Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 02:58 PM EDT

PDB ID	:	4POG
Title	:	MCM-ssDNA co-crystal structure
Authors	:	Froelich, C.A.; Kang, S.; Epling, L.B.; Bell, S.P.; Enemark, E.J.
Deposited on	:	2014-02-25
Resolution	:	3.20 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:

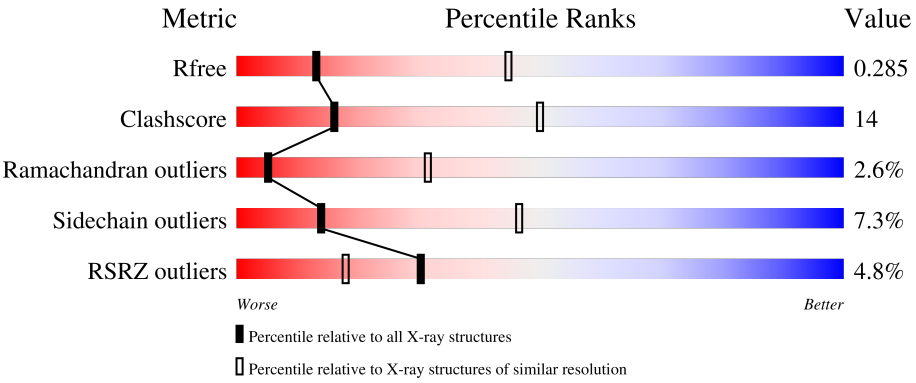
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	257	6% 70% 26%
1	B	257	3% 65% 28% 5%
1	C	257	4% 69% 25% 5%
1	D	257	4% 65% 30% 5%
1	E	257	5% 67% 30%

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Mol	Chain	Length	Quality of chain
1	F	257	2% 68% 28%
1	G	257	5% 56% 34% 7%
1	H	257	9% 65% 29% 5%
1	I	257	7% 67% 28%
1	J	257	5% 67% 28%
1	K	257	2% 63% 31% 5%
1	L	257	4% 63% 31% 5%
2	V	30	10% 87%
2	X	30	17% 77%
2	Y	30	23% 10% 63%
2	Z	30	3% 10% 13% 77%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24942 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 Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	B	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	C	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	D	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	E	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	F	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	G	249	Total	C	N	O	S	0	0	0
			1884	1188	325	362	9			
1	H	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	I	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	J	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	K	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	L	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8U3I4
A	1	VAL	-	expression tag	UNP Q8U3I4
B	0	SER	-	expression tag	UNP Q8U3I4
B	1	VAL	-	expression tag	UNP Q8U3I4
C	0	SER	-	expression tag	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	VAL	-	expression tag	UNP Q8U3I4
D	0	SER	-	expression tag	UNP Q8U3I4
D	1	VAL	-	expression tag	UNP Q8U3I4
E	0	SER	-	expression tag	UNP Q8U3I4
E	1	VAL	-	expression tag	UNP Q8U3I4
F	0	SER	-	expression tag	UNP Q8U3I4
F	1	VAL	-	expression tag	UNP Q8U3I4
G	0	SER	-	expression tag	UNP Q8U3I4
G	1	VAL	-	expression tag	UNP Q8U3I4
H	0	SER	-	expression tag	UNP Q8U3I4
H	1	VAL	-	expression tag	UNP Q8U3I4
I	0	SER	-	expression tag	UNP Q8U3I4
I	1	VAL	-	expression tag	UNP Q8U3I4
J	0	SER	-	expression tag	UNP Q8U3I4
J	1	VAL	-	expression tag	UNP Q8U3I4
K	0	SER	-	expression tag	UNP Q8U3I4
K	1	VAL	-	expression tag	UNP Q8U3I4
L	0	SER	-	expression tag	UNP Q8U3I4
L	1	VAL	-	expression tag	UNP Q8U3I4

- Molecule 2 is a DNA chain called 30-mer oligo(dT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	7	Total	C	N	O	P	0	0	0
			141	70	14	50	7			
2	V	4	Total	C	N	O	P	0	0	0
			81	40	8	29	4			
2	Y	11	Total	C	N	O	P	0	0	0
			221	110	22	78	11			
2	Z	7	Total	C	N	O	P	0	0	0
			141	70	14	50	7			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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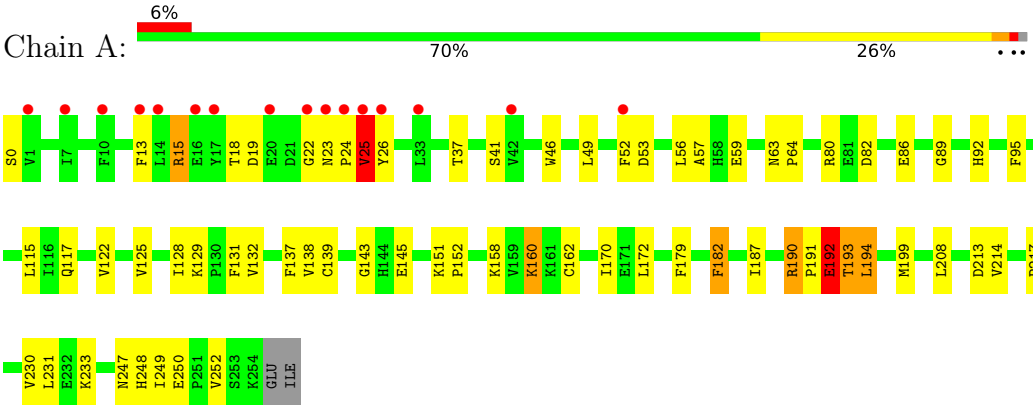
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	K	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

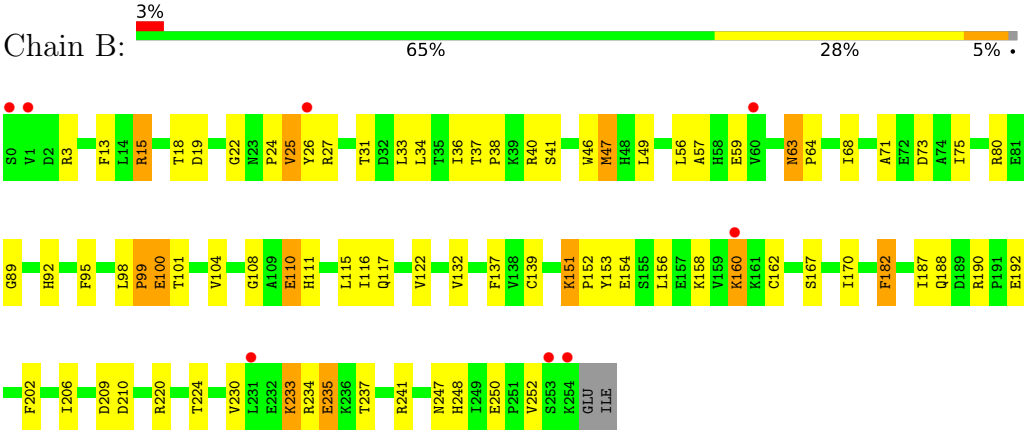
• Molecule 1: Cell division control protein 21

Chain A:



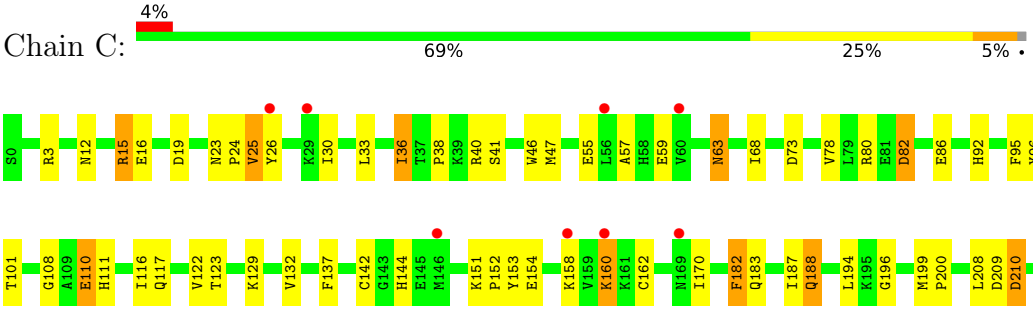
• Molecule 1: Cell division control protein 21

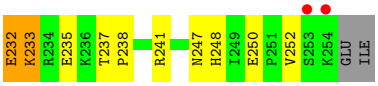
Chain B:



• Molecule 1: Cell division control protein 21

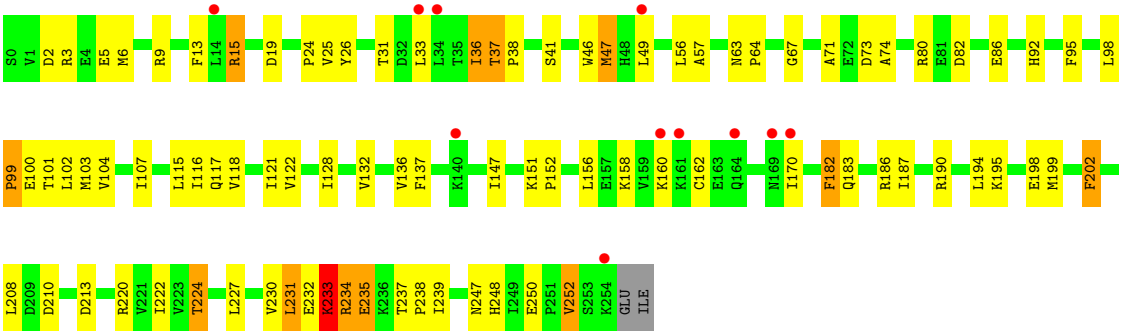
Chain C:





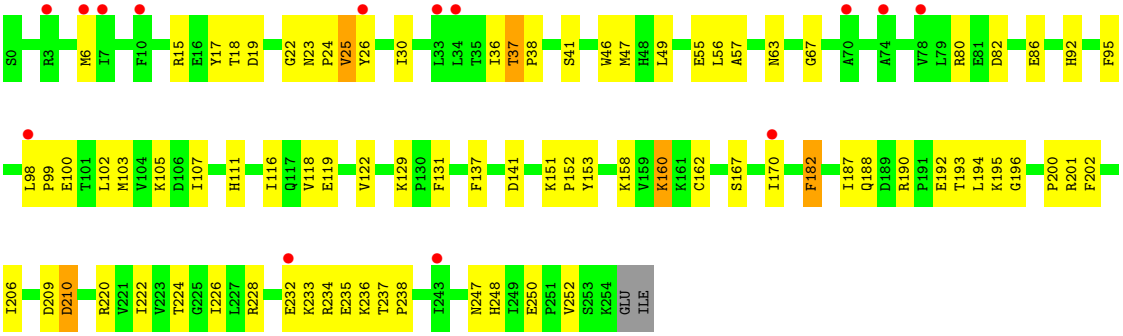
• Molecule 1: Cell division control protein 21

Chain D:



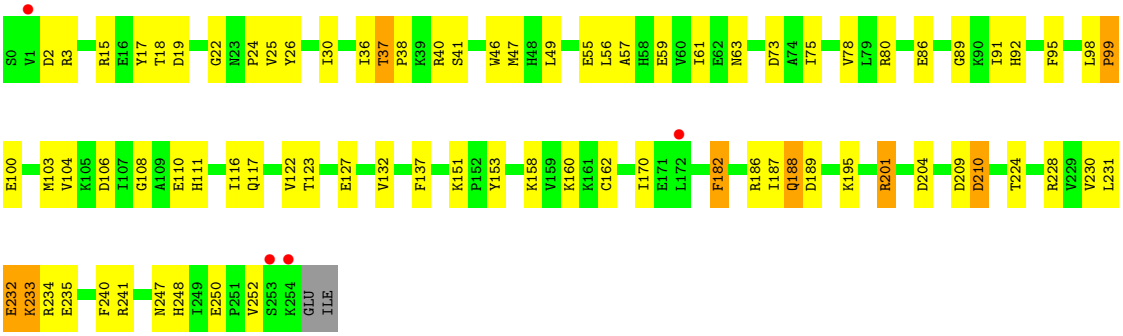
• Molecule 1: Cell division control protein 21

Chain E:



