



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2017 – 08:38 PM EDT

PDB ID : 5MV3  
Title : ACC1 Fab fragment in complex with CII583-591 (CG10)  
Authors : Dobritsch, D.; Holmdahl, R.; Ge, C.  
Deposited on : unknown  
Resolution : 2.95 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](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

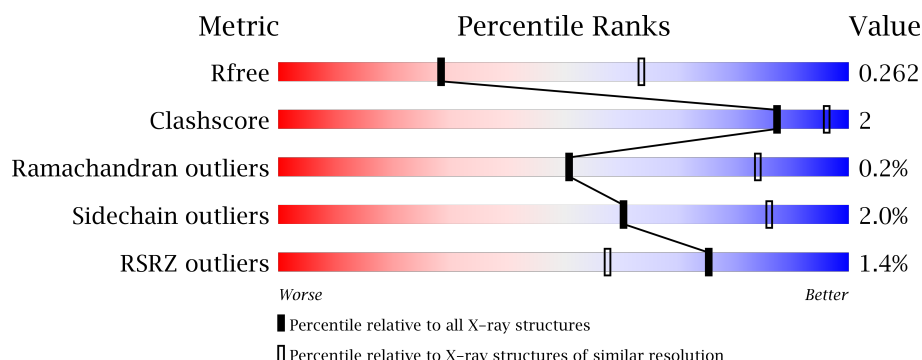
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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.



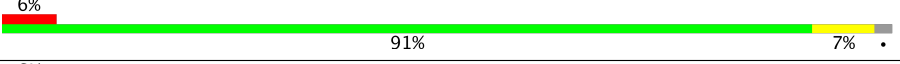




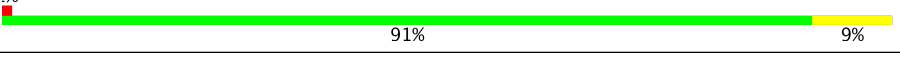

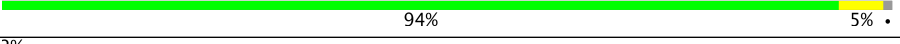
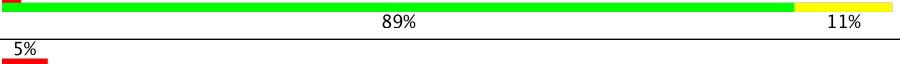
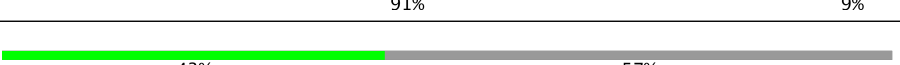







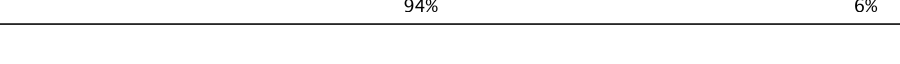

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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	
1	C	218	
1	F	218	
1	I	218	
1	O	218	

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Mol	Chain	Length	Quality of chain
1	R	218	
1	U	218	
2	B	218	
2	D	218	
2	G	218	
2	J	218	
2	M	218	
2	P	218	
2	S	218	
2	V	218	
3	E	30	
3	H	30	
3	K	30	
3	N	30	
3	Q	30	
3	T	30	
3	W	30	
3	X	30	
4	L	220	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26921 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 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1629	1028	271	322	8			
1	C	213	Total	C	N	O	S	0	0	0
			1614	1020	268	318	8			
1	F	216	Total	C	N	O	S	0	0	0
			1629	1028	271	322	8			
1	I	215	Total	C	N	O	S	0	0	0
			1625	1026	270	321	8			
1	O	215	Total	C	N	O	S	0	0	0
			1625	1026	270	321	8			
1	R	214	Total	C	N	O	S	0	0	0
			1613	1019	269	317	8			
1	U	211	Total	C	N	O	S	0	0	0
			1597	1008	266	315	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1666	1038	282	339	7			
2	D	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	G	217	Total	C	N	O	S	0	0	0
			1660	1035	281	338	6			
2	J	218	Total	C	N	O	S	0	0	0
			1666	1038	282	339	7			
2	M	218	Total	C	N	O	S	0	0	0
			1666	1038	282	339	7			
2	P	215	Total	C	N	O	S	0	0	0
			1643	1026	278	333	6			
2	S	218	Total	C	N	O	S	0	0	0
			1666	1038	282	339	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	218	Total	C	N	O	S	0	0	0
			1666	1038	282	339	7			

- Molecule 3 is a protein called synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	14	Total	C	N	O		0	0	0
			87	54	17	16				
3	E	13	Total	C	N	O		0	0	0
			84	52	16	16				
3	H	12	Total	C	N	O		0	0	0
			76	47	15	14				
3	K	13	Total	C	N	O		0	0	0
			83	52	16	15				
3	N	13	Total	C	N	O		0	0	0
			83	52	16	15				
3	Q	12	Total	C	N	O		0	0	0
			76	47	15	14				
3	T	12	Total	C	N	O		0	0	0
			76	47	15	14				
3	W	12	Total	C	N	O		0	0	0
			76	47	15	14				

