



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 AM UTC

PDB ID : 6JW4 / pdb_00006jw4
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

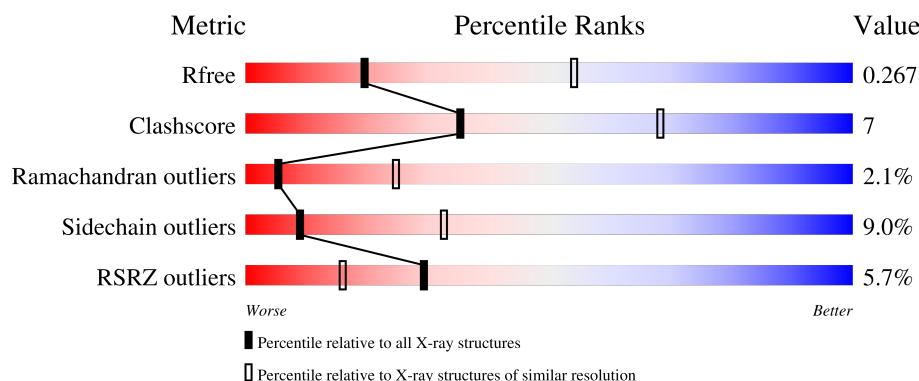
1 Overall quality at a glance

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.



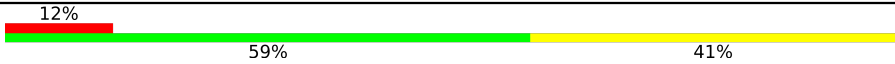
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 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 $\leq 5\%$. 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	
1	B	499	
1	E	499	
1	H	499	
2	C	17	

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Mol	Chain	Length	Quality of chain
2	F	17	
2	I	17	
2	K	17	
3	D	17	
3	G	17	
3	J	17	
3	L	17	

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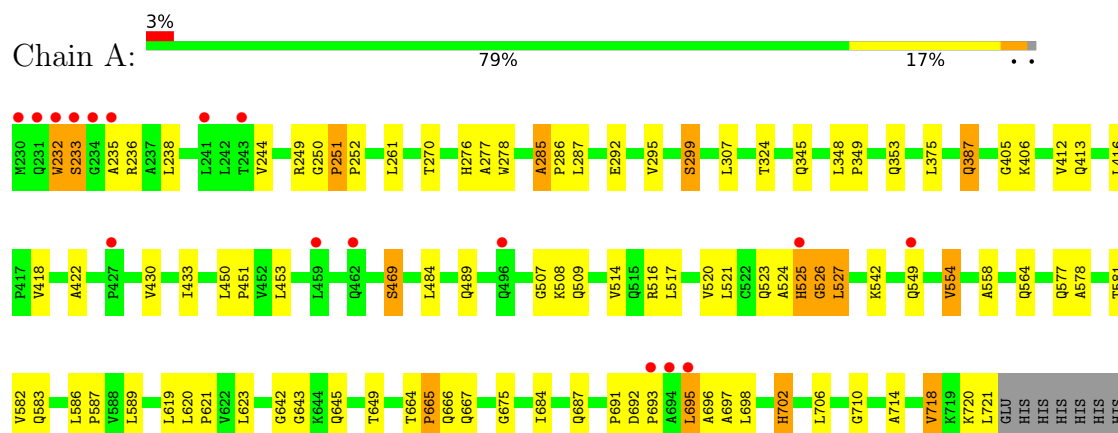
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	17	Total	C	N	O	P	0	0	0
			355	167	79	93	16			