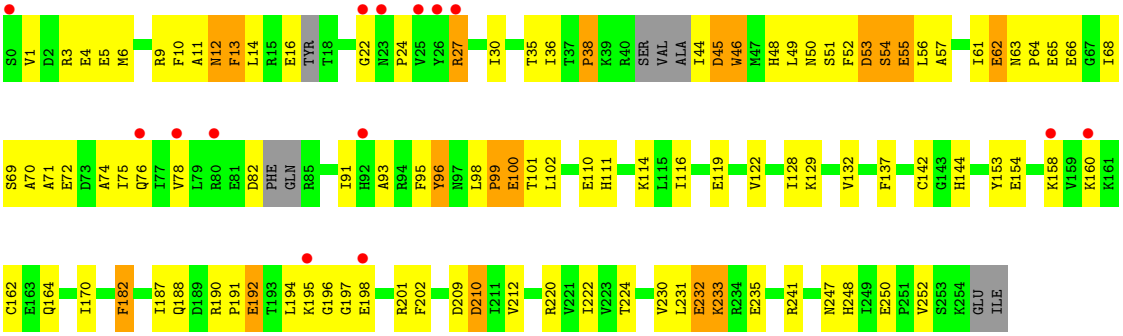
• Molecule 1: Cell division control protein 21

Chain F:



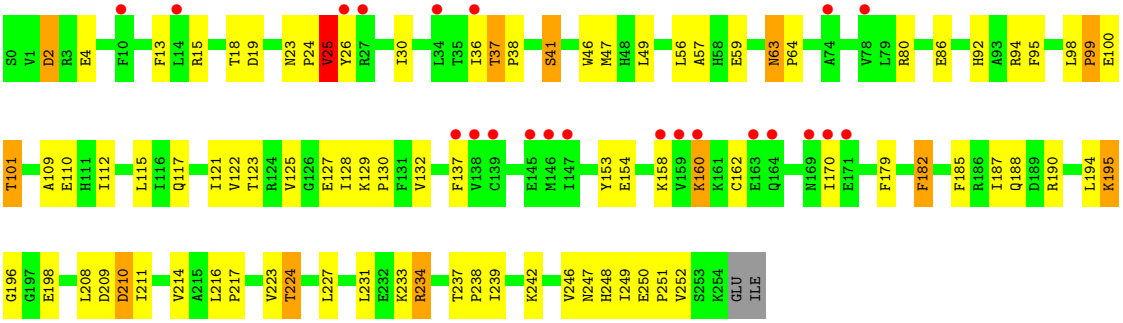
• Molecule 1: Cell division control protein 21

Chain G:



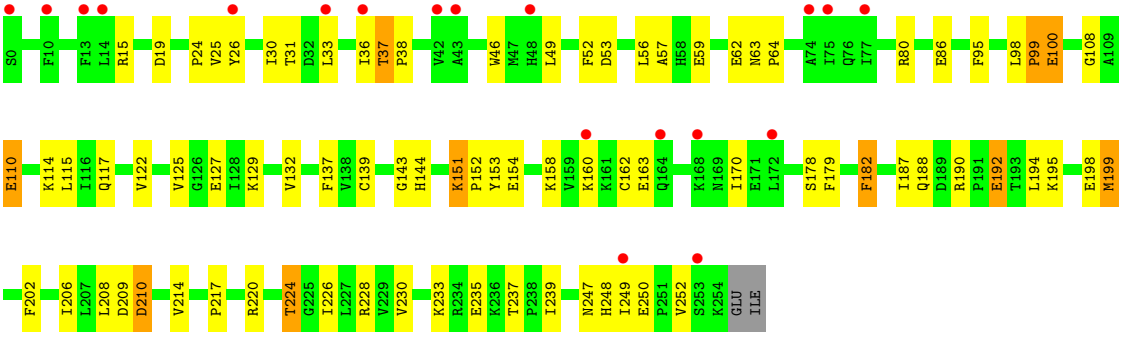
• Molecule 1: Cell division control protein 21

Chain H:



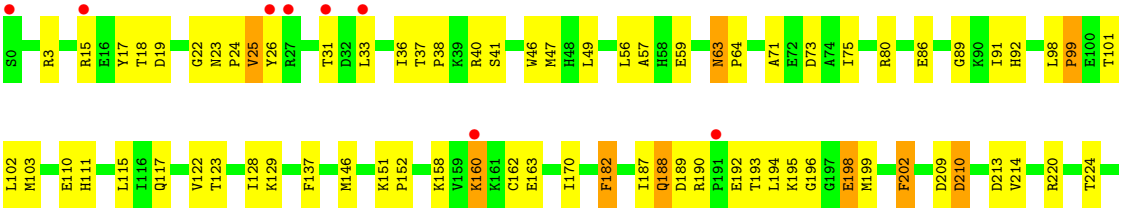
• Molecule 1: Cell division control protein 21

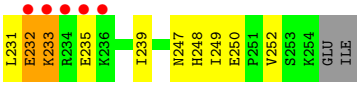
Chain I:



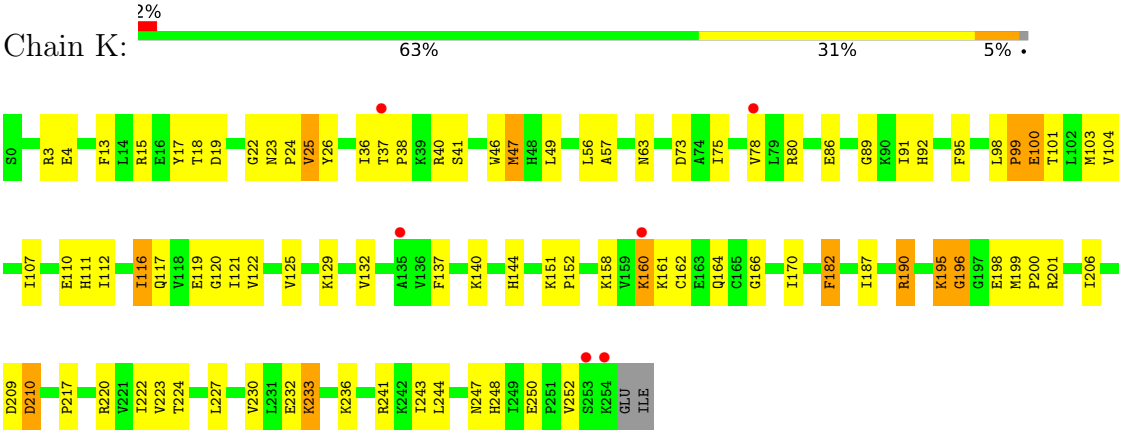
• Molecule 1: Cell division control protein 21

Chain J:

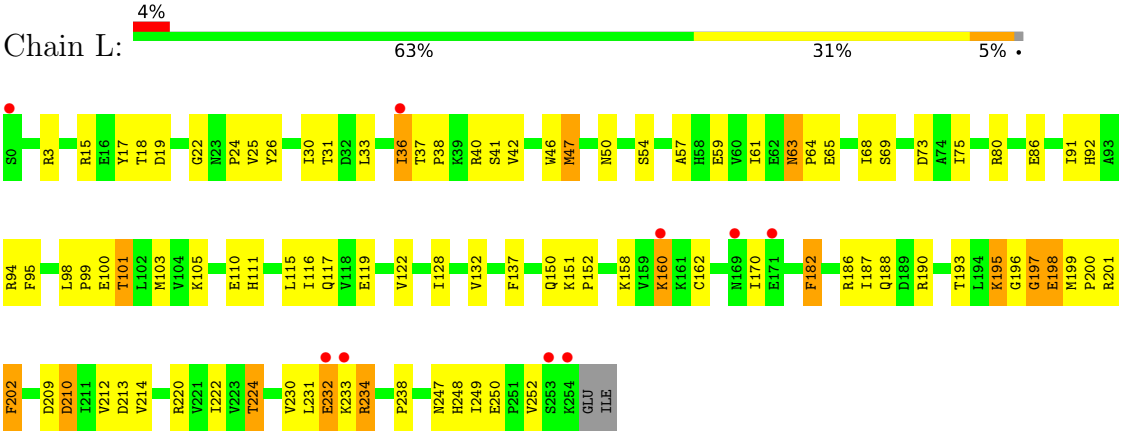




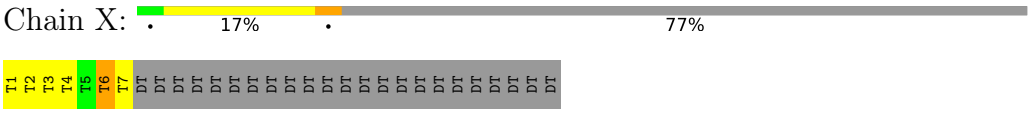
• Molecule 1: Cell division control protein 21



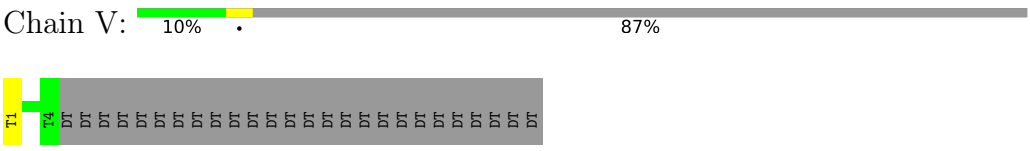
• Molecule 1: Cell division control protein 21



• Molecule 2: 30-mer oligo(dT)



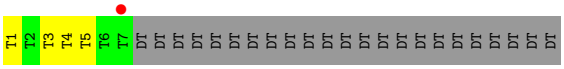
• Molecule 2: 30-mer oligo(dT)



• Molecule 2: 30-mer oligo(dT)

• Molecule 2: 30-mer oligo(dT)

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.28Å 113.40Å 196.85Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	48.51 – 3.20 48.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.51-3.20) 99.6 (48.52-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.257 , 0.294 0.249 , 0.285	Depositor DCC
R_{free} test set	3376 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	81.0	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24942	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.41	0/2077	0.57	0/2805
1	B	0.40	0/2077	0.57	0/2805
1	C	0.39	0/2077	0.56	0/2805
1	D	0.42	0/2077	0.57	0/2805
1	E	0.39	0/2077	0.54	0/2805
1	F	0.39	0/2077	0.56	0/2805
1	G	0.41	0/1909	0.63	2/2579 (0.1%)
1	H	0.47	0/2077	0.62	0/2805
1	I	0.40	0/2077	0.55	0/2805
1	J	0.41	0/2077	0.55	0/2805
1	K	0.50	0/2077	0.65	0/2805
1	L	0.46	0/2077	0.61	0/2805
2	V	1.47	1/88 (1.1%)	1.48	0/132
2	X	1.15	1/154 (0.6%)	1.46	1/234 (0.4%)
2	Y	1.01	1/242 (0.4%)	1.57	5/370 (1.4%)
2	Z	1.15	1/154 (0.6%)	1.36	0/234
All	All	0.45	4/25394 (0.0%)	0.63	8/34404 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	1	DT	OP3-P	-11.02	1.48	1.61
2	X	1	DT	OP3-P	-10.94	1.48	1.61
2	Y	1	DT	OP3-P	-10.85	1.48	1.61
2	Z	1	DT	OP3-P	-10.85	1.48	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	6	DT	C4-C5-C7	6.18	122.71	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	10	DT	C4-C5-C7	6.08	122.65	119.00
1	G	24	PRO	N-CA-CB	5.96	110.45	103.30
1	G	38	PRO	N-CA-CB	5.72	110.16	103.30
2	Y	6	DT	C6-C5-C7	-5.52	119.59	122.90
2	Y	6	DT	C4-C5-C7	5.32	122.19	119.00
2	Y	5	DT	N3-C4-O4	5.29	123.07	119.90
2	Y	10	DT	C6-C5-C7	-5.01	119.89	122.90

There are no chirality outliers.

There are no planarity outliers.

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	2042	0	2052	44	0
1	B	2042	0	2052	62	0
1	C	2042	0	2052	56	0
1	D	2042	0	2052	61	0
1	E	2042	0	2052	48	0
1	F	2042	0	2052	54	0
1	G	1884	0	1797	88	0
1	H	2042	0	2052	70	0
1	I	2042	0	2052	54	0
1	J	2042	0	2052	52	0
1	K	2042	0	2052	64	0
1	L	2042	0	2052	67	0
2	V	81	0	49	0	0
2	X	141	0	85	6	0
2	Y	221	0	133	14	0
2	Z	141	0	85	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	24942	0	24721	719	0

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 14.

