



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:40 am BST

PDB ID : 6JW4  
Title : Degenerate RVD RG forms a distinct loop conformation  
Authors : Liu, L.; Yi, C.  
Deposited on : 2019-04-18  
Resolution : 3.09 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

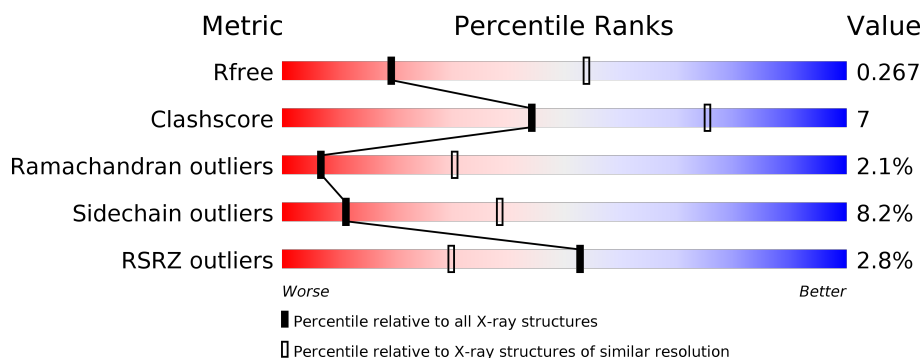
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 Å.

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









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	499	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	499	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	499	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
1	H	499	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>..</div> </div> </div>
2	C	17	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>35%</div> </div> </div>
2	F	17	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>41%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	17	 76% 24%
2	K	17	 6% 65% 29% 6%
3	D	17	 6% 82% 18%
3	G	17	 6% 71% 29%
3	J	17	 82% 18%
3	L	17	 6% 76% 24%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17036 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 TAL effector.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3567	2229	666	660	12			
1	B	492	Total	C	N	O	S	0	0	0
			3567	2229	666	660	12			
1	E	492	Total	C	N	O	S	0	0	0
			3567	2229	666	660	12			
1	H	492	Total	C	N	O	S	0	0	0
			3567	2229	666	660	12			

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*(5HC)P\*GP\*CP\*GP\*TP\*CP\*TP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	C	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	F	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			
2	K	17	Total	C	N	O	P	0	0	0
			337	163	50	108	16			

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*CP\*GP\*CP\*GP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			
3	D	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			
3	G	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			

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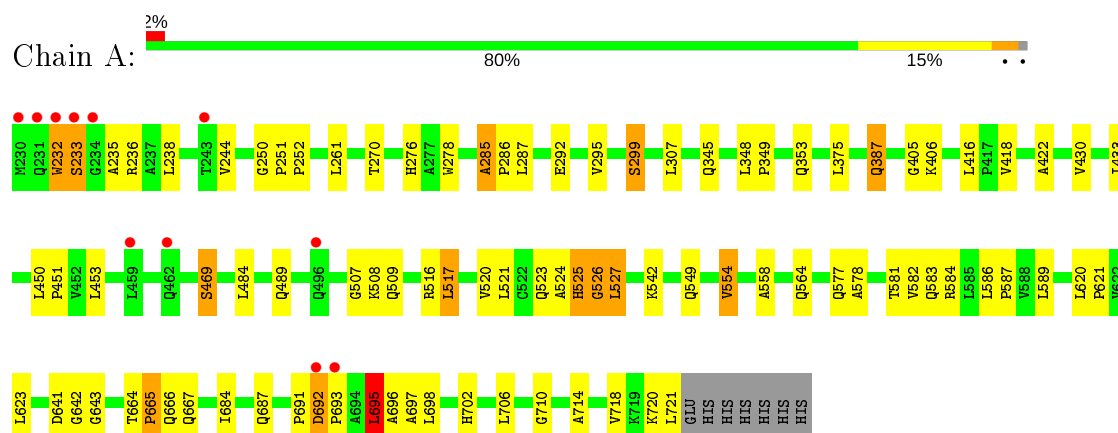
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			

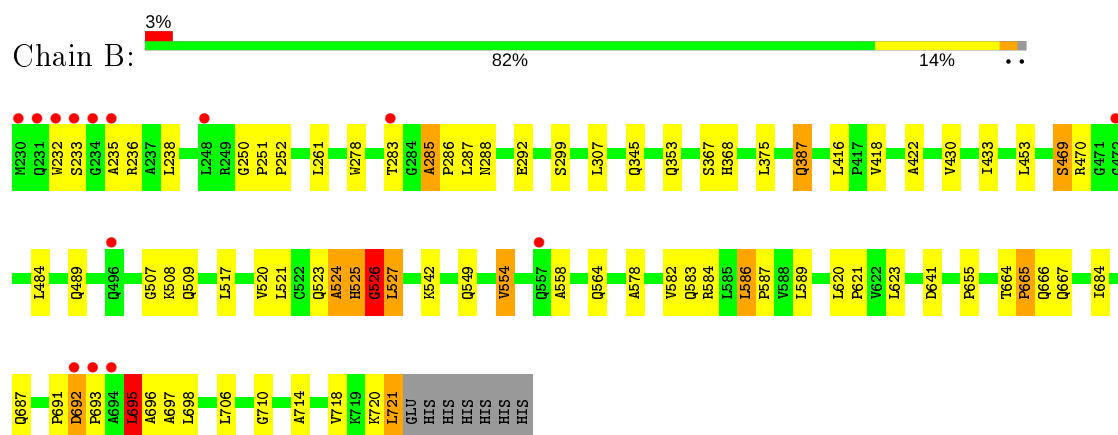
### 3 Residue-property plots [i](#)

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.

