



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:41 AM GMT

PDB ID : 2DTU
Title : Crystal structure of the beta hairpin loop deletion variant of RB69 gp43 in complex with DNA containing an abasic site analog
Authors : Aller, P.; Hogg, M.; Konigsberg, W.; Wallace, S.S.; Doubie, S.
Deposited on : 2006-07-15
Resolution : 2.37 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

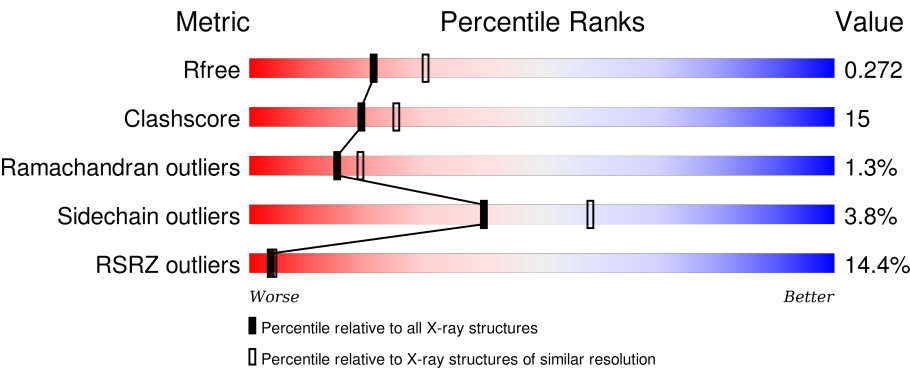
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	E	18	<div><div>6%</div><div>17%</div><div>78%</div><div>6%</div></div>
1	G	18	<div><div>6%</div><div>28%</div><div>56%</div><div>11%</div><div>6%</div></div>
1	I	18	<div><div>6%</div><div>39%</div><div>50%</div><div>6%</div><div>6%</div></div>
1	K	18	<div><div>17%</div><div>28%</div><div>72%</div></div>
2	F	15	<div><div>7%</div><div>13%</div><div>87%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	15	<div><div></div><div>13%</div><div>13%</div><div>80%</div><div>7%</div></div>
2	J	15	<div><div></div><div>20%</div><div>40%</div><div>27%</div><div>13%</div></div>
2	L	15	<div><div></div><div>33%</div><div>100%</div></div>
3	A	896	<div><div></div><div>7%</div><div>74%</div><div>24%</div><div>•</div></div>
3	B	896	<div><div></div><div>18%</div><div>72%</div><div>26%</div><div>•</div></div>
3	C	896	<div><div></div><div>3%</div><div>76%</div><div>21%</div><div>•</div></div>
3	D	896	<div><div></div><div>30%</div><div>57%</div><div>39%</div><div>• •</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32454 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 DNA chain called 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*C P*AP*GP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	G	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	I	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	K	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	J	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	L	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	896	Total	C	N	O	S	0	0	0
			7281	4678	1209	1362	32			
3	B	896	Total	C	N	O	S	0	0	0
			7235	4649	1201	1353	32			
3	C	892	Total	C	N	O	S	0	0	0
			7238	4650	1200	1357	31			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	891	Total	C	N	O	S	0	0	0
			7191	4619	1192	1349	31			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	253	GLY	ILE	ENGINEERED	UNP Q38087
A	?	-	GLU	DELETION	UNP Q38087
A	?	-	ASN	DELETION	UNP Q38087
A	?	-	MET	DELETION	UNP Q38087
A	?	-	TYR	DELETION	UNP Q38087
A	?	-	GLY	DELETION	UNP Q38087
A	?	-	SER	DELETION	UNP Q38087
A	?	-	ARG	DELETION	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
B	222	ALA	ASP	ENGINEERED	UNP Q38087
B	253	GLY	ILE	ENGINEERED	UNP Q38087
B	?	-	GLU	DELETION	UNP Q38087
B	?	-	ASN	DELETION	UNP Q38087
B	?	-	MET	DELETION	UNP Q38087
B	?	-	TYR	DELETION	UNP Q38087
B	?	-	GLY	DELETION	UNP Q38087
B	?	-	SER	DELETION	UNP Q38087
B	?	-	ARG	DELETION	UNP Q38087
B	327	ALA	ASP	ENGINEERED	UNP Q38087
C	222	ALA	ASP	ENGINEERED	UNP Q38087
C	253	GLY	ILE	ENGINEERED	UNP Q38087
C	?	-	GLU	DELETION	UNP Q38087
C	?	-	ASN	DELETION	UNP Q38087
C	?	-	MET	DELETION	UNP Q38087
C	?	-	TYR	DELETION	UNP Q38087
C	?	-	GLY	DELETION	UNP Q38087
C	?	-	SER	DELETION	UNP Q38087
C	?	-	ARG	DELETION	UNP Q38087
C	327	ALA	ASP	ENGINEERED	UNP Q38087
D	222	ALA	ASP	ENGINEERED	UNP Q38087
D	253	GLY	ILE	ENGINEERED	UNP Q38087
D	?	-	GLU	DELETION	UNP Q38087
D	?	-	ASN	DELETION	UNP Q38087
D	?	-	MET	DELETION	UNP Q38087
D	?	-	TYR	DELETION	UNP Q38087

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	DELETION	UNP Q38087
D	?	-	SER	DELETION	UNP Q38087
D	?	-	ARG	DELETION	UNP Q38087
D	327	ALA	ASP	ENGINEERED	UNP Q38087

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	251	Total 251	O 251	0	0
4	B	195	Total 195	O 195	0	0
4	C	272	Total 272	O 272	0	0
4	D	38	Total 38	O 38	0	0
4	E	9	Total 9	O 9	0	0
4	F	10	Total 10	O 10	0	0
4	G	15	Total 15	O 15	0	0
4	H	8	Total 8	O 8	0	0
4	I	31	Total 31	O 31	0	0
4	J	18	Total 18	O 18	0	0
4	K	10	Total 10	O 10	0	0

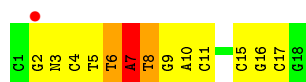
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'



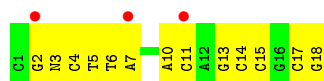
- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

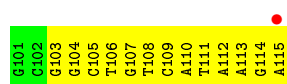


- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

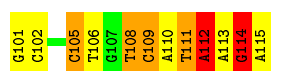
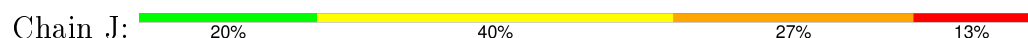




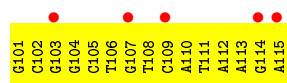
- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'



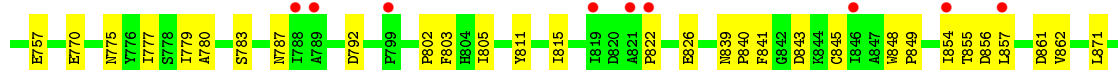
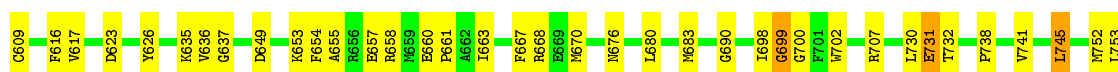
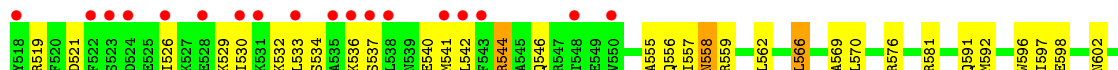
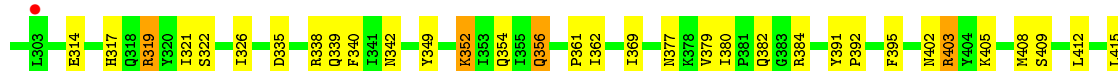
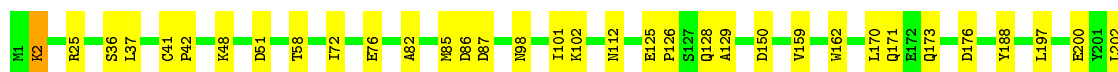
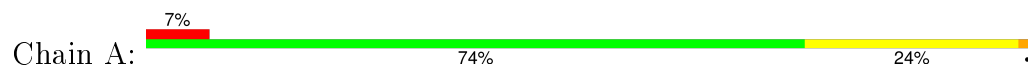
- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

