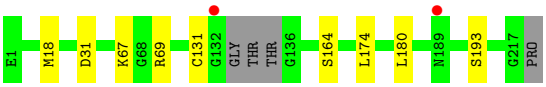




• Molecule 1: ACC1 Fab fragment heavy chain

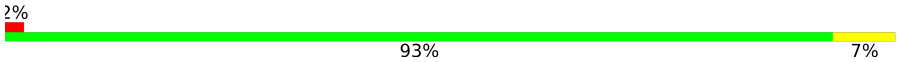
Chain O:

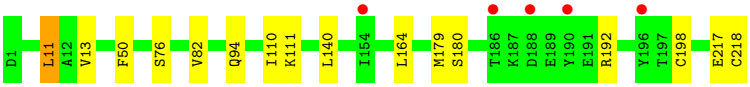




• Molecule 2: ACC1 Fab fragment light chain

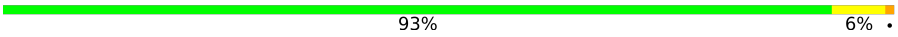
Chain B:

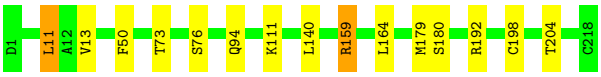




• Molecule 2: ACC1 Fab fragment light chain

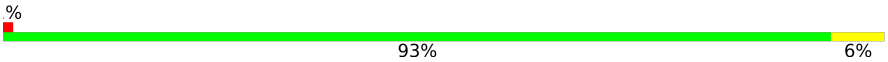
Chain D:

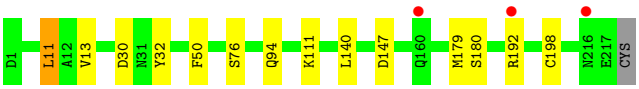




• Molecule 2: ACC1 Fab fragment light chain

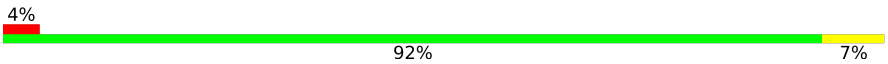
Chain F:

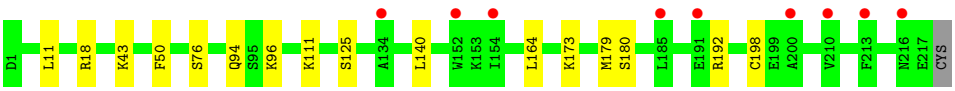




• Molecule 2: ACC1 Fab fragment light chain

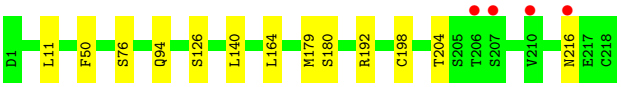
Chain H:





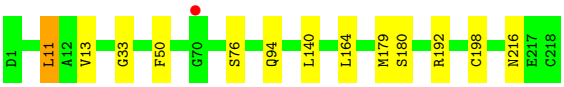
• Molecule 2: ACC1 Fab fragment light chain

Chain J: 2% 94% 6%



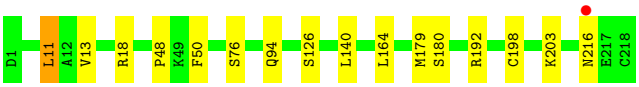
• Molecule 2: ACC1 Fab fragment light chain

Chain L: 94% 6%



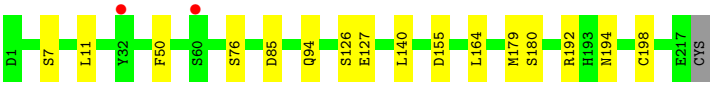
• Molecule 2: ACC1 Fab fragment light chain

Chain N: 93% 7%



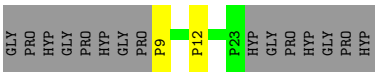
• Molecule 2: ACC1 Fab fragment light chain