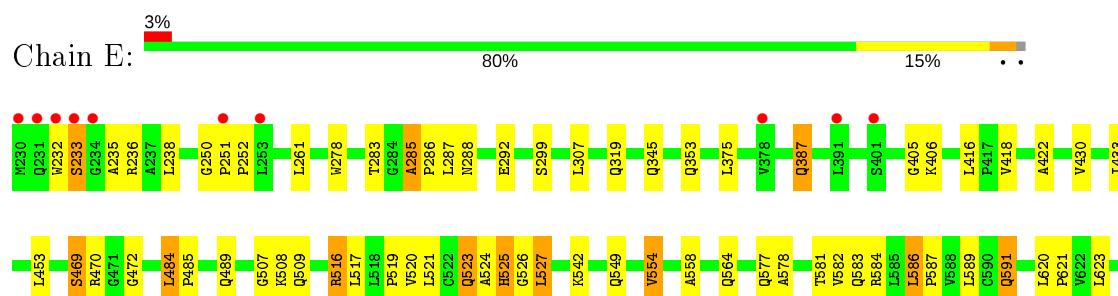
#### • Molecule 1: TAL effector

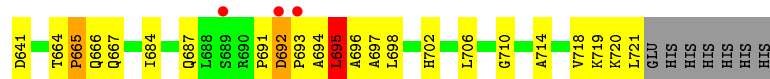


#### • Molecule 1: TAL effector

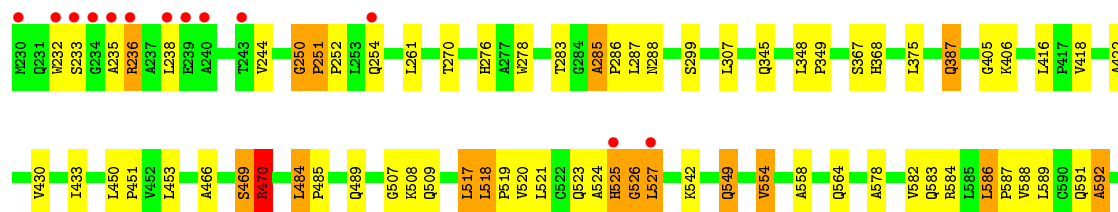
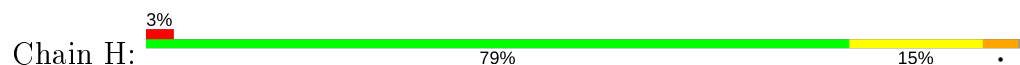


#### • Molecule 1: TAL effector





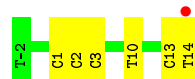
• Molecule 1: TAL effector



• Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*(5HC)P\*GP\*CP\*GP\*TP\*CP\*TP\*CP\*T)-3')



• Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*(5HC)P\*GP\*CP\*GP\*TP\*CP\*TP\*CP\*T)-3')

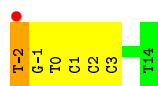


• Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*(5HC)P\*GP\*CP\*GP\*TP\*CP\*TP\*CP\*T)-3')

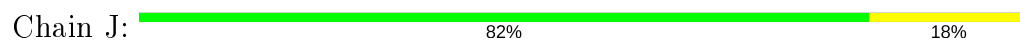


• Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*(5HC)P\*GP\*CP\*GP\*TP\*CP\*TP\*CP\*T)-3')

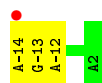
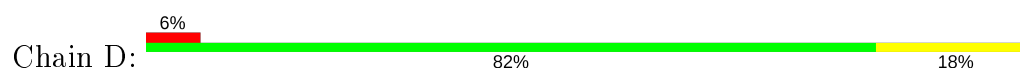




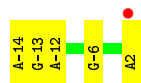
- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*CP\*GP\*CP\*GP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3')



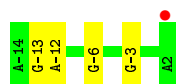
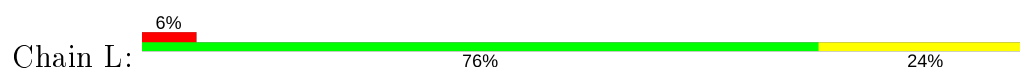
- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*CP\*GP\*CP\*GP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3')



- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*CP\*GP\*CP\*GP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3')



- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*CP\*GP\*CP\*GP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.05Å 93.97Å 167.69Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	163.51 – 3.09 39.56 – 3.09	Depositor EDS
% Data completeness (in resolution range)	86.9 (163.51-3.09) 87.0 (39.56-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.243 , 0.275 0.240 , 0.267	Depositor DCC
$R_{free}$ test set	2320 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4489e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 5HC