All (719) 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:X:6:DT:H2"	2:X:7:DT:H5"	1.46	0.97
1:L:41:SER:HB3	1:L:92:HIS:HB2	1.48	0.95
1:G:11:ALA:HA	1:G:14:LEU:HD12	1.51	0.93
1:G:72:GLU:O	1:G:75:ILE:HG22	1.74	0.87
1:I:188:GLN:HB3	1:I:202:PHE:HB3	1.56	0.87
1:J:49:LEU:HD11	1:J:56:LEU:HD23	1.56	0.87
1:G:9:ARG:HH12	1:G:55:GLU:HB2	1.41	0.86
1:L:234:ARG:HD3	1:L:234:ARG:H	1.42	0.85
1:K:190:ARG:HE	1:K:220:ARG:HE	1.27	0.80
2:Y:7:DT:H3'	2:Y:8:DT:H5'	1.62	0.79
1:G:233:LYS:HE2	2:Y:11:DT:OP2	1.83	0.78
1:B:188:GLN:HB3	1:B:202:PHE:HB3	1.64	0.78
1:H:122:VAL:HA	1:H:187:ILE:HG22	1.65	0.77
1:K:80:ARG:HG3	1:K:86:GLU:HG2	1.66	0.77
1:B:49:LEU:HD11	1:B:56:LEU:HD23	1.67	0.77
1:H:98:LEU:HD12	1:H:117:GLN:HB2	1.67	0.77
1:B:80:ARG:HG3	1:B:86:GLU:HG2	1.66	0.77
1:D:202:PHE:H	1:D:202:PHE:HD1	1.33	0.77
1:F:201:ARG:HH11	1:F:201:ARG:HG3	1.49	0.76
1:H:123:THR:HG21	1:H:188:GLN:HG2	1.65	0.76
1:H:98:LEU:HB3	1:H:99:PRO:HD2	1.67	0.76
1:D:186:ARG:HD3	1:D:202:PHE:HD2	1.50	0.76
2:Y:3:DT:H3'	2:Y:4:DT:H5'	1.69	0.75
1:C:80:ARG:HG3	1:C:86:GLU:HG2	1.68	0.75
1:H:80:ARG:HG3	1:H:86:GLU:HG2	1.68	0.75
1:C:24:PRO:O	1:C:26:TYR:N	2.20	0.75
1:E:188:GLN:HB3	1:E:202:PHE:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:3:DT:H3'	2:Z:4:DT:H5'	1.69	0.74
1:A:80:ARG:HG3	1:A:86:GLU:HG2	1.68	0.74
1:E:119:GLU:HG3	1:E:222:ILE:HG12	1.70	0.74
1:H:49:LEU:HD11	1:H:56:LEU:HD23	1.70	0.74
1:G:54:SER:HA	1:G:57:ALA:HB3	1.70	0.73
2:Y:8:DT:H5"	2:Y:10:DT:H71	1.70	0.73
1:D:80:ARG:HG3	1:D:86:GLU:HG2	1.69	0.73
1:L:80:ARG:HG3	1:L:86:GLU:HG2	1.70	0.72
1:F:80:ARG:HG3	1:F:86:GLU:HG2	1.71	0.71
1:G:11:ALA:HB2	1:G:74:ALA:HB1	1.72	0.71
1:H:234:ARG:H	1:H:234:ARG:HD3	1.56	0.71
1:K:230:VAL:HG23	1:K:241:ARG:HB3	1.72	0.71
1:J:194:LEU:HD23	1:J:196:GLY:H	1.55	0.71
1:F:49:LEU:HD11	1:F:56:LEU:HD23	1.72	0.70
1:E:80:ARG:HG3	1:E:86:GLU:HG2	1.71	0.70
1:H:214:VAL:HG21	1:H:249:ILE:HG21	1.73	0.70
1:J:231:LEU:HB2	1:J:235:GLU:HG2	1.74	0.70
1:C:41:SER:HB3	1:C:92:HIS:HB2	1.73	0.70
1:K:40:ARG:HH11	1:K:209:ASP:CG	1.95	0.70
1:H:41:SER:HB3	1:H:92:HIS:HB2	1.74	0.69
1:D:36:ILE:O	1:D:38:PRO:HD3	1.93	0.69
1:B:41:SER:HB3	1:B:92:HIS:HB2	1.72	0.69
1:D:49:LEU:HD11	1:D:56:LEU:HD23	1.75	0.69
1:G:49:LEU:CD1	1:G:57:ALA:HB2	2.22	0.69
1:J:80:ARG:HG3	1:J:86:GLU:HG2	1.75	0.68
1:L:24:PRO:O	1:L:26:TYR:N	2.26	0.68
1:L:98:LEU:HB3	1:L:99:PRO:HD2	1.75	0.68
1:I:80:ARG:HG3	1:I:86:GLU:HG2	1.75	0.68
1:K:41:SER:HB3	1:K:92:HIS:HB2	1.75	0.68
1:C:231:LEU:HB2	1:C:235:GLU:HG2	1.76	0.68
1:G:61:ILE:HD11	1:G:98:LEU:HD13	1.76	0.68
1:K:98:LEU:HB3	1:K:99:PRO:HD2	1.75	0.68
2:X:4:DT:H2"	2:X:6:DT:O4	1.94	0.68
1:D:122:VAL:HA	1:D:187:ILE:HG22	1.76	0.67
1:H:109:ALA:O	1:H:112:ILE:HG13	1.95	0.67
1:F:188:GLN:HG3	1:F:189:ASP:O	1.95	0.67
1:G:44:ILE:HG21	1:G:95:PHE:HA	1.76	0.67
1:F:98:LEU:HD12	1:F:117:GLN:HB2	1.76	0.67
1:I:190:ARG:CZ	1:I:220:ARG:HE	2.08	0.67
1:K:190:ARG:NE	1:K:220:ARG:HE	1.93	0.67
1:F:201:ARG:HH11	1:F:201:ARG:CG	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ASN:O	1:C:16:GLU:HB2	1.95	0.66
1:B:98:LEU:HD12	1:B:117:GLN:HB2	1.78	0.66
1:B:85:ARG:HD3	1:G:54:SER:HB2	1.76	0.65
1:D:231:LEU:HD12	1:D:231:LEU:H	1.61	0.65
1:G:162:CYS:HB2	1:G:170:ILE:HD11	1.77	0.65
2:Y:8:DT:H2'	2:Y:10:DT:O4	1.97	0.65
1:H:224:THR:HG23	1:H:247:ASN:HB3	1.78	0.65
1:G:69:SER:O	1:G:72:GLU:HB2	1.95	0.65
1:G:1:VAL:CG1	1:G:5:GLU:HG3	2.27	0.64
1:B:139:CYS:SG	1:B:167:SER:OG	2.55	0.64
1:B:160:LYS:H	1:B:160:LYS:HD3	1.62	0.64
1:L:94:ARG:HH11	1:L:94:ARG:HG2	1.63	0.64
1:G:4:GLU:CD	1:G:4:GLU:H	2.01	0.64
1:L:41:SER:HA	1:L:91:ILE:HG23	1.79	0.64
1:K:125:VAL:HG22	1:K:217:PRO:HD3	1.80	0.64
1:H:123:THR:CG2	1:H:188:GLN:HG2	2.28	0.64
1:H:160:LYS:H	1:H:160:LYS:HD3	1.63	0.63
1:E:201:ARG:HD3	1:F:127:GLU:HA	1.80	0.63
1:B:190:ARG:CZ	1:B:220:ARG:HE	2.12	0.63
1:G:224:THR:HG22	1:G:248:HIS:HB3	1.81	0.63
1:B:40:ARG:HH11	1:B:209:ASP:CG	2.02	0.63
1:I:188:GLN:HB3	1:I:202:PHE:CB	2.27	0.63
1:I:214:VAL:HG21	1:I:249:ILE:HG21	1.80	0.62
1:A:122:VAL:HA	1:A:187:ILE:HG22	1.82	0.62
1:D:160:LYS:H	1:D:160:LYS:HD3	1.64	0.62
1:J:64:PRO:HB3	1:J:115:LEU:HB2	1.81	0.62
1:K:122:VAL:HA	1:K:187:ILE:HG22	1.81	0.62
1:L:47:MET:HA	1:L:47:MET:HE3	1.81	0.62
1:G:64:PRO:O	1:G:68:ILE:HG13	2.00	0.62
1:F:224:THR:HG23	1:F:247:ASN:HB3	1.80	0.62
1:G:231:LEU:HB2	1:G:235:GLU:HG2	1.81	0.62
1:J:214:VAL:HG21	1:J:249:ILE:HG21	1.81	0.62
1:L:18:THR:HB	1:L:22:GLY:HA2	1.80	0.62
1:E:192:GLU:HG3	1:E:193:THR:H	1.65	0.61
1:K:120:GLY:HA3	1:K:187:ILE:HD12	1.82	0.61
1:E:192:GLU:HG3	1:E:193:THR:N	2.14	0.61
1:G:72:GLU:HG2	1:G:93:ALA:CB	2.29	0.61
1:J:98:LEU:HD12	1:J:117:GLN:HB2	1.83	0.61
1:G:49:LEU:HD12	1:G:57:ALA:HB2	1.83	0.61
1:E:49:LEU:HD11	1:E:56:LEU:HD23	1.82	0.61
1:F:24:PRO:O	1:F:26:TYR:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:LEU:HD12	1:I:117:GLN:HB2	1.82	0.61
1:C:98:LEU:HB3	1:C:99:PRO:HD2	1.81	0.61
1:B:132:VAL:O	1:B:132:VAL:HG13	2.00	0.61
1:G:72:GLU:HG2	1:G:93:ALA:HB2	1.81	0.61
1:H:112:ILE:HA	1:H:227:LEU:HD12	1.83	0.60
1:D:36:ILE:HG23	1:D:37:THR:HG22	1.83	0.60
1:J:224:THR:HG22	1:J:248:HIS:HB3	1.83	0.60
1:A:224:THR:HG23	1:A:247:ASN:HB3	1.83	0.60
1:B:122:VAL:HA	1:B:187:ILE:HG22	1.84	0.60
1:F:160:LYS:HD3	1:F:160:LYS:H	1.66	0.60
1:L:26:TYR:O	1:L:30:ILE:HG13	2.02	0.60
1:F:95:PHE:H	1:F:247:ASN:HD21	1.48	0.60
1:F:36:ILE:O	1:F:38:PRO:HD3	2.01	0.60
1:K:125:VAL:CG2	1:K:217:PRO:HD3	2.32	0.60
1:F:123:THR:HG21	1:F:188:GLN:NE2	2.17	0.60
1:L:160:LYS:H	1:L:160:LYS:HD3	1.67	0.60
1:C:182:PHE:C	1:C:182:PHE:CD2	2.75	0.59
1:E:98:LEU:HB3	1:E:99:PRO:HD2	1.84	0.59
1:J:190:ARG:NH2	1:J:220:ARG:HE	2.00	0.59
1:K:98:LEU:HD12	1:K:117:GLN:HB2	1.82	0.59
1:I:36:ILE:O	1:I:38:PRO:HD3	2.02	0.59
1:H:24:PRO:O	1:H:26:TYR:N	2.35	0.59
1:E:190:ARG:CZ	1:E:220:ARG:HE	2.15	0.59
1:J:137:PHE:CZ	1:J:158:LYS:HA	2.37	0.59
1:L:186:ARG:HD3	1:L:202:PHE:HD2	1.67	0.59
1:C:123:THR:HG21	1:C:188:GLN:NE2	2.18	0.59
1:F:137:PHE:CZ	1:F:158:LYS:HA	2.38	0.59
1:C:80:ARG:HG3	1:C:86:GLU:CG	2.32	0.58
1:C:160:LYS:H	1:C:160:LYS:HD3	1.66	0.58
1:H:237:THR:HG23	1:H:239:ILE:H	1.68	0.58
1:C:224:THR:CG2	1:C:248:HIS:HB3	2.33	0.58
1:F:122:VAL:HA	1:F:187:ILE:HG22	1.85	0.58
1:H:125:VAL:HG22	1:H:217:PRO:HD3	1.84	0.58
1:L:47:MET:HA	1:L:47:MET:CE	2.33	0.58
1:I:239:ILE:HG21	1:J:129:LYS:HD3	1.84	0.58
1:D:107:ILE:HD11	1:D:118:VAL:HG21	1.85	0.58
1:A:160:LYS:HD3	1:A:160:LYS:H	1.68	0.58
1:I:98:LEU:HB3	1:I:99:PRO:HD2	1.86	0.58
1:B:162:CYS:HB2	1:B:170:ILE:HD11	1.86	0.58
1:J:36:ILE:O	1:J:38:PRO:HD3	2.04	0.58
1:J:98:LEU:HB3	1:J:99:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:ARG:HE	1:K:220:ARG:NE	2.00	0.58
1:L:190:ARG:CZ	1:L:220:ARG:HE	2.17	0.58
2:X:2:DT:H2"	2:X:3:DT:H5"	1.84	0.58
1:H:195:LYS:O	1:H:198:GLU:HG3	2.04	0.57
1:C:95:PHE:H	1:C:247:ASN:HD21	1.52	0.57
1:E:122:VAL:HA	1:E:187:ILE:HG22	1.85	0.57
1:E:224:THR:HG22	1:E:248:HIS:HB3	1.85	0.57
1:K:49:LEU:HD11	1:K:56:LEU:HD23	1.86	0.57
1:D:41:SER:HB3	1:D:92:HIS:HB2	1.86	0.57
1:D:136:VAL:HG22	1:D:147:ILE:HG12	1.85	0.57
1:I:64:PRO:HB3	1:I:115:LEU:HB2	1.86	0.57
1:J:41:SER:HB3	1:J:92:HIS:HB2	1.86	0.57
1:L:36:ILE:O	1:L:38:PRO:HD3	2.04	0.57
1:L:234:ARG:HD3	1:L:234:ARG:N	2.18	0.57
1:D:224:THR:HG23	1:D:247:ASN:HB3	1.86	0.57
1:G:46:TRP:CZ2	1:G:57:ALA:HB1	2.39	0.57
1:G:61:ILE:HD11	1:G:98:LEU:CD1	2.35	0.57
1:H:125:VAL:CG2	1:H:217:PRO:HD3	2.34	0.57
1:L:95:PHE:O	1:L:224:THR:HG21	2.05	0.57
1:A:18:THR:HB	1:A:22:GLY:HA2	1.87	0.57
1:J:192:GLU:HG2	1:J:193:THR:N	2.20	0.57
1:E:160:LYS:H	1:E:160:LYS:HD3	1.69	0.56
1:G:44:ILE:O	1:G:96:TYR:CE1	2.58	0.56
1:H:98:LEU:HB3	1:H:99:PRO:CD	2.35	0.56
1:J:160:LYS:H	1:J:160:LYS:HD3	1.70	0.56
1:K:182:PHE:C	1:K:182:PHE:CD2	2.78	0.56
1:A:98:LEU:HD12	1:A:117:GLN:HB2	1.86	0.56
1:B:47:MET:HA	1:B:47:MET:HE3	1.86	0.56
1:G:9:ARG:NH1	1:G:55:GLU:HB2	2.15	0.56
1:H:23:ASN:HB3	1:H:25:VAL:HG13	1.87	0.56
1:J:248:HIS:HE1	1:J:250:GLU:HB2	1.69	0.56
1:C:95:PHE:O	1:C:224:THR:HG21	2.05	0.56
1:G:45:ASP:HA	1:G:96:TYR:O	2.04	0.56
2:Y:4:DT:H3'	2:Y:6:DT:H72	1.87	0.56
1:F:41:SER:HB3	1:F:92:HIS:HB2	1.87	0.56
1:I:239:ILE:CG2	1:J:129:LYS:HD3	2.36	0.56
1:A:182:PHE:CD2	1:A:182:PHE:C	2.78	0.56
1:D:182:PHE:C	1:D:182:PHE:CD2	2.78	0.56
1:F:17:TYR:O	1:F:24:PRO:HA	2.06	0.56
1:I:95:PHE:O	1:I:224:THR:HG21	2.06	0.56
1:L:3:ARG:NH1	1:L:73:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:TRP:CE3	1:D:99:PRO:HD3	2.41	0.55
1:E:26:TYR:O	1:E:30:ILE:HG13	2.05	0.55
1:K:24:PRO:O	1:K:26:TYR:N	2.39	0.55
1:A:224:THR:HG22	1:A:248:HIS:HB3	1.88	0.55
1:I:224:THR:HG22	1:I:248:HIS:HB3	1.87	0.55
1:A:24:PRO:O	1:A:26:TYR:N	2.39	0.55
1:B:18:THR:HB	1:B:22:GLY:HA2	1.88	0.55
1:C:230:VAL:HG23	1:C:241:ARG:HB3	1.89	0.55
1:G:46:TRP:HZ2	1:G:57:ALA:O	1.88	0.55
1:G:48:HIS:O	1:G:51:SER:OG	2.23	0.55
1:G:132:VAL:HG13	1:G:132:VAL:O	2.06	0.55
1:A:125:VAL:HG22	1:A:217:PRO:HD3	1.88	0.55
1:E:36:ILE:O	1:E:38:PRO:HD3	2.07	0.55
1:F:95:PHE:H	1:F:247:ASN:ND2	2.05	0.55
1:I:49:LEU:HD11	1:I:56:LEU:HD23	1.88	0.55
1:D:190:ARG:NE	1:D:220:ARG:HE	2.05	0.55
1:G:44:ILE:HG12	1:G:45:ASP:H	1.72	0.55
1:D:95:PHE:H	1:D:247:ASN:HD21	1.54	0.55
1:K:140:LYS:HA	1:K:140:LYS:HE2	1.89	0.55
1:B:36:ILE:O	1:B:38:PRO:HD3	2.07	0.54
1:D:46:TRP:CZ3	1:D:99:PRO:HD3	2.42	0.54
1:E:24:PRO:O	1:E:26:TYR:N	2.39	0.54
1:H:46:TRP:CE2	1:H:57:ALA:HB1	2.41	0.54
1:H:95:PHE:H	1:H:247:ASN:HD21	1.53	0.54
1:A:231:LEU:HD21	1:B:156:LEU:HD22	1.89	0.54
1:C:224:THR:HG22	1:C:248:HIS:HB3	1.87	0.54
1:A:190:ARG:O	1:A:192:GLU:N	2.41	0.54
1:A:162:CYS:HB2	1:A:170:ILE:HD11	1.88	0.54
1:K:119:GLU:HG3	1:K:222:ILE:HG12	1.88	0.54
1:K:199:MET:HG3	1:K:200:PRO:HD2	1.88	0.54
1:K:152:PRO:HB2	1:K:206:ILE:HG21	1.89	0.54
1:L:214:VAL:HG21	1:L:249:ILE:HG21	1.89	0.54
1:D:95:PHE:O	1:D:224:THR:HG21	2.08	0.54
1:I:224:THR:HG23	1:I:247:ASN:HB3	1.90	0.54
1:K:190:ARG:HH21	1:K:220:ARG:NE	2.06	0.54
1:B:85:ARG:HD3	1:G:54:SER:CB	2.38	0.54
1:B:137:PHE:CZ	1:B:158:LYS:HA	2.42	0.54
1:I:151:LYS:HG2	1:I:153:TYR:CZ	2.42	0.54
1:L:137:PHE:CZ	1:L:158:LYS:HA	2.43	0.53
1:C:96:TYR:HB3	1:C:248:HIS:CD2	2.42	0.53
1:K:224:THR:HG23	1:K:247:ASN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LEU:HB3	1:D:99:PRO:HD2	1.90	0.53
1:F:46:TRP:CE2	1:F:57:ALA:HB1	2.44	0.53
1:J:24:PRO:O	1:J:26:TYR:N	2.41	0.53
1:J:224:THR:CG2	1:J:248:HIS:HB3	2.39	0.53
1:K:190:ARG:HH21	1:K:220:ARG:HE	1.56	0.53
1:J:128:ILE:HD11	1:J:213:ASP:HB2	1.90	0.53
1:L:119:GLU:HG3	1:L:222:ILE:HG12	1.91	0.53
1:D:24:PRO:O	1:D:26:TYR:N	2.41	0.53
1:D:98:LEU:HD12	1:D:117:GLN:HB2	1.90	0.53
1:D:234:ARG:O	1:D:235:GLU:HG2	2.09	0.53
1:I:99:PRO:HG2	1:I:100:GLU:H	1.74	0.53
1:B:224:THR:HG22	1:B:248:HIS:HB3	1.91	0.53