Chain P: % 92% 7%



• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain X: 43% 7% 50%

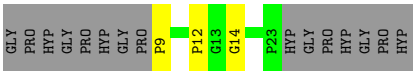


• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain Q: 40% 10% 50%

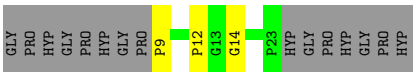
• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain R: 40% 10% 50%



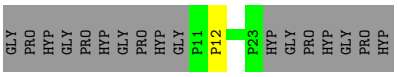
• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain S:



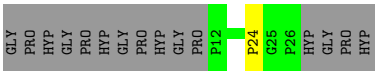
• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain T:



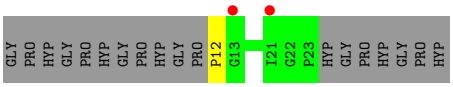
• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain U:



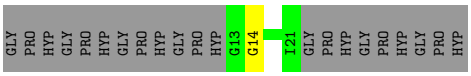
• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain V:



• Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	148.86Å 156.01Å 156.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.70 47.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.09-2.70) 100.0 (47.30-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.206 , 0.228 0.208 , 0.230	Depositor DCC
R_{free} test set	4864 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 27.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k 0.018 for -l,-k,-h 0.019 for k,h,-l 0.012 for k,l,h 0.012 for l,h,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27447	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.52	0/1669	0.81	4/2277 (0.2%)
1	C	0.51	0/1681	0.97	5/2295 (0.2%)
1	E	0.56	0/1662	0.82	3/2267 (0.1%)
1	G	0.50	0/1640	0.78	2/2237 (0.1%)
1	I	0.58	1/1681 (0.1%)	0.81	3/2295 (0.1%)
1	K	0.52	0/1669	0.69	0/2277
1	M	0.52	1/1669 (0.1%)	0.95	4/2277 (0.2%)
1	O	0.50	0/1654	0.98	3/2255 (0.1%)
2	B	0.51	0/1703	0.70	1/2310 (0.0%)
2	D	0.58	0/1703	0.74	1/2310 (0.0%)
2	F	0.51	0/1697	0.71	2/2302 (0.1%)
2	H	0.49	0/1697	0.71	2/2302 (0.1%)
2	J	0.50	0/1703	0.69	1/2310 (0.0%)
2	L	0.49	0/1703	0.69	2/2310 (0.1%)
2	N	0.47	0/1703	0.69	2/2310 (0.1%)
2	P	0.57	1/1697 (0.1%)	0.81	3/2302 (0.1%)
3	Q	0.71	0/79	0.67	0/102
3	R	0.71	0/80	0.81	0/106
3	S	0.81	0/80	1.00	0/106
3	T	0.64	0/76	0.86	0/100
3	U	0.80	0/80	0.73	0/106
3	V	0.59	0/69	0.87	0/92
3	W	0.66	0/57	0.89	0/75
3	X	0.72	0/80	0.79	0/106
All	All	0.53	3/27532 (0.0%)	0.79	38/37429 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	I	0	1
1	K	0	1
2	B	0	1
2	J	0	1
2	L	0	1
2	N	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	127	GLU	CD-OE1	5.84	1.32	1.25
1	M	42	GLU	CD-OE1	5.55	1.31	1.25
1	I	91	GLU	CD-OE1	5.07	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	69	ARG	NE-CZ-NH2	-22.13	109.23	120.30
1	C	69	ARG	NE-CZ-NH1	22.08	131.34	120.30
1	O	69	ARG	NE-CZ-NH1	21.98	131.29	120.30
1	M	69	ARG	NE-CZ-NH1	21.57	131.09	120.30
1	M	69	ARG	NE-CZ-NH2	-21.42	109.59	120.30