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

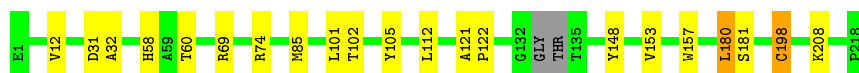
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	220	Total	C	N	O	S	0	0	0
			1655	1044	275	328	8			

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

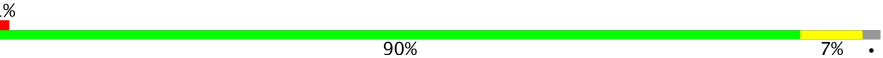
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

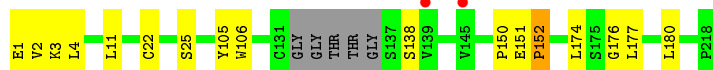
- Molecule 1: heavy chain of ACC1 Fab fragment

Chain A: 




- Molecule 1: heavy chain of ACC1 Fab fragment

Chain C: 




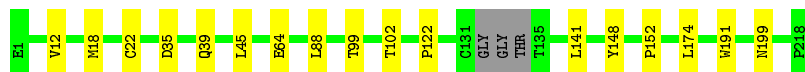
- Molecule 1: heavy chain of ACC1 Fab fragment

Chain F: 



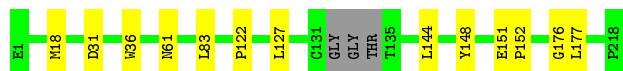
- Molecule 1: heavy chain of ACC1 Fab fragment

Chain I: 




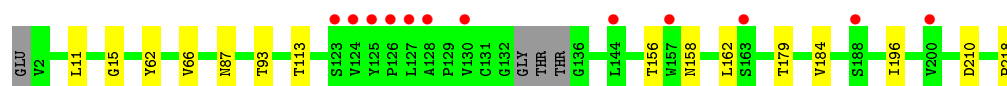
- Molecule 1: heavy chain of ACC1 Fab fragment

Chain O: 

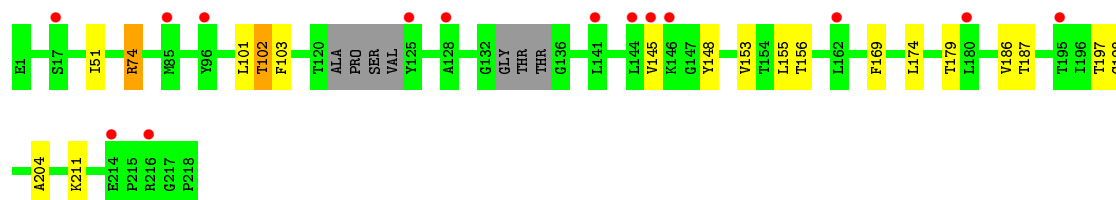
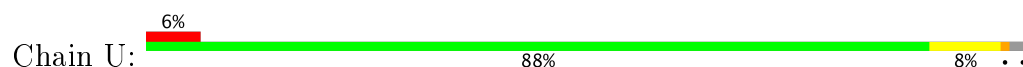


- Molecule 1: heavy chain of ACC1 Fab fragment

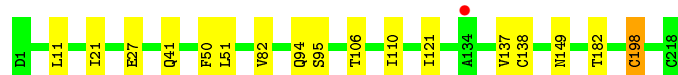
Chain R: 



- Molecule 1: heavy chain of ACC1 Fab fragment



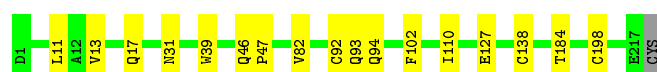
- Molecule 2: light chain of ACC1 Fab fragment



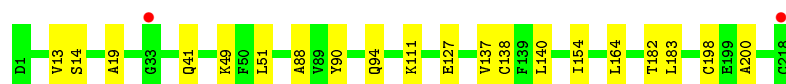
- Molecule 2: light chain of ACC1 Fab fragment



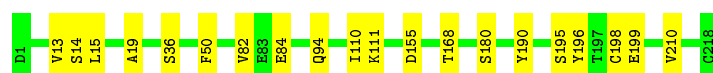
- Molecule 2: light chain of ACC1 Fab fragment



- Molecule 2: light chain of ACC1 Fab fragment



- Molecule 2: light chain of ACC1 Fab fragment




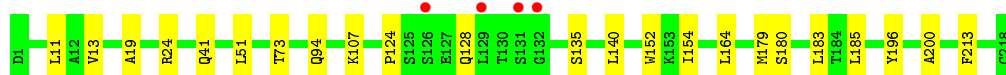
- Molecule 2: light chain of ACC1 Fab fragment