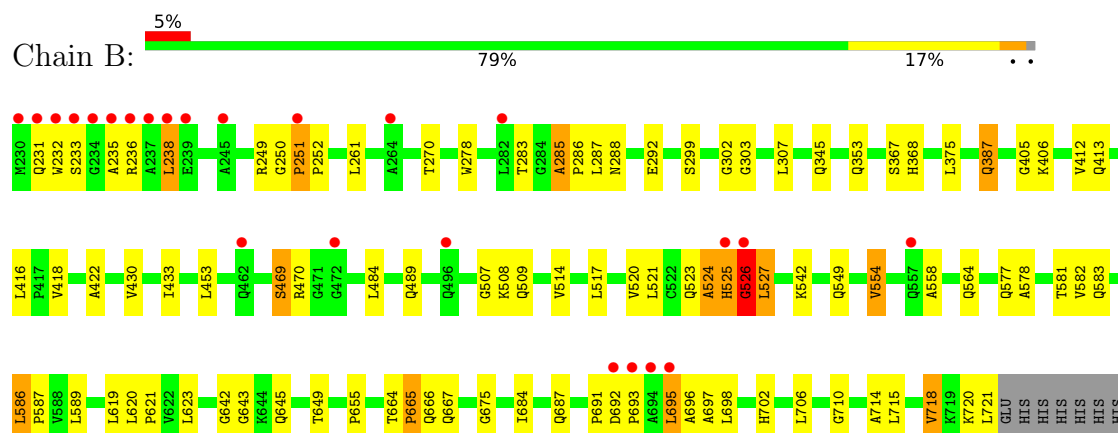
3 Residue-property plots

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.

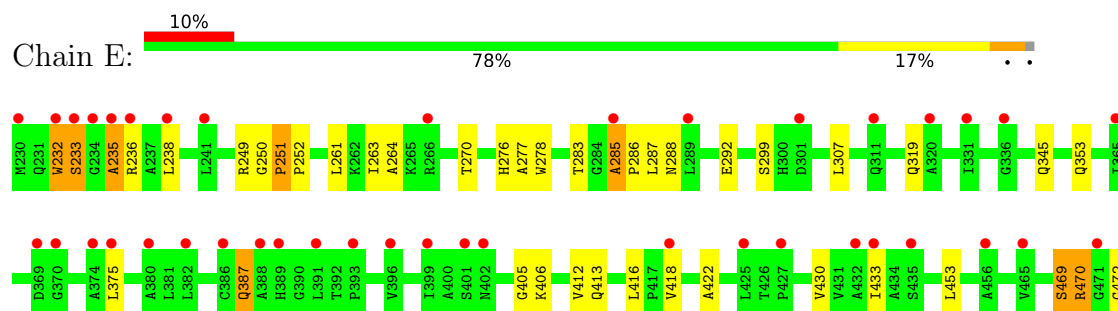
• Molecule 1: TAL effector

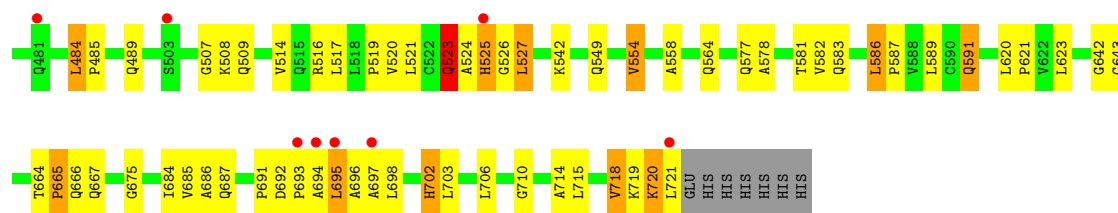


• Molecule 1: TAL effector

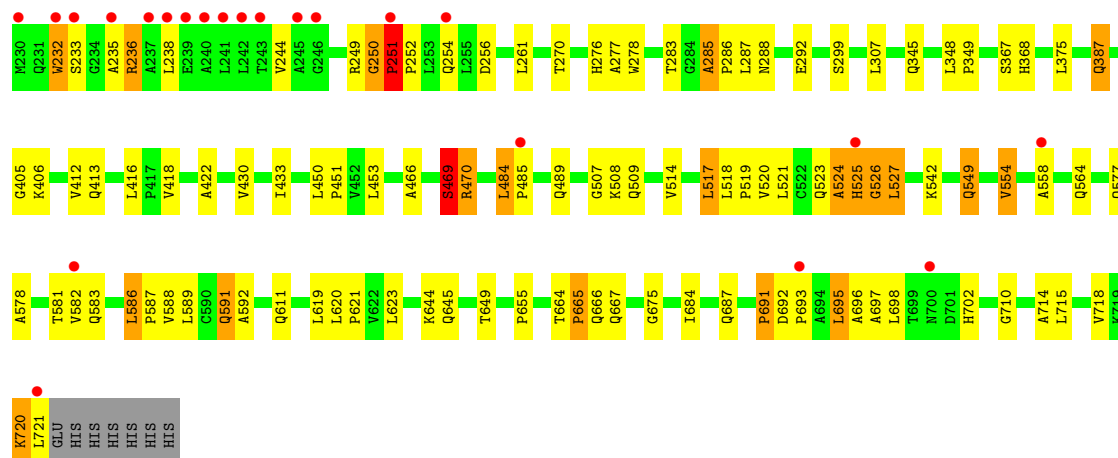
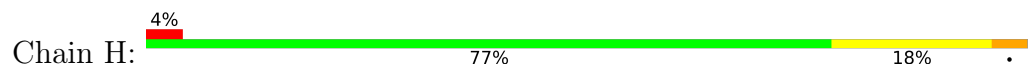