1	C	69	ARG	NE-CZ-NH2	-21.33	109.63	120.30
2	P	192	ARG	NE-CZ-NH2	16.04	128.32	120.30
1	E	69	ARG	NE-CZ-NH2	13.41	127.01	120.30
1	I	69	ARG	NE-CZ-NH2	13.17	126.88	120.30
1	G	69	ARG	NE-CZ-NH2	12.98	126.79	120.30
1	A	69	ARG	NE-CZ-NH2	12.23	126.42	120.30
1	G	69	ARG	NE-CZ-NH1	-12.17	114.21	120.30
1	E	69	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	I	69	ARG	NE-CZ-NH1	-11.87	114.37	120.30
1	A	69	ARG	NE-CZ-NH1	-11.70	114.45	120.30
2	P	192	ARG	NE-CZ-NH1	-10.47	115.07	120.30
1	M	69	ARG	CD-NE-CZ	7.33	133.87	123.60
1	C	69	ARG	CD-NE-CZ	7.21	133.69	123.60
1	O	69	ARG	CD-NE-CZ	7.20	133.67	123.60
1	E	119	THR	CA-CB-CG2	6.95	122.13	112.40
2	F	192	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	H	18	ARG	NE-CZ-NH2	5.86	123.23	120.30
2	J	192	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	174	LEU	CA-CB-CG	5.54	128.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	192	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	N	18	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	192	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	P	85	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	31	ASP	CB-CG-OD1	-5.24	113.59	118.30
2	F	192	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	L	192	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	52	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	I	210	ASP	CB-CG-OD2	5.16	122.95	118.30
2	D	159	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	52	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	M	174	LEU	CA-CB-CG	5.02	126.86	115.30
2	N	192	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	L	192	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	217	GLU	Peptide
1	C	135	THR	Peptide
1	I	135	THR	Peptide
2	J	216	ASN	Peptide
1	K	52	ARG	Sidechain
2	L	216	ASN	Peptide
2	N	216	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1629	0	1589	2	0
1	C	1640	0	1600	10	0
1	E	1622	0	1583	1	0
1	G	1601	0	1563	6	0
1	I	1640	0	1600	8	0
1	K	1629	0	1589	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1629	0	1589	2	0
1	O	1615	0	1576	2	1
2	B	1666	0	1597	7	0
2	D	1666	0	1597	13	0
2	F	1660	0	1593	5	0
2	H	1660	0	1593	5	0
2	J	1666	0	1597	5	0
2	L	1666	0	1597	7	0
2	N	1666	0	1597	10	0
2	P	1660	0	1593	6	0
3	Q	95	0	95	1	0
3	R	95	0	96	1	0
3	S	95	0	95	1	0
3	T	83	0	85	0	0
3	U	95	0	95	0	0
3	V	76	0	79	0	0
3	W	57	0	60	1	0
3	X	95	0	96	0	0
4	A	37	0	0	0	0
4	B	38	0	0	0	0
4	C	18	0	0	1	0
4	D	64	0	0	0	0
4	E	42	0	0	0	0
4	F	24	0	0	0	0
4	G	21	0	0	0	0
4	H	12	0	0	0	0
4	I	37	0	0	0	0
4	J	25	0	0	0	0
4	K	17	0	0	0	0
4	L	28	0	0	0	0
4	M	15	0	0	0	0
4	N	19	0	0	0	0
4	O	10	0	0	0	0
4	P	22	0	0	0	0
4	Q	3	0	0	0	0
4	R	2	0	0	0	0
4	S	2	0	0	0	0
4	T	3	0	0	0	0
4	U	1	0	0	0	0
4	X	1	0	0	0	0
All	All	27447	0	26154	64	1