Chain P:  94% 5%

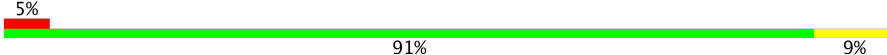


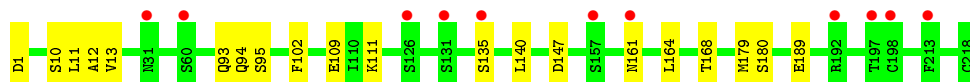
- Molecule 2: light chain of ACC1 Fab fragment

Chain S:  2% 89% 11%




- Molecule 2: light chain of ACC1 Fab fragment

Chain V:  5% 91% 9%



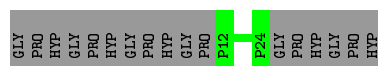
- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,

Chain X:  37% 10% 53%



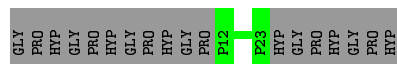
- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,

Chain E:  43% 57%



- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,

Chain H:  40% 60%



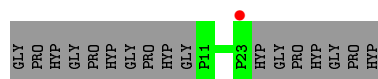
- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,

Chain K:  43% 57%





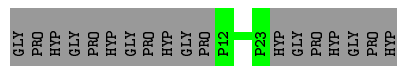
- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,



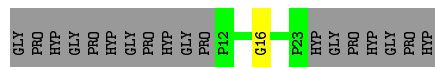
- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,



- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,



- Molecule 3: synthetic peptide containing the CII583-591 epitope of collagen type II, Collagen alpha-1(II) chain, synthetic peptide containing the CII583-591 epitope of collagen type II,



- Molecule 4: heavy chain of ACC1 Fab fragment



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.35Å 92.84Å 121.71Å 92.50° 106.53° 104.31°	Depositor
Resolution (Å)	50.01 – 2.95 48.85 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.01-2.95) 95.0 (48.85-2.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.202 , 0.261 0.204 , 0.262	Depositor DCC
$R_{free}$ test set	3639 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 19.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/1669	0.70	1/2277 (0.0%)
1	C	0.51	0/1654	0.73	0/2257
1	F	0.53	0/1669	0.71	1/2277 (0.0%)
1	I	0.53	0/1665	0.74	0/2272
1	O	0.50	0/1665	0.69	0/2272
1	R	0.56	1/1653 (0.1%)	0.71	1/2255 (0.0%)
1	U	0.48	0/1635	0.69	0/2227
2	B	0.52	0/1703	0.73	1/2310 (0.0%)
2	D	0.57	1/1697 (0.1%)	0.73	0/2302
2	G	0.56	2/1697 (0.1%)	0.72	0/2302
2	J	0.49	0/1703	0.70	0/2310
2	M	0.52	0/1703	0.72	0/2310
2	P	0.50	0/1680	0.71	0/2279
2	S	0.53	0/1703	0.71	0/2310
2	V	0.48	0/1703	0.69	0/2310
3	E	0.46	0/69	0.81	0/92
3	H	0.57	0/69	0.73	0/92
3	K	0.54	0/76	0.83	0/100
3	N	0.63	0/76	0.76	0/100
3	Q	0.65	0/69	0.79	0/92
3	T	0.54	0/69	0.73	0/92
3	W	0.51	0/69	0.87	0/92
3	X	0.59	0/80	0.65	0/106
4	L	0.52	0/1696	0.74	0/2316
All	All	0.52	4/27472 (0.0%)	0.71	4/37352 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	127	GLU	CG-CD	9.28	1.65	1.51
2	G	127	GLU	CD-OE2	8.58	1.35	1.25
1	R	218	PRO	C-O	5.73	1.34	1.23
2	G	127	GLU	CG-CD	5.67	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	GLU	OE1-CD-OE2	-7.65	114.12	123.30
1	A	69	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	F	69	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	R	210	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	152	PRO	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	1629	0	1589	11	1
1	C	1614	0	1577	8	0
1	F	1629	0	1590	10	0
1	I	1625	0	1586	7	0
1	O	1625	0	1587	6	0
1	R	1613	0	1573	7	0
1	U	1597	0	1555	13	0
2	B	1666	0	1597	5	0
2	D	1660	0	1593	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1660	0	1593	9	0
2	J	1666	0	1597	9	0
2	M	1666	0	1597	8	0
2	P	1643	0	1581	4	0
2	S	1666	0	1597	13	0
2	V	1666	0	1597	10	1
3	E	84	0	86	0	0
3	H	76	0	79	0	0
3	K	83	0	84	0	0
3	N	83	0	85	0	0
3	Q	76	0	79	2	0
3	T	76	0	79	0	0
3	W	76	0	78	1	0
3	X	87	0	87	3	0
4	L	1655	0	1618	8	0
All	All	26921	0	26084	127	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 2.