• Molecule 1: TAL effector





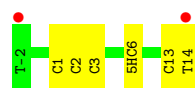
● Molecule 1: TAL effector



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



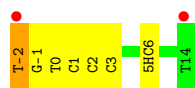
● Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



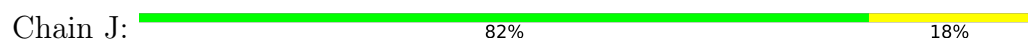
● Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



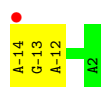
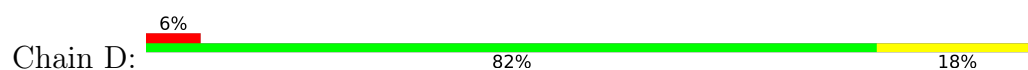
- Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*(5HC)P*GP*CP*GP*TP*CP*TP*CP*T)-3')



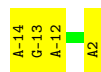
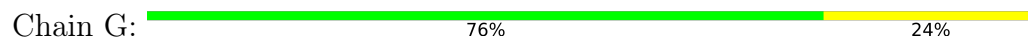
- Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')



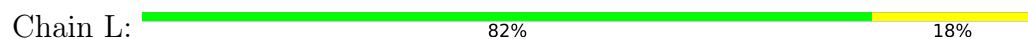
- Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*CP*GP*CP*GP*AP*AP*GP*GP*GP*AP*CP*A)-3')



- 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, α , β , γ	94.05Å 93.97Å 167.69Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	163.51 – 3.09 163.51 – 3.09	Depositor EDS
% Data completeness (in resolution range)	86.9 (163.51-3.09) 87.0 (163.51-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.77	0/3618	0.97	6/4941 (0.1%)
1	B	0.75	1/3618 (0.0%)	0.96	4/4941 (0.1%)
1	E	0.71	0/3618	0.95	8/4941 (0.2%)
1	H	0.75	0/3618	0.98	7/4941 (0.1%)
2	C	0.60	0/349	0.89	0/533
2	F	0.56	0/349	0.86	0/533
2	I	0.62	0/349	0.88	0/533
2	K	0.60	0/349	1.04	2/533 (0.4%)
3	D	0.46	0/402	0.69	0/620
3	G	0.43	0/402	0.76	0/620
3	J	0.46	0/402	0.72	0/620
3	L	0.49	0/402	0.72	0/620
All	All	0.71	1/17476 (0.0%)	0.94	27/24376 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	GLY	N-CA	-5.46	1.37	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	GLN	N-CA-C	-12.13	92.01	108.38
1	B	523	GLN	N-CA-C	-11.48	91.84	108.60
1	H	251	PRO	N-CA-C	9.13	121.84	110.70
1	B	251	PRO	N-CA-C	8.82	121.46	110.70
1	E	251	PRO	N-CA-C	8.46	121.02	110.70
1	A	251	PRO	N-CA-C	8.40	120.95	110.70
1	H	524	ALA	N-CA-C	-8.04	100.53	110.41
1	E	523	GLN	N-CA-C	-7.41	99.28	109.95
1	H	232	TRP	N-CA-C	7.22	120.42	109.23
2	K	-2	DT	N1-C1'-C2'	6.77	123.65	113.50
1	E	232	TRP	N-CA-C	6.59	119.47	108.13
1	A	232	TRP	CA-CB-CG	6.32	125.61	113.60
2	K	-2	DT	C2'-C3'-O3'	6.07	120.61	111.50
1	A	249	ARG	N-CA-C	-5.92	104.95	111.82
1	H	249	ARG	N-CA-C	-5.88	105.00	111.82
1	E	249	ARG	N-CA-C	-5.84	105.04	111.82
1	H	469	SER	N-CA-C	-5.75	97.78	108.02
1	E	472	GLY	N-CA-C	-5.73	99.60	113.18
1	E	235	ALA	N-CA-C	5.73	117.71	108.32
1	A	675	GLY	N-CA-C	-5.66	106.10	112.33
1	A	232	TRP	N-CA-C	5.48	117.32	108.34
1	B	249	ARG	N-CA-C	-5.27	105.71	111.82
1	E	720	LYS	N-CA-C	-5.25	99.91	109.56
1	B	675	GLY	N-CA-C	-5.15	106.67	112.33
1	H	591	GLN	N-CA-C	-5.12	100.82	109.07
1	H	675	GLY	N-CA-C	-5.01	106.81	112.33
1	E	675	GLY	N-CA-C	-5.01	106.82	112.33