1:K:161:LYS:HG3	1:K:166:GLY:O	2.10	0.52
1:L:122:VAL:HA	1:L:187:ILE:HG22	1.90	0.52
1:A:152:PRO:HG3	1:A:208:LEU:HD11	1.91	0.52
1:L:101:THR:HB	1:L:117:GLN:HE21	1.74	0.52
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.90	0.52
1:K:162:CYS:HB2	1:K:170:ILE:HD11	1.91	0.52
2:Y:8:DT:H5"	2:Y:10:DT:C7	2.40	0.52
1:F:40:ARG:O	1:F:91:ILE:HA	2.09	0.52
1:I:152:PRO:HB2	1:I:206:ILE:HD13	1.92	0.52
1:B:234:ARG:O	1:B:235:GLU:HB2	2.09	0.52
1:D:128:ILE:HD11	1:D:213:ASP:HB2	1.90	0.52
1:L:182:PHE:C	1:L:182:PHE:CD2	2.83	0.52
1:J:224:THR:HG23	1:J:247:ASN:HB3	1.92	0.52
1:L:224:THR:CG2	1:L:248:HIS:HB3	2.39	0.52
1:G:49:LEU:HD12	1:G:57:ALA:CB	2.39	0.52
1:G:142:CYS:SG	1:G:144:HIS:HB2	2.50	0.52
1:C:108:GLY:HA3	1:C:110:GLU:OE2	2.10	0.52
1:H:224:THR:HG22	1:H:248:HIS:N	2.25	0.52
1:D:186:ARG:CD	1:D:202:PHE:HD2	2.23	0.52
1:G:190:ARG:NH2	1:G:192:GLU:HG3	2.25	0.52
1:H:209:ASP:HB3	1:H:210:ASP:OD1	2.09	0.52
1:D:13:PHE:CE1	1:D:49:LEU:HA	2.44	0.51
1:E:226:ILE:HD12	1:E:228:ARG:HH21	1.75	0.51
1:J:102:LEU:HD11	1:J:111:HIS:CD2	2.44	0.51
1:J:239:ILE:HD11	1:K:182:PHE:CE1	2.45	0.51
1:C:129:LYS:HE3	2:Z:5:DT:OP2	2.10	0.51
1:C:137:PHE:CZ	1:C:158:LYS:HA	2.45	0.51
1:K:46:TRP:CE2	1:K:57:ALA:HB1	2.45	0.51
1:D:64:PRO:HB3	1:D:115:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:TYR:O	1:F:30:ILE:HG13	2.09	0.51
1:G:102:LEU:HD11	1:G:111:HIS:CD2	2.45	0.51
1:D:162:CYS:HB2	1:D:170:ILE:HD11	1.92	0.51
1:K:248:HIS:HE1	1:K:250:GLU:HB2	1.76	0.51
1:B:64:PRO:HB3	1:B:115:LEU:HB2	1.92	0.51
1:G:248:HIS:HE1	1:G:250:GLU:HB2	1.74	0.51
1:K:243:ILE:HG22	1:K:244:LEU:N	2.25	0.51
1:A:41:SER:HB3	1:A:92:HIS:HB2	1.91	0.51
1:B:98:LEU:HB3	1:B:99:PRO:HD2	1.92	0.51
1:D:248:HIS:HE1	1:D:250:GLU:HB2	1.76	0.51
1:A:224:THR:CG2	1:A:248:HIS:HB3	2.41	0.51
1:E:46:TRP:CE2	1:E:57:ALA:HB1	2.45	0.51
1:G:1:VAL:HG13	1:G:5:GLU:CG	2.41	0.51
1:B:46:TRP:CE2	1:B:57:ALA:HB1	2.45	0.51
1:F:162:CYS:HB2	1:F:170:ILE:HD11	1.92	0.51
1:K:112:ILE:HA	1:K:227:LEU:HD12	1.92	0.51
1:C:68:ILE:HG12	1:C:95:PHE:HE1	1.76	0.51
1:H:95:PHE:H	1:H:247:ASN:ND2	2.09	0.51
1:H:242:LYS:NZ	1:I:127:GLU:OE1	2.44	0.51
2:X:6:DT:C2'	2:X:7:DT:H5"	2.29	0.51
1:C:111:HIS:HB3	1:C:116:ILE:HG21	1.92	0.50
1:A:138:VAL:HG22	1:A:145:GLU:HG2	1.92	0.50
1:C:46:TRP:CE2	1:C:57:ALA:HB1	2.45	0.50
1:K:144:HIS:ND1	1:K:164:GLN:HB2	2.26	0.50
1:D:202:PHE:CD1	1:D:202:PHE:N	2.77	0.50
1:F:103:MET:HB2	1:F:106:ASP:OD2	2.12	0.50
1:F:224:THR:HG22	1:F:248:HIS:HB3	1.93	0.50
1:I:132:VAL:HB	1:I:179:PHE:CE1	2.46	0.50
1:J:102:LEU:HD11	1:J:111:HIS:NE2	2.27	0.50
1:L:224:THR:HG22	1:L:248:HIS:N	2.26	0.50
1:B:71:ALA:O	1:B:75:ILE:HG13	2.11	0.50
1:G:50:ASN:HA	1:G:54:SER:OG	2.12	0.50
1:H:36:ILE:O	1:H:38:PRO:HD3	2.12	0.50
1:I:24:PRO:O	1:I:26:TYR:N	2.45	0.50
1:I:153:TYR:CE1	1:I:154:GLU:HG3	2.46	0.50
1:L:186:ARG:CD	1:L:202:PHE:HD2	2.24	0.50
2:Y:4:DT:H2"	2:Y:5:DT:OP1	2.10	0.50
1:F:36:ILE:HG23	1:F:37:THR:HG22	1.94	0.50
1:F:224:THR:CG2	1:F:248:HIS:HB3	2.42	0.50
1:G:122:VAL:HA	1:G:187:ILE:HG22	1.93	0.50
1:H:153:TYR:CE1	1:H:154:GLU:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:239:ILE:HG21	1:I:129:LYS:HD2	1.93	0.50
1:A:125:VAL:CG2	1:A:217:PRO:HD3	2.41	0.50
1:L:232:GLU:HG2	1:L:233:LYS:H	1.76	0.50
1:I:36:ILE:HG23	1:I:37:THR:HG22	1.93	0.50
1:L:199:MET:HG2	1:L:200:PRO:HD2	1.92	0.50
1:E:102:LEU:HD11	1:E:111:HIS:CD2	2.46	0.50
1:E:194:LEU:HD21	1:E:200:PRO:HA	1.93	0.50
1:D:190:ARG:HE	1:D:220:ARG:HE	1.57	0.50
1:I:160:LYS:H	1:I:160:LYS:HD3	1.76	0.50
1:A:137:PHE:CZ	1:A:158:LYS:HA	2.47	0.49
1:B:24:PRO:O	1:B:26:TYR:N	2.44	0.49
1:G:190:ARG:NE	1:G:220:ARG:HH21	2.10	0.49
1:H:122:VAL:CA	1:H:187:ILE:HG22	2.40	0.49
1:J:182:PHE:C	1:J:182:PHE:CD2	2.85	0.49
1:E:151:LYS:HG2	1:E:153:TYR:CZ	2.47	0.49
1:H:127:GLU:HG2	1:H:128:ILE:N	2.27	0.49
1:I:182:PHE:C	1:I:182:PHE:CD2	2.86	0.49
1:K:160:LYS:HD3	1:K:160:LYS:H	1.76	0.49
1:K:232:GLU:O	1:K:233:LYS:C	2.50	0.49
1:L:17:TYR:O	1:L:24:PRO:HA	2.12	0.49
1:H:132:VAL:HG13	1:H:132:VAL:O	2.12	0.49
1:K:224:THR:HG22	1:K:248:HIS:N	2.27	0.49
1:C:122:VAL:HA	1:C:187:ILE:HG22	1.94	0.49
1:H:223:VAL:HG12	1:H:249:ILE:HG13	1.95	0.49
1:G:160:LYS:H	1:G:160:LYS:HD3	1.76	0.49
1:J:122:VAL:HA	1:J:187:ILE:HG22	1.94	0.49
1:L:132:VAL:O	1:L:132:VAL:HG13	2.12	0.49
1:B:182:PHE:C	1:B:182:PHE:CD2	2.86	0.49
1:I:198:GLU:O	1:I:199:MET:HB2	2.12	0.49
1:J:56:LEU:O	1:J:59:GLU:HB2	2.12	0.49
1:C:237:THR:HB	1:C:238:PRO:HD2	1.95	0.49
1:G:74:ALA:C	1:G:76:GLN:H	2.15	0.49
1:H:208:LEU:O	1:H:211:ILE:HG13	2.13	0.49
1:J:46:TRP:CE2	1:J:57:ALA:HB1	2.47	0.49
1:F:182:PHE:C	1:F:182:PHE:CD2	2.86	0.49
1:H:46:TRP:NE1	1:H:57:ALA:HB1	2.28	0.49
1:F:201:ARG:CG	1:F:201:ARG:NH1	2.72	0.49
1:A:95:PHE:H	1:A:247:ASN:HD21	1.59	0.49
1:C:41:SER:CB	1:C:92:HIS:HB2	2.43	0.49
1:C:162:CYS:HB2	1:C:170:ILE:HD11	1.95	0.49
1:C:248:HIS:HE1	1:C:250:GLU:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:GLU:HG2	1:G:114:LYS:HD2	1.95	0.49
2:Y:8:DT:O2	2:Y:9:DT:H72	2.13	0.49
1:A:190:ARG:HD3	1:A:192:GLU:HG2	1.95	0.48
1:E:162:CYS:HB2	1:E:170:ILE:HD11	1.93	0.48
1:H:129:LYS:O	1:H:182:PHE:HB3	2.12	0.48
1:D:47:MET:HA	1:D:47:MET:CE	2.42	0.48
1:E:237:THR:OG1	1:E:238:PRO:HD2	2.13	0.48
1:D:222:ILE:HD11	1:D:252:VAL:HG11	1.95	0.48
1:I:62:GLU:HA	1:I:114:LYS:HD2	1.95	0.48
1:D:36:ILE:HG23	1:D:37:THR:H	1.78	0.48
1:F:186:ARG:HB2	1:F:204:ASP:OD1	2.12	0.48
1:G:190:ARG:HB3	1:G:192:GLU:HG2	1.96	0.48
1:H:182:PHE:C	1:H:182:PHE:CD2	2.86	0.48
1:I:192:GLU:C	1:I:194:LEU:H	2.16	0.48
1:I:224:THR:CG2	1:I:248:HIS:HB3	2.43	0.48
1:B:15:ARG:HH21	1:B:82:ASP:CG	2.17	0.48
1:D:99:PRO:HG2	1:D:100:GLU:H	1.78	0.48
1:E:209:ASP:HB3	1:E:210:ASP:H	1.47	0.48
1:E:224:THR:HG23	1:E:247:ASN:HB3	1.94	0.48
1:K:190:ARG:NH2	1:K:220:ARG:HE	2.12	0.48
1:B:47:MET:HA	1:B:47:MET:CE	2.43	0.48
1:C:30:ILE:HA	1:C:33:LEU:HD12	1.96	0.48
1:D:186:ARG:HD3	1:D:202:PHE:CD2	2.41	0.48
1:E:248:HIS:HE1	1:E:250:GLU:HB2	1.79	0.48
1:G:11:ALA:O	1:G:14:LEU:HB2	2.13	0.48
1:I:162:CYS:HB2	1:I:170:ILE:HD11	1.95	0.48
1:E:182:PHE:C	1:E:182:PHE:CD2	2.86	0.48
1:F:103:MET:HG2	1:F:189:ASP:OD1	2.13	0.48
1:G:153:TYR:CE1	1:G:154:GLU:HG3	2.49	0.48
1:I:46:TRP:CE3	1:I:99:PRO:HD3	2.49	0.48
1:C:224:THR:HG23	1:C:247:ASN:HB3	1.96	0.47
1:G:63:ASN:N	1:G:64:PRO:HD3	2.29	0.47
1:I:31:THR:C	1:I:33:LEU:H	2.16	0.47
1:I:122:VAL:HA	1:I:187:ILE:HG22	1.95	0.47
1:F:46:TRP:CE3	1:F:99:PRO:HD3	2.49	0.47
1:I:190:ARG:NH1	1:I:220:ARG:HH21	2.12	0.47
1:B:68:ILE:HG12	1:B:95:PHE:HE1	1.78	0.47
1:G:78:VAL:HG12	1:G:78:VAL:O	2.13	0.47
1:L:210:ASP:OD1	1:L:210:ASP:N	2.38	0.47
1:E:137:PHE:CZ	1:E:158:LYS:HA	2.49	0.47
1:F:231:LEU:HB2	1:F:235:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:PRO:HG3	1:C:208:LEU:HD11	1.95	0.47
1:G:182:PHE:C	1:G:182:PHE:CD2	2.87	0.47
1:H:237:THR:OG1	1:H:238:PRO:HD2	2.15	0.47
1:B:233:LYS:HG3	1:B:234:ARG:H	1.80	0.47
1:E:224:THR:CG2	1:E:248:HIS:HB3	2.44	0.47
1:H:101:THR:HB	1:H:117:GLN:HE21	1.79	0.47
1:H:210:ASP:OD1	1:H:210:ASP:N	2.38	0.47
1:I:226:ILE:HD12	1:I:228:ARG:HH21	1.80	0.47
1:K:230:VAL:CG2	1:K:241:ARG:HB3	2.41	0.47
2:Y:3:DT:H3'	2:Y:4:DT:C5'	2.43	0.47
1:J:23:ASN:C	1:J:25:VAL:H	2.18	0.47
1:B:248:HIS:HE1	1:B:250:GLU:HB2	1.80	0.47
1:H:26:TYR:O	1:H:30:ILE:HG13	2.14	0.47
1:L:64:PRO:HB3	1:L:115:LEU:HB2	1.97	0.47
2:X:6:DT:H2"	2:X:7:DT:C5'	2.33	0.47
1:B:224:THR:HG23	1:B:247:ASN:HB3	1.95	0.46
1:C:3:ARG:NH1	1:C:73:ASP:OD2	2.48	0.46
1:K:95:PHE:H	1:K:247:ASN:HD21	1.63	0.46
1:B:99:PRO:HG2	1:B:100:GLU:H	1.80	0.46
1:E:152:PRO:HB2	1:E:206:ILE:HG21	1.98	0.46
1:I:190:ARG:NH2	1:I:220:ARG:HE	2.12	0.46
1:L:224:THR:HG22	1:L:248:HIS:HB3	1.98	0.46
1:L:224:THR:HG23	1:L:247:ASN:HB3	1.97	0.46
1:A:0:SER:HB3	1:G:22:GLY:HA2	1.96	0.46
1:A:172:LEU:HD21	1:F:240:PHE:HZ	1.81	0.46
1:F:46:TRP:CZ3	1:F:99:PRO:HD3	2.50	0.46
1:H:239:ILE:CG2	1:I:129:LYS:HD2	2.45	0.46
1:I:26:TYR:O	1:I:30:ILE:HG13	2.15	0.46
1:K:125:VAL:HG22	1:K:217:PRO:CD	2.45	0.46
1:G:44:ILE:HG22	1:G:96:TYR:HD1	1.79	0.46
1:L:128:ILE:HD11	1:L:213:ASP:HB2	1.98	0.46
1:L:151:LYS:HG3	1:L:152:PRO:HD2	1.98	0.46
1:E:17:TYR:O	1:E:24:PRO:HA	2.16	0.46
1:H:214:VAL:HG21	1:H:249:ILE:CG2	2.45	0.46
1:K:36:ILE:O	1:K:38:PRO:HD3	2.15	0.46
1:B:190:ARG:HB2	1:B:192:GLU:HG2	1.98	0.46
1:C:132:VAL:O	1:C:132:VAL:HG13	2.16	0.46
1:H:64:PRO:HG3	1:H:115:LEU:N	2.30	0.46
1:A:131:PHE:O	1:A:179:PHE:HA	2.16	0.46
1:A:158:LYS:NZ	1:F:235:GLU:O	2.49	0.46
1:B:210:ASP:OD1	1:B:210:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:TYR:HB3	1:C:248:HIS:CG	2.51	0.46
1:F:248:HIS:HE1	1:F:250:GLU:HB2	1.81	0.46
1:H:36:ILE:HG23	1:H:37:THR:HG22	1.97	0.46
1:H:248:HIS:HE1	1:H:250:GLU:HB2	1.81	0.46
1:C:153:TYR:CE1	1:C:154:GLU:HG3	2.51	0.46
1:L:248:HIS:HE1	1:L:250:GLU:HB2	1.81	0.46
1:B:13:PHE:CE1	1:B:49:LEU:HA	2.50	0.46
1:G:1:VAL:HG11	1:G:5:GLU:HG3	1.98	0.46
1:H:137:PHE:CZ	1:H:158:LYS:HA	2.51	0.46
1:L:46:TRP:CE2	1:L:57:ALA:HB1	2.51	0.46
1:L:132:VAL:HG13	1:L:150:GLN:HG3	1.97	0.46
1:L:186:ARG:HD3	1:L:202:PHE:CD2	2.47	0.46
2:Z:3:DT:H3'	2:Z:4:DT:C5'	2.43	0.46
1:A:224:THR:HG22	1:A:248:HIS:N	2.31	0.46
1:C:224:THR:HG22	1:C:248:HIS:N	2.31	0.46
1:L:94:ARG:HG2	1:L:94:ARG:NH1	2.29	0.46
1:L:103:MET:HE2	1:L:105:LYS:HG2	1.98	0.46
1:L:232:GLU:CG	1:L:233:LYS:H	2.29	0.46
1:F:232:GLU:O	1:F:234:ARG:N	2.49	0.45
1:G:61:ILE:HG22	1:G:114:LYS:HB3	1.98	0.45
1:G:233:LYS:CE	2:Y:11:DT:OP2	2.59	0.45
1:K:195:LYS:HG3	1:K:196:GLY:H	1.81	0.45
1:E:23:ASN:C	1:E:25:VAL:H	2.19	0.45
1:J:209:ASP:HB3	1:J:210:ASP:OD1	2.15	0.45
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.96	0.45
1:G:111:HIS:HB3	1:G:116:ILE:HG21	1.99	0.45
1:I:137:PHE:CZ	1:I:158:LYS:HA	2.51	0.45
1:L:95:PHE:H	1:L:247:ASN:ND2	2.14	0.45
1:C:209:ASP:HB3	1:C:210:ASP:H	1.52	0.45
1:E:95:PHE:H	1:E:247:ASN:HD21	1.63	0.45
1:F:95:PHE:O	1:F:224:THR:HG21	2.16	0.45
1:F:224:THR:HG22	1:F:248:HIS:N	2.31	0.45
1:J:198:GLU:HB2	1:J:199:MET:H	1.56	0.45
1:B:15:ARG:NH2	1:B:82:ASP:OD1	2.50	0.45
1:E:103:MET:HE2	1:E:105:LYS:HG2	1.98	0.45
1:G:44:ILE:HD13	1:G:95:PHE:HA	1.99	0.45
1:H:194:LEU:O	1:H:195:LYS:HE2	2.16	0.45
1:J:162:CYS:HB2	1:J:170:ILE:HD11	1.97	0.45
1:J:232:GLU:O	1:J:233:LYS:C	2.54	0.45
1:K:132:VAL:O	1:K:132:VAL:HG13	2.16	0.45
1:K:137:PHE:CZ	1:K:158:LYS:HA	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:O	1:G:55:GLU:HG2	2.17	0.45
1:B:151:LYS:HG3	1:B:152:PRO:HD2	1.99	0.45
1:G:71:ALA:O	1:G:75:ILE:HB	2.17	0.45
1:G:232:GLU:O	1:G:233:LYS:C	2.55	0.45
1:J:151:LYS:HG3	1:J:152:PRO:HD2	1.98	0.45
1:J:224:THR:HG22	1:J:248:HIS:N	2.32	0.45
1:A:132:VAL:O	1:A:132:VAL:HG13	2.17	0.45
1:A:139:CYS:O	1:A:143:GLY:HA2	2.16	0.45
1:A:248:HIS:HE1	1:A:250:GLU:HB2	1.82	0.45