All (127) 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:U:174:LEU:HD13	2:V:164:LEU:HD11	1.48	0.96
1:F:12:VAL:HG11	1:F:88:LEU:HD13	1.73	0.69
2:S:13:VAL:HG21	2:S:19:ALA:HB2	1.77	0.67
2:V:11:LEU:HD12	2:V:13:VAL:HG23	1.76	0.67
2:G:46:GLN:HG3	2:G:47:PRO:HD2	1.77	0.66
4:L:113:THR:HG21	4:L:150:PRO:HB3	1.79	0.65
2:J:13:VAL:HG21	2:J:19:ALA:HB2	1.82	0.62
2:S:183:LEU:HD21	2:S:185:LEU:HD21	1.82	0.62
2:S:196:TYR:HB2	2:S:213:PHE:CE1	2.35	0.61
2:V:140:LEU:HD13	2:V:179:MET:CE	2.30	0.61
2:D:140:LEU:HD23	2:D:148:ILE:HD13	1.86	0.58
2:S:41:GLN:HB2	2:S:51:LEU:HD11	1.86	0.58
2:V:140:LEU:HD13	2:V:179:MET:HE2	1.85	0.57
2:S:140:LEU:HD13	2:S:179:MET:CE	2.35	0.57
2:S:128:GLN:HE22	2:S:135:SER:HB2	1.71	0.56
1:A:32:ALA:HA	3:X:14:GLY:HA2	1.87	0.55
2:S:11:LEU:CD1	2:S:13:VAL:HG23	2.37	0.55
2:V:11:LEU:CD1	2:V:13:VAL:HG23	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:140:LEU:HD13	2:S:179:MET:HE2	1.89	0.54
1:F:174:LEU:HD11	2:G:184:THR:HG21	1.89	0.54
1:R:162:LEU:HD13	1:R:184:VAL:HG21	1.88	0.54
2:J:140:LEU:HD21	2:J:200:ALA:HB2	1.90	0.54
2:S:154:ILE:HG23	2:S:196:TYR:CE1	2.44	0.53
1:A:208:LYS:O	1:F:209:VAL:HA	2.08	0.53
1:F:119:THR:CG2	1:F:205:SER:HB3	2.39	0.52
2:M:199:GLU:HG2	2:M:210:VAL:HG22	1.91	0.52
4:L:147:GLY:HA2	4:L:177:LEU:HD23	1.89	0.52
2:P:82:VAL:CG1	2:P:110:ILE:HD12	2.40	0.52
1:A:148:TYR:CE1	1:A:153:VAL:HG13	2.46	0.51
1:C:176:GLY:O	1:C:177:LEU:HD12	2.11	0.50
2:D:43:LYS:O	2:D:46:GLN:HB2	2.11	0.50
2:J:88:ALA:HB3	2:J:90:TYR:CE1	2.46	0.50
1:F:93:THR:HG23	1:F:113:THR:HA	1.94	0.50
1:O:122:PRO:HB3	1:O:148:TYR:HB3	1.92	0.50
1:U:148:TYR:OH	1:U:204:ALA:HB3	2.12	0.50
4:L:147:GLY:CA	4:L:177:LEU:HD23	2.42	0.49
1:C:3:LYS:O	1:C:4:LEU:HD23	2.12	0.49
2:G:11:LEU:HD12	2:G:13:VAL:HG23	1.93	0.49
4:L:162:LEU:O	4:L:162:LEU:HD12	2.13	0.49
2:J:41:GLN:HB2	2:J:51:LEU:HD11	1.95	0.49
2:M:190:TYR:HA	2:M:196:TYR:OH	2.13	0.49
2:B:82:VAL:CG1	2:B:110:ILE:HD12	2.43	0.49
2:M:155:ASP:HA	2:M:195:SER:HB3	1.94	0.48
1:U:51:ILE:HD13	1:U:74:ARG:HG2	1.95	0.48
2:D:140:LEU:HD23	2:D:148:ILE:CD1	2.43	0.48
2:D:199:GLU:HG2	2:D:210:VAL:HG12	1.94	0.48
3:X:13:GLY:O	3:X:16:GLY:N	2.47	0.48
2:S:140:LEU:HD21	2:S:200:ALA:HB2	1.95	0.47
1:U:197:THR:HA	1:U:211:LYS:O	2.15	0.47
4:L:169:PHE:CD1	2:M:168:THR:HG23	2.48	0.47
1:A:31:ASP:O	3:X:14:GLY:HA3	2.15	0.47
2:J:137:VAL:HG22	2:J:182:THR:HG23	1.96	0.47
1:O:127:LEU:HD11	1:O:144:LEU:HB2	1.96	0.47
1:A:121:ALA:HB3	1:F:206:SER:HB3	1.97	0.46
2:S:152:TRP:CB	2:S:183:LEU:HD13	2.45	0.46
1:R:62:TYR:HB3	1:R:66:VAL:HG23	1.96	0.46
1:U:148:TYR:CD2	1:U:153:VAL:HG22	2.50	0.46
1:O:151:GLU:HB2	1:O:152:PRO:HA	1.97	0.46
2:J:154:ILE:HD11	2:J:183:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:VAL:HG11	1:C:105:TYR:CG	2.51	0.46
1:O:36:TRP:CG	1:O:83:LEU:HD22	2.51	0.46
1:R:179:THR:HG21	2:S:164:LEU:HD13	1.98	0.46
2:B:21:ILE:HG23	2:B:106:THR:HG21	1.98	0.46
2:V:12:ALA:HA	2:V:109:GLU:O	2.16	0.46
2:B:137:VAL:HG22	2:B:182:THR:HG23	1.98	0.45
2:G:11:LEU:CD1	2:G:13:VAL:HG23	2.45	0.45
2:M:82:VAL:CG1	2:M:110:ILE:HD12	2.46	0.45
1:C:174:LEU:HD12	1:C:174:LEU:O	2.17	0.45
1:F:12:VAL:HG11	1:F:88:LEU:CD1	2.44	0.45
1:I:174:LEU:HD13	2:J:164:LEU:HD11	1.98	0.45
1:A:157:TRP:CZ3	1:A:198:CYS:HB2	2.52	0.45
1:U:102:THR:HG22	1:U:103:PHE:N	2.33	0.44
1:F:11:LEU:HD12	1:F:113:THR:O	2.18	0.44
2:D:112:ARG:HG2	2:D:113:ALA:N	2.32	0.44
1:C:11:LEU:HB2	1:C:150:PRO:HG3	1.99	0.44
2:D:197:THR:HG23	2:D:212:SER:HB2	2.00	0.44
2:D:82:VAL:CG1	2:D:110:ILE:HD12	2.48	0.44
2:G:39:TRP:CZ3	2:G:92:CYS:HB3	2.52	0.44
2:J:14:SER:HA	2:J:111:LYS:HB3	1.99	0.44
1:I:122:PRO:HB3	1:I:148:TYR:HB3	2.00	0.43
1:R:162:LEU:HD12	1:R:162:LEU:O	2.18	0.43
1:A:58:HIS:HD2	1:A:74:ARG:HD3	1.82	0.43
2:J:13:VAL:HG21	2:J:19:ALA:CB	2.47	0.43
1:R:93:THR:HG23	1:R:113:THR:HA	1.99	0.43
2:G:93:GLN:HG3	2:G:102:PHE:CE2	2.53	0.43
2:B:121:ILE:HD13	2:B:198:CYS:HB3	2.01	0.43
2:P:167:TRP:CD1	2:P:179:MET:HB3	2.54	0.43
1:A:121:ALA:HB1	1:A:122:PRO:HD2	2.00	0.42
1:I:12:VAL:HG11	1:I:88:LEU:HD12	2.01	0.42
4:L:151:GLU:HB2	4:L:152:PRO:HA	2.00	0.42
2:M:14:SER:HA	2:M:111:LYS:HB2	2.01	0.42
2:V:93:GLN:HG3	2:V:102:PHE:CE2	2.54	0.42
1:F:2:VAL:HA	1:F:26:GLY:HA3	2.01	0.42
1:C:151:GLU:HG2	1:C:152:PRO:HA	2.02	0.42
2:V:140:LEU:HD13	2:V:179:MET:HE1	2.01	0.42
1:O:31:ASP:O	3:Q:14:GLY:HA3	2.18	0.42
2:S:24:ARG:HA	2:S:73:THR:O	2.19	0.42
1:U:169:PHE:CE2	2:V:180:SER:HB3	2.54	0.42
2:G:82:VAL:CG1	2:G:110:ILE:HD12	2.49	0.42
2:M:15:LEU:HD21	2:M:84:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:140:LEU:HD12	2:P:140:LEU:N	2.35	0.42
2:B:41:GLN:HB2	2:B:51:LEU:HD11	2.00	0.42
2:G:13:VAL:CG1	2:G:17:GLN:HB2	2.50	0.42
1:A:180:LEU:HD12	1:A:181:SER:N	2.35	0.41
1:I:141:LEU:HD11	1:I:191:TRP:CD1	2.55	0.41
1:U:197:THR:HG23	1:U:211:LYS:O	2.19	0.41
1:A:85:MET:CE	1:A:112:LEU:HD22	2.50	0.41
1:C:180:LEU:C	1:C:180:LEU:HD12	2.41	0.41
2:G:46:GLN:CG	2:G:47:PRO:HD2	2.47	0.41
1:O:176:GLY:O	1:O:177:LEU:HD12	2.20	0.41
3:Q:12:HYP:OD1	3:Q:17:LEU:HD23	2.19	0.41
1:I:39:GLN:HB2	1:I:45:LEU:HD23	2.02	0.41
1:C:106:TRP:CE3	2:D:48:PRO:HD2	2.55	0.41
2:M:13:VAL:HG21	2:M:19:ALA:HB2	2.02	0.41
1:U:145:VAL:O	1:U:179:THR:HA	2.21	0.41
1:A:101:LEU:HD22	1:A:105:TYR:CE2	2.55	0.41
4:L:162:LEU:CD1	4:L:184:VAL:HG21	2.51	0.41
1:I:35:ASP:HB2	1:I:99:THR:OG1	2.20	0.41
1:U:169:PHE:CD1	2:V:168:THR:HG23	2.56	0.41
1:R:15:GLY:HA2	1:R:87:ASN:HA	2.03	0.41
1:U:101:LEU:HD23	3:W:16:GLY:HA2	2.03	0.41
4:L:218:PRO:O	2:P:18:ARG:NH2	2.50	0.40
1:R:158:ASN:HD21	1:R:196:ILE:HA	1.86	0.40
1:I:64:GLU:OE1	1:I:64:GLU:N	2.53	0.40
1:U:186:VAL:HG12	1:U:187:THR:H	1.87	0.40
1:F:20:LEU:HD22	1:F:110:THR:HG21	2.03	0.40
1:U:155:LEU:HD23	1:U:156:THR:N	2.37	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:A:60:THR:OG1	2:V:10:SER:OG[1_665]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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