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

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Mol	Chain	Res	Type	Group
1	H	250	GLY	Peptide
1	H	251	PRO	Peptide
1	H	526	GLY	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	3567	0	3720	50	26
1	B	3567	0	3720	45	0
1	E	3567	0	3720	49	0
1	H	3567	0	3720	69	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	246	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 (246) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:524:ALA:C	1:H:526:GLY:H	1.92	0.75
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:E:524:ALA:O	1:E:526:GLY:N	2.27	0.68
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:B:235:ALA:C	1:B:236:ARG:HG3	2.23	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:524:ALA:C	1:H:526:GLY:N	2.60	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
1:E:525:HIS:O	1:E:526:GLY:C	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:666:GLN:CD	1:E:666:GLN:H	2.12	0.56
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
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:A:666:GLN:CD	1:A:666:GLN:H	2.14	0.55
1:B:526:GLY:C	1:B:527:LEU:HD13	2.32	0.54
1:A:720:LYS:O	1:A:721:LEU:HG	2.07	0.54
1:B:666:GLN:H	1:B:666:GLN:CD	2.16	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:666:GLN:CD	1:H:666:GLN:H	2.16	0.54
1:H:710:GLY:HA3	1:H:714:ALA:HB2	1.89	0.53
1:B:718:VAL:C	1:B:720:LYS:H	2.15	0.53
1:H:507:GLY:O	1:H:508:LYS:C	2.51	0.53
1:H:691:PRO:O	1:H:695:LEU:HD12	2.09	0.53
1:A:525:HIS:O	1:A:526:GLY:C	2.52	0.53
1:B:664:THR:O	1:B:665:PRO:C	2.51	0.53
1:B:507:GLY:O	1:B:508:LYS:C	2.52	0.52
1:E:718:VAL:C	1:E:720:LYS:H	2.17	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:507:GLY:O	1:E:508:LYS:C	2.53	0.51
1:E:664:THR:O	1:E:665:PRO:C	2.53	0.51
1:E:710:GLY:HA3	1:E:714:ALA:HB2	1.93	0.51
2:C:14:DT:H4'	2:C:14:DT:OP1	2.10	0.51
1:B:433:ILE:HA	1:B:469:SER:HB3	1.93	0.51
1:H:718:VAL:O	1:H:718:VAL:CG1	2.58	0.51
1:A:721:LEU:CD2	2:F:14:DT:C5	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLY:O	1:A:508:LYS:C	2.54	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:A:664:THR:O	1:A:665:PRO:C	2.55	0.49
2:F:-1:DG:C2	3:G:2:DA:C2	3.01	0.49
1:B:710:GLY:HA3	1:B:714:ALA:HB2	1.93	0.49
1:H:698:LEU:N	1:H:698:LEU:HD12	2.27	0.49
1:B:525:HIS:O	1:B:526:GLY:C	2.54	0.48
2:C:14:DT:C4	3:D:-14:DA:N6	2.79	0.48
1:H:695:LEU:O	1:H:696:ALA:C	2.56	0.48
1:H:664:THR:O	1:H:665:PRO:C	2.55	0.48
2:C:14:DT:OP1	2:C:14:DT:C4'	2.61	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:E:526:GLY:C	1:E:527:LEU:HD13	2.39	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
1:E:695:LEU:O	1:E:696:ALA:C	2.56	0.48
1:A:526:GLY:C	1:A:527:LEU:HD13	2.39	0.47
2:C:13:DC:C4	2:C:14:DT:C4	3.03	0.47
1:A:292:GLU:H	1:A:292:GLU:CD	2.22	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:A:416:LEU:HD23	1:A:430:VAL:HG11	1.97	0.47
2:I:14:DT:OP1	2:I:14:DT:C4'	2.63	0.47
1:B:517:LEU:HD23	1:B:517:LEU:HA	1.75	0.47
1:E:416:LEU:HD23	1:E:430:VAL:HG11	1.97	0.47
1:H:692:ASP:O	1:H:695:LEU:CD1	2.62	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
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:405:GLY:O	1:A:406:LYS:C	2.58	0.46
1:A:695:LEU:O	1:A:696:ALA:C	2.58	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
1:E:292:GLU:H	1:E:292:GLU:CD	2.24	0.46
1:E:405:GLY:O	1:E:406:LYS:C	2.57	0.46
3:L:-13:DG:H2''	3:L:-12:DA:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:405:GLY:O	1:H:406:LYS:C	2.59	0.46
3:G:-13:DG:H2''	3:G:-12:DA:OP2	2.16	0.46
1:H:526:GLY:C	1:H:527:LEU:HD13	2.41	0.46
1:A:517:LEU:HA	1:A:520:VAL:CG1	2.46	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:N	1:H:698:LEU:CD1	2.79	0.45
1:A:509:GLN:HB3	1:A:542:LYS:HD3	1.99	0.45