1:B:56:LEU:O	1:B:59:GLU:HB2	2.16	0.45
1:C:95:PHE:H	1:C:247:ASN:ND2	2.14	0.45
1:J:103:MET:HG2	1:J:189:ASP:OD1	2.16	0.45
1:D:238:PRO:HB2	1:E:131:PHE:CE1	2.52	0.45
1:G:74:ALA:C	1:G:76:GLN:N	2.70	0.45
1:L:128:ILE:HG23	1:L:212:VAL:HG11	1.99	0.45
1:E:95:PHE:O	1:E:224:THR:HG21	2.17	0.45
1:G:1:VAL:HG13	1:G:5:GLU:HG3	1.99	0.45
1:G:46:TRP:C	1:G:48:HIS:H	2.20	0.45
1:H:162:CYS:HB2	1:H:170:ILE:HD11	1.98	0.45
1:K:18:THR:HB	1:K:22:GLY:HA2	1.98	0.45
1:K:99:PRO:HG2	1:K:100:GLU:H	1.81	0.45
1:L:41:SER:HA	1:L:91:ILE:CG2	2.44	0.45
1:C:182:PHE:CD2	1:C:183:GLN:N	2.85	0.45
1:C:199:MET:O	1:C:200:PRO:C	2.55	0.45
1:C:231:LEU:CB	1:C:235:GLU:HG2	2.46	0.45
1:I:248:HIS:HE1	1:I:250:GLU:HB2	1.82	0.45
1:J:31:THR:C	1:J:33:LEU:H	2.21	0.45
1:K:95:PHE:O	1:K:224:THR:HG21	2.17	0.45
1:D:195:LYS:O	1:D:198:GLU:HG3	2.16	0.44
1:E:18:THR:HB	1:E:22:GLY:HA2	1.99	0.44
1:G:10:PHE:CD2	1:G:70:ALA:HB3	2.53	0.44
1:G:61:ILE:CD1	1:G:98:LEU:CD1	2.95	0.44
1:L:111:HIS:HB3	1:L:116:ILE:HG21	1.99	0.44
1:H:185:PHE:CZ	1:H:246:VAL:HG21	2.53	0.44
1:I:46:TRP:CZ3	1:I:99:PRO:HD3	2.53	0.44
1:B:95:PHE:H	1:B:247:ASN:HD21	1.63	0.44
1:B:230:VAL:O	1:B:241:ARG:N	2.35	0.44
1:D:71:ALA:O	1:D:74:ALA:HB3	2.18	0.44
1:G:230:VAL:HG23	1:G:241:ARG:HB3	1.99	0.44
1:K:122:VAL:HG22	1:K:187:ILE:HG22	1.99	0.44
1:A:193:THR:O	1:A:194:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ARG:NH1	1:B:73:ASP:OD2	2.50	0.44
1:B:59:GLU:O	1:B:63:ASN:N	2.50	0.44
1:F:3:ARG:NH1	1:F:73:ASP:OD2	2.50	0.44
1:G:27:ARG:HA	1:G:30:ILE:CB	2.48	0.44
1:C:15:ARG:NH2	1:C:82:ASP:OD1	2.50	0.44
1:K:98:LEU:HB3	1:K:99:PRO:CD	2.46	0.44
1:D:47:MET:HA	1:D:47:MET:HE3	2.00	0.44
1:D:137:PHE:CZ	1:D:158:LYS:HA	2.53	0.44
1:G:9:ARG:HB3	1:G:56:LEU:HD22	1.99	0.44
1:D:15:ARG:HH21	1:D:82:ASP:CG	2.21	0.44
1:G:12:ASN:O	1:G:13:PHE:C	2.55	0.44
1:G:197:GLY:HA3	1:H:216:LEU:HD13	2.00	0.44
1:I:209:ASP:HB3	1:I:210:ASP:H	1.50	0.44
1:J:18:THR:HB	1:J:22:GLY:HA2	1.99	0.44
1:F:18:THR:HB	1:F:22:GLY:HA2	1.99	0.44
1:A:15:ARG:NH2	1:A:82:ASP:OD1	2.50	0.44
1:C:98:LEU:HB3	1:C:99:PRO:CD	2.48	0.44
1:D:237:THR:HA	1:D:238:PRO:HD3	1.84	0.44
1:B:152:PRO:HB2	1:B:206:ILE:HG21	2.00	0.43
1:E:46:TRP:CE3	1:E:99:PRO:HD3	2.52	0.43
1:E:151:LYS:HG3	1:E:152:PRO:HD2	1.98	0.43
1:G:52:PHE:HD2	1:G:53:ASP:HB2	1.83	0.43
1:G:98:LEU:O	1:G:99:PRO:C	2.56	0.43
1:I:108:GLY:HA3	1:I:110:GLU:OE2	2.17	0.43
1:B:195:LYS:H	1:B:195:LYS:HD2	1.83	0.43
1:H:2:ASP:OD2	1:H:4:GLU:HG2	2.18	0.43
1:H:46:TRP:CE3	1:H:99:PRO:HD3	2.53	0.43
1:L:31:THR:C	1:L:33:LEU:H	2.22	0.43
1:L:188:GLN:HB2	1:L:201:ARG:O	2.18	0.43
1:B:194:LEU:O	1:B:195:LYS:C	2.57	0.43
1:C:23:ASN:C	1:C:25:VAL:H	2.21	0.43
1:G:3:ARG:NH1	1:G:69:SER:OG	2.51	0.43
1:L:162:CYS:HB2	1:L:170:ILE:HD11	2.00	0.43
1:B:190:ARG:NH1	1:B:220:ARG:HE	2.16	0.43
1:D:152:PRO:HG3	1:D:208:LEU:HD11	2.00	0.43
1:J:71:ALA:O	1:J:75:ILE:HG13	2.19	0.43
2:Y:8:DT:H2"	2:Y:9:DT:OP1	2.17	0.43
1:B:111:HIS:HB3	1:B:116:ILE:HG21	2.00	0.43
1:D:224:THR:HG22	1:D:248:HIS:N	2.34	0.43
1:F:230:VAL:HG23	1:F:241:ARG:HB3	2.00	0.43
1:A:95:PHE:O	1:A:224:THR:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:ILE:HD11	1:F:98:LEU:HD22	2.00	0.43
1:G:224:THR:HG23	1:G:247:ASN:HB3	2.00	0.43
1:H:49:LEU:HG	1:H:57:ALA:HB2	2.01	0.43
1:B:195:LYS:C	1:B:197:GLY:H	2.22	0.43
1:C:194:LEU:HD11	1:C:200:PRO:HA	2.01	0.43
1:D:6:MET:HE1	1:D:67:GLY:HA2	2.00	0.43
1:D:64:PRO:HG3	1:D:115:LEU:N	2.34	0.43
1:G:72:GLU:HG2	1:G:93:ALA:HB3	1.98	0.43
1:H:64:PRO:HB3	1:H:115:LEU:HB2	2.01	0.43
1:J:232:GLU:OE2	1:K:129:LYS:HD3	2.18	0.43
1:K:3:ARG:O	1:K:4:GLU:C	2.57	0.43
1:B:153:TYR:CE1	1:B:154:GLU:HG3	2.53	0.43
1:D:95:PHE:H	1:D:247:ASN:ND2	2.17	0.43
1:I:46:TRP:CE2	1:I:57:ALA:HB1	2.53	0.43
1:I:214:VAL:HG21	1:I:249:ILE:CG2	2.46	0.43
1:J:40:ARG:HA	1:J:91:ILE:HD12	2.00	0.43
1:K:13:PHE:CZ	1:K:26:TYR:CE2	3.06	0.43
1:K:104:VAL:HA	1:K:107:ILE:CD1	2.49	0.43
1:A:46:TRP:CE2	1:A:57:ALA:HB1	2.53	0.43
1:A:56:LEU:O	1:A:59:GLU:HB2	2.19	0.43
1:B:132:VAL:O	1:B:132:VAL:CG1	2.67	0.43
1:F:209:ASP:HB3	1:F:210:ASP:H	1.47	0.43
1:G:129:LYS:O	1:G:182:PHE:HB3	2.19	0.43
1:F:132:VAL:HG13	1:F:132:VAL:O	2.18	0.43
1:F:232:GLU:O	1:F:233:LYS:C	2.57	0.43
1:H:13:PHE:CE1	1:H:49:LEU:HA	2.53	0.43
1:L:61:ILE:HA	1:L:115:LEU:HB3	2.01	0.43
2:X:6:DT:H6	2:X:6:DT:H2'	1.66	0.43
1:D:233:LYS:HG2	1:D:234:ARG:HE	1.83	0.42
1:F:75:ILE:HA	1:F:78:VAL:HG22	2.01	0.42
1:G:70:ALA:C	1:G:72:GLU:H	2.21	0.42
1:K:209:ASP:HB3	1:K:210:ASP:OD1	2.18	0.42
1:A:128:ILE:HD11	1:A:213:ASP:HB2	2.01	0.42
1:I:125:VAL:HG22	1:I:217:PRO:HD3	2.01	0.42
1:L:98:LEU:HB3	1:L:99:PRO:CD	2.47	0.42
1:G:100:GLU:HG3	1:G:100:GLU:O	2.20	0.42
1:G:137:PHE:CZ	1:G:158:LYS:HA	2.54	0.42
1:B:108:GLY:HA3	1:B:110:GLU:OE2	2.18	0.42
1:C:30:ILE:HD13	1:C:78:VAL:HG21	2.01	0.42
1:J:188:GLN:HA	1:J:202:PHE:HA	2.01	0.42
1:K:227:LEU:HD22	1:K:227:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:209:ASP:HB3	1:L:210:ASP:H	1.47	0.42
1:L:209:ASP:HB3	1:L:210:ASP:OD1	2.20	0.42
1:A:214:VAL:HG21	1:A:249:ILE:HG21	2.02	0.42
1:B:224:THR:CG2	1:B:248:HIS:HB3	2.50	0.42
1:C:36:ILE:O	1:C:38:PRO:HD3	2.20	0.42
1:D:3:ARG:NH1	1:D:73:ASP:OD2	2.53	0.42
1:H:231:LEU:N	1:H:231:LEU:HD12	2.35	0.42
1:K:190:ARG:CZ	1:K:220:ARG:HE	2.32	0.42
1:K:224:THR:HG22	1:K:248:HIS:HB3	2.00	0.42
1:A:129:LYS:O	1:A:182:PHE:HB3	2.20	0.42
1:D:182:PHE:CD2	1:D:183:GLN:N	2.88	0.42
1:J:123:THR:HG21	1:J:188:GLN:NE2	2.35	0.42
1:K:40:ARG:O	1:K:91:ILE:HA	2.19	0.42
1:L:214:VAL:HG21	1:L:249:ILE:CG2	2.49	0.42
1:E:46:TRP:NE1	1:E:57:ALA:HB1	2.35	0.42
1:F:153:TYR:OH	1:F:228:ARG:NH1	2.53	0.42
1:K:3:ARG:NH1	1:K:73:ASP:OD2	2.53	0.42
1:L:59:GLU:O	1:L:63:ASN:N	2.52	0.42
1:B:31:THR:C	1:B:33:LEU:H	2.22	0.42
1:B:46:TRP:CE3	1:B:99:PRO:HD3	2.55	0.42
1:C:142:CYS:SG	1:C:144:HIS:HB2	2.60	0.42
1:I:52:PHE:HD2	1:I:53:ASP:HB2	1.84	0.42
1:K:23:ASN:C	1:K:25:VAL:H	2.23	0.42
1:A:13:PHE:CE1	1:A:49:LEU:HA	2.55	0.42
1:C:59:GLU:O	1:C:63:ASN:N	2.53	0.42
1:D:46:TRP:CE2	1:D:57:ALA:HB1	2.55	0.42
1:F:56:LEU:O	1:F:59:GLU:HB2	2.19	0.42
1:H:132:VAL:HB	1:H:179:PHE:CE1	2.54	0.42
1:E:41:SER:HB3	1:E:92:HIS:HB2	2.01	0.41
1:G:128:ILE:HG23	1:G:212:VAL:HG11	2.02	0.41
1:L:50:ASN:OD1	1:L:54:SER:HB2	2.19	0.41
1:D:132:VAL:O	1:D:132:VAL:HG13	2.19	0.41
1:H:94:ARG:NH2	1:H:211:ILE:HG12	2.34	0.41
1:I:152:PRO:HG3	1:I:208:LEU:HD11	2.01	0.41
1:A:192:GLU:HB2	1:A:193:THR:H	1.70	0.41
1:B:104:VAL:HG11	1:B:202:PHE:HA	2.02	0.41
1:C:68:ILE:HG12	1:C:95:PHE:CE1	2.55	0.41
1:D:238:PRO:HB2	1:E:131:PHE:CD1	2.55	0.41
1:E:6:MET:HE1	1:E:67:GLY:HA2	2.02	0.41
1:G:144:HIS:ND1	1:G:164:GLN:HB2	2.36	0.41
1:G:188:GLN:HB3	1:G:202:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:LYS:HA	1:H:130:PRO:HD3	1.88	0.41
1:I:139:CYS:O	1:I:143:GLY:HA2	2.20	0.41
1:J:146:MET:CE	1:J:163:GLU:HB2	2.50	0.41
1:L:132:VAL:O	1:L:150:GLN:HB2	2.20	0.41
1:C:224:THR:HG21	1:C:248:HIS:HB3	2.02	0.41
1:G:119:GLU:HG3	1:G:222:ILE:HG12	2.02	0.41
1:I:56:LEU:O	1:I:59:GLU:HB2	2.20	0.41
1:K:47:MET:HE3	1:K:47:MET:HA	2.02	0.41
1:B:46:TRP:CE3	1:B:47:MET:HE3	2.56	0.41
1:E:107:ILE:HD11	1:E:118:VAL:HG21	2.02	0.41
1:F:111:HIS:HB3	1:F:116:ILE:HG21	2.01	0.41
1:G:191:PRO:HA	1:G:194:LEU:HD12	2.01	0.41
1:H:250:GLU:HA	1:H:251:PRO:HD3	1.93	0.41
1:J:56:LEU:O	1:J:59:GLU:N	2.52	0.41
1:D:102:LEU:HD12	1:D:116:ILE:HD12	2.01	0.41
1:E:141:ASP:OD1	1:E:167:SER:HB2	2.20	0.41
1:H:125:VAL:HG22	1:H:217:PRO:CD	2.50	0.41
2:Y:4:DT:H3'	2:Y:6:DT:C7	2.51	0.41
1:A:23:ASN:C	1:A:25:VAL:H	2.24	0.41
1:E:46:TRP:CZ3	1:E:99:PRO:HD3	2.56	0.41
1:G:6:MET:SD	1:G:66:GLU:HB3	2.61	0.41
1:G:209:ASP:HB3	1:G:210:ASP:H	1.50	0.41
1:H:59:GLU:O	1:H:63:ASN:N	2.54	0.41
1:H:92:HIS:CD2	1:H:210:ASP:OD1	2.74	0.41
1:D:5:GLU:HG2	1:D:9:ARG:HG3	2.02	0.41
1:H:224:THR:CG2	1:H:248:HIS:HB3	2.51	0.41
1:I:235:GLU:O	1:I:235:GLU:HG2	2.20	0.41
1:J:187:ILE:O	1:J:187:ILE:HG13	2.21	0.41
1:K:223:VAL:HG21	1:K:244:LEU:CD2	2.51	0.41
1:C:238:PRO:HD3	1:D:156:LEU:N	2.36	0.41
1:D:31:THR:C	1:D:33:LEU:H	2.24	0.41
1:D:103:MET:O	1:D:104:VAL:C	2.59	0.41
1:G:12:ASN:O	1:G:16:GLU:HG2	2.21	0.41
1:G:44:ILE:HG21	1:G:95:PHE:CA	2.48	0.41
1:J:3:ARG:NH1	1:J:73:ASP:OD2	2.54	0.41
1:J:17:TYR:O	1:J:24:PRO:HA	2.20	0.41
1:K:104:VAL:HA	1:K:107:ILE:HD11	2.03	0.41
1:L:101:THR:HB	1:L:117:GLN:NE2	2.34	0.41
1:L:198:GLU:H	1:L:198:GLU:HG3	1.53	0.41
1:L:202:PHE:N	1:L:202:PHE:CD1	2.89	0.41
1:K:75:ILE:HA	1:K:78:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PRO:HB2	1:A:226:ILE:HD11	2.03	0.40
1:C:231:LEU:HD12	1:C:235:GLU:HB3	2.03	0.40
1:D:224:THR:CG2	1:D:248:HIS:HB3	2.51	0.40
1:D:239:ILE:HG22	1:E:129:LYS:HB2	2.04	0.40
1:E:36:ILE:HG23	1:E:37:THR:HG22	2.02	0.40
1:H:18:THR:HA	1:H:23:ASN:O	2.20	0.40
1:H:209:ASP:HB3	1:H:210:ASP:H	1.50	0.40
1:J:41:SER:CB	1:J:92:HIS:HB2	2.51	0.40
1:A:52:PHE:HD2	1:A:53:ASP:HB2	1.87	0.40
1:A:64:PRO:HB3	1:A:115:LEU:HB2	2.02	0.40
1:B:24:PRO:O	1:B:27:ARG:N	2.49	0.40
1:F:232:GLU:O	1:F:235:GLU:N	2.49	0.40
1:G:12:ASN:HD22	1:G:12:ASN:HA	1.64	0.40
1:I:144:HIS:CE1	1:I:163:GLU:HB3	2.56	0.40
1:J:59:GLU:O	1:J:63:ASN:N	2.54	0.40
1:J:209:ASP:HB3	1:J:210:ASP:H	1.52	0.40
1:L:40:ARG:HA	1:L:91:ILE:HD12	2.03	0.40
1:L:42:VAL:CG2	1:L:75:ILE:HD13	2.51	0.40
1:L:195:LYS:O	1:L:197:GLY:N	2.50	0.40
1:B:46:TRP:NE1	1:B:57:ALA:HB1	2.37	0.40
1:C:232:GLU:O	1:C:233:LYS:C	2.59	0.40
1:I:99:PRO:CG	1:I:100:GLU:H	2.35	0.40
1:L:65:GLU:O	1:L:69:SER:HB2	2.22	0.40
1:C:98:LEU:HD12	1:C:117:GLN:HB2	2.02	0.40
1:F:108:GLY:HA3	1:F:110:GLU:OE2	2.21	0.40
1:H:129:LYS:HE3	2:Y:9:DT:OP2	2.21	0.40
1:K:17:TYR:O	1:K:24:PRO:HA	2.22	0.40
1:B:195:LYS:O	1:B:197:GLY:N	2.54	0.40
1:C:30:ILE:HD13	1:C:78:VAL:CG2	2.52	0.40
1:C:40:ARG:HH11	1:C:209:ASP:CG	2.24	0.40
1:E:111:HIS:HB3	1:E:116:ILE:HG21	2.03	0.40
1:F:103:MET:O	1:F:104:VAL:C	2.60	0.40
1:G:70:ALA:C	1:G:72:GLU:N	2.75	0.40
1:H:224:THR:CG2	1:H:247:ASN:HB3	2.48	0.40
1:K:111:HIS:HB3	1:K:116:ILE:HG21	2.02	0.40
1:L:68:ILE:HG12	1:L:95:PHE:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/257 (98%)	219 (87%)	26 (10%)	8 (3%)	4	26
1	B	253/257 (98%)	219 (87%)	26 (10%)	8 (3%)	4	26
1	C	253/257 (98%)	223 (88%)	25 (10%)	5 (2%)	7	38
1	D	253/257 (98%)	221 (87%)	26 (10%)	6 (2%)	6	34
1	E	253/257 (98%)	220 (87%)	26 (10%)	7 (3%)	5	29
1	F	253/257 (98%)	224 (88%)	24 (10%)	5 (2%)	7	38
1	G	241/257 (94%)	191 (79%)	38 (16%)	12 (5%)	2	16
1	H	253/257 (98%)	227 (90%)	21 (8%)	5 (2%)	7	38
1	I	253/257 (98%)	221 (87%)	26 (10%)	6 (2%)	6	34
1	J	253/257 (98%)	225 (89%)	23 (9%)	5 (2%)	7	38
1	K	253/257 (98%)	218 (86%)	29 (12%)	6 (2%)	6	34
1	L	253/257 (98%)	219 (87%)	27 (11%)	7 (3%)	5	29
All	All	3024/3084 (98%)	2627 (87%)	317 (10%)	80 (3%)	5	31