of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/218 (97%)	202 (95%)	9 (4%)	1 (0%)	32	71
1	C	209/218 (96%)	205 (98%)	3 (1%)	1 (0%)	32	71
1	F	212/218 (97%)	205 (97%)	7 (3%)	0	100	100
1	I	211/218 (97%)	202 (96%)	8 (4%)	1 (0%)	32	71
1	O	211/218 (97%)	203 (96%)	8 (4%)	0	100	100
1	R	210/218 (96%)	203 (97%)	7 (3%)	0	100	100
1	U	205/218 (94%)	194 (95%)	10 (5%)	1 (0%)	32	71
2	B	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
2	D	215/218 (99%)	209 (97%)	6 (3%)	0	100	100
2	G	215/218 (99%)	206 (96%)	9 (4%)	0	100	100
2	J	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
2	M	216/218 (99%)	212 (98%)	4 (2%)	0	100	100
2	P	213/218 (98%)	206 (97%)	7 (3%)	0	100	100
2	S	216/218 (99%)	205 (95%)	10 (5%)	1 (0%)	32	71
2	V	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	E	11/30 (37%)	10 (91%)	1 (9%)	0	100	100
3	H	10/30 (33%)	9 (90%)	1 (10%)	0	100	100
3	K	10/30 (33%)	10 (100%)	0	0	100	100
3	N	10/30 (33%)	10 (100%)	0	0	100	100
3	Q	10/30 (33%)	10 (100%)	0	0	100	100
3	T	10/30 (33%)	10 (100%)	0	0	100	100
3	W	10/30 (33%)	10 (100%)	0	0	100	100
3	X	11/30 (37%)	10 (91%)	1 (9%)	0	100	100
4	L	218/220 (99%)	212 (97%)	5 (2%)	1 (0%)	32	71
All	All	3493/3730 (94%)	3366 (96%)	121 (4%)	6 (0%)	51	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	102	THR