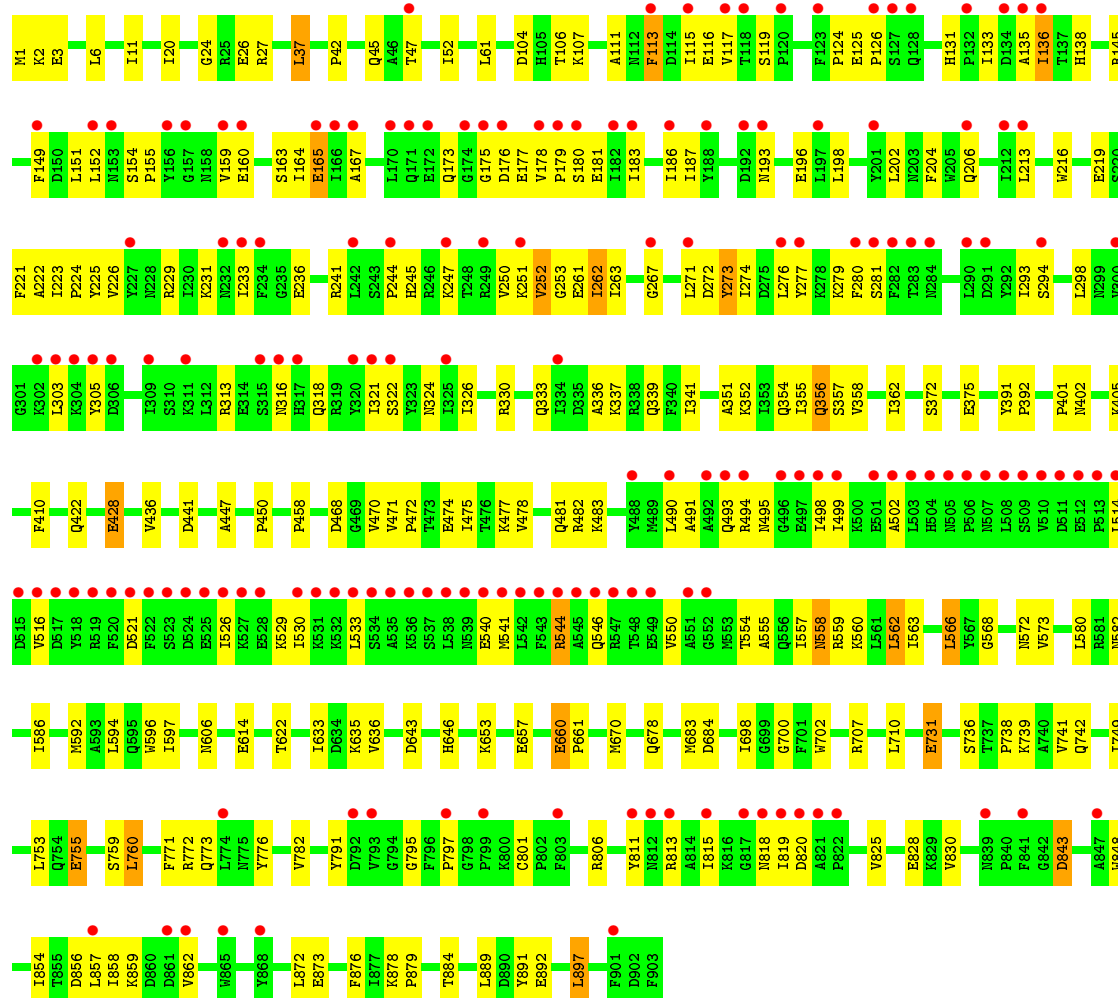


- Molecule 3: DNA polymerase

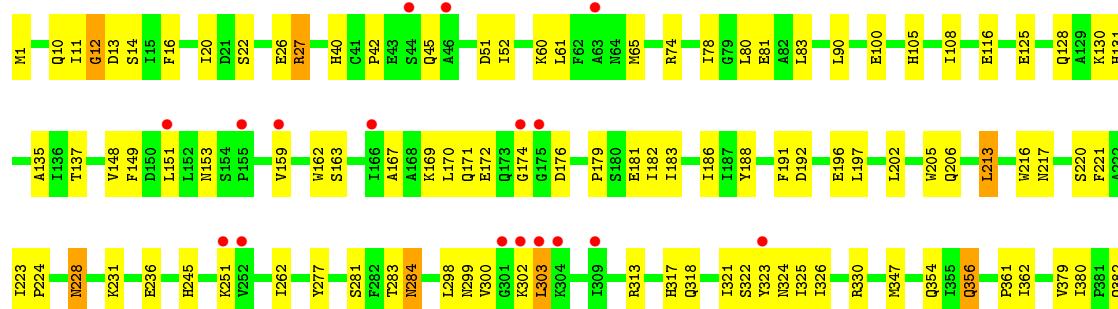
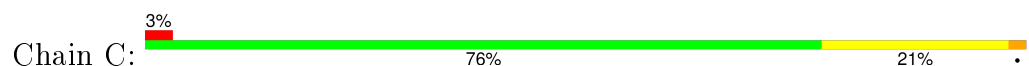


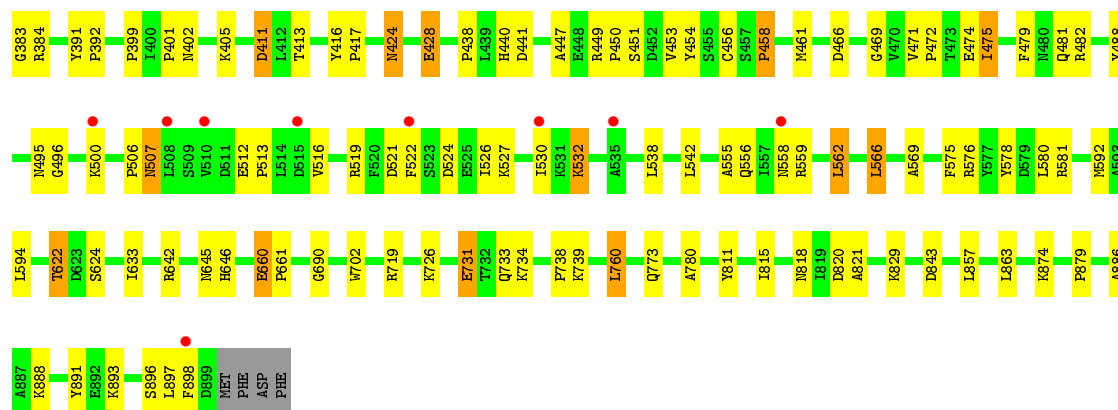


• Molecule 3: DNA polymerase

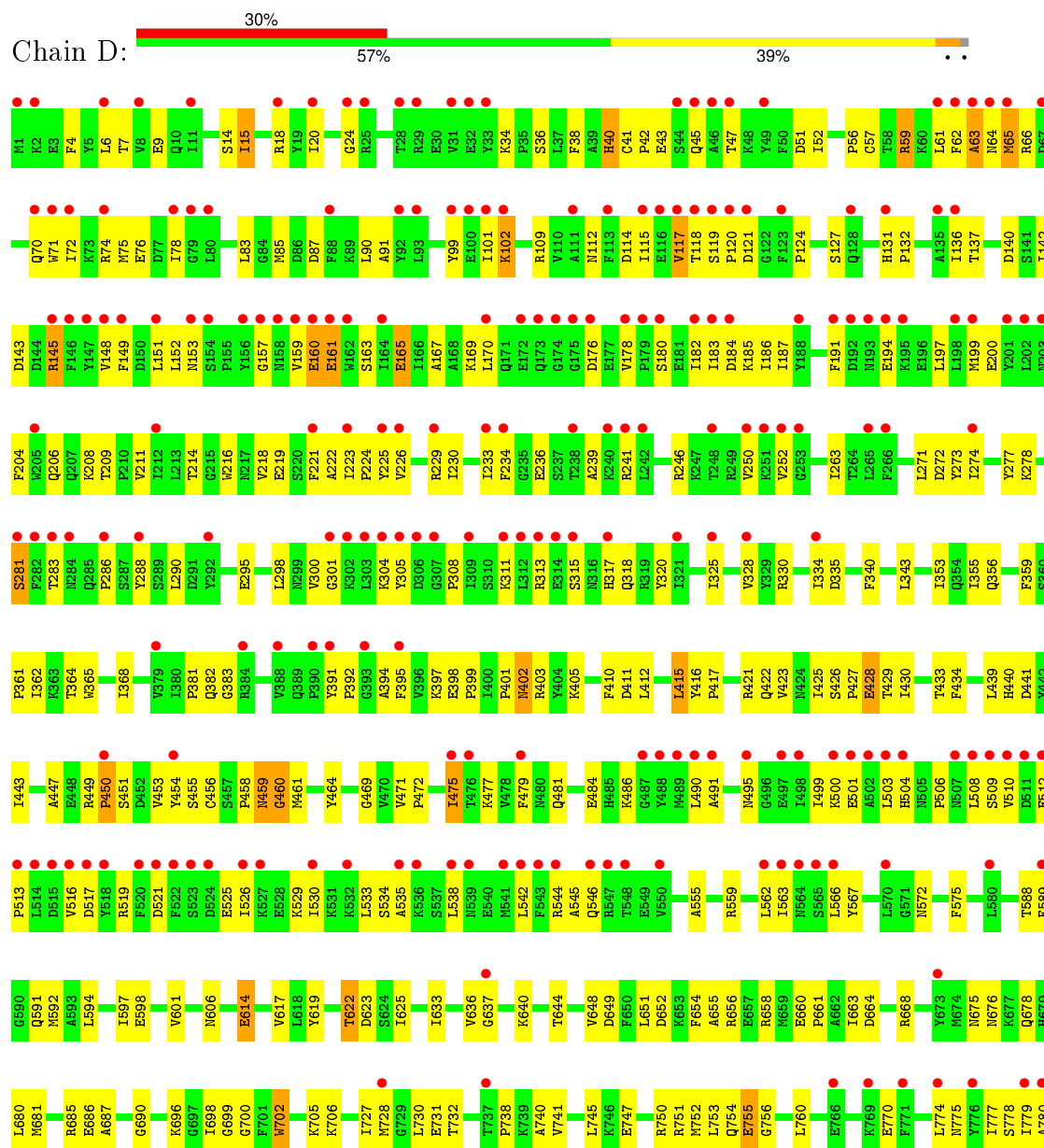


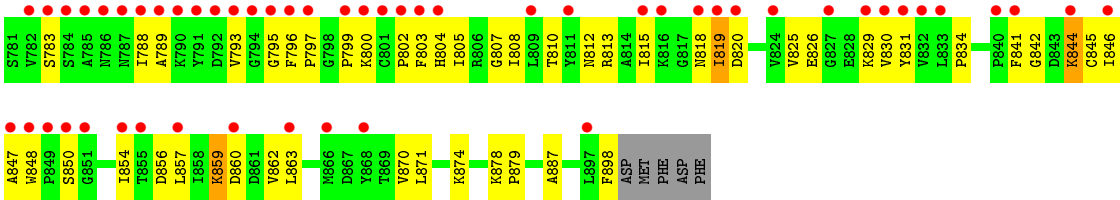
• Molecule 3: DNA polymerase





● Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.07Å 123.06Å 164.56Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	50.00 – 2.37 48.64 – 2.38	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.37) 94.2 (48.64-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.268 0.227 , 0.272	Depositor DCC
R_{free} test set	18819 reflections (9.45%)	DCC
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 396029 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32454	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 3DR

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	E	0.49	0/384	1.35	1/588 (0.2%)
1	G	0.55	0/384	1.44	5/588 (0.9%)
1	I	0.63	0/384	1.42	5/588 (0.9%)
1	K	0.40	0/384	1.26	0/588
2	F	0.42	0/346	1.28	0/533
2	H	0.50	0/346	1.29	1/533 (0.2%)
2	J	0.68	0/346	1.40	6/533 (1.1%)
2	L	0.38	0/346	1.21	0/533
3	A	0.42	0/7461	0.57	0/10092
3	B	0.38	0/7414	0.53	0/10036
3	C	0.41	0/7416	0.57	0/10032
3	D	0.29	0/7369	0.45	0/9980
All	All	0.39	0/32580	0.66	18/44624 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
1	I	0	1
2	J	0	2
All	All	0	5

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6	DT	C4'-C3'-C2'	6.36	108.82	103.10
1	G	7	DA	C4'-C3'-O3'	5.95	124.58	109.70
1	E	7	DA	C4'-C3'-C2'	5.75	108.28	103.10
2	J	109	DC	O4'-C1'-C2'	5.64	110.42	105.90
1	I	7	DA	C4'-C3'-C2'	5.50	108.05	103.10
2	J	111	DT	O4'-C1'-C2'	5.48	110.28	105.90
2	J	114	DG	O4'-C1'-N9	5.38	111.77	108.00
2	H	109	DC	O4'-C1'-N1	5.30	111.71	108.00
1	G	7	DA	C4'-C3'-C2'	5.30	107.87	103.10
2	J	105	DC	C4'-C3'-C2'	5.27	107.84	103.10
1	G	8	DT	C4'-C3'-C2'	5.21	107.79	103.10
1	I	7	DA	C4'-C3'-O3'	5.19	122.69	112.30
1	G	6	DT	C4'-C3'-O3'	5.12	122.54	112.30
1	I	15	DC	C4'-C3'-C2'	5.09	107.68	103.10
1	I	17	DC	O4'-C1'-N1	5.08	111.56	108.00
2	J	108	DT	O4'-C1'-N1	5.02	111.52	108.00
1	I	9	DG	N9-C1'-C2'	5.01	122.12	112.60
2	J	112	DA	C4'-C3'-C2'	5.01	107.61	103.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	7	DA	Sidechain
1	G	7	DA	Sidechain
1	I	7	DA	Sidechain
2	J	112	DA	Sidechain
2	J	114	DG	Sidechain

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	E	355	0	200	17	0
1	G	355	0	200	16	0
1	I	355	0	200	10	0
1	K	355	0	200	18	0
2	F	308	0	170	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	308	0	170	20	0
2	J	308	0	170	21	0
2	L	308	0	170	17	0
3	A	7281	0	7136	177	0
3	B	7235	0	7052	190	0
3	C	7238	0	7101	151	0
3	D	7191	0	7005	289	0
4	A	251	0	0	18	0
4	B	195	0	0	19	0
4	C	272	0	0	18	0
4	D	38	0	0	9	0
4	E	9	0	0	0	0
4	F	10	0	0	1	0
4	G	15	0	0	1	0
4	H	8	0	0	3	0
4	I	31	0	0	1	0
4	J	18	0	0	5	0
4	K	10	0	0	4	0
All	All	32454	0	29774	930	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 15.