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	0/3618	0.70	4/4941 (0.1%)
1	B	0.50	1/3618 (0.0%)	0.70	3/4941 (0.1%)
1	E	0.47	0/3618	0.69	3/4941 (0.1%)
1	H	0.50	0/3618	0.70	3/4941 (0.1%)
2	C	0.75	1/349 (0.3%)	0.88	0/533
2	F	0.68	1/349 (0.3%)	0.85	0/533
2	I	0.77	0/349	0.88	0/533
2	K	0.82	1/349 (0.3%)	0.97	1/533 (0.2%)
3	D	0.55	0/402	0.77	0/620
3	G	0.51	0/402	0.78	1/620 (0.2%)
3	J	0.57	0/402	0.77	0/620
3	L	0.60	0/402	0.77	1/620 (0.2%)
All	All	0.53	4/17476 (0.0%)	0.72	16/24376 (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	A	0	3
1	B	0	3
1	E	0	3
1	H	0	3
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	GLY	N-CA	-5.74	1.37	1.46
2	C	10	DT	O3'-P	-5.24	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	10	DT	O3'-P	-5.23	1.54	1.61
2	K	-2	DT	C1'-N1	5.04	1.55	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	523	GLN	N-CA-C	-7.09	91.84	111.00
1	A	523	GLN	N-CA-C	-7.03	92.01	111.00
1	A	232	TRP	CA-CB-CG	6.27	125.61	113.70
1	B	721	LEU	CA-CB-CG	6.08	129.29	115.30
1	E	516	ARG	NE-CZ-NH2	6.01	123.31	120.30
2	K	-2	DT	N1-C1'-C2'	5.82	123.65	112.60
1	H	592	ALA	N-CA-CB	5.54	117.85	110.10
1	H	470	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	E	695	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	517	LEU	CB-CG-CD1	5.41	120.19	111.00
1	E	472	GLY	N-CA-C	-5.40	99.60	113.10
1	H	518	LEU	CB-CG-CD1	5.37	120.13	111.00
1	A	695	LEU	CA-CB-CG	5.27	127.43	115.30
3	L	-6	DG	C1'-O4'-C4'	-5.26	104.84	110.10
3	G	-6	DG	C1'-O4'-C4'	-5.06	105.04	110.10
1	B	695	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	GLY	Peptide
1	A	251	PRO	Peptide
1	A	526	GLY	Peptide
1	B	250	GLY	Peptide
1	B	251	PRO	Peptide
1	B	526	GLY	Peptide
1	E	250	GLY	Peptide
1	E	251	PRO	Peptide
1	E	470	ARG	Peptide
1	H	250	GLY	Peptide
1	H	251	PRO	Peptide
1	H	526	GLY	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	3567	0	3720	47	26
1	B	3567	0	3720	36	0
1	E	3567	0	3720	42	0
1	H	3567	0	3720	62	7
2	C	337	0	195	9	0
2	F	337	0	195	10	0
2	I	337	0	195	4	0
2	K	337	0	195	11	17
3	D	355	0	189	5	0
3	G	355	0	189	3	0
3	J	355	0	189	1	1
3	L	355	0	189	1	9
All	All	17036	0	16416	220	33

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 7.