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Mol	Chain	Res	Type
1	A	102	THR
1	I	102	THR
1	U	102	THR
2	S	124	PRO
1	C	152	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/185 (100%)	181 (98%)	3 (2%)	68	89
1	C	183/185 (99%)	179 (98%)	4 (2%)	57	85
1	F	184/185 (100%)	181 (98%)	3 (2%)	68	89
1	I	184/185 (100%)	181 (98%)	3 (2%)	68	89
1	O	184/185 (100%)	182 (99%)	2 (1%)	78	92
1	R	182/185 (98%)	180 (99%)	2 (1%)	78	92
1	U	180/185 (97%)	178 (99%)	2 (1%)	78	92
2	B	188/188 (100%)	181 (96%)	7 (4%)	39	74
2	D	187/188 (100%)	184 (98%)	3 (2%)	68	89
2	G	187/188 (100%)	183 (98%)	4 (2%)	59	85
2	J	188/188 (100%)	183 (97%)	5 (3%)	50	81
2	M	188/188 (100%)	183 (97%)	5 (3%)	50	81
2	P	185/188 (98%)	181 (98%)	4 (2%)	57	85
2	S	188/188 (100%)	185 (98%)	3 (2%)	68	89
2	V	188/188 (100%)	180 (96%)	8 (4%)	33	70
3	E	6/12 (50%)	6 (100%)	0	100	100
3	H	6/12 (50%)	6 (100%)	0	100	100
3	K	7/12 (58%)	7 (100%)	0	100	100
3	N	7/12 (58%)	7 (100%)	0	100	100
3	Q	6/12 (50%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	6/12 (50%)	6 (100%)	0	100	100
3	W	6/12 (50%)	6 (100%)	0	100	100
3	X	7/12 (58%)	7 (100%)	0	100	100
4	L	187/187 (100%)	185 (99%)	2 (1%)	78	92
All	All	3018/3082 (98%)	2958 (98%)	60 (2%)	60	86