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 (64) 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:M:174:LEU:HD13	2:N:164:LEU:HD11	1.61	0.79
2:F:32:TYR:HA	1:I:161:SER:O	1.90	0.72
1:O:174:LEU:HD13	2:P:164:LEU:HD11	1.74	0.68
1:A:174:LEU:HD13	2:B:164:LEU:HD11	1.75	0.67
2:J:204:THR:O	2:L:33:GLY:N	2.30	0.65
1:C:174:LEU:HB2	2:D:164:LEU:HD11	1.79	0.65
2:F:30:ASP:HB3	1:I:164:SER:OG	1.96	0.64
1:I:61:ASN:HD21	2:P:7:SER:HB2	1.64	0.63
1:C:75:ASP:OD1	2:N:203:LYS:HE3	2.00	0.62
2:P:155:ASP:OD1	2:P:194:ASN:OD1	2.19	0.61
1:G:154:THR:HG22	1:G:201:ALA:HB3	1.83	0.59
2:D:192:ARG:O	2:D:192:ARG:HG3	2.04	0.56
2:D:73:THR:OG1	1:I:193:SER:CB	2.54	0.55
2:D:73:THR:OG1	1:I:193:SER:OG	2.17	0.55
2:D:73:THR:HG1	1:I:193:SER:CB	2.20	0.54
2:H:140:LEU:HD13	2:H:179:MET:HE2	1.89	0.54
2:L:140:LEU:HD13	2:L:179:MET:HE2	1.90	0.54
2:J:164:LEU:C	2:J:164:LEU:HD23	2.29	0.53
2:D:140:LEU:HD13	2:D:179:MET:HE2	1.91	0.53
2:D:204:THR:O	1:G:1:GLU:N	2.37	0.53
2:P:140:LEU:HD13	2:P:179:MET:HE2	1.90	0.53
1:C:174:LEU:HD13	2:D:164:LEU:HD11	1.91	0.52
2:N:140:LEU:HD13	2:N:179:MET:HE2	1.91	0.52
1:E:31:ASP:O	3:R:14:GLY:HA3	2.10	0.51
2:D:73:THR:OG1	1:I:193:SER:HB3	2.10	0.51
1:C:78:ARG:NH1	2:N:203:LYS:O	2.44	0.51
1:C:124:VAL:HG21	1:C:209:VAL:HG11	1.93	0.50
2:J:140:LEU:HD13	2:J:179:MET:HE2	1.94	0.50
1:G:154:THR:CG2	1:G:201:ALA:HB3	2.43	0.49
1:C:134:THR:HG21	4:C:312:HOH:O	2.13	0.48
1:C:57:ASN:HB3	2:N:11:LEU:HD23	1.95	0.48
1:C:174:LEU:HD22	2:D:164:LEU:CD1	2.44	0.48
2:B:140:LEU:HD13	2:B:179:MET:HE2	1.95	0.47
2:F:140:LEU:HD13	2:F:179:MET:HE2	1.96	0.47
2:J:204:THR:O	2:L:33:GLY:CA	2.63	0.47
1:A:131:CYS:HB3	2:B:218:CYS:HB3	1.73	0.46
2:H:140:LEU:HD13	2:H:179:MET:CE	2.46	0.46
2:B:140:LEU:HD13	2:B:179:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:TRP:CE3	2:N:48:PRO:HD2	2.51	0.45
2:P:140:LEU:HD13	2:P:179:MET:CE	2.47	0.44
1:G:126:PRO:O	2:H:125:SER:HB3	2.18	0.44
2:L:140:LEU:HD13	2:L:179:MET:CE	2.46	0.44
1:O:31:ASP:O	3:W:14:GLY:HA3	2.17	0.44
1:C:57:ASN:CB	2:N:11:LEU:HD23	2.48	0.43
2:N:140:LEU:HD13	2:N:179:MET:CE	2.47	0.43
2:D:140:LEU:HD13	2:D:179:MET:CE	2.48	0.43
2:F:140:LEU:HD13	2:F:179:MET:CE	2.49	0.42
2:L:11:LEU:HD22	2:L:13:VAL:CG2	2.49	0.42
2:B:140:LEU:HD12	2:B:140:LEU:N	2.35	0.42
2:F:11:LEU:HD22	2:F:13:VAL:CG2	2.50	0.41
1:G:31:ASP:O	3:S:14:GLY:HA3	2.20	0.41
2:J:140:LEU:HD13	2:J:179:MET:CE	2.49	0.41
2:D:140:LEU:N	2:D:140:LEU:HD12	2.36	0.41
1:K:174:LEU:HD13	2:L:164:LEU:HD11	2.03	0.41
1:C:31:ASP:O	3:Q:14:GLY:HA3	2.21	0.41
2:L:140:LEU:N	2:L:140:LEU:HD12	2.35	0.41
2:N:11:LEU:HD22	2:N:13:VAL:CG2	2.50	0.41
2:H:140:LEU:N	2:H:140:LEU:HD12	2.35	0.41
2:N:140:LEU:HD12	2:N:140:LEU:N	2.36	0.41
2:B:82:VAL:CG1	2:B:110:ILE:HD12	2.51	0.41
2:D:11:LEU:HD22	2:D:13:VAL:CG2	2.51	0.41
1:G:174:LEU:HD13	2:H:164:LEU:HD11	2.02	0.40
1:I:61:ASN:ND2	2:P:7:SER:HB2	2.35	0.40
2:B:11:LEU:HD22	2:B:13:VAL:CG2	2.52	0.40