All (220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:-1:DG:C2'	2:K:0:DT:H5'	1.67	1.23
2:K:-1:DG:H2'	2:K:0:DT:H5'	1.29	1.06
2:K:-1:DG:C2'	2:K:0:DT:C5'	2.50	0.89
2:C:14:DT:O4	3:D:-14:DA:N6	2.09	0.85
1:B:521:LEU:O	1:B:526:GLY:HA3	1.80	0.82
1:A:285:ALA:HB1	1:A:286:PRO:HD2	1.61	0.80
1:H:285:ALA:HB1	1:H:286:PRO:HD2	1.62	0.80
1:B:285:ALA:HB1	1:B:286:PRO:HD2	1.62	0.79
1:E:285:ALA:HB1	1:E:286:PRO:HD2	1.61	0.79
1:H:524:ALA:O	1:H:526:GLY:N	2.17	0.78
1:H:718:VAL:HG12	1:H:718:VAL:O	1.88	0.74
2:K:-1:DG:C3'	2:K:0:DT:H5'	2.18	0.73
3:G:-14:DA:H4'	3:G:-13:DG:OP1	1.88	0.72
1:H:524:ALA:C	1:H:526:GLY:H	1.92	0.70
1:E:524:ALA:O	1:E:526:GLY:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:ALA:HB1	1:H:286:PRO:CD	2.24	0.68
1:A:521:LEU:O	1:A:526:GLY:HA3	1.95	0.67
1:A:285:ALA:HB1	1:A:286:PRO:CD	2.24	0.67
1:E:587:PRO:O	1:E:591:GLN:HG2	1.95	0.67
1:B:524:ALA:O	1:B:526:GLY:N	2.27	0.67
2:K:-1:DG:H2''	2:K:0:DT:C5'	2.25	0.66
1:E:285:ALA:HB1	1:E:286:PRO:CD	2.24	0.66
1:B:285:ALA:HB1	1:B:286:PRO:CD	2.25	0.65
2:K:-1:DG:H2''	2:K:0:DT:H5'	1.73	0.65
1:A:524:ALA:O	1:A:526:GLY:N	2.31	0.64
1:E:521:LEU:O	1:E:526:GLY:HA3	1.98	0.63
1:A:696:ALA:O	1:A:698:LEU:N	2.32	0.63
1:H:519:PRO:O	1:H:523:GLN:HB2	1.99	0.62
1:H:521:LEU:O	1:H:526:GLY:HA3	1.99	0.62
1:B:696:ALA:O	1:B:698:LEU:N	2.32	0.62
1:E:696:ALA:O	1:E:698:LEU:N	2.32	0.62
2:F:13:DC:C5	2:F:14:DT:C2	2.87	0.62
1:H:692:ASP:O	1:H:695:LEU:HD13	2.00	0.61
1:H:696:ALA:O	1:H:698:LEU:N	2.32	0.61
1:B:517:LEU:HD23	1:B:520:VAL:CG1	2.31	0.60
1:H:517:LEU:HD22	1:H:521:LEU:HD11	1.83	0.60
1:H:588:VAL:O	1:H:591:GLN:O	2.20	0.60
1:B:554:VAL:O	1:B:558:ALA:HB3	2.03	0.59
1:H:720:LYS:O	1:H:721:LEU:HG	2.03	0.59
1:A:554:VAL:O	1:A:558:ALA:HB3	2.02	0.59
2:K:-1:DG:C3'	2:K:0:DT:C5'	2.81	0.58
1:H:519:PRO:O	1:H:523:GLN:N	2.35	0.58
1:B:235:ALA:C	1:B:236:ARG:HG3	2.23	0.58
1:E:554:VAL:O	1:E:558:ALA:HB3	2.04	0.58
1:H:517:LEU:HA	1:H:520:VAL:HG12	1.86	0.58
1:E:319:GLN:HB3	1:H:422:ALA:HB2	1.85	0.58
1:H:517:LEU:HD21	1:H:549:GLN:HB2	1.86	0.57
1:H:554:VAL:O	1:H:558:ALA:HB3	2.04	0.57
1:A:517:LEU:HA	1:A:520:VAL:HG12	1.87	0.57
1:E:720:LYS:O	1:E:721:LEU:HG	2.04	0.56
1:H:466:ALA:O	1:H:469:SER:O	2.23	0.56
1:H:693:PRO:O	1:H:695:LEU:HD22	2.06	0.56
1:E:517:LEU:HA	1:E:520:VAL:HG12	1.87	0.56
2:C:13:DC:C4	2:C:14:DT:O4	2.58	0.56
2:F:13:DC:C5	2:F:14:DT:N3	2.74	0.56
1:A:710:GLY:HA3	1:A:714:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:GLN:HB3	1:H:422:ALA:CB	2.35	0.55
1:H:469:SER:O	1:H:470:ARG:HG2	2.05	0.55
1:H:591:GLN:N	1:H:591:GLN:OE1	2.39	0.55
1:H:524:ALA:C	1:H:526:GLY:N	2.60	0.55
1:A:720:LYS:O	1:A:721:LEU:HG	2.07	0.54
1:E:525:HIS:O	1:E:526:GLY:C	2.45	0.54
2:C:13:DC:C5	2:C:14:DT:C4	2.95	0.54
1:H:517:LEU:HD23	1:H:521:LEU:HG	1.90	0.54
1:H:710:GLY:HA3	1:H:714:ALA:HB2	1.89	0.53
1:H:691:PRO:O	1:H:695:LEU:HD12	2.09	0.53
1:E:666:GLN:H	1:E:666:GLN:CD	2.12	0.52
1:H:578:ALA:O	1:H:582:VAL:HG23	2.09	0.52
1:B:517:LEU:HA	1:B:520:VAL:HG12	1.91	0.52
3:D:-14:DA:C8	3:D:-13:DG:C5	2.98	0.52
1:H:587:PRO:O	1:H:591:GLN:OE1	2.28	0.52
1:A:516:ARG:NH2	1:A:517:LEU:HD13	2.26	0.51
1:H:433:ILE:HA	1:H:469:SER:HB3	1.92	0.51
1:E:710:GLY:HA3	1:E:714:ALA:HB2	1.93	0.51
2:C:14:DT:OP1	2:C:14:DT:H4'	2.10	0.51
1:A:666:GLN:CD	1:A:666:GLN:H	2.14	0.51
1:B:433:ILE:HA	1:B:469:SER:HB3	1.93	0.51
1:H:718:VAL:CG1	1:H:718:VAL:O	2.58	0.51
1:A:721:LEU:CD2	2:F:14:DT:C5	2.95	0.50
1:B:526:GLY:C	1:B:527:LEU:HD13	2.32	0.50
1:A:702:HIS:CE1	1:E:702:HIS:CE1	3.00	0.50
1:A:433:ILE:HA	1:A:469:SER:HB3	1.94	0.50
1:B:666:GLN:CD	1:B:666:GLN:H	2.16	0.49
2:F:-1:DG:C2	3:G:2:DA:C2	3.01	0.49
1:H:666:GLN:CD	1:H:666:GLN:H	2.16	0.49
1:B:710:GLY:HA3	1:B:714:ALA:HB2	1.93	0.49
1:H:698:LEU:HD12	1:H:698:LEU:N	2.27	0.49
2:C:14:DT:C4	3:D:-14:DA:N6	2.79	0.48
1:B:718:VAL:C	1:B:720:LYS:H	2.15	0.48
1:H:507:GLY:O	1:H:508:LYS:C	2.51	0.48
2:C:14:DT:OP1	2:C:14:DT:C4'	2.61	0.48
1:A:525:HIS:O	1:A:526:GLY:C	2.52	0.48
3:D:-14:DA:H8	3:D:-13:DG:C4	2.31	0.48
1:E:433:ILE:HA	1:E:469:SER:HB3	1.95	0.48
1:B:664:THR:O	1:B:665:PRO:C	2.51	0.48
1:H:693:PRO:O	1:H:695:LEU:HD13	2.13	0.48
1:E:519:PRO:O	1:E:523:GLN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:GLY:O	1:B:508:LYS:C	2.52	0.47
2:C:13:DC:C4	2:C:14:DT:C4	3.03	0.47
1:E:718:VAL:C	1:E:720:LYS:H	2.17	0.47
1:E:578:ALA:O	1:E:582:VAL:HG23	2.15	0.47
1:A:235:ALA:O	1:A:236:ARG:HB2	2.14	0.47
2:C:1:DC:H2''	2:C:2:DC:O5'	2.15	0.47
1:E:416:LEU:HD23	1:E:430:VAL:HG11	1.97	0.47
1:E:664:THR:O	1:E:665:PRO:C	2.53	0.47
1:H:692:ASP:O	1:H:695:LEU:CD1	2.62	0.47
1:A:416:LEU:HD23	1:A:430:VAL:HG11	1.97	0.47
1:B:517:LEU:HD23	1:B:517:LEU:HA	1.75	0.47
2:I:14:DT:C4'	2:I:14:DT:OP1	2.63	0.47