All (930) 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)
3:A:85:MET:HE2	3:A:87:ASP:H	1.18	1.03
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.43	1.01
1:G:6:DT:H2'	1:G:7:DA:H5"	1.40	1.00
1:G:6:DT:C2'	1:G:7:DA:H5"	1.91	1.00
2:J:108:DT:H2"	2:J:109:DC:H5"	1.46	0.97
3:B:481:GLN:HE21	3:B:559:ARG:HE	1.13	0.97
3:A:2:LYS:HD2	3:A:2:LYS:H	1.33	0.91
3:D:194:GLU:HG2	3:D:229:ARG:HH21	1.35	0.91
3:C:356:GLN:H	3:C:356:GLN:HE21	1.16	0.89
1:I:3:3DR:H2"	1:I:4:DC:H5'	1.55	0.88
3:A:698:ILE:HG13	3:A:698:ILE:O	1.75	0.87
3:D:112:ASN:HB3	3:D:214:THR:HG23	1.55	0.86
3:D:85:MET:HE2	3:D:87:ASP:H	1.39	0.86
3:B:606:ASN:HD21	3:B:614:GLU:H	1.19	0.86
3:B:499:ILE:HA	3:B:530:ILE:HD11	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:412:LEU:HB2	3:D:623:ASP:HB2	1.58	0.86
3:C:163:SER:H	3:C:318:GLN:HE22	1.23	0.85
3:D:422:GLN:HE22	3:D:681:MET:HG2	1.42	0.83
3:B:115:ILE:HD11	3:B:133:ILE:HG21	1.59	0.83
3:C:74:ARG:HD3	4:C:1164:HOH:O	1.77	0.83
3:D:819:ILE:HG22	3:D:820:ASP:H	1.44	0.82
3:B:261:GLU:HG3	3:B:262:ILE:H	1.44	0.82
3:C:303:LEU:H	3:C:303:LEU:HD22	1.45	0.81
2:H:103:DG:H2''	2:H:104:DG:H5'	1.62	0.81
2:J:110:DA:H2''	2:J:111:DT:H5''	1.64	0.80
3:B:475:ILE:HD13	3:B:566:LEU:HD12	1.63	0.80
3:C:356:GLN:NE2	3:C:356:GLN:H	1.79	0.80
3:D:295:GLU:HG2	3:D:301:GLY:HA2	1.64	0.79
3:C:167:ALA:HA	3:C:176:ASP:HB2	1.66	0.78
3:B:2:LYS:HD3	4:B:1077:HOH:O	1.82	0.78
3:B:481:GLN:NE2	3:B:559:ARG:HE	1.80	0.78
3:D:458:PRO:HB2	3:D:588:THR:HG22	1.64	0.78
3:B:116:GLU:HB2	3:B:135:ALA:HB3	1.64	0.78
2:J:108:DT:H2''	2:J:109:DC:C5'	2.13	0.78
3:D:751:ARG:HA	3:D:755:GLU:HG3	1.66	0.78
3:B:559:ARG:O	3:B:563:ILE:HG12	1.84	0.77
3:A:792:ASP:HB2	4:A:927:HOH:O	1.84	0.77
3:C:302:LYS:HE2	3:C:302:LYS:HA	1.66	0.77
3:A:481:GLN:HE21	3:A:559:ARG:HE	1.33	0.77
3:D:402:ASN:ND2	3:D:403:ARG:H	1.83	0.76
3:C:298:LEU:HB2	3:C:300:VAL:HG12	1.65	0.76
3:C:495:ASN:HD21	3:C:522:PHE:H	1.33	0.76
3:B:897:LEU:H	3:B:897:LEU:HD23	1.51	0.76
3:B:321:ILE:HD12	4:B:1074:HOH:O	1.87	0.75
1:E:6:DT:H2''	1:E:7:DA:H5''	1.69	0.74
3:B:223:ILE:HB	3:B:224:PRO:HD3	1.69	0.74
3:B:273:TYR:HA	3:B:276:LEU:HD12	1.68	0.74
3:C:354:GLN:HB3	3:C:356:GLN:HE22	1.53	0.74
3:C:482:ARG:HE	3:C:556:GLN:HE21	1.36	0.73
3:A:206:GLN:NE2	3:A:241:ARG:HE	1.86	0.73
3:A:699:GLY:N	4:A:998:HOH:O	2.21	0.73
3:B:222:ALA:O	3:B:226:VAL:HG23	1.89	0.73
3:A:602:ASN:HD21	3:A:617:VAL:H	1.35	0.72
3:B:133:ILE:HD11	3:B:198:LEU:HD21	1.70	0.72
3:C:78:ILE:HG13	3:C:80:LEU:HD23	1.71	0.72
3:B:336:ALA:HB3	3:B:337:LYS:HE3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:500:LYS:HA	3:D:503:LEU:HD12	1.71	0.72
3:C:231:LYS:HG3	3:C:236:GLU:HA	1.69	0.72
3:D:740:ALA:HB2	3:D:778:SER:HB3	1.71	0.71
3:B:231:LYS:HG3	3:B:236:GLU:HA	1.72	0.71
3:A:581:ARG:HD3	4:A:1102:HOH:O	1.90	0.71
3:B:273:TYR:HB3	4:B:1083:HOH:O	1.91	0.70
3:D:308:PRO:HG2	3:D:311:LYS:HB2	1.74	0.70
3:C:411:ASP:OD1	3:C:624:SER:HB3	1.91	0.70
3:A:698:ILE:C	4:A:998:HOH:O	2.29	0.70
3:D:298:LEU:HB2	3:D:300:VAL:HG12	1.72	0.70
3:A:698:ILE:O	3:A:753:LEU:HA	1.92	0.69
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.74	0.69
3:D:530:ILE:HA	3:D:533:LEU:HD13	1.73	0.69
1:E:5:DT:H2"	1:E:6:DT:H5'	1.73	0.69
3:C:516:VAL:HG11	3:C:526:ILE:HD13	1.74	0.69
1:E:6:DT:H2"	1:E:7:DA:C5'	2.22	0.69
2:H:112:DA:H2"	2:H:113:DA:H5'	1.74	0.69
3:A:649:ASP:O	3:A:653:LYS:HG2	1.92	0.69
3:A:471:VAL:HB	3:A:472:PRO:HD3	1.75	0.69
3:B:11:ILE:HD13	3:B:247:LYS:HG3	1.74	0.69
3:D:170:LEU:HD12	3:D:170:LEU:H	1.58	0.69
3:D:660:GLU:HG2	4:D:915:HOH:O	1.92	0.68
3:D:399:PRO:HB3	3:D:619:TYR:HD2	1.58	0.68
1:K:5:DT:H2"	1:K:6:DT:H5'	1.74	0.68
3:C:441:ASP:HB3	3:C:447:ALA:HB2	1.74	0.68
3:B:167:ALA:HA	3:B:177:GLU:OE2	1.93	0.68
2:J:108:DT:C2'	2:J:109:DC:H5"	2.21	0.68
1:K:6:DT:H1'	3:D:706:LYS:HE3	1.75	0.68
3:D:530:ILE:HG13	3:D:533:LEU:HD22	1.74	0.68
3:A:775:ASN:OD1	3:A:777:ILE:HG22	1.94	0.68
3:A:540:GLU:O	3:A:544:ARG:HD3	1.93	0.68
3:A:85:MET:HE2	3:A:87:ASP:N	2.03	0.67
1:K:15:DC:H5"	4:K:457:HOH:O	1.94	0.67
1:I:10:DA:H2"	1:I:11:DC:H5"	1.75	0.67
3:D:223:ILE:HB	3:D:224:PRO:HD3	1.74	0.67
3:D:731:GLU:HG3	3:D:879:PRO:HB3	1.75	0.67
3:D:598:GLU:HG3	3:D:617:VAL:HG11	1.76	0.67
4:F:120:HOH:O	3:A:783:SER:HA	1.95	0.67
3:C:526:ILE:HD12	4:C:1045:HOH:O	1.94	0.67
3:A:354:GLN:HB3	3:A:356:GLN:HE22	1.59	0.67
3:D:860:ASP:H	3:D:863:LEU:HD23	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:516:VAL:HG11	3:D:526:ILE:HG21	1.77	0.67
3:A:602:ASN:ND2	3:A:616:PHE:H	1.92	0.66
3:D:830:VAL:HA	3:D:850:SER:HB3	1.78	0.66
3:C:148:VAL:HG13	4:C:1125:HOH:O	1.96	0.66
3:A:72:ILE:O	3:A:76:GLU:HG3	1.95	0.66
3:A:481:GLN:NE2	3:A:559:ARG:HE	1.93	0.66
3:C:81:GLU:HG2	3:C:83:LEU:CD1	2.26	0.66
3:A:526:ILE:HG23	3:A:529:LYS:HD2	1.77	0.65
3:D:738:PRO:HG2	3:D:741:VAL:HB	1.77	0.65
3:B:738:PRO:HG2	3:B:741:VAL:HB	1.77	0.65
1:G:6:DT:H6	1:G:6:DT:H5''	1.62	0.65
3:D:41:CYS:HB2	3:D:45:GLN:HG3	1.78	0.65
2:H:112:DA:H2''	2:H:113:DA:C5'	2.25	0.65
3:D:700:GLY:HA2	3:D:753:LEU:HD22	1.79	0.65
3:D:118:THR:HG21	3:D:313:ARG:HB3	1.79	0.65
3:B:119:SER:HB3	3:B:124:PRO:HD3	1.77	0.65
3:C:283:THR:HB	4:C:1145:HOH:O	1.95	0.65
3:D:606:ASN:HD21	3:D:614:GLU:H	1.45	0.65
2:J:114:DG:H2''	2:J:115:DA:O5'	1.96	0.64
3:D:149:PHE:HB3	3:D:197:LEU:HD21	1.79	0.64
2:F:110:DA:H1'	2:F:111:DT:H5''	1.79	0.64
3:C:277:TYR:O	3:C:281:SER:HB3	1.97	0.64
3:D:398:GLU:OE1	3:D:705:LYS:HE3	1.97	0.64
3:B:540:GLU:HB3	3:B:544:ARG:NH1	2.13	0.64
3:D:512:GLU:HG3	3:D:513:PRO:HD2	1.78	0.64
3:A:848:TRP:HB2	3:A:849:PRO:HD2	1.80	0.64
2:J:110:DA:H2''	2:J:111:DT:C5'	2.28	0.64
3:A:598:GLU:HG3	3:A:617:VAL:HG11	1.79	0.64
1:K:5:DT:H2''	1:K:6:DT:C5'	2.28	0.63
2:F:113:DA:H3'	2:F:114:DG:H5''	1.80	0.63