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	233	LYS
1	B	25	VAL
1	B	233	LYS
1	C	25	VAL
1	C	196	GLY
1	C	233	LYS
1	D	25	VAL
1	E	25	VAL
1	E	196	GLY
1	F	25	VAL
1	F	233	LYS

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Mol	Chain	Res	Type
1	G	36	ILE
1	G	99	PRO
1	G	100	GLU
1	G	233	LYS
1	H	19	ASP
1	H	25	VAL
1	H	233	LYS
1	I	25	VAL
1	I	195	LYS
1	I	199	MET
1	I	233	LYS
1	J	25	VAL
1	J	233	LYS
1	K	25	VAL
1	K	196	GLY
1	K	233	LYS
1	L	25	VAL
1	A	19	ASP
1	A	191	PRO
1	A	192	GLU
1	A	194	LEU
1	B	196	GLY
1	D	19	ASP
1	D	233	LYS
1	D	235	GLU
1	E	195	LYS
1	E	233	LYS
1	F	19	ASP
1	G	35	THR
1	H	196	GLY
1	I	19	ASP
1	J	19	ASP
1	K	19	ASP
1	L	19	ASP
1	L	197	GLY
1	L	231	LEU
1	A	193	THR
1	B	19	ASP
1	C	19	ASP
1	E	19	ASP
1	E	235	GLU
1	G	27	ARG