1:B:578:ALA:O	1:B:582:VAL:HG23	2.15	0.47
2:F:1:DC:H2''	2:F:2:DC:O5'	2.14	0.47
1:E:507:GLY:O	1:E:508:LYS:C	2.53	0.46
2:I:1:DC:H2''	2:I:2:DC:O5'	2.15	0.46
2:K:1:DC:H2''	2:K:2:DC:O5'	2.14	0.46
1:A:578:ALA:O	1:A:582:VAL:HG23	2.14	0.46
1:B:416:LEU:HD23	1:B:430:VAL:HG11	1.96	0.46
1:E:285:ALA:CB	1:E:286:PRO:HD2	2.41	0.46
3:L:-13:DG:H2''	3:L:-12:DA:OP2	2.15	0.46
1:H:235:ALA:O	1:H:236:ARG:HB2	2.15	0.46
1:H:418:VAL:O	1:H:422:ALA:HB3	2.16	0.46
1:A:577:GLN:O	1:A:581:THR:OG1	2.29	0.46
1:H:285:ALA:CB	1:H:286:PRO:CD	2.93	0.46
3:G:-13:DG:H2''	3:G:-12:DA:OP2	2.16	0.46
1:A:517:LEU:HA	1:A:520:VAL:CG1	2.46	0.45
1:A:507:GLY:O	1:A:508:LYS:C	2.54	0.45
1:A:516:ARG:NH2	1:A:517:LEU:CD1	2.80	0.45
1:E:285:ALA:CB	1:E:286:PRO:CD	2.93	0.45
1:E:418:VAL:O	1:E:422:ALA:HB3	2.16	0.45
1:H:416:LEU:HD23	1:H:430:VAL:HG11	1.98	0.45
1:H:698:LEU:CD1	1:H:698:LEU:N	2.79	0.45
1:A:509:GLN:HB3	1:A:542:LYS:HD3	1.99	0.45
1:B:706:LEU:HD21	1:B:718:VAL:HG21	1.99	0.45
1:A:664:THR:O	1:A:665:PRO:C	2.55	0.45
1:A:586:LEU:HB3	1:A:587:PRO:CD	2.46	0.45
1:A:706:LEU:HD21	1:A:718:VAL:HG21	1.98	0.45
1:B:285:ALA:CB	1:B:286:PRO:CD	2.94	0.45
3:J:-13:DG:H2''	3:J:-12:DA:OP2	2.17	0.45
1:B:418:VAL:O	1:B:422:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:LEU:HA	1:E:520:VAL:CG1	2.47	0.44
2:K:2:DC:H2"	2:K:3:DC:O5'	2.18	0.44
1:A:285:ALA:CB	1:A:286:PRO:CD	2.93	0.44
1:A:721:LEU:HD22	2:F:14:DT:C5	2.53	0.44
3:D:-13:DG:H2"	3:D:-12:DA:OP2	2.16	0.44
1:A:721:LEU:HD23	2:F:14:DT:C5	2.52	0.44
1:H:620:LEU:HB3	1:H:621:PRO:CD	2.47	0.44
1:H:664:THR:O	1:H:665:PRO:C	2.55	0.44
2:K:-1:DG:H2"	2:K:0:DT:H5"	1.98	0.44
1:B:292:GLU:OE2	1:B:292:GLU:N	2.45	0.44
1:B:509:GLN:HB3	1:B:542:LYS:HD3	1.98	0.44
2:I:2:DC:H2"	2:I:3:DC:O5'	2.18	0.44
1:H:285:ALA:CB	1:H:286:PRO:HD2	2.40	0.44
1:A:418:VAL:O	1:A:422:ALA:HB3	2.17	0.44
1:H:695:LEU:O	1:H:696:ALA:C	2.56	0.44
1:E:695:LEU:O	1:E:696:ALA:C	2.56	0.44
1:A:721:LEU:HA	2:F:14:DT:C6	2.52	0.44
1:H:517:LEU:HA	1:H:520:VAL:CG1	2.47	0.43
1:B:285:ALA:CB	1:B:286:PRO:HD2	2.41	0.43
1:E:586:LEU:HB3	1:E:587:PRO:CD	2.48	0.43
1:E:509:GLN:HB3	1:E:542:LYS:HD3	2.01	0.43
1:E:526:GLY:C	1:E:527:LEU:HD13	2.39	0.43
1:H:586:LEU:HB3	1:H:587:PRO:CD	2.49	0.43
1:H:692:ASP:HB3	1:H:693:PRO:HD2	1.99	0.43
1:E:620:LEU:HB3	1:E:621:PRO:CD	2.48	0.43
1:E:692:ASP:HB3	1:E:693:PRO:HD2	2.00	0.43
1:A:693:PRO:O	1:A:695:LEU:N	2.52	0.43
2:C:2:DC:H2"	2:C:3:DC:O5'	2.18	0.43
1:A:292:GLU:OE2	1:A:292:GLU:N	2.42	0.43
1:A:526:GLY:C	1:A:527:LEU:HD13	2.39	0.43
1:E:706:LEU:HD21	1:E:718:VAL:HG21	2.00	0.43
1:A:285:ALA:CB	1:A:286:PRO:HD2	2.40	0.42
1:A:292:GLU:CD	1:A:292:GLU:H	2.22	0.42
1:B:620:LEU:HB3	1:B:621:PRO:CD	2.50	0.42
1:B:692:ASP:HB3	1:B:693:PRO:HD2	2.00	0.42
1:B:520:VAL:O	1:B:524:ALA:HB3	2.20	0.42
1:B:525:HIS:O	1:B:526:GLY:C	2.54	0.42
1:E:484:LEU:N	1:E:485:PRO:HD2	2.34	0.42
1:E:693:PRO:O	1:E:695:LEU:N	2.52	0.42
1:H:348:LEU:HB3	1:H:349:PRO:HD3	2.02	0.42
1:B:517:LEU:HA	1:B:520:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:PRO:O	1:B:695:LEU:N	2.52	0.42
1:A:620:LEU:HB3	1:A:621:PRO:CD	2.50	0.42
1:B:586:LEU:HB3	1:B:587:PRO:CD	2.50	0.42
1:B:664:THR:O	1:B:667:GLN:N	2.52	0.42
1:H:509:GLN:HB3	1:H:542:LYS:HD3	2.00	0.42
1:A:244:VAL:HG13	1:A:276:HIS:HB2	2.01	0.42
1:A:692:ASP:HB3	1:A:693:PRO:HD2	2.01	0.42
1:A:695:LEU:O	1:A:696:ALA:C	2.58	0.42
1:A:405:GLY:O	1:A:406:LYS:C	2.58	0.41
1:E:235:ALA:O	1:E:236:ARG:CG	2.68	0.41
1:E:292:GLU:OE2	1:E:292:GLU:N	2.44	0.41
1:H:526:GLY:C	1:H:527:LEU:HD13	2.41	0.41
1:E:664:THR:O	1:E:667:GLN:N	2.51	0.41
1:E:292:GLU:H	1:E:292:GLU:CD	2.24	0.41
1:E:405:GLY:O	1:E:406:LYS:C	2.57	0.41
1:H:611:GLN:HB3	1:H:644:LYS:HD3	2.02	0.41
2:K:-2:DT:O2	2:K:-1:DG:C8	2.72	0.41
1:H:664:THR:O	1:H:667:GLN:N	2.52	0.41
1:H:720:LYS:HG3	1:H:720:LYS:O	2.21	0.41
1:A:664:THR:O	1:A:667:GLN:N	2.53	0.41
1:B:367:SER:O	1:B:368:HIS:CG	2.74	0.41
1:H:405:GLY:O	1:H:406:LYS:C	2.59	0.41
1:H:484:LEU:N	1:H:485:PRO:HD2	2.36	0.41
1:H:517:LEU:HD22	1:H:521:LEU:CD1	2.50	0.41
1:H:244:VAL:HG13	1:H:276:HIS:HB2	2.02	0.41
1:H:283:THR:O	1:H:288:ASN:HA	2.19	0.41
1:H:693:PRO:O	1:H:695:LEU:N	2.52	0.41
1:H:367:SER:O	1:H:368:HIS:CG	2.74	0.41
1:H:517:LEU:CD2	1:H:521:LEU:HG	2.50	0.41
1:A:348:LEU:HB3	1:A:349:PRO:HD3	2.03	0.41
2:I:14:DT:H4'	2:I:14:DT:OP1	2.20	0.41
1:E:577:GLN:O	1:E:581:THR:OG1	2.30	0.40
2:F:2:DC:H2''	2:F:3:DC:O5'	2.20	0.40
1:A:642:GLY:O	1:A:643:GLY:C	2.59	0.40
1:B:283:THR:O	1:B:288:ASN:HA	2.22	0.40
1:E:283:THR:O	1:E:288:ASN:HA	2.21	0.40
1:H:450:LEU:N	1:H:451:PRO:CD	2.85	0.40
1:A:450:LEU:N	1:A:451:PRO:CD	2.84	0.40
1:B:695:LEU:O	1:B:696:ALA:C	2.59	0.40
1:A:295:VAL:O	1:A:299:SER:OG	2.38	0.40
1:A:721:LEU:HA	2:F:14:DT:C5	2.55	0.40