3:B:52:ILE:HD12	3:B:428:GLU:HG3	1.81	0.63
3:A:653:LYS:O	3:A:657:GLU:HG2	1.98	0.63
3:A:422:GLN:NE2	3:A:680:LEU:H	1.96	0.63
3:A:514:LEU:HD12	3:A:530:ILE:HG12	1.80	0.63
2:J:112:DA:H2'	4:J:405:HOH:O	1.98	0.63
2:F:110:DA:H2''	2:F:111:DT:C5'	2.28	0.63
3:A:2:LYS:CD	3:A:2:LYS:H	2.06	0.62
3:B:606:ASN:ND2	3:B:614:GLU:H	1.95	0.62
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.80	0.62
2:F:103:DG:H2''	2:F:104:DG:H5'	1.82	0.62
3:A:82:ALA:O	3:A:382:GLN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:530:ILE:HG23	3:C:538:LEU:HD21	1.80	0.62
2:H:105:DC:H2'	2:H:106:DT:H72	1.80	0.62
3:C:482:ARG:HH21	3:C:556:GLN:NE2	1.97	0.62
3:D:660:GLU:HB2	3:D:661:PRO:HD3	1.82	0.62
3:C:191:PHE:HD2	3:C:196:GLU:HG3	1.63	0.62
3:A:395:PHE:HB2	3:A:591:GLN:CG	2.25	0.62
3:A:2:LYS:HG2	3:A:102:LYS:HE3	1.81	0.62
3:D:433:THR:HG22	3:D:461:MET:HE1	1.82	0.62
3:B:482:ARG:NH2	3:B:560:LYS:HD3	2.14	0.61
3:D:434:PHE:CZ	3:D:460:GLY:HA2	2.35	0.61
3:C:888:LYS:HE3	4:C:918:HOH:O	1.99	0.61
3:D:362:ILE:HG23	3:D:575:PHE:HD1	1.63	0.61
3:C:1:MET:HG2	3:C:22:SER:O	2.00	0.61
2:J:115:DA:H2'	4:J:414:HOH:O	1.98	0.61
2:H:104:DG:H2''	2:H:105:DC:O5'	2.00	0.61
3:D:230:ILE:HG23	3:D:234:PHE:HD2	1.66	0.61
3:D:51:ASP:HB2	4:D:912:HOH:O	2.01	0.61
2:L:112:DA:H2''	2:L:113:DA:H5'	1.82	0.61
3:B:635:LYS:HG2	3:D:898:PHE:CD2	2.35	0.61
3:D:151:LEU:HD11	3:D:194:GLU:HA	1.83	0.61
3:C:148:VAL:HG22	4:C:1125:HOH:O	2.00	0.61
3:C:401:PRO:O	3:C:402:ASN:HB2	2.01	0.61
3:D:812:ASN:HA	3:D:815:ILE:HG12	1.83	0.61
3:D:859:LYS:HD3	3:D:860:ASP:HB2	1.81	0.61
3:B:514:LEU:HG	3:B:533:LEU:HD21	1.82	0.61
2:F:103:DG:H2'	2:F:104:DG:C8	2.35	0.61
3:C:347:MET:HE3	3:C:562:LEU:HD13	1.81	0.61
3:B:606:ASN:HD21	3:B:614:GLU:N	1.97	0.60
1:K:17:DC:H2''	1:K:18:DG:OP1	2.01	0.60
3:D:286:PRO:O	3:D:829:LYS:HD2	2.01	0.60
1:K:4:DC:H42	2:L:114:DG:H1	1.49	0.60
3:D:401:PRO:HA	3:D:702:TRP:O	2.01	0.60
3:B:202:LEU:O	3:B:206:GLN:HG2	2.01	0.60
3:B:24:GLY:HA3	3:B:107:LYS:HE3	1.83	0.60
3:B:490:LEU:HA	3:B:493:GLN:HG2	1.83	0.60
3:C:169:LYS:HE2	3:C:174:GLY:H	1.66	0.60
3:D:535:ALA:HA	3:D:538:LEU:HB2	1.84	0.60
3:C:424:ASN:HD21	3:C:469:GLY:H	1.48	0.60
3:B:154:SER:HB2	3:B:155:PRO:HD2	1.82	0.60
3:D:140:ASP:HB3	3:D:143:ASP:HB2	1.84	0.60
3:A:176:ASP:HA	3:A:319:ARG:NH2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:271:LEU:HD21	3:D:356:GLN:HA	1.84	0.60
3:B:582:ASN:O	3:B:586:ILE:HG13	2.02	0.60
3:D:87:ASP:OD1	3:D:90:LEU:HD13	2.01	0.60
3:B:825:VAL:HB	3:B:828:GLU:HG3	1.84	0.60
2:J:110:DA:C2'	2:J:111:DT:H5''	2.32	0.60
2:J:101:DG:H2'	2:J:102:DC:C5	2.36	0.60
3:C:815:ILE:HG23	3:C:821:ALA:HB3	1.84	0.60
3:A:441:ASP:HB3	3:A:447:ALA:HB2	1.83	0.59
3:B:391:TYR:HB2	3:B:392:PRO:HD2	1.83	0.59
3:D:416:TYR:HB2	3:D:417:PRO:HD3	1.83	0.59
1:E:5:DT:H2''	1:E:6:DT:C5'	2.32	0.59
3:D:434:PHE:CE1	3:D:460:GLY:HA2	2.37	0.59
3:C:52:ILE:HD12	3:C:428:GLU:HG3	1.82	0.59
3:D:449:ARG:HH21	3:D:675:ASN:HB2	1.65	0.59
3:B:261:GLU:HG3	3:B:262:ILE:N	2.17	0.59
3:D:698:ILE:HG12	3:D:752:MET:O	2.02	0.59
3:D:131:HIS:HB3	3:D:132:PRO:HD2	1.85	0.59
3:A:556:GLN:HE22	3:A:557:ILE:HD13	1.67	0.59
3:A:698:ILE:CA	4:A:998:HOH:O	2.49	0.59
3:B:772:ARG:HG2	4:B:1043:HOH:O	2.03	0.59
3:D:854:ILE:HD12	3:D:859:LYS:HB2	1.85	0.59
3:C:60:LYS:C	4:C:1100:HOH:O	2.41	0.58
3:B:136:ILE:HG23	3:B:149:PHE:HB2	1.84	0.58
3:D:405:LYS:O	3:D:690:GLY:HA2	2.03	0.58
3:D:471:VAL:HB	3:D:472:PRO:HD3	1.86	0.58
3:D:90:LEU:HG	3:D:353:ILE:HG22	1.85	0.58
3:D:102:LYS:HB2	3:D:102:LYS:NZ	2.18	0.58
2:H:110:DA:H2''	2:H:111:DT:O5'	2.02	0.58
2:F:110:DA:H2''	2:F:111:DT:H5'	1.84	0.58
3:C:284:ASN:HD21	3:C:829:LYS:HZ2	1.52	0.58
3:D:503:LEU:O	3:D:506:PRO:HD3	2.04	0.58
3:A:41:CYS:HB2	3:A:42:PRO:HD2	1.84	0.58
3:A:354:GLN:HB3	3:A:356:GLN:NE2	2.17	0.58
3:D:395:PHE:HB2	3:D:591:GLN:HG2	1.86	0.58
3:B:797:PRO:HG3	3:B:806:ARG:NH1	2.19	0.58
3:A:839:ASN:HD22	3:A:841:PHE:HB2	1.69	0.58
3:A:403:ARG:HD2	3:A:887:ALA:O	2.04	0.58
1:I:10:DA:H2''	1:I:11:DC:C5'	2.34	0.58
3:B:470:VAL:O	3:B:474:GLU:HG2	2.04	0.57
3:D:115:ILE:HG22	3:D:136:ILE:HG12	1.86	0.57
3:C:78:ILE:CG1	3:C:80:LEU:HD23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:760:LEU:HD13	3:B:891:TYR:HA	1.87	0.57
3:A:202:LEU:O	3:A:206:GLN:HG2	2.05	0.57
3:B:322:SER:O	3:B:326:ILE:HG12	2.03	0.57
3:C:216:TRP:O	3:C:217:ASN:HB2	2.05	0.57
3:B:339:GLN:HB3	4:B:1056:HOH:O	2.04	0.57
3:A:395:PHE:CB	3:A:591:GLN:HG3	2.26	0.57
3:B:219:GLU:HG2	3:B:262:ILE:HG23	1.86	0.56
3:D:359:PHE:O	3:D:361:PRO:HD3	2.05	0.56
3:B:178:VAL:HB	3:B:179:PRO:HA	1.86	0.56
3:D:236:GLU:HA	3:D:239:ALA:HB3	1.88	0.56
3:D:664:ASP:O	3:D:668:ARG:HG3	2.05	0.56
3:D:698:ILE:O	3:D:753:LEU:HA	2.05	0.56
2:J:101:DG:H2'	2:J:102:DC:C6	2.41	0.56
3:D:405:LYS:O	3:D:699:GLY:HA3	2.05	0.56
3:A:408:MET:HE1	3:A:655:ALA:HB2	1.86	0.56
3:B:279:LYS:HE3	3:B:280:PHE:CZ	2.39	0.56
3:C:302:LYS:HG2	3:C:330:ARG:HH12	1.71	0.56
3:B:897:LEU:HD12	3:D:636:VAL:HG11	1.88	0.56
3:C:159:VAL:HG21	3:C:317:HIS:CD2	2.40	0.56
3:D:696:LYS:O	3:D:756:GLY:HA2	2.05	0.56
1:E:18:DG:H3'	1:E:18:DG:OP1	2.06	0.56
3:D:545:ALA:HB1	4:D:923:HOH:O	2.04	0.56
3:A:402:ASN:HA	3:A:886:ALA:O	2.06	0.56
1:I:7:DA:H2'	1:I:8:DT:H72	1.88	0.56
2:J:111:DT:H2''	2:J:112:DA:H8	1.71	0.56
3:A:362:ILE:HD11	3:A:569:ALA:HA	1.88	0.56
3:A:51:ASP:HA	3:A:379:VAL:HG22	1.87	0.56
3:C:481:GLN:HE21	3:C:559:ARG:HE	1.53	0.56
3:C:507:ASN:HD22	3:C:507:ASN:N	2.04	0.56
4:K:596:HOH:O	3:D:800:LYS:HG3	2.06	0.56
3:D:856:ASP:HA	3:D:859:LYS:HG2	1.88	0.55
3:D:597:ILE:O	3:D:601:VAL:HG23	2.06	0.55
3:A:112:ASN:HB3	4:A:1119:HOH:O	2.05	0.55
3:B:326:ILE:O	3:B:330:ARG:HG2	2.06	0.55
3:A:249:ARG:HB3	3:A:264:THR:HG23	1.89	0.55
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.42	0.55