All (1) 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:K:28:THR:OG1	1:O:164:SER:OG[3_555]	2.01	0.19

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	212/218 (97%)	206 (97%)	6 (3%)	0	100	100
1	C	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
1	E	211/218 (97%)	205 (97%)	6 (3%)	0	100	100
1	G	207/218 (95%)	202 (98%)	5 (2%)	0	100	100
1	I	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
1	K	212/218 (97%)	206 (97%)	6 (3%)	0	100	100
1	M	212/218 (97%)	206 (97%)	6 (3%)	0	100	100
1	O	210/218 (96%)	204 (97%)	6 (3%)	0	100	100
2	B	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
2	D	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
2	F	215/218 (99%)	210 (98%)	5 (2%)	0	100	100
2	H	215/218 (99%)	210 (98%)	5 (2%)	0	100	100
2	J	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
2	L	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
2	N	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
2	P	215/218 (99%)	210 (98%)	5 (2%)	0	100	100
3	Q	11/30 (37%)	11 (100%)	0	0	100	100
3	R	12/30 (40%)	12 (100%)	0	0	100	100
3	S	12/30 (40%)	11 (92%)	1 (8%)	0	100	100
3	T	10/30 (33%)	10 (100%)	0	0	100	100
3	U	12/30 (40%)	12 (100%)	0	0	100	100
3	V	10/30 (33%)	10 (100%)	0	0	100	100
3	W	7/30 (23%)	7 (100%)	0	0	100	100
3	X	12/30 (40%)	12 (100%)	0	0	100	100
All	All	3507/3728 (94%)	3418 (98%)	89 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/185 (100%)	180 (98%)	4 (2%)	52	79
1	C	185/185 (100%)	181 (98%)	4 (2%)	52	79
1	E	183/185 (99%)	177 (97%)	6 (3%)	38	67
1	G	181/185 (98%)	177 (98%)	4 (2%)	52	79
1	I	185/185 (100%)	178 (96%)	7 (4%)	33	62
1	K	184/185 (100%)	178 (97%)	6 (3%)	38	67
1	M	184/185 (100%)	181 (98%)	3 (2%)	62	85
1	O	182/185 (98%)	177 (97%)	5 (3%)	44	74
2	B	188/188 (100%)	181 (96%)	7 (4%)	34	63
2	D	188/188 (100%)	180 (96%)	8 (4%)	29	57
2	F	187/188 (100%)	179 (96%)	8 (4%)	29	57
2	H	187/188 (100%)	177 (95%)	10 (5%)	22	48
2	J	188/188 (100%)	181 (96%)	7 (4%)	34	63
2	L	188/188 (100%)	182 (97%)	6 (3%)	39	68
2	N	188/188 (100%)	181 (96%)	7 (4%)	34	63
2	P	187/188 (100%)	180 (96%)	7 (4%)	34	63
3	Q	7/12 (58%)	7 (100%)	0	100	100
3	R	7/12 (58%)	7 (100%)	0	100	100
3	S	7/12 (58%)	7 (100%)	0	100	100
3	T	7/12 (58%)	7 (100%)	0	100	100
3	U	7/12 (58%)	7 (100%)	0	100	100
3	V	6/12 (50%)	6 (100%)	0	100	100
3	W	5/12 (42%)	5 (100%)	0	100	100
3	X	7/12 (58%)	7 (100%)	0	100	100
All	All	3022/3080 (98%)	2923 (97%)	99 (3%)	38	67