All (33) 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:236:ARG:CZ	3:L:-3:DG:OP2[2_545]	0.47	1.73
1:A:232:TRP:NE1	2:K:-2:DT:N1[2_545]	0.58	1.62
1:A:232:TRP:NE1	2:K:-2:DT:C6[2_545]	0.96	1.24
1:A:232:TRP:CD1	2:K:-2:DT:C6[2_545]	1.10	1.10
1:A:236:ARG:NH1	3:L:-3:DG:OP2[2_545]	1.17	1.03
1:H:254:GLN:OE1	1:H:525:HIS:ND1[2_655]	1.36	0.84
1:A:232:TRP:CD1	2:K:-2:DT:N1[2_545]	1.39	0.81
1:A:236:ARG:NH1	3:L:-3:DG:P[2_545]	1.49	0.71
1:A:232:TRP:NE1	2:K:-2:DT:C2[2_545]	1.49	0.71
1:A:236:ARG:NH2	3:L:-3:DG:OP2[2_545]	1.50	0.70
1:A:236:ARG:NE	3:L:-3:DG:OP2[2_545]	1.54	0.66
1:A:232:TRP:CE2	2:K:-2:DT:N1[2_545]	1.63	0.57
1:A:236:ARG:CZ	3:L:-3:DG:P[2_545]	1.79	0.41
1:H:250:GLY:O	1:H:525:HIS:NE2[2_655]	1.82	0.38
1:A:232:TRP:CE2	2:K:-2:DT:C6[2_545]	1.83	0.37
1:A:232:TRP:CD1	2:K:-2:DT:C1'[2_545]	1.84	0.36
1:A:236:ARG:NH2	3:L:-3:DG:P[2_545]	1.85	0.35
1:A:232:TRP:NE1	2:K:-2:DT:C5[2_545]	1.85	0.35
1:A:232:TRP:CE2	2:K:-2:DT:C2[2_545]	1.87	0.33
1:H:250:GLY:O	1:H:525:HIS:CE1[2_655]	1.89	0.31
1:A:232:TRP:CZ2	2:K:-2:DT:N3[2_545]	1.91	0.29
3:J:-3:DG:OP1	1:H:236:ARG:NH1[2_545]	1.96	0.24
1:A:232:TRP:CG	2:K:-2:DT:C6[2_545]	1.96	0.24
1:A:236:ARG:NH2	3:L:-3:DG:O5'[2_545]	2.02	0.18
1:A:232:TRP:CD1	2:K:-2:DT:O4'[2_545]	2.03	0.17
1:A:232:TRP:NE1	2:K:-2:DT:N3[2_545]	2.07	0.13
1:A:236:ARG:NH1	3:L:-3:DG:OP1[2_545]	2.08	0.12
1:H:251:PRO:CA	1:H:525:HIS:CG[2_655]	2.09	0.11
1:A:232:TRP:NE1	2:K:-2:DT:C1'[2_545]	2.09	0.11
1:A:232:TRP:CE2	2:K:-2:DT:N3[2_545]	2.11	0.09
1:H:251:PRO:CA	1:H:525:HIS:CD2[2_655]	2.13	0.07
1:H:254:GLN:OE1	1:H:525:HIS:CE1[2_655]	2.17	0.03
1:A:232:TRP:CE2	2:K:-2:DT:C5[2_545]	2.18	0.02