3:D:805:ILE:HA	3:D:808:ILE:HD12	1.88	0.55
3:C:148:VAL:HG23	3:C:188:TYR:HA	1.88	0.55
3:A:202:LEU:CD1	3:A:242:LEU:HD13	2.36	0.55
2:H:109:DC:H2''	2:H:110:DA:H5'	1.89	0.55
3:A:249:ARG:HH11	3:A:251:LYS:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:272:ASP:OD1	3:D:274:ILE:HG22	2.06	0.55
3:C:303:LEU:HB2	3:C:323:TYR:OH	2.07	0.55
3:C:61:LEU:N	4:C:1100:HOH:O	2.39	0.55
1:G:8:DT:H2'	1:G:9:DG:C8	2.42	0.55
3:D:109:ARG:HB3	3:D:211:VAL:HG23	1.87	0.55
3:D:206:GLN:HE22	3:D:241:ARG:HE	1.55	0.55
3:A:654:PHE:O	3:A:658:ARG:HB2	2.07	0.55
3:D:426:SER:OG	3:D:427:PRO:HD2	2.07	0.55
3:B:336:ALA:CB	3:B:337:LYS:HE3	2.37	0.55
3:D:250:VAL:HG12	3:D:263:ILE:HD12	1.89	0.55
3:A:482:ARG:HE	3:A:556:GLN:HE21	1.54	0.54
3:A:732:THR:HG22	3:A:745:LEU:HB3	1.87	0.54
3:C:475:ILE:HG12	3:C:566:LEU:HD12	1.90	0.54
3:A:223:ILE:HB	3:A:224:PRO:HD3	1.89	0.54
2:F:103:DG:H2''	2:F:104:DG:C5'	2.37	0.54
3:A:482:ARG:HE	3:A:556:GLN:HG2	1.72	0.54
3:A:779:ILE:O	3:A:871:LEU:HD21	2.07	0.54
3:B:2:LYS:HA	4:B:1077:HOH:O	2.07	0.54
3:B:897:LEU:HD23	3:B:897:LEU:N	2.22	0.54
3:C:313:ARG:O	3:C:317:HIS:HB2	2.08	0.54
3:D:66:ARG:HH21	3:D:70:GLN:NE2	2.05	0.54
3:A:25:ARG:HD2	4:A:926:HOH:O	2.08	0.54
3:B:47:THR:HB	4:B:1059:HOH:O	2.08	0.54
3:D:229:ARG:NE	3:D:233:ILE:HD11	2.22	0.54
3:A:555:ALA:O	3:A:559:ARG:HG2	2.08	0.54
3:A:822:PRO:HD2	3:A:855:THR:HB	1.88	0.54
1:G:15:DC:H5''	4:G:515:HOH:O	2.08	0.54
3:D:509:SER:HA	3:D:534:SER:HB3	1.89	0.54
3:D:151:LEU:HD23	3:D:152:LEU:N	2.22	0.54
3:D:4:PHE:HB3	3:D:101:ILE:HG21	1.90	0.54
3:D:216:TRP:H	3:D:218:VAL:HG13	1.73	0.54
3:D:364:THR:O	3:D:368:ILE:HG13	2.08	0.54
3:B:516:VAL:HG11	3:B:526:ILE:HD13	1.89	0.54
3:A:542:LEU:O	3:A:546:GLN:HG3	2.07	0.54
3:B:26:GLU:O	3:B:27:ARG:HG2	2.08	0.54
3:C:469:GLY:C	3:C:472:PRO:HD2	2.29	0.54
1:K:2:DG:C3'	1:K:3:3DR:H5'	2.38	0.54
3:A:222:ALA:O	3:A:226:VAL:HG23	2.08	0.54
3:A:98:ASN:HB3	4:A:1126:HOH:O	2.07	0.54
2:J:105:DC:P	4:J:206:HOH:O	2.66	0.53
2:L:105:DC:H2'	2:L:106:DT:H72	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:DA:H2''	2:F:113:DA:O4'	2.08	0.53
2:H:105:DC:H2'	2:H:106:DT:C7	2.39	0.53
3:D:368:ILE:HD13	3:D:562:LEU:HD21	1.91	0.53
3:D:441:ASP:HB3	3:D:447:ALA:HB2	1.90	0.53
3:C:438:PRO:HD2	3:C:441:ASP:OD1	2.08	0.53
3:D:182:ILE:O	3:D:186:ILE:HG13	2.08	0.53
3:C:354:GLN:HB3	3:C:356:GLN:NE2	2.23	0.53
1:E:6:DT:H2''	1:E:7:DA:O5'	2.08	0.53
3:B:326:ILE:CG2	3:B:330:ARG:HE	2.22	0.53
3:D:241:ARG:HA	3:D:241:ARG:CZ	2.39	0.53
3:B:472:PRO:O	3:B:475:ILE:HG22	2.08	0.53
3:A:284:ASN:HA	3:A:288:TYR:OH	2.08	0.53
3:A:731:GLU:H	3:A:731:GLU:CD	2.10	0.53
3:B:478:VAL:HG13	3:B:559:ARG:HD2	1.90	0.52
3:D:422:GLN:NE2	3:D:681:MET:HG2	2.18	0.52
3:D:397:LYS:O	3:D:399:PRO:HD3	2.09	0.52
3:C:475:ILE:CG1	3:C:566:LEU:HD12	2.38	0.52
3:B:731:GLU:HG3	3:B:879:PRO:CB	2.39	0.52
3:C:299:ASN:HB3	4:C:927:HOH:O	2.07	0.52
3:C:516:VAL:CG1	3:C:526:ILE:HD13	2.39	0.52
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.91	0.52
3:B:250:VAL:HA	3:B:263:ILE:HG22	1.90	0.52
3:C:27:ARG:HB3	3:C:27:ARG:HH11	1.74	0.52
3:B:333:GLN:O	3:B:337:LYS:HG2	2.08	0.52
3:A:507:ASN:HD22	3:A:532:LYS:HA	1.74	0.52
3:A:839:ASN:ND2	3:A:841:PHE:HB2	2.24	0.52
3:B:219:GLU:HA	3:B:223:ILE:HD12	1.90	0.52
3:B:514:LEU:HD13	3:B:526:ILE:HG23	1.90	0.52
3:A:338:ARG:HB3	3:A:340:PHE:CE1	2.44	0.52
3:A:101:ILE:HD11	3:A:349:TYR:O	2.09	0.52
3:D:271:LEU:HD11	3:D:355:ILE:HG22	1.90	0.52
3:A:245:HIS:HE1	4:A:938:HOH:O	1.92	0.52
3:C:874:LYS:HB2	4:C:1151:HOH:O	2.07	0.52
3:B:145:ARG:HD2	3:B:187:ILE:HD11	1.91	0.52
3:A:285:GLN:HB3	3:A:292:TYR:HE2	1.75	0.52
3:B:294:SER:O	3:B:298:LEU:HB2	2.10	0.52
3:D:194:GLU:HG2	3:D:229:ARG:NH2	2.15	0.52
3:D:656:ARG:HA	3:D:660:GLU:HG3	1.91	0.52
3:C:738:PRO:HB3	3:C:780:ALA:O	2.10	0.52
3:C:78:ILE:CD1	3:C:80:LEU:HD23	2.39	0.52
3:C:221:PHE:O	3:C:224:PRO:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:755:GLU:HB3	3:B:759:SER:HB3	1.91	0.52
3:A:609:CYS:HA	3:A:635:LYS:HE3	1.91	0.52
3:C:642:ARG:HH11	3:C:646:HIS:CD2	2.27	0.52
3:C:81:GLU:HG2	3:C:83:LEU:HD11	1.91	0.52
3:D:594:LEU:O	3:D:597:ILE:HG22	2.09	0.52
3:D:36:SER:HB3	3:D:59:ARG:HD3	1.92	0.52
3:B:491:ALA:HA	3:B:494:ARG:HH11	1.73	0.52
3:C:495:ASN:ND2	3:C:522:PHE:H	2.05	0.52
3:D:167:ALA:HB2	3:D:318:GLN:HE22	1.74	0.52
3:D:403:ARG:HD2	3:D:887:ALA:O	2.10	0.51
3:D:148:VAL:HG21	3:D:325:ILE:HD11	1.93	0.51
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.91	0.51
3:A:566:LEU:O	3:A:570:LEU:HD23	2.10	0.51
3:B:316:ASN:C	3:B:318:GLN:H	2.14	0.51
1:E:15:DC:H2''	1:E:16:DG:O5'	2.09	0.51
3:D:863:LEU:HD22	3:D:863:LEU:H	1.74	0.51
3:D:793:VAL:HG22	3:D:796:PHE:O	2.10	0.51
3:B:700:GLY:HA3	3:B:710:LEU:HD23	1.92	0.51
3:B:818:ASN:HD21	3:B:857:LEU:HD11	1.74	0.51
3:D:109:ARG:NH1	3:D:142:ILE:HD11	2.25	0.51
3:A:556:GLN:NE2	3:A:557:ILE:HD13	2.26	0.51
2:J:113:DA:H2''	2:J:114:DG:H5''	1.93	0.51
2:H:114:DG:H2''	2:H:115:DA:C8	2.46	0.51
3:A:356:GLN:NE2	3:A:356:GLN:H	2.08	0.51
3:D:802:PRO:HD2	3:D:805:ILE:HG13	1.92	0.51
3:B:163:SER:H	3:B:318:GLN:HE21	1.57	0.51
3:C:760:LEU:HD13	3:C:891:TYR:HA	1.92	0.51
3:C:284:ASN:HD21	3:C:829:LYS:NZ	2.07	0.51
3:D:475:ILE:O	3:D:475:ILE:HD13	2.10	0.51
3:B:560:LYS:NZ	4:B:1071:HOH:O	2.36	0.51
3:D:517:ASP:OD2	3:D:519:ARG:HB2	2.09	0.51
1:G:7:DA:H2'	1:G:8:DT:H72	1.93	0.51
3:A:698:ILE:O	3:A:698:ILE:CG1	2.54	0.51
3:C:221:PHE:C	3:C:224:PRO:HD2	2.31	0.51
3:D:132:PRO:HG2	4:D:920:HOH:O	2.09	0.51
3:A:730:LEU:HD22	3:A:883:PHE:CE1	2.46	0.50
3:B:356:GLN:O	3:B:357:SER:HB2	2.11	0.50
3:B:450:PRO:HG2	4:B:965:HOH:O	2.09	0.50
3:C:451:SER:HB3	3:C:456:CYS:SG	2.51	0.50
3:C:555:ALA:O	3:C:559:ARG:HG2	2.12	0.50
3:D:273:TYR:OH	3:D:335:ASP:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:PRO:HB3	3:C:181:GLU:OE1	2.10	0.50