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Mol	Chain	Res	Type
1	G	54	SER
1	B	89	GLY
1	B	195	LYS
1	B	235	GLU
1	D	232	GLU
1	E	232	GLU
1	G	198	GLU
1	H	99	PRO
1	I	99	PRO
1	L	232	GLU
1	A	89	GLY
1	C	99	PRO
1	G	38	PRO
1	G	62	GLU
1	G	196	GLY
1	K	99	PRO
1	F	89	GLY
1	J	89	GLY
1	J	99	PRO
1	D	99	PRO
1	B	99	PRO
1	K	89	GLY
1	F	99	PRO
1	G	91	ILE
1	L	238	PRO
1	L	196	GLY

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	230/233 (99%)	216 (94%)	14 (6%)	18 54
1	B	230/233 (99%)	215 (94%)	15 (6%)	17 51
1	C	230/233 (99%)	213 (93%)	17 (7%)	13 46
1	D	230/233 (99%)	209 (91%)	21 (9%)	9 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	230/233 (99%)	217 (94%)	13 (6%)	20 56
1	F	230/233 (99%)	215 (94%)	15 (6%)	17 51
1	G	195/233 (84%)	177 (91%)	18 (9%)	9 33
1	H	230/233 (99%)	211 (92%)	19 (8%)	11 40
1	I	230/233 (99%)	216 (94%)	14 (6%)	18 54
1	J	230/233 (99%)	215 (94%)	15 (6%)	17 51
1	K	230/233 (99%)	210 (91%)	20 (9%)	10 37
1	L	230/233 (99%)	211 (92%)	19 (8%)	11 40
All	All	2725/2796 (98%)	2525 (93%)	200 (7%)	14 46