## 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	490/499 (98%)	437 (89%)	45 (9%)	8 (2%)	9	37
1	B	490/499 (98%)	433 (88%)	46 (9%)	11 (2%)	6	29
1	E	490/499 (98%)	437 (89%)	43 (9%)	10 (2%)	7	31
1	H	490/499 (98%)	438 (89%)	40 (8%)	12 (2%)	6	27
All	All	1960/1996 (98%)	1745 (89%)	174 (9%)	41 (2%)	7	30

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ALA
1	A	525	HIS
1	B	285	ALA
1	B	525	HIS
1	B	526	GLY
1	E	233	SER
1	E	285	ALA
1	E	525	HIS
1	H	233	SER
1	H	285	ALA
1	H	470	ARG
1	H	592	ALA
1	A	233	SER
1	A	691	PRO
1	B	691	PRO
1	E	691	PRO
1	H	252	PRO
1	H	525	HIS
1	A	252	PRO
1	B	252	PRO
1	E	252	PRO
1	E	719	LYS

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Mol	Chain	Res	Type
1	H	691	PRO
1	A	697	ALA
1	B	232	TRP
1	B	524	ALA
1	B	697	ALA
1	E	697	ALA
1	H	236	ARG
1	A	387	GLN
1	B	387	GLN
1	E	694	ALA
1	E	387	GLN
1	H	387	GLN
1	H	697	ALA
1	B	665	PRO
1	E	665	PRO
1	H	665	PRO
1	A	665	PRO
1	B	655	PRO
1	H	655	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	376/384 (98%)	347 (92%)	29 (8%)	13	41
1	B	376/384 (98%)	345 (92%)	31 (8%)	11	38
1	E	376/384 (98%)	343 (91%)	33 (9%)	10	36
1	H	376/384 (98%)	345 (92%)	31 (8%)	11	38
All	All	1504/1536 (98%)	1380 (92%)	124 (8%)	11	38

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	SER
1	A	238	LEU

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Mol	Chain	Res	Type
1	A	261	LEU
1	A	270	THR
1	A	278	TRP
1	A	287	LEU
1	A	299	SER
1	A	307	LEU
1	A	345	GLN
1	A	353	GLN
1	A	375	LEU
1	A	387	GLN
1	A	453	LEU
1	A	469	SER
1	A	484	LEU
1	A	489	GLN
1	A	527	LEU
1	A	549	GLN
1	A	554	VAL
1	A	564	GLN
1	A	583	GLN
1	A	584	ARG
1	A	589	LEU
1	A	623	LEU
1	A	641	ASP
1	A	684	ILE
1	A	687	GLN
1	A	692	ASP
1	A	695	LEU
1	B	233	SER
1	B	238	LEU
1	B	261	LEU
1	B	278	TRP
1	B	287	LEU
1	B	299	SER
1	B	307	LEU
1	B	345	GLN
1	B	353	GLN
1	B	375	LEU
1	B	387	GLN
1	B	453	LEU
1	B	469	SER
1	B	470	ARG
1	B	484	LEU

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Mol	Chain	Res	Type
1	B	489	GLN
1	B	527	LEU
1	B	549	GLN
1	B	554	VAL
1	B	564	GLN
1	B	583	GLN
1	B	584	ARG
1	B	586	LEU
1	B	589	LEU
1	B	623	LEU
1	B	641	ASP
1	B	684	ILE
1	B	687	GLN
1	B	692	ASP
1	B	695	LEU
1	B	721	LEU
1	E	232	TRP
1	E	233	SER
1	E	238	LEU
1	E	261	LEU
1	E	278	TRP
1	E	287	LEU
1	E	299	SER
1	E	307	LEU
1	E	345	GLN
1	E	353	GLN
1	E	375	LEU
1	E	387	GLN
1	E	453	LEU
1	E	469	SER
1	E	484	LEU
1	E	489	GLN
1	E	516	ARG
1	E	523	GLN
1	E	527	LEU
1	E	549	GLN
1	E	554	VAL
1	E	564	GLN
1	E	583	GLN
1	E	584	ARG
1	E	586	LEU
1	E	589	LEU