3:B:731:GLU:HG3	3:B:879:PRO:HB3	1.93	0.50
3:C:645:ASN:ND2	3:C:719:ARG:HH11	2.09	0.50
3:A:482:ARG:HG2	3:A:482:ARG:HH11	1.76	0.50
3:B:313:ARG:HG2	3:B:313:ARG:HH11	1.77	0.50
3:D:47:THR:HG21	3:D:57:CYS:H	1.75	0.50
3:D:72:ILE:HG22	3:D:76:GLU:OE2	2.11	0.50
3:D:637:GLY:O	3:D:640:LYS:HB2	2.11	0.50
3:D:277:TYR:O	3:D:281:SER:HB2	2.12	0.50
3:D:439:LEU:O	3:D:443:ILE:HG13	2.12	0.50
3:D:197:LEU:O	3:D:197:LEU:HD23	2.12	0.50
3:C:424:ASN:HD22	3:C:472:PRO:HG2	1.77	0.50
3:D:7:THR:HG22	3:D:18:ARG:HB2	1.92	0.50
2:H:109:DC:H2''	2:H:110:DA:C5'	2.42	0.50
3:A:412:LEU:HG	3:A:683:MET:HG2	1.93	0.50
3:D:508:LEU:N	3:D:508:LEU:HD22	2.27	0.50
3:B:499:ILE:HA	3:B:530:ILE:CD1	2.37	0.50
3:C:726:LYS:HE3	4:C:1054:HOH:O	2.12	0.50
3:C:171:GLN:HE22	3:C:303:LEU:HB3	1.77	0.50
2:H:102:DC:H2''	2:H:103:DG:C8	2.46	0.50
3:D:863:LEU:N	3:D:863:LEU:HD22	2.27	0.50
3:A:517:ASP:OD2	3:A:519:ARG:HB2	2.11	0.50
3:D:458:PRO:HG3	3:D:592:MET:SD	2.51	0.50
1:K:11:DC:H4'	3:D:803:PHE:HB2	1.94	0.50
3:D:109:ARG:HD2	3:D:209:THR:O	2.12	0.50
3:A:221:PHE:O	3:A:224:PRO:HD2	2.12	0.50
3:C:496:GLY:O	3:C:500:LYS:HG2	2.12	0.50
2:F:108:DT:H2''	2:F:109:DC:O5'	2.12	0.50
3:D:330:ARG:O	3:D:334:ILE:HG13	2.12	0.50
3:C:302:LYS:HD2	3:C:326:ILE:HD13	1.93	0.50
3:B:356:GLN:C	3:B:358:VAL:H	2.14	0.50
3:A:48:LYS:HZ1	3:A:377:ASN:ND2	2.10	0.50
3:D:542:LEU:O	3:D:546:GLN:HG3	2.11	0.50
3:B:273:TYR:HA	3:B:276:LEU:HB2	1.94	0.49
3:B:660:GLU:HB3	3:B:661:PRO:HD3	1.93	0.49
2:J:112:DA:H2''	2:J:113:DA:H5'	1.94	0.49
3:B:159:VAL:HG13	3:B:313:ARG:HH12	1.78	0.49
3:D:411:ASP:HB2	3:D:686:GLU:OE1	2.11	0.49
3:D:422:GLN:HG3	3:D:678:GLN:O	2.13	0.49
3:C:191:PHE:CD2	3:C:196:GLU:HG3	2.46	0.49
3:B:555:ALA:O	3:B:559:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:322:SER:O	3:C:326:ILE:HG23	2.12	0.49
3:C:300:VAL:HG13	3:C:300:VAL:O	2.11	0.49
2:H:112:DA:C2'	2:H:113:DA:H5'	2.41	0.49
3:C:362:ILE:HD13	3:C:569:ALA:HB1	1.95	0.49
3:B:483:LYS:NZ	3:B:483:LYS:HB3	2.27	0.49
3:A:481:GLN:HE21	3:A:559:ARG:NE	2.07	0.49
3:D:831:TYR:CD1	3:D:850:SER:HA	2.48	0.49
3:D:145:ARG:HG2	3:D:187:ILE:HD11	1.93	0.49
3:D:469:GLY:C	3:D:472:PRO:HD2	2.33	0.49
3:B:707:ARG:HD2	4:B:1050:HOH:O	2.12	0.49
3:D:165:GLU:CD	3:D:165:GLU:H	2.15	0.49
3:A:101:ILE:HG12	4:A:1047:HOH:O	2.12	0.49
3:D:633:ILE:HG13	3:D:651:LEU:HD21	1.94	0.49
3:D:71:TRP:O	3:D:75:MET:HG2	2.12	0.49
3:D:222:ALA:O	3:D:226:VAL:HG23	2.11	0.49
3:D:191:PHE:HB2	3:D:197:LEU:HD12	1.94	0.49
3:A:731:GLU:HG3	3:A:879:PRO:CB	2.43	0.49
1:E:12:DA:H2''	1:E:13:DG:O5'	2.13	0.49
3:C:488:TYR:CD1	3:C:519:ARG:HB3	2.48	0.49
3:B:405:LYS:HA	3:B:698:ILE:O	2.12	0.49
3:A:856:ASP:O	3:A:857:LEU:HB2	2.13	0.49
3:D:313:ARG:HD3	3:D:320:TYR:CE2	2.48	0.48
3:D:362:ILE:HD11	3:D:572:ASN:HD22	1.78	0.48
3:D:204:PHE:HE1	3:D:208:LYS:HD2	1.78	0.48
3:D:509:SER:HA	3:D:534:SER:CB	2.43	0.48
3:B:458:PRO:HG3	3:B:592:MET:SD	2.52	0.48
3:D:727:ILE:HG23	3:D:730:LEU:HD12	1.95	0.48
3:B:303:LEU:HD22	3:B:303:LEU:H	1.78	0.48
1:K:14:DC:H2''	1:K:15:DC:O5'	2.14	0.48
3:A:530:ILE:HA	3:A:533:LEU:HD13	1.95	0.48
3:B:372:SER:O	3:B:375:GLU:HG2	2.13	0.48
3:C:453:VAL:HG23	3:C:454:TYR:CG	2.48	0.48
3:A:405:LYS:O	3:A:690:GLY:HA2	2.14	0.48
3:D:137:THR:HG21	3:D:325:ILE:HA	1.95	0.48
3:A:757:GLU:HB2	3:A:889:LEU:HD22	1.93	0.48
3:C:361:PRO:HG3	4:C:1143:HOH:O	2.12	0.48
3:A:362:ILE:CD1	3:A:569:ALA:HA	2.43	0.48
3:D:813:ARG:NH2	3:D:842:GLY:HA3	2.28	0.48
1:G:2:DG:H5'	1:G:3:3DR:H5'	1.95	0.48
1:G:3:3DR:H2''	1:G:4:DC:O4'	2.13	0.48
2:F:115:DA:H62	3:A:282:PHE:HE2	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ILE:HD12	3:C:16:PHE:CD2	2.48	0.48
3:D:102:LYS:O	3:D:102:LYS:HD3	2.14	0.48
2:L:102:DC:H2''	2:L:103:DG:C8	2.49	0.48
3:B:355:ILE:C	3:B:356:GLN:O	2.51	0.48
1:G:10:DA:H1'	1:G:11:DC:H5'	1.94	0.48
3:A:802:PRO:HG2	3:A:805:ILE:HD12	1.94	0.48
3:B:193:ASN:ND2	3:B:196:GLU:H	2.12	0.48
3:D:300:VAL:O	3:D:300:VAL:HG13	2.14	0.48
3:A:902:ASP:O	3:A:903:PHE:HB2	2.14	0.48
3:D:219:GLU:HG2	3:D:219:GLU:O	2.14	0.48
3:B:124:PRO:HB2	3:B:225:TYR:CE1	2.47	0.48
3:D:450:PRO:HB2	3:D:456:CYS:SG	2.53	0.48
3:C:52:ILE:HB	3:C:428:GLU:HG2	1.95	0.48
3:B:554:THR:O	3:B:557:ILE:HG22	2.14	0.48
3:B:401:PRO:O	3:B:402:ASN:HB2	2.13	0.48
3:D:750:ARG:HG3	3:D:754:GLN:NE2	2.29	0.48
3:C:12:GLY:O	3:C:13:ASP:HB2	2.13	0.48
3:B:45:GLN:HG3	3:B:45:GLN:O	2.14	0.48
3:D:402:ASN:ND2	3:D:403:ARG:N	2.59	0.47
3:C:495:ASN:HD21	3:C:522:PHE:N	2.04	0.47
3:D:503:LEU:HG	3:D:538:LEU:HB3	1.95	0.47
1:K:13:DG:H2''	1:K:14:DC:C6	2.48	0.47
2:H:108:DT:H5''	4:H:575:HOH:O	2.13	0.47
3:C:382:GLN:HG2	3:C:383:GLY:N	2.28	0.47
1:E:4:DC:H2'	1:E:5:DT:H71	1.96	0.47
3:D:41:CYS:CB	3:D:45:GLN:HG3	2.43	0.47
4:K:745:HOH:O	3:D:361:PRO:HD2	2.14	0.47
3:D:38:PHE:CZ	3:D:59:ARG:HG2	2.48	0.47
3:D:481:GLN:HB3	3:D:559:ARG:HE	1.79	0.47
3:D:61:LEU:HD23	3:D:62:PHE:N	2.29	0.47
3:B:354:GLN:HG3	4:B:907:HOH:O	2.14	0.47
2:H:110:DA:H2'	2:H:111:DT:H71	1.96	0.47
3:B:660:GLU:CB	3:B:661:PRO:HD3	2.44	0.47
3:B:277:TYR:O	3:B:281:SER:HB2	2.15	0.47
3:B:164:ILE:HG23	3:B:165:GLU:OE1	2.14	0.47
3:D:52:ILE:HD12	3:D:428:GLU:HG3	1.96	0.47
3:B:164:ILE:HG13	3:B:183:ILE:HD11	1.96	0.47
3:C:202:LEU:O	3:C:206:GLN:HG2	2.14	0.47
3:D:484:GLU:HG2	4:D:927:HOH:O	2.15	0.47
3:A:369:ILE:HG12	3:A:474:GLU:HG2	1.96	0.47
2:H:112:DA:H2''	2:H:113:DA:H5''	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ARG:NH1	3:C:27:ARG:HB3	2.30	0.47
3:A:415:LEU:HD22	3:A:623:ASP:HB3	1.95	0.47
3:D:362:ILE:HD11	3:D:572:ASN:ND2	2.29	0.47
3:C:402:ASN:HA	3:C:886:ALA:O	2.14	0.47
3:B:529:LYS:O	3:B:533:LEU:HG	2.15	0.47
2:J:105:DC:H2'	2:J:106:DT:C6	2.50	0.47
3:B:355:ILE:O	3:B:356:GLN:O	2.32	0.47