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET

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Mol	Chain	Res	Type
1	A	131	CYS
1	A	138	SER
1	A	193	SER
2	B	11	LEU
2	B	50	PHE
2	B	76	SER
2	B	94	GLN
2	B	111	LYS
2	B	180	SER
2	B	198	CYS
1	C	18	MET
1	C	131	CYS
1	C	180	LEU
1	C	193	SER
2	D	11	LEU
2	D	50	PHE
2	D	76	SER
2	D	94	GLN
2	D	111	LYS
2	D	159	ARG
2	D	180	SER
2	D	198	CYS
1	E	1	GLU
1	E	18	MET
1	E	119	THR
1	E	131	CYS
1	E	180	LEU
1	E	193	SER
2	F	11	LEU
2	F	50	PHE
2	F	76	SER
2	F	94	GLN
2	F	111	LYS
2	F	147	ASP
2	F	180	SER
2	F	198	CYS
1	G	18	MET
1	G	135	THR
1	G	180	LEU
1	G	193	SER
2	H	11	LEU
2	H	43	LYS

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Mol	Chain	Res	Type
2	H	50	PHE
2	H	76	SER
2	H	94	GLN
2	H	96	LYS
2	H	111	LYS
2	H	173	LYS
2	H	180	SER
2	H	198	CYS
1	I	18	MET
1	I	54	LYS
1	I	131	CYS
1	I	134	THR
1	I	180	LEU
1	I	189	ASN
1	I	193	SER
2	J	11	LEU
2	J	50	PHE
2	J	76	SER
2	J	94	GLN
2	J	126	SER
2	J	180	SER
2	J	198	CYS
1	K	18	MET
1	K	131	CYS
1	K	138	SER
1	K	180	LEU
1	K	189	ASN
1	K	193	SER
2	L	11	LEU
2	L	50	PHE
2	L	76	SER
2	L	94	GLN
2	L	180	SER
2	L	198	CYS
1	M	18	MET
1	M	131	CYS
1	M	193	SER
2	N	11	LEU
2	N	50	PHE
2	N	76	SER
2	N	94	GLN
2	N	126	SER