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Mol	Chain	Res	Type
1	E	591	GLN
1	E	623	LEU
1	E	641	ASP
1	E	684	ILE
1	E	687	GLN
1	E	692	ASP
1	E	695	LEU
1	H	232	TRP
1	H	238	LEU
1	H	261	LEU
1	H	270	THR
1	H	278	TRP
1	H	287	LEU
1	H	299	SER
1	H	307	LEU
1	H	345	GLN
1	H	375	LEU
1	H	387	GLN
1	H	453	LEU
1	H	469	SER
1	H	484	LEU
1	H	489	GLN
1	H	517	LEU
1	H	518	LEU
1	H	527	LEU
1	H	549	GLN
1	H	554	VAL
1	H	564	GLN
1	H	583	GLN
1	H	584	ARG
1	H	586	LEU
1	H	589	LEU
1	H	623	LEU
1	H	641	ASP
1	H	684	ILE
1	H	687	GLN
1	H	695	LEU
1	H	720	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	538	HIS
1	A	687	GLN
1	A	700	ASN
1	A	702	HIS
1	B	538	HIS
1	B	687	GLN
1	B	700	ASN
1	B	702	HIS
1	E	311	GLN
1	E	523	GLN
1	E	538	HIS
1	E	606	ASN
1	E	687	GLN
1	E	700	ASN
1	E	702	HIS
1	H	538	HIS
1	H	606	ASN
1	H	687	GLN
1	H	700	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z  > 2$
2	5HC	C	6	3,2	16,22,23	1.13	1 (6%)	20,31,34	0.93	0
2	5HC	F	6	3,2	16,22,23	1.16	1 (6%)	20,31,34	1.17	2 (10%)
2	5HC	I	6	3,2	16,22,23	1.11	1 (6%)	20,31,34	1.32	1 (5%)
2	5HC	K	6	3,2	16,22,23	1.19	1 (6%)	20,31,34	0.99	1 (5%)



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
2	5HC	C	6	3,2	-	0/6/23/24	0/2/2/2
2	5HC	F	6	3,2	-	0/6/23/24	0/2/2/2
2	5HC	I	6	3,2	-	0/6/23/24	0/2/2/2
2	5HC	K	6	3,2	-	0/6/23/24	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6	5HC	C5-C4	2.79	1.47	1.42
2	K	6	5HC	C5-C4	2.67	1.47	1.42
2	C	6	5HC	C5-C4	2.53	1.47	1.42
2	I	6	5HC	C5-C4	2.02	1.46	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	5HC	C2-N3-C4	4.38	121.31	116.02
2	F	6	5HC	C2-N3-C4	2.64	119.20	116.02
2	K	6	5HC	C2-N3-C4	2.38	118.88	116.02
2	F	6	5HC	O5-C5M-C5	-2.09	105.97	111.87

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	492/499 (98%)	-0.04	11 (2%) 62 41	31, 60, 102, 192	0
1	B	492/499 (98%)	0.01	14 (2%) 53 30	32, 58, 116, 224	0
1	E	492/499 (98%)	0.13	13 (2%) 56 33	39, 83, 128, 175	0
1	H	492/499 (98%)	0.03	15 (3%) 50 27	40, 70, 116, 185	0
2	C	16/17 (94%)	-0.24	1 (6%) 20 8	36, 45, 106, 116	0
2	F	16/17 (94%)	0.34	1 (6%) 20 8	42, 64, 144, 165	0
2	I	16/17 (94%)	-0.28	0 100 100	29, 44, 91, 109	0
2	K	16/17 (94%)	0.08	1 (6%) 20 8	31, 49, 131, 168	0
3	D	17/17 (100%)	-0.31	1 (5%) 22 10	38, 57, 93, 114	0
3	G	17/17 (100%)	-0.01	1 (5%) 22 10	46, 70, 122, 143	0
3	J	17/17 (100%)	-0.46	0 100 100	34, 50, 87, 102	0
3	L	17/17 (100%)	-0.05	1 (5%) 22 10	38, 57, 120, 131	0
All	All	2100/2132 (98%)	0.02	59 (2%) 53 30	29, 67, 121, 224	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	SER	10.2
1	B	231	GLN	9.5
1	H	232	TRP	7.2
1	E	233	SER	7.1
1	B	232	TRP	7.1
1	H	235	ALA	7.0
1	E	234	GLY	6.9
1	B	230	MET	6.9
1	A	233	SER	6.7
1	B	234	GLY	6.3
1	B	693	PRO	6.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	692	ASP	5.7
1	H	234	GLY	5.6
1	H	236	ARG	5.5
1	E	230	MET	5.3
2	F	14	DT	5.3
1	A	230	MET	5.3
1	A	693	PRO	5.3
1	E	232	TRP	5.1
1	A	231	GLN	4.8
1	B	235	ALA	4.7
1	H	233	SER	4.6
1	H	239	GLU	4.3
1	A	234	GLY	4.2
2	K	-2	DT	3.9
1	B	694	ALA	3.9
1	A	692	ASP	3.6
3	G	2	DA	3.4
1	H	240	ALA	3.3
1	H	693	PRO	3.2
1	H	243	THR	3.1
1	B	248	LEU	3.1
3	L	2	DA	3.1
1	E	401	SER	3.0
1	A	232	TRP	2.7
1	H	230	MET	2.7
1	B	557	GLN	2.5
1	E	391	LEU	2.5
1	H	238	LEU	2.5
1	B	283	THR	2.5
1	E	692	ASP	2.4
1	H	254	GLN	2.4
1	A	462	GLN	2.4
1	B	472	GLY	2.4
1	E	689	SER	2.3
1	E	253	LEU	2.3
1	E	378	VAL	2.3
1	A	243	THR	2.2
2	C	14	DT	2.2
1	H	660	ALA	2.2
3	D	-14	DA	2.1
1	A	459	LEU	2.1
1	H	527	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	231	GLN	2.1
1	H	525	HIS	2.1
1	E	251	PRO	2.1
1	B	496	GLN	2.0
1	A	496	GLN	2.0
1	E	693	PRO	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	5HC	K	6	21/22	0.96	0.16	30,35,43,47	0
2	5HC	F	6	21/22	0.97	0.15	43,46,51,53	0
2	5HC	I	6	21/22	0.98	0.16	27,30,34,35	0
2	5HC	C	6	21/22	0.98	0.17	31,34,39,41	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.