1:A:642:GLY:O	1:A:643:GLY:C	2.59	0.45
1:B:706:LEU:HD21	1:B:718:VAL:HG21	1.99	0.45
1:B:695:LEU:O	1:B:696:ALA:C	2.59	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
3:J:-13:DG:H2''	3:J:-12:DA:OP2	2.17	0.45
1:B:285:ALA:CB	1:B:286:PRO:CD	2.94	0.45
1:B:412:VAL:O	1:B:413:GLN:C	2.60	0.45
1:A:412:VAL:O	1:A:413:GLN:C	2.59	0.44
1:B:418:VAL:O	1:B:422:ALA:HB3	2.17	0.44
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:693:PRO:C	1:H:695:LEU:HD13	2.42	0.44
1:B:292:GLU:H	1:B:292:GLU:CD	2.24	0.44
2:K:-1:DG:H2''	2:K:0:DT:H5''	1.98	0.44
2:I:2:DC:H2''	2:I:3:DC:O5'	2.18	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
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:A:721:LEU:HA	2:F:14:DT:C6	2.52	0.44
1:B:645:GLN:O	1:B:649:THR:OG1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:718:VAL:C	1:B:720:LYS:N	2.76	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: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:E:412:VAL:O	1:E:413:GLN:C	2.60	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:H:645:GLN:O	1:H:649:THR:OG1	2.35	0.43
1:A:292:GLU:OE2	1:A:292:GLU:N	2.42	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: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:405:GLY:O	1:B:406:LYS:C	2.62	0.42
1:B:520:VAL:O	1:B:524:ALA:HB3	2.20	0.42
1:B:642:GLY:O	1:B:643:GLY:C	2.62	0.42
1:E:685:VAL:O	1:E:686:ALA:C	2.62	0.42
1:E:484:LEU:N	1:E:485:PRO:HD2	2.34	0.42
1:E:642:GLY:O	1:E:643:GLY:C	2.62	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
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:577:GLN:O	1:B:581:THR:OG1	2.29	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:H:577:GLN:O	1:H:581:THR:OG1	2.31	0.42
1:A:692:ASP:HB3	1:A:693:PRO:HD2	2.01	0.42
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:E:523:GLN:O	1:E:524:ALA:C	2.59	0.41
1:E:664:THR:O	1:E:667:GLN:N	2.51	0.41
1:H:276:HIS:O	1:H:277:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:412:VAL:O	1:H:413:GLN:C	2.62	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:A:645:GLN:O	1:A:649:THR:OG1	2.35	0.41
1:H:256:ASP:OD1	1:H:256:ASP:C	2.63	0.41
1:H:664:THR:O	1:H:667:GLN:N	2.52	0.41
1:H:720:LYS:O	1:H:720:LYS:HG3	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: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:A:348:LEU:HB3	1:A:349:PRO:HD3	2.03	0.41
1:B:302:GLY:O	1:B:303:GLY:C	2.63	0.41
1:E:702:HIS:O	1:E:703:LEU:C	2.63	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
2:I:14:DT:OP1	2:I:14:DT:H4'	2.20	0.41
1:H:292:GLU:H	1:H:292:GLU:CD	2.24	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:B:283:THR:O	1:B:288:ASN:HA	2.22	0.40
1:E:263:ILE:O	1:E:264:ALA:C	2.65	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: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
1:B:236:ARG:C	1:B:238:LEU:H	2.29	0.40
1:E:276:HIS:O	1:E:277:ALA:C	2.63	0.40
1:A:276:HIS:O	1:A:277:ALA:C	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:232:TRP:NE1	2:K:-2:DT:C2[2_545]	1.49	0.71
1:A:236:ARG:NH1	3:L:-3:DG:P[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:232:TRP:NE1	2:K:-2:DT:C5[2_545]	1.85	0.35
1:A:236:ARG:NH2	3:L:-3:DG:P[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
1:A:232:TRP:CG	2:K:-2:DT:C6[2_545]	1.96	0.24
3:J:-3:DG:OP1	1:H:236:ARG:NH1[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:A:232:TRP:NE1	2:K:-2:DT:C1'[2_545]	2.09	0.11
1:H:251:PRO:CA	1:H:525:HIS:CG[2_655]	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%)	7	30
1	B	490/499 (98%)	433 (88%)	46 (9%)	11 (2%)	5	24
1	E	490/499 (98%)	437 (89%)	43 (9%)	10 (2%)	6	25
1	H	490/499 (98%)	438 (89%)	40 (8%)	12 (2%)	4	22
All	All	1960/1996 (98%)	1745 (89%)	174 (9%)	41 (2%)	5	25