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Mol	Chain	Res	Type
2	N	180	SER
2	N	198	CYS
1	O	18	MET
1	O	67	LYS
1	O	131	CYS
1	O	180	LEU
1	O	193	SER
2	P	11	LEU
2	P	50	PHE
2	P	76	SER
2	P	94	GLN
2	P	126	SER
2	P	180	SER
2	P	198	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	141	ASN
2	D	141	ASN
1	I	61	ASN
1	M	167	HIS
2	N	31	ASN
2	N	141	ASN
2	N	142	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	T	12	3	6,8,9	1.29	1 (16%)	5,10,12	1.15	0
3	HYP	X	9	3	6,8,9	0.99	0	5,10,12	2.08	2 (40%)
3	HYP	V	12	3	6,8,9	0.47	0	5,10,12	2.84	2 (40%)
3	HYP	Q	9	3	6,8,9	0.60	0	5,10,12	2.58	3 (60%)
3	HYP	X	12	3	6,8,9	1.26	1 (16%)	5,10,12	1.48	0
3	HYP	R	12	3	6,8,9	1.25	1 (16%)	5,10,12	1.38	1 (20%)
3	HYP	S	12	3	6,8,9	1.25	1 (16%)	5,10,12	1.29	1 (20%)
3	HYP	R	9	3	6,8,9	0.63	0	5,10,12	2.44	1 (20%)
3	HYP	U	24	3	6,8,9	0.37	0	5,10,12	2.15	3 (60%)
3	HYP	Q	12	3	6,8,9	1.28	1 (16%)	5,10,12	1.13	0
3	HYP	U	12	3	6,8,9	1.28	0	5,10,12	1.01	0
3	HYP	S	9	3	6,8,9	0.56	0	5,10,12	2.43	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	HYP	T	12	3	-	0/0/11/13	0/1/1/1
3	HYP	X	9	3	-	0/0/11/13	0/1/1/1
3	HYP	V	12	3	-	0/0/11/13	0/1/1/1
3	HYP	Q	9	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
3	HYP	S	12	3	-	0/0/11/13	0/1/1/1
3	HYP	R	9	3	-	0/0/11/13	0/1/1/1
3	HYP	U	24	3	-	0/0/11/13	0/1/1/1
3	HYP	Q	12	3	-	0/0/11/13	0/1/1/1
3	HYP	U	12	3	-	0/0/11/13	0/1/1/1
3	HYP	S	9	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	T	12	HYP	CD-N	2.24	1.55	1.47
3	Q	12	HYP	CD-N	2.24	1.55	1.47
3	S	12	HYP	CD-N	2.13	1.54	1.47
3	R	12	HYP	CD-N	2.12	1.54	1.47
3	X	12	HYP	CD-N	2.07	1.54	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	12	HYP	CG-CB-CA	5.38	110.76	103.96
3	R	9	HYP	CG-CB-CA	4.57	109.73	103.96
3	S	9	HYP	CB-CG-CD	4.50	108.78	103.27
3	Q	9	HYP	CG-CB-CA	4.37	109.48	103.96
3	Q	9	HYP	O-C-CA	-3.04	116.82	124.78
3	V	12	HYP	O-C-CA	-3.02	116.86	124.78
3	X	9	HYP	CB-CG-CD	3.01	106.95	103.27
3	U	24	HYP	CG-CB-CA	2.93	107.66	103.96
3	U	24	HYP	O-C-CA	-2.83	117.36	124.78
3	X	9	HYP	CG-CB-CA	-2.76	100.47	103.96
3	U	24	HYP	CB-CG-CD	2.52	106.35	103.27
3	S	9	HYP	CG-CB-CA	-2.31	101.05	103.96
3	S	12	HYP	O-C-CA	-2.24	118.91	124.78
3	R	12	HYP	O-C-CA	-2.18	119.05	124.78
3	Q	9	HYP	OD1-CG-CD	2.07	114.88	110.35