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	25	VAL
1	A	37	THR
1	A	63	ASN
1	A	100	GLU
1	A	101	THR
1	A	151	LYS
1	A	160	LYS
1	A	182	PHE
1	A	190	ARG
1	A	192	GLU
1	A	199	MET
1	A	230	VAL
1	A	252	VAL
1	B	15	ARG
1	B	25	VAL
1	B	37	THR
1	B	47	MET
1	B	63	ASN
1	B	100	GLU
1	B	101	THR
1	B	110	GLU
1	B	151	LYS
1	B	160	LYS
1	B	182	PHE
1	B	194	LEU

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Mol	Chain	Res	Type
1	B	195	LYS
1	B	237	THR
1	B	252	VAL
1	C	15	ARG
1	C	36	ILE
1	C	47	MET
1	C	55	GLU
1	C	63	ASN
1	C	82	ASP
1	C	100	GLU
1	C	101	THR
1	C	110	GLU
1	C	151	LYS
1	C	160	LYS
1	C	182	PHE
1	C	188	GLN
1	C	210	ASP
1	C	230	VAL
1	C	232	GLU
1	C	252	VAL
1	D	2	ASP
1	D	15	ARG
1	D	36	ILE
1	D	37	THR
1	D	47	MET
1	D	63	ASN
1	D	101	THR
1	D	121	ILE
1	D	151	LYS
1	D	182	PHE
1	D	194	LEU
1	D	199	MET
1	D	202	PHE
1	D	210	ASP
1	D	224	THR
1	D	227	LEU
1	D	230	VAL
1	D	231	LEU
1	D	233	LYS
1	D	234	ARG
1	D	252	VAL
1	E	15	ARG

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Mol	Chain	Res	Type
1	E	37	THR
1	E	47	MET
1	E	55	GLU
1	E	63	ASN
1	E	82	ASP
1	E	100	GLU
1	E	160	LYS
1	E	182	PHE
1	E	210	ASP
1	E	234	ARG
1	E	236	LYS
1	E	252	VAL
1	F	2	ASP
1	F	15	ARG
1	F	37	THR
1	F	47	MET
1	F	55	GLU
1	F	63	ASN
1	F	100	GLU
1	F	151	LYS
1	F	182	PHE
1	F	188	GLN
1	F	195	LYS
1	F	201	ARG
1	F	210	ASP
1	F	232	GLU
1	F	252	VAL
1	G	12	ASN
1	G	13	PHE
1	G	45	ASP
1	G	46	TRP
1	G	53	ASP
1	G	55	GLU
1	G	65	GLU
1	G	82	ASP
1	G	96	TYR
1	G	101	THR
1	G	110	GLU
1	G	182	PHE
1	G	192	GLU
1	G	195	LYS
1	G	201	ARG

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Mol	Chain	Res	Type
1	G	210	ASP
1	G	232	GLU
1	G	252	VAL
1	H	2	ASP
1	H	15	ARG
1	H	25	VAL
1	H	37	THR
1	H	41	SER
1	H	47	MET
1	H	63	ASN
1	H	100	GLU
1	H	101	THR
1	H	110	GLU
1	H	121	ILE
1	H	160	LYS
1	H	182	PHE
1	H	190	ARG
1	H	195	LYS
1	H	210	ASP
1	H	224	THR
1	H	234	ARG
1	H	252	VAL
1	I	15	ARG
1	I	37	THR
1	I	63	ASN
1	I	100	GLU
1	I	110	GLU
1	I	151	LYS
1	I	178	SER
1	I	182	PHE
1	I	192	GLU
1	I	210	ASP
1	I	224	THR
1	I	230	VAL
1	I	237	THR
1	I	252	VAL
1	J	15	ARG
1	J	37	THR
1	J	47	MET
1	J	63	ASN
1	J	101	THR
1	J	110	GLU

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Mol	Chain	Res	Type
1	J	160	LYS
1	J	182	PHE
1	J	188	GLN
1	J	195	LYS
1	J	198	GLU
1	J	202	PHE
1	J	210	ASP
1	J	232	GLU
1	J	252	VAL
1	K	15	ARG
1	K	37	THR
1	K	47	MET
1	K	63	ASN
1	K	100	GLU
1	K	101	THR
1	K	103	MET
1	K	110	GLU
1	K	116	ILE
1	K	121	ILE
1	K	151	LYS
1	K	160	LYS
1	K	182	PHE
1	K	190	ARG
1	K	195	LYS
1	K	198	GLU
1	K	201	ARG
1	K	210	ASP
1	K	236	LYS
1	K	252	VAL
1	L	15	ARG
1	L	36	ILE
1	L	37	THR
1	L	47	MET
1	L	63	ASN
1	L	100	GLU
1	L	101	THR
1	L	110	GLU
1	L	160	LYS
1	L	182	PHE
1	L	193	THR
1	L	195	LYS
1	L	198	GLU

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Mol	Chain	Res	Type
1	L	202	PHE
1	L	210	ASP
1	L	224	THR
1	L	230	VAL
1	L	234	ARG
1	L	252	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	B	188	GLN
1	B	247	ASN
1	C	188	GLN
1	C	247	ASN
1	D	247	ASN
1	E	188	GLN
1	E	247	ASN
1	F	188	GLN
1	F	247	ASN
1	G	12	ASN
1	G	48	HIS
1	G	58	HIS
1	G	188	GLN
1	G	247	ASN
1	H	63	ASN
1	H	247	ASN
1	I	12	ASN
1	J	188	GLN
1	J	248	HIS
1	K	188	GLN
1	K	247	ASN
1	L	247	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	255/257 (99%)	0.21	16 (6%) 20 11	65, 120, 219, 325	0
1	B	255/257 (99%)	0.13	8 (3%) 49 32	65, 113, 189, 316	0
1	C	255/257 (99%)	0.11	10 (3%) 39 25	74, 112, 192, 268	0
1	D	255/257 (99%)	0.08	11 (4%) 35 22	67, 112, 200, 251	0
1	E	255/257 (99%)	0.33	14 (5%) 25 14	69, 128, 219, 278	0
1	F	255/257 (99%)	0.02	4 (1%) 72 59	69, 116, 197, 270	0
1	G	249/257 (96%)	0.30	14 (5%) 24 13	75, 136, 219, 279	0
1	H	255/257 (99%)	0.39	22 (8%) 10 5	59, 117, 272, 410	0
1	I	255/257 (99%)	0.40	19 (7%) 14 8	75, 148, 274, 362	0
1	J	255/257 (99%)	0.22	13 (5%) 28 16	71, 119, 214, 329	0
1	K	255/257 (99%)	0.13	6 (2%) 59 44	60, 108, 191, 266	0
1	L	255/257 (99%)	0.14	9 (3%) 44 28	58, 102, 198, 344	0
2	V	4/30 (13%)	0.39	0 100 100	109, 118, 146, 179	0
2	X	7/30 (23%)	0.55	0 100 100	104, 139, 191, 219	0
2	Y	11/30 (36%)	0.47	0 100 100	163, 184, 240, 246	0
2	Z	7/30 (23%)	0.81	1 (14%) 2 1	138, 187, 215, 219	0
All	All	3083/3204 (96%)	0.21	147 (4%) 30 18	58, 119, 224, 410	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	159	VAL	10.6
1	L	253	SER	9.5
1	F	254	LYS	8.9
1	H	158	LYS	8.1
1	K	253	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	F	253	SER	6.8
1	A	24	PRO	6.8
1	I	0	SER	6.7
1	H	170	ILE	6.7
1	H	146	MET	6.2
1	H	147	ILE	6.0
1	H	138	VAL	5.5
1	H	137	PHE	5.4
1	A	16	GLU	5.3
1	B	253	SER	5.2
1	G	0	SER	4.9
1	B	254	LYS	4.9
1	H	160	LYS	4.7
1	D	33	LEU	4.5
1	L	254	LYS	4.4
1	C	253	SER	4.4
1	I	36	ILE	4.4
1	C	254	LYS	4.3
1	I	10	PHE	4.2
1	I	43	ALA	4.2
1	I	164	GLN	4.2
1	I	26	TYR	4.1
1	A	14	LEU	4.1
1	L	160	LYS	4.1
1	I	14	LEU	4.1
1	E	10	PHE	4.0
1	H	169	ASN	4.0
1	L	232	GLU	3.9
1	E	33	LEU	3.8
1	G	25	VAL	3.8
1	I	75	ILE	3.8
1	E	170	ILE	3.7
1	C	60	VAL	3.7
1	J	236	LYS	3.6
1	J	234	ARG	3.6
1	F	172	LEU	3.6
1	J	233	LYS	3.6
1	A	22	GLY	3.4
1	G	198	GLU	3.4
1	A	33	LEU	3.3
1	J	26	TYR	3.2
1	D	14	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	139	CYS	3.2
1	H	171	GLU	3.2
1	D	170	ILE	3.1
1	D	140	LYS	3.1
1	H	78	VAL	3.1
1	E	98	LEU	3.1
1	K	135	ALA	3.0
1	A	26	TYR	3.0
1	B	0	SER	3.0
1	H	145	GLU	3.0
1	G	76	GLN	3.0
1	C	160	LYS	3.0
1	G	26	TYR	3.0
1	L	233	LYS	3.0
1	J	27	ARG	2.9
1	J	31	THR	2.9
1	H	36	ILE	2.9
1	A	23	ASN	2.9
1	G	80	ARG	2.9
1	J	160	LYS	2.9
1	G	160	LYS	2.9
1	I	48	HIS	2.9
1	J	191	PRO	2.9
1	A	17	TYR	2.8
1	I	253	SER	2.8
1	L	0	SER	2.8
1	I	74	ALA	2.8
1	A	1	VAL	2.7
1	B	160	LYS	2.7
1	G	195	LYS	2.7
1	I	77	ILE	2.7
1	C	169	ASN	2.7
1	B	60	VAL	2.6
1	J	232	GLU	2.6
1	H	163	GLU	2.6
1	A	10	PHE	2.6
1	L	36	ILE	2.6
1	D	169	ASN	2.6
1	C	146	MET	2.6
1	K	254	LYS	2.5
1	J	0	SER	2.5
1	B	1	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	78	VAL	2.5
1	G	158	LYS	2.5
1	H	34	LEU	2.5
1	G	27	ARG	2.5
1	I	33	LEU	2.5
1	I	42	VAL	2.5
1	E	243	ILE	2.4
1	A	13	PHE	2.4
1	E	232	GLU	2.4
1	I	160	LYS	2.4
1	L	169	ASN	2.4
1	C	26	TYR	2.4
1	K	78	VAL	2.4
1	B	26	TYR	2.4
1	C	56	LEU	2.4
1	J	235	GLU	2.4
1	C	29	LYS	2.4
1	D	160	LYS	2.4
1	A	42	VAL	2.3
1	K	160	LYS	2.3
2	Z	7	DT	2.3
1	E	70	ALA	2.3
1	E	3	ARG	2.3
1	J	33	LEU	2.3
1	A	25	VAL	2.3
1	I	168	LYS	2.3
1	D	34	LEU	2.3
1	H	14	LEU	2.3
1	A	7	ILE	2.3
1	F	1	VAL	2.3
1	A	52	PHE	2.3
1	I	249	ILE	2.2
1	H	27	ARG	2.2
1	A	20	GLU	2.2
1	E	26	TYR	2.2
1	H	74	ALA	2.2
1	H	10	PHE	2.2
1	H	26	TYR	2.2
1	G	23	ASN	2.2
1	D	164	GLN	2.2
1	E	34	LEU	2.2
1	H	164	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	6	MET	2.1
1	E	7	ILE	2.1
1	D	49	LEU	2.1
1	J	15	ARG	2.1
1	C	158	LYS	2.1
1	I	13	PHE	2.1
1	G	92	HIS	2.1
1	G	22	GLY	2.1
1	D	254	LYS	2.1
1	L	171	GLU	2.1
1	E	78	VAL	2.1
1	K	37	THR	2.1
1	B	231	LEU	2.1
1	E	74	ALA	2.0
1	D	161	LYS	2.0
1	I	172	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	E	301	1/1	0.65	0.11	218,218,218,218	0
3	ZN	F	301	1/1	0.69	0.07	206,206,206,206	0
3	ZN	C	301	1/1	0.80	0.04	188,188,188,188	0
3	ZN	I	301	1/1	0.82	0.12	260,260,260,260	0
3	ZN	D	301	1/1	0.83	0.11	190,190,190,190	0
3	ZN	H	301	1/1	0.91	0.07	311,311,311,311	0
3	ZN	A	301	1/1	0.91	0.21	176,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	L	301	1/1	0.92	0.16	201,201,201,201	0
3	ZN	J	301	1/1	0.94	0.15	169,169,169,169	0
3	ZN	K	301	1/1	0.95	0.12	179,179,179,179	0
3	ZN	G	301	1/1	0.97	0.23	181,181,181,181	0
3	ZN	B	301	1/1	0.99	0.21	159,159,159,159	0

6.5 Other polymers (i)

There are no such residues in this entry.