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
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

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Mol	Chain	Res	Type
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%)	345 (92%)	31 (8%)	10	36
1	B	376/384 (98%)	341 (91%)	35 (9%)	8	31
1	E	376/384 (98%)	340 (90%)	36 (10%)	8	30
1	H	376/384 (98%)	343 (91%)	33 (9%)	9	33
All	All	1504/1536 (98%)	1369 (91%)	135 (9%)	9	33

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	SER
1	A	238	LEU
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	324	THR
1	A	345	GLN
1	A	353	GLN
1	A	375	LEU
1	A	387	GLN

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Mol	Chain	Res	Type
1	A	453	LEU
1	A	469	SER
1	A	484	LEU
1	A	489	GLN
1	A	514	VAL
1	A	527	LEU
1	A	549	GLN
1	A	554	VAL
1	A	564	GLN
1	A	583	GLN
1	A	589	LEU
1	A	619	LEU
1	A	623	LEU
1	A	684	ILE
1	A	687	GLN
1	A	695	LEU
1	A	702	HIS
1	A	718	VAL
1	B	231	GLN
1	B	233	SER
1	B	238	LEU
1	B	261	LEU
1	B	270	THR
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
1	B	489	GLN
1	B	514	VAL
1	B	527	LEU
1	B	549	GLN
1	B	554	VAL
1	B	564	GLN
1	B	583	GLN

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Mol	Chain	Res	Type
1	B	586	LEU
1	B	589	LEU
1	B	619	LEU
1	B	623	LEU
1	B	684	ILE
1	B	687	GLN
1	B	695	LEU
1	B	702	HIS
1	B	715	LEU
1	B	718	VAL
1	B	721	LEU
1	E	232	TRP
1	E	233	SER
1	E	238	LEU
1	E	261	LEU
1	E	270	THR
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	470	ARG
1	E	484	LEU
1	E	489	GLN
1	E	514	VAL
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	586	LEU
1	E	589	LEU
1	E	591	GLN
1	E	623	LEU
1	E	684	ILE