3:C:362:ILE:HD12	3:C:575:PHE:HB2	1.96	0.47
3:C:137:THR:OG1	3:C:324:ASN:ND2	2.48	0.47
3:D:423:VAL:HB	3:D:425:ILE:HG13	1.96	0.47
3:C:20:ILE:HD13	3:C:26:GLU:HA	1.97	0.47
1:K:10:DA:OP1	3:D:878:LYS:HG2	2.14	0.47
3:D:455:SER:OG	3:D:676:ASN:HA	2.13	0.47
3:B:272:ASP:OD1	3:B:274:ILE:HG22	2.15	0.47
3:C:731:GLU:CD	3:C:731:GLU:H	2.17	0.47
3:D:819:ILE:HG22	3:D:820:ASP:N	2.23	0.47
2:F:113:DA:H2'	2:F:114:DG:C8	2.50	0.47
3:D:18:ARG:HH12	3:D:209:THR:HB	1.80	0.47
3:B:596:TRP:CE2	3:B:670:MET:HB2	2.50	0.47
3:D:38:PHE:CE2	3:D:59:ARG:HG2	2.49	0.47
1:G:4:DC:H2'	1:G:5:DT:C6	2.50	0.47
3:D:834:PRO:HD2	3:D:871:LEU:HD13	1.97	0.47
3:B:351:ALA:O	3:B:352:LYS:HB2	2.14	0.47
3:D:459:ASN:HD22	3:D:459:ASN:N	2.13	0.47
3:D:180:SER:O	3:D:183:ILE:HG22	2.14	0.47
1:E:7:DA:H2''	1:E:8:DT:C6	2.51	0.46
3:C:231:LYS:HG3	3:C:236:GLU:CA	2.42	0.46
3:A:269:SER:OG	3:A:356:GLN:NE2	2.48	0.46
3:C:83:LEU:HB3	3:C:379:VAL:HG12	1.97	0.46
3:D:810:THR:HG23	3:D:813:ARG:HH21	1.81	0.46
3:C:731:GLU:HA	3:C:734:LYS:HG3	1.98	0.46
3:D:52:ILE:HG12	4:D:912:HOH:O	2.15	0.46
3:D:458:PRO:HG2	3:D:589:PHE:HA	1.96	0.46
1:K:6:DT:O2	3:D:706:LYS:HE3	2.15	0.46
3:C:481:GLN:NE2	3:C:559:ARG:HE	2.12	0.46
3:D:775:ASN:OD1	3:D:777:ILE:HG13	2.14	0.46
3:C:660:GLU:CB	3:C:661:PRO:HD3	2.45	0.46
3:D:412:LEU:HD13	3:D:415:LEU:HD13	1.98	0.46
3:C:303:LEU:CD2	3:C:303:LEU:H	2.23	0.46
1:K:4:DC:H2'	1:K:5:DT:C6	2.51	0.46
3:B:52:ILE:HD12	3:B:428:GLU:CG	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:281:SER:OG	3:D:283:THR:HG22	2.14	0.46
3:B:151:LEU:HD23	3:B:152:LEU:N	2.30	0.46
3:B:252:VAL:HG12	3:B:252:VAL:O	2.16	0.46
3:D:159:VAL:HB	3:D:317:HIS:CD2	2.51	0.46
3:B:362:ILE:HD11	3:B:572:ASN:HB3	1.98	0.46
3:D:191:PHE:HZ	3:D:200:GLU:HG2	1.81	0.46
3:C:284:ASN:ND2	3:C:829:LYS:HZ2	2.12	0.46
3:C:458:PRO:HG3	3:C:592:MET:SD	2.55	0.46
3:A:494:ARG:HD2	3:A:521:ASP:OD1	2.16	0.46
3:A:247:LYS:HG3	3:A:266:PHE:CD1	2.50	0.46
3:B:633:ILE:O	3:B:636:VAL:HG22	2.15	0.46
3:A:263:ILE:N	3:A:263:ILE:HD12	2.31	0.46
3:A:241:ARG:NE	4:A:1105:HOH:O	2.49	0.46
3:D:512:GLU:CG	3:D:513:PRO:HD2	2.44	0.46
3:B:514:LEU:HB2	3:B:541:MET:HE3	1.97	0.46
3:A:566:LEU:HD13	3:A:570:LEU:HD23	1.98	0.46
3:D:391:TYR:HB2	3:D:392:PRO:HD2	1.97	0.46
3:C:594:LEU:HD22	3:C:622:THR:O	2.16	0.46
3:B:791:TYR:CD2	3:B:801:CYS:HA	2.50	0.46
3:C:170:LEU:HD23	4:C:1112:HOH:O	2.15	0.46
3:A:206:GLN:HE21	3:A:241:ARG:HE	1.63	0.46
3:D:41:CYS:SG	3:D:45:GLN:HG3	2.56	0.46
3:B:494:ARG:HG3	3:B:495:ASN:N	2.30	0.46
3:B:568:GLY:HA3	4:B:1016:HOH:O	2.16	0.46
1:K:13:DG:H2"	1:K:14:DC:H6	1.81	0.46
3:D:206:GLN:NE2	3:D:241:ARG:HE	2.13	0.46
3:A:811:TYR:O	3:A:815:ILE:HG12	2.16	0.46
3:C:893:LYS:HE3	4:C:1134:HOH:O	2.16	0.46
3:D:430:ILE:HG22	4:D:936:HOH:O	2.16	0.46
3:D:807:GLY:HA2	3:D:845:CYS:O	2.15	0.46
3:A:129:ALA:HA	3:A:225:TYR:CE1	2.51	0.46
1:K:10:DA:H2"	1:K:11:DC:O5'	2.15	0.46
3:D:453:VAL:HG23	3:D:454:TYR:CD2	2.51	0.46
1:G:6:DT:C3'	1:G:7:DA:H5"	2.46	0.45
3:D:544:ARG:HH11	3:D:544:ARG:HG3	1.81	0.45
3:A:86:ASP:OD1	3:A:86:ASP:N	2.49	0.45
3:A:636:VAL:O	3:A:636:VAL:HG12	2.16	0.45
3:A:352:LYS:CE	4:A:1069:HOH:O	2.63	0.45
2:J:113:DA:H2'	4:J:629:HOH:O	2.17	0.45
3:D:516:VAL:HG11	3:D:526:ILE:CG2	2.46	0.45
3:D:145:ARG:HG3	3:D:185:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:625:ILE:O	3:D:625:ILE:HG13	2.16	0.45
3:D:34:LYS:HG3	3:D:64:ASN:HA	1.98	0.45
3:B:471:VAL:N	3:B:472:PRO:HD2	2.31	0.45
3:B:231:LYS:HG3	3:B:236:GLU:CA	2.43	0.45
3:D:398:GLU:HA	3:D:705:LYS:HE2	1.98	0.45
3:B:180:SER:O	3:B:183:ILE:HG22	2.16	0.45
3:D:644:THR:O	3:D:648:VAL:HG23	2.17	0.45
3:D:422:GLN:NE2	3:D:680:LEU:H	2.13	0.45
3:D:295:GLU:CG	3:D:301:GLY:HA2	2.42	0.45
3:A:533:LEU:HB3	3:A:537:SER:OG	2.16	0.45
3:D:451:SER:HB3	3:D:456:CYS:SG	2.56	0.45
3:B:494:ARG:HG3	3:B:495:ASN:ND2	2.32	0.45
3:C:149:PHE:N	3:C:149:PHE:CD1	2.84	0.45
3:C:558:ASN:HD22	3:C:558:ASN:HA	1.66	0.45
1:G:6:DT:C2'	1:G:7:DA:C5'	2.80	0.45
2:F:104:DG:H2''	2:F:105:DC:O5'	2.15	0.45
3:B:251:LYS:HG3	3:B:252:VAL:H	1.82	0.45
3:D:429:THR:O	3:D:464:TYR:HD1	1.99	0.45
2:H:103:DG:H2''	2:H:104:DG:C5'	2.40	0.45
3:D:439:LEU:HD11	3:D:592:MET:HB2	1.98	0.45
3:D:738:PRO:HB3	3:D:780:ALA:C	2.36	0.45
3:D:738:PRO:HB3	3:D:780:ALA:O	2.17	0.45
3:D:85:MET:HG2	3:D:91:ALA:HB2	1.99	0.45
3:B:684:ASP:HB2	4:B:1051:HOH:O	2.16	0.45
3:B:771:PHE:CE2	3:B:872:LEU:HB2	2.52	0.45
3:D:433:THR:CG2	3:D:461:MET:HE1	2.47	0.45
3:D:800:LYS:N	3:D:800:LYS:HD2	2.32	0.45
3:A:745:LEU:HD13	3:A:876:PHE:CD1	2.52	0.45
3:B:573:VAL:HG13	4:B:989:HOH:O	2.16	0.45
3:B:749:ILE:O	3:B:753:LEU:HG	2.17	0.45
3:D:365:TRP:CE2	3:D:566:LEU:HD23	2.52	0.45
3:B:273:TYR:HE2	3:B:341:ILE:HG12	1.82	0.45
3:D:830:VAL:HG22	3:D:831:TYR:N	2.31	0.45
1:I:7:DA:H2'	1:I:8:DT:C7	2.46	0.45
3:A:802:PRO:CG	3:A:805:ILE:HD12	2.48	0.45
3:C:405:LYS:O	3:C:690:GLY:HA2	2.17	0.45
3:D:278:LYS:HG2	3:D:288:TYR:CE2	2.52	0.45
3:D:112:ASN:HB3	3:D:214:THR:CG2	2.38	0.44
3:B:472:PRO:HA	3:B:475:ILE:HG22	1.99	0.44
3:C:302:LYS:CG	3:C:330:ARG:HH12	2.28	0.44
3:D:655:ALA:O	3:D:660:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:119:SER:HB2	3:B:124:PRO:HB3	1.99	0.44
2:L:111:DT:H2''	2:L:112:DA:C8	2.52	0.44
3:B:339:GLN:HB2	4:B:1092:HOH:O	2.16	0.44
3:B:104:ASP:OD1	3:B:106:THR:OG1	2.31	0.44
3:B:546:GLN:O	3:B:550:VAL:HG23	2.16	0.44
2:H:113:DA:H5'	4:H:758:HOH:O	2.15	0.44
3:A:653:LYS:HD3	4:A:1043:HOH:O	2.17	0.44
1:K:13:DG:H2''	1:K:14:DC:O5'	2.15	0.44
3:D:4:PHE:HB3	3:D:101:ILE:CG2	2.48	0.44
2:L:108:DT:H2''	2:L:109:DC:O5'	2.17	0.44
3:A:231:LYS:O	3:A:234:PHE:O	2.35	0.44
1:K:6:DT:H2''	1:K:7:DA:O5'	2.18	0.44
2:L:114:DG:H2''	2:L:115:DA:O5'	2.17	0.44
1:I:7:DA:H2''	1:I:8:DT:C6	2.53	0.44
3:D:486:LYS:O	3:D:490:LEU:HG	2.18	0.44