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	216/218 (99%)	-0.37	0	100	100	28, 50, 75, 99	0
1	C	218/218 (100%)	-0.32	1 (0%)	91	92	29, 55, 81, 99	0
1	E	215/218 (98%)	-0.41	0	100	100	29, 47, 83, 106	0
1	G	211/218 (96%)	0.06	7 (3%)	46	46	28, 74, 121, 131	0
1	I	218/218 (100%)	-0.34	1 (0%)	91	92	23, 43, 91, 105	0
1	K	216/218 (99%)	-0.29	1 (0%)	91	92	35, 54, 79, 103	0
1	M	216/218 (99%)	-0.31	0	100	100	39, 58, 79, 98	0
1	O	214/218 (98%)	-0.08	2 (0%)	84	85	39, 65, 99, 117	0
2	B	218/218 (100%)	-0.20	5 (2%)	60	62	25, 47, 107, 132	0
2	D	218/218 (100%)	-0.40	0	100	100	25, 43, 65, 78	0
2	F	217/218 (99%)	-0.20	3 (1%)	75	77	29, 56, 104, 127	0
2	H	217/218 (99%)	0.12	9 (4%)	37	36	31, 67, 133, 157	0
2	J	218/218 (100%)	-0.20	4 (1%)	68	70	26, 58, 103, 118	0
2	L	218/218 (100%)	-0.12	1 (0%)	91	92	38, 59, 84, 109	0
2	N	218/218 (100%)	-0.22	1 (0%)	91	92	39, 60, 80, 101	0
2	P	217/218 (99%)	-0.16	2 (0%)	84	85	34, 54, 99, 114	0
3	Q	13/30 (43%)	-0.37	0	100	100	40, 48, 93, 128	0
3	R	13/30 (43%)	-0.17	0	100	100	38, 46, 90, 94	0
3	S	13/30 (43%)	-0.13	0	100	100	33, 44, 101, 102	0
3	T	12/30 (40%)	-0.15	0	100	100	47, 59, 86, 95	0
3	U	13/30 (43%)	0.28	0	100	100	58, 65, 93, 93	0
3	V	11/30 (36%)	0.28	2 (18%)	1	1	57, 65, 97, 103	0
3	W	9/30 (30%)	-0.18	0	100	100	50, 54, 62, 66	0
3	X	13/30 (43%)	-0.05	0	100	100	40, 50, 95, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3562/3728 (95%)	-0.21	39 (1%) 80 82	23, 55, 103, 157	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	132	GLY	6.3
1	G	186	VAL	4.6
2	J	206	THR	4.1
2	H	213	PHE	3.8
1	O	189	ASN	3.5
2	H	191	GLU	3.4
1	C	1	GLU	3.4
2	P	32	TYR	3.1
2	H	134	ALA	3.1
2	N	216	ASN	2.9
1	G	197	THR	2.9
2	J	207	SER	2.8
2	B	154	ILE	2.7
2	H	152	TRP	2.7
2	P	60	SER	2.7
1	G	141	LEU	2.7
2	B	188	ASP	2.6
2	H	216	ASN	2.5
1	I	134	THR	2.5
1	K	135	THR	2.5
2	J	216	ASN	2.5
2	B	196	TYR	2.5
2	F	216	ASN	2.5
1	G	212	LYS	2.4
2	H	210	VAL	2.4
2	F	160	GLN	2.4
1	G	124	VAL	2.4
2	L	70	GLY	2.3
3	V	13	GLY	2.3
1	G	187	THR	2.3
2	B	186	THR	2.3
2	H	185	LEU	2.2
2	H	200	ALA	2.2
2	F	192	ARG	2.2
3	V	21	ILE	2.2
2	B	190	TYR	2.1
1	G	144	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	154	ILE	2.1
2	J	210	VAL	2.1

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	HYP	X	9	8/9	0.61	0.29	106,109,115,117	0
3	HYP	R	9	8/9	0.69	0.25	99,101,103,103	0
3	HYP	Q	9	8/9	0.75	0.18	94,104,109,110	0
3	HYP	U	12	8/9	0.85	0.22	84,90,91,92	0
3	HYP	S	9	8/9	0.86	0.15	97,112,129,131	0
3	HYP	U	24	8/9	0.88	0.20	93,93,94,94	0
3	HYP	V	12	8/9	0.89	0.20	77,77,78,78	0
3	HYP	R	12	8/9	0.91	0.16	67,72,77,78	0
3	HYP	X	12	8/9	0.92	0.17	69,73,77,79	0
3	HYP	Q	12	8/9	0.93	0.13	56,64,72,72	0
3	HYP	T	12	8/9	0.94	0.16	74,76,81,82	0
3	HYP	S	12	8/9	0.94	0.15	64,69,76,77	0

6.3 Carbohydrates (i)

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.