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	180	LEU
1	A	198	CYS
2	B	11	LEU
2	B	50	PHE
2	B	94	GLN
2	B	95	SER
2	B	138	CYS
2	B	149	ASN
2	B	198	CYS
1	C	1	GLU
1	C	22	CYS
1	C	25	SER
1	C	138	SER
2	D	94	GLN
2	D	138	CYS
2	D	198	CYS
1	F	17	SER
1	F	31	ASP
1	F	193	SER
2	G	31	ASN
2	G	94	GLN
2	G	138	CYS
2	G	198	CYS
1	I	18	MET
1	I	22	CYS
1	I	199	ASN
2	J	49	LYS
2	J	94	GLN
2	J	127	GLU
2	J	138	CYS
2	J	198	CYS

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Mol	Chain	Res	Type
4	L	174	LEU
4	L	197	THR
2	M	36	SER
2	M	50	PHE
2	M	94	GLN
2	M	180	SER
2	M	198	CYS
1	O	18	MET
1	O	61	ASN
2	P	14	SER
2	P	94	GLN
2	P	138	CYS
2	P	180	SER
1	R	11	LEU
1	R	156	THR
2	S	94	GLN
2	S	107	LYS
2	S	180	SER
1	U	74	ARG
1	U	198	CYS
2	V	1	ASP
2	V	94	GLN
2	V	95	SER
2	V	111	LYS
2	V	135	SER
2	V	147	ASP
2	V	161	ASN
2	V	189	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
2	B	142	ASN
1	C	56	ASN
2	D	149	ASN
2	G	31	ASN
4	L	167	HIS
2	S	128	GLN
2	V	161	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	E	12	3	7,8,9	0.70	0	5,10,12	2.00	3 (60%)
3	HYP	E	24	3	7,8,9	0.42	0	5,10,12	1.75	3 (60%)
3	HYP	H	12	3	7,8,9	0.68	0	5,10,12	1.91	3 (60%)
3	HYP	K	12	3	7,8,9	1.14	1 (14%)	5,10,12	1.91	2 (40%)
3	HYP	N	12	3	7,8,9	0.65	0	5,10,12	1.97	3 (60%)
3	HYP	Q	12	3	7,8,9	0.63	0	5,10,12	2.03	3 (60%)
3	HYP	T	12	3	7,8,9	0.62	0	5,10,12	2.04	3 (60%)
3	HYP	W	12	3	7,8,9	0.74	0	5,10,12	1.83	2 (40%)
3	HYP	X	12	3	7,8,9	0.99	0	5,10,12	1.50	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	E	12	3	-	0/0/11/13	0/1/1/1
3	HYP	E	24	3	-	0/0/11/13	0/1/1/1
3	HYP	H	12	3	-	0/0/11/13	0/1/1/1
3	HYP	K	12	3	-	0/0/11/13	0/1/1/1
3	HYP	N	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	T	12	3	-	0/0/11/13	0/1/1/1
3	HYP	W	12	3	-	0/0/11/13	0/1/1/1
3	HYP	X	12	3	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	12	HYP	CA-C	2.63	1.53	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	12	HYP	O-C-CA	-2.50	119.31	125.15
3	K	12	HYP	O-C-CA	-2.45	119.45	125.15
3	N	12	HYP	O-C-CA	-2.39	119.57	125.15
3	H	12	HYP	O-C-CA	-2.36	119.66	125.15
3	X	12	HYP	O-C-CA	-2.34	119.68	125.15
3	E	24	HYP	O-C-CA	-2.32	119.75	125.15
3	T	12	HYP	O-C-CA	-2.28	119.84	125.15
3	Q	12	HYP	O-C-CA	-2.27	119.87	125.15
3	E	12	HYP	O-C-CA	-2.16	120.11	125.15
3	E	24	HYP	CG-CB-CA	2.05	106.63	103.93
3	H	12	HYP	CG-CB-CA	2.20	106.83	103.93
3	X	12	HYP	CG-CB-CA	2.23	106.87	103.93
3	N	12	HYP	CG-CB-CA	2.25	106.89	103.93
3	E	24	HYP	CB-CG-CD	2.33	106.41	103.33
3	N	12	HYP	CB-CG-CD	2.47	106.59	103.33
3	H	12	HYP	CB-CG-CD	2.68	106.88	103.33
3	E	12	HYP	CB-CG-CD	2.71	106.91	103.33
3	T	12	HYP	CB-CG-CD	2.76	106.98	103.33
3	Q	12	HYP	CG-CB-CA	2.77	107.59	103.93
3	Q	12	HYP	CB-CG-CD	2.78	107.00	103.33
3	E	12	HYP	CG-CB-CA	2.81	107.64	103.93
3	T	12	HYP	CG-CB-CA	2.81	107.64	103.93
3	W	12	HYP	CB-CG-CD	3.16	107.51	103.33
3	K	12	HYP	CB-CG-CD	3.41	107.84	103.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	12	HYP	1	0