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Mol	Chain	Res	Type
1	E	687	GLN
1	E	695	LEU
1	E	702	HIS
1	E	715	LEU
1	E	718	VAL
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	514	VAL
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	586	LEU
1	H	589	LEU
1	H	619	LEU
1	H	623	LEU
1	H	684	ILE
1	H	687	GLN
1	H	695	LEU
1	H	702	HIS
1	H	715	LEU
1	H	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	276	HIS
1	A	300	HIS
1	A	538	HIS
1	A	549	GLN
1	A	573	ASN
1	A	591	GLN
1	A	661	HIS
1	A	702	HIS
1	B	254	GLN
1	B	276	HIS
1	B	300	HIS
1	B	311	GLN
1	B	457	HIS
1	B	538	HIS
1	B	549	GLN
1	B	591	GLN
1	B	661	HIS
1	B	700	ASN
1	B	702	HIS
1	E	254	GLN
1	E	276	HIS
1	E	300	HIS
1	E	353	GLN
1	E	373	GLN
1	E	441	GLN
1	E	538	HIS
1	E	549	GLN
1	E	606	ASN
1	E	661	HIS
1	E	700	ASN
1	E	702	HIS
1	H	254	GLN
1	H	276	HIS
1	H	300	HIS
1	H	311	GLN
1	H	353	GLN
1	H	373	GLN
1	H	538	HIS
1	H	549	GLN
1	H	606	ASN
1	H	661	HIS

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	I	6	3,2	18,22,23	1.03	1 (5%)	22,31,34	0.98	1 (4%)
2	5HC	K	6	3,2	18,22,23	1.13	1 (5%)	22,31,34	1.10	3 (13%)
2	5HC	F	6	3,2	18,22,23	0.99	1 (5%)	22,31,34	1.23	3 (13%)
2	5HC	C	6	3,2	18,22,23	0.98	1 (5%)	22,31,34	1.17	3 (13%)

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	I	6	3,2	-	0/9/23/24	0/2/2/2
2	5HC	K	6	3,2	-	0/9/23/24	0/2/2/2
2	5HC	F	6	3,2	-	0/9/23/24	0/2/2/2
2	5HC	C	6	3,2	-	0/9/23/24	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	6	5HC	C6-N1	-3.40	1.32	1.38
2	F	6	5HC	C6-N1	-2.79	1.33	1.38
2	I	6	5HC	C6-N1	-2.59	1.33	1.38
2	C	6	5HC	C6-N1	-2.31	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	5HC	C5-C6-N1	-2.79	119.19	122.94
2	C	6	5HC	C5-C6-N1	-2.71	119.29	122.94
2	I	6	5HC	O2-C2-N3	-2.48	118.42	122.33
2	K	6	5HC	C5-C6-N1	-2.39	119.73	122.94
2	F	6	5HC	N1-C2-N3	2.38	122.93	118.80
2	C	6	5HC	O2-C2-N3	-2.32	118.67	122.33
2	F	6	5HC	O2-C2-N3	-2.31	118.69	122.33
2	K	6	5HC	O2-C2-N3	-2.21	118.85	122.33
2	K	6	5HC	N1-C2-N3	2.19	122.60	118.80
2	C	6	5HC	C4-N3-C2	-2.08	117.92	120.81