3:C:130:LYS:HG3	3:C:131:HIS:N	2.31	0.44
3:B:3:GLU:HG3	3:B:20:ILE:O	2.18	0.44
3:D:20:ILE:HD11	3:D:24:GLY:HA2	1.99	0.44
2:F:105:DC:H2'	2:F:106:DT:H72	1.99	0.44
3:D:109:ARG:HH12	3:D:142:ILE:HD11	1.83	0.44
3:D:6:LEU:HB2	3:D:18:ARG:O	2.17	0.44
3:A:745:LEU:HD12	3:A:745:LEU:HA	1.83	0.44
3:D:779:ILE:O	3:D:871:LEU:HD21	2.17	0.44
3:A:698:ILE:HG12	3:A:752:MET:O	2.17	0.44
3:D:652:ASP:OD1	3:D:656:ARG:NH1	2.46	0.44
3:B:6:LEU:CD1	3:B:26:GLU:HG3	2.48	0.44
2:L:101:DG:H2''	2:L:102:DC:C6	2.53	0.44
3:D:163:SER:HB3	3:D:165:GLU:OE1	2.17	0.44
3:D:566:LEU:C	3:D:566:LEU:HD13	2.37	0.44
3:A:506:PRO:HG3	4:A:1153:HOH:O	2.16	0.44
3:C:125:GLU:HG3	4:C:1142:HOH:O	2.17	0.44
2:F:113:DA:H3'	2:F:114:DG:C5'	2.45	0.44
3:B:876:PHE:O	3:B:879:PRO:HG2	2.18	0.44
3:D:841:PHE:CZ	3:D:862:VAL:HG22	2.52	0.44
3:C:818:ASN:ND2	3:C:857:LEU:HD11	2.32	0.44
2:L:115:DA:H2''	3:D:567:TYR:HD2	1.82	0.44
3:B:326:ILE:HG23	3:B:330:ARG:HE	1.81	0.44
3:A:101:ILE:HD12	3:A:349:TYR:HD1	1.83	0.44
3:C:197:LEU:C	3:C:197:LEU:HD23	2.38	0.44
3:A:277:TYR:C	3:A:279:LYS:H	2.20	0.44
3:D:731:GLU:HG3	3:D:879:PRO:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:338:ARG:HB3	3:A:340:PHE:CD1	2.53	0.44
3:A:322:SER:O	3:A:326:ILE:HG12	2.16	0.44
3:C:512:GLU:HB3	3:C:513:PRO:HD2	1.99	0.44
3:D:844:LYS:N	3:D:844:LYS:HD3	2.33	0.44
3:D:40:HIS:ND1	3:D:83:LEU:HD11	2.32	0.44
3:D:783:SER:O	3:D:829:LYS:HB3	2.17	0.44
3:D:63:ALA:HB3	3:D:66:ARG:HG2	1.99	0.44
1:E:14:DC:H2'	1:E:15:DC:C5	2.53	0.44
3:B:594:LEU:O	3:B:597:ILE:HG22	2.18	0.44
3:B:811:TYR:O	3:B:815:ILE:HG12	2.17	0.44
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.99	0.44
3:D:525:GLU:O	3:D:529:LYS:HG3	2.17	0.44
1:G:7:DA:H2'	1:G:8:DT:C7	2.48	0.43
1:E:8:DT:H4'	3:A:707:ARG:CD	2.47	0.43
3:D:178:VAL:HG11	3:D:186:ILE:HD11	1.99	0.43
3:A:48:LYS:NZ	3:A:377:ASN:CG	2.71	0.43
1:G:10:DA:H2''	1:G:11:DC:O5'	2.18	0.43
1:G:16:DG:H2''	1:G:17:DC:O5'	2.18	0.43
3:B:858:ILE:O	3:B:862:VAL:HG23	2.17	0.43
3:A:85:MET:HE3	3:A:576:ARG:NH2	2.33	0.43
3:D:530:ILE:O	3:D:533:LEU:HB2	2.18	0.43
3:C:186:ILE:HG23	4:C:1125:HOH:O	2.18	0.43
3:D:597:ILE:HD11	3:D:663:ILE:HG23	2.00	0.43
3:B:42:PRO:HG2	3:B:45:GLN:HG2	2.00	0.43
3:D:14:SER:HA	3:D:65:MET:HG2	1.99	0.43
3:C:10:GLN:HG3	3:C:65:MET:CE	2.48	0.43
3:D:495:ASN:O	3:D:499:ILE:HG13	2.18	0.43
3:A:36:SER:O	3:A:37:LEU:HD23	2.18	0.43
3:C:251:LYS:HB2	3:C:262:ILE:HG13	1.99	0.43
3:C:380:ILE:HD12	3:C:576:ARG:NE	2.32	0.43
3:D:151:LEU:HD23	3:D:153:ASN:H	1.82	0.43
3:B:245:HIS:O	3:B:247:LYS:HG2	2.18	0.43
3:D:143:ASP:OD2	3:D:208:LYS:HE2	2.16	0.43
3:D:72:ILE:O	3:D:76:GLU:HG3	2.18	0.43
3:D:459:ASN:HD22	3:D:459:ASN:H	1.66	0.43
3:D:114:ASP:HB3	3:D:328:VAL:HG13	2.00	0.43
2:J:111:DT:H2''	2:J:112:DA:C8	2.51	0.43
3:C:81:GLU:HG2	3:C:83:LEU:HD12	1.99	0.43
3:A:730:LEU:HB3	3:A:883:PHE:CZ	2.53	0.43
3:D:117:VAL:HG13	3:D:124:PRO:HG3	2.00	0.43
3:D:410:PHE:CD2	3:D:685:ARG:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:221:PHE:O	3:D:225:TYR:HB2	2.19	0.43
1:E:8:DT:H4'	3:A:707:ARG:HD2	2.00	0.43
3:B:410:PHE:HB3	3:B:683:MET:HG2	1.99	0.43
3:B:795:GLY:O	3:B:813:ARG:HD3	2.19	0.43
3:D:160:GLU:HB3	3:D:161:GLU:H	1.62	0.43
3:A:300:VAL:O	3:A:300:VAL:HG23	2.18	0.43
2:H:113:DA:H2''	2:H:114:DG:O5'	2.18	0.43
3:D:878:LYS:N	3:D:879:PRO:HD2	2.33	0.43
3:A:249:ARG:HG2	3:A:250:VAL:N	2.33	0.43
3:D:555:ALA:O	3:D:559:ARG:HG2	2.18	0.43
3:C:461:MET:CE	3:C:581:ARG:HD2	2.49	0.43
3:C:205:TRP:HH2	3:C:213:LEU:HD11	1.84	0.43
3:B:111:ALA:HB1	3:B:138:HIS:NE2	2.33	0.43
3:B:271:LEU:HB3	3:B:276:LEU:HD11	2.01	0.43
2:H:113:DA:H3'	4:H:758:HOH:O	2.18	0.43
3:B:279:LYS:HE3	3:B:280:PHE:CE2	2.54	0.43
3:D:477:LYS:O	3:D:481:GLN:HG3	2.18	0.43
3:C:416:TYR:HB2	3:C:417:PRO:HD3	2.00	0.43
3:C:105:HIS:HA	3:C:108:ILE:HD12	2.01	0.43
3:A:700:GLY:HA2	3:A:753:LEU:HD22	2.00	0.43
3:D:458:PRO:HB2	3:D:588:THR:CG2	2.42	0.43
3:C:495:ASN:HD21	3:C:521:ASP:HA	1.83	0.43
3:B:131:HIS:HB2	3:B:225:TYR:OH	2.19	0.43
3:A:458:PRO:HG3	3:A:592:MET:SD	2.59	0.43
3:A:596:TRP:CE2	3:A:670:MET:HB2	2.54	0.43
3:C:532:LYS:N	3:C:532:LYS:HD2	2.34	0.43
3:A:405:LYS:HA	4:A:998:HOH:O	2.19	0.43
3:D:559:ARG:O	3:D:563:ILE:HG13	2.19	0.43
3:B:356:GLN:O	3:B:358:VAL:N	2.52	0.43
3:A:494:ARG:O	3:A:498:ILE:HG12	2.19	0.43
3:C:262:ILE:O	3:C:262:ILE:HG13	2.19	0.43
3:B:830:VAL:HB	3:B:848:TRP:O	2.18	0.43
3:A:214:THR:OG1	3:A:215:GLY:N	2.51	0.43
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.99	0.43
3:D:456:CYS:HA	3:D:461:MET:O	2.18	0.42
3:D:381:PRO:HG3	4:D:912:HOH:O	2.19	0.42
3:A:482:ARG:HG2	3:A:482:ARG:NH1	2.34	0.42
3:C:284:ASN:ND2	3:C:829:LYS:NZ	2.66	0.42
3:B:251:LYS:C	3:B:253:GLY:H	2.22	0.42
3:D:15:ILE:HD13	3:D:15:ILE:C	2.40	0.42
3:B:244:PRO:HG2	3:B:267:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:340:PHE:HD1	3:D:343:LEU:HD12	1.84	0.42
3:D:394:ALA:HB1	3:D:622:THR:HA	2.01	0.42
4:K:745:HOH:O	3:D:362:ILE:HG13	2.18	0.42
1:I:6:DT:H2''	1:I:7:DA:H5''	2.01	0.42
1:K:2:DG:H3'	1:K:3:3DR:H5'	2.01	0.42
2:L:104:DG:H2''	2:L:105:DC:O5'	2.19	0.42
2:L:106:DT:H2''	2:L:107:DG:C8	2.54	0.42
3:A:129:ALA:HA	3:A:225:TYR:CZ	2.54	0.42
3:A:391:TYR:HB2	3:A:392:PRO:HD2	2.00	0.42
3:B:739:LYS:HD3	3:B:742:GLN:OE1	2.19	0.42
3:B:202:LEU:HD23	3:B:241:ARG:HH21	1.83	0.42
3:A:221:PHE:C	3:A:224:PRO:HD2	2.39	0.42
3:B:313:ARG:NH1	3:B:313:ARG:HG2	2.33	0.42
3:B:468:ASP:HB2	4:B:957:HOH:O	2.20	0.42
3:B:422:GLN:HG3	3:B:678:GLN:O	2.20	0.42
3:A:380:ILE:HD12	3:A:576:ARG:CZ	2.49	0.42
3:D:500:LYS:O	3:D:503:LEU:HB2	2.19	0.42
3:D:230:ILE:HG23	3:D:234:PHE:CD2	2.51	0.42
3:D:102:LYS:HB2	3:D:102:LYS:HZ3	1.83	0.42
3:B:806:ARG:HD3	3:B:843:ASP:OD1	2.20	0.42
3:A:170:LEU:HB2	3:A:173:GLN:HE21	1.84	0.42
3:B:186:ILE:HG22	4:B:1053:