## 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 [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, 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	216/218 (99%)	-0.37	0 100 100	39, 70, 107, 141	0
1	C	213/218 (97%)	-0.17	2 (0%) 84 69	39, 80, 117, 140	0
1	F	216/218 (99%)	-0.39	0 100 100	48, 71, 106, 121	0
1	I	215/218 (98%)	-0.49	0 100 100	46, 64, 87, 106	0
1	O	215/218 (98%)	-0.28	0 100 100	46, 79, 110, 132	0
1	R	214/218 (98%)	0.33	12 (5%) 25 14	50, 103, 136, 162	0
1	U	211/218 (96%)	0.37	14 (6%) 19 11	65, 116, 166, 190	0
2	B	218/218 (100%)	-0.28	1 (0%) 90 79	33, 72, 124, 144	0
2	D	217/218 (99%)	-0.37	0 100 100	35, 61, 108, 123	0
2	G	217/218 (99%)	-0.38	0 100 100	44, 66, 106, 125	0
2	J	218/218 (100%)	-0.34	2 (0%) 84 69	41, 66, 98, 117	0
2	M	218/218 (100%)	-0.34	0 100 100	44, 65, 107, 125	0
2	P	215/218 (98%)	-0.35	0 100 100	46, 74, 102, 114	0
2	S	218/218 (100%)	-0.19	4 (1%) 69 50	38, 75, 130, 145	0
2	V	218/218 (100%)	0.05	11 (5%) 30 18	45, 87, 153, 174	0
3	E	11/30 (36%)	-0.32	0 100 100	46, 60, 100, 112	0
3	H	11/30 (36%)	-0.42	0 100 100	66, 73, 101, 113	0
3	K	12/30 (40%)	-0.29	0 100 100	67, 71, 108, 115	0
3	N	12/30 (40%)	0.40	1 (8%) 12 6	52, 65, 104, 106	0
3	Q	11/30 (36%)	-0.26	0 100 100	56, 64, 89, 94	0
3	T	11/30 (36%)	-0.19	0 100 100	60, 73, 106, 125	0
3	W	11/30 (36%)	-0.05	0 100 100	74, 84, 116, 127	0
3	X	13/30 (43%)	-0.11	0 100 100	59, 71, 94, 102	0
4	L	220/220 (100%)	-0.38	1 (0%) 90 79	45, 69, 98, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3551/3730 (95%)	-0.22	48 (1%) 75 58	33, 73, 128, 190	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	23	PRO	5.1
1	R	200	VAL	4.9
1	U	17	SER	4.2
1	R	144	LEU	4.0
1	U	125	TYR	4.0
1	R	188	SER	3.9
1	R	163	SER	3.7
1	U	145	VAL	3.7
1	U	128	ALA	3.5
1	R	123	SER	3.5
2	V	31	ASN	3.3
1	U	141	LEU	3.2
2	J	33	GLY	3.2
1	U	180	LEU	3.2
2	V	126	SER	3.0
2	V	157	SER	3.0
2	S	126	SER	3.0
1	R	125	TYR	3.0
1	R	127	LEU	2.9
1	U	195	THR	2.9
2	J	218	CYS	2.8
1	R	128	ALA	2.8
1	R	126	PRO	2.8
1	U	146	LYS	2.6
1	U	96	TYR	2.5
1	R	124	VAL	2.5
2	V	131	SER	2.5
1	R	130	VAL	2.4
2	S	132	GLY	2.4
1	U	214	GLU	2.4
1	U	85	MET	2.4
2	B	134	ALA	2.3
2	V	197	THR	2.3
2	V	213	PHE	2.3
1	U	144	LEU	2.3
2	V	135	SER	2.2
1	C	139	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	216	ARG	2.2
1	R	157	TRP	2.2
4	L	175	SER	2.2
2	V	198	CYS	2.1
2	S	129	LEU	2.1
1	C	145	VAL	2.1
2	S	131	SER	2.0
2	V	60	SER	2.0
2	V	192	ARG	2.0
1	U	162	LEU	2.0
2	V	161	ASN	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. 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	E	12	8/9	0.91	0.21	-	88,96,101,109	0
3	HYP	X	12	8/9	0.89	0.16	-	72,76,82,84	0
3	HYP	N	12	8/9	0.90	0.23	-	89,95,99,99	0
3	HYP	Q	12	8/9	0.72	0.46	-	102,107,111,111	0
3	HYP	T	12	8/9	0.73	0.55	-	97,105,114,115	0
3	HYP	W	12	8/9	0.86	0.40	-	104,107,111,111	0
3	HYP	H	12	8/9	0.88	0.27	-	89,96,100,102	0
3	HYP	K	12	8/9	0.86	0.17	-	92,96,102,102	0
3	HYP	E	24	8/9	0.86	0.19	-	95,100,104,107	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.