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	492/499 (98%)	0.28	17 (3%)	47	27	31, 60, 102, 192	0
1	B	492/499 (98%)	0.33	24 (4%)	35	18	32, 58, 116, 224	0
1	E	492/499 (98%)	0.74	49 (9%)	12	6	39, 83, 128, 175	0
1	H	492/499 (98%)	0.49	22 (4%)	38	20	40, 70, 116, 185	0
2	C	16/17 (94%)	0.09	2 (12%)	8	5	36, 45, 106, 116	0
2	F	16/17 (94%)	0.94	2 (12%)	8	5	42, 64, 144, 165	0
2	I	16/17 (94%)	0.17	0	100	100	29, 44, 91, 109	0
2	K	16/17 (94%)	0.51	2 (12%)	8	5	31, 49, 131, 168	0
3	D	17/17 (100%)	0.06	1 (5%)	28	15	38, 57, 93, 114	0
3	G	17/17 (100%)	0.41	0	100	100	46, 70, 122, 143	0
3	J	17/17 (100%)	0.06	0	100	100	34, 50, 87, 102	0
3	L	17/17 (100%)	0.52	0	100	100	38, 57, 120, 131	0
All	All	2100/2132 (98%)	0.45	119 (5%)	29	16	29, 67, 121, 224	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	MET	8.8
1	B	235	ALA	6.7
1	H	242	LEU	6.5
1	H	230	MET	5.7
1	H	241	LEU	5.4
1	B	230	MET	5.2
1	A	233	SER	5.2
1	B	236	ARG	5.0
1	H	232	TRP	4.8
1	E	230	MET	4.8
1	A	235	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	237	ALA	4.4
1	H	238	LEU	4.4
1	B	557	GLN	4.3
1	B	694	ALA	4.3
1	B	233	SER	4.2
2	F	14	DT	4.0
1	A	693	PRO	4.0
1	B	238	LEU	3.9
1	E	721	LEU	3.9
1	E	233	SER	3.8
1	B	234	GLY	3.7
1	B	693	PRO	3.6
1	A	694	ALA	3.6
1	B	462	GLN	3.5
1	H	240	ALA	3.4
1	E	401	SER	3.4
1	H	239	GLU	3.4
1	H	235	ALA	3.4
1	E	695	LEU	3.2
1	H	251	PRO	3.2
1	H	245	ALA	3.2
1	H	254	GLN	3.1
1	A	232	TRP	3.1
1	E	693	PRO	3.1
2	K	14	DT	3.1
1	B	232	TRP	3.1
1	E	336	GLY	3.1
1	E	365	ILE	3.0
2	K	-2	DT	3.0
1	H	582	VAL	3.0
1	A	241	LEU	2.9
1	E	235	ALA	2.9
1	E	236	ARG	2.9
1	B	239	GLU	2.8
1	H	243	THR	2.8
1	H	721	LEU	2.8
1	E	234	GLY	2.8
1	E	232	TRP	2.7
1	H	693	PRO	2.7
1	E	433	ILE	2.7
1	E	266	ARG	2.7
1	B	695	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	472	GLY	2.7
3	D	-14	DA	2.7
1	A	234	GLY	2.6
1	E	471	GLY	2.6
1	E	391	LEU	2.6
1	A	462	GLN	2.6
1	E	301	ASP	2.6
1	A	525	HIS	2.5
1	B	525	HIS	2.5
1	A	496	GLN	2.5
1	E	402	ASN	2.5
1	E	465	VAL	2.5
1	B	282	LEU	2.5
1	E	503	SER	2.4
1	E	388	ALA	2.4
1	E	481	GLN	2.4
1	B	251	PRO	2.3
1	E	694	ALA	2.3
1	A	231	GLN	2.3
1	B	231	GLN	2.3
1	A	427	PRO	2.3
1	B	264	ALA	2.3
1	H	558	ALA	2.3
1	H	233	SER	2.3
1	A	459	LEU	2.3
1	E	456	ALA	2.3
1	E	389	HIS	2.3
1	E	382	LEU	2.2
1	B	692	ASP	2.2
1	E	370	GLY	2.2
1	A	695	LEU	2.2
1	E	320	ALA	2.2
1	E	525	HIS	2.2
1	E	396	VAL	2.2
1	E	425	LEU	2.2
1	E	386	CYS	2.2
1	E	393	PRO	2.2
1	E	311	GLN	2.2
1	B	245	ALA	2.2
1	E	432	ALA	2.2
1	H	237	ALA	2.2
1	H	700	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	243	THR	2.1
1	E	289	LEU	2.1
1	E	285	ALA	2.1
1	E	369	ASP	2.1
1	E	331	ILE	2.1
1	E	375	LEU	2.1
2	C	14	DT	2.1
1	E	238	LEU	2.1
1	E	374	ALA	2.1
1	E	697	ALA	2.1
1	E	418	VAL	2.1
2	F	-1	DG	2.1
1	A	549	GLN	2.1
2	C	-2	DT	2.1
1	E	380	ALA	2.1
1	B	496	GLN	2.1
1	B	526	GLY	2.1
1	H	246	GLY	2.1
1	H	485	PRO	2.1
1	E	435	SER	2.0
1	H	525	HIS	2.0
1	E	427	PRO	2.0
1	E	241	LEU	2.0
1	E	399	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5HC	F	6	21/22	0.94	0.09	43,46,51,53	0
2	5HC	K	6	21/22	0.95	0.09	30,35,43,47	0
2	5HC	I	6	21/22	0.97	0.08	27,30,34,35	0
2	5HC	C	6	21/22	0.97	0.08	31,34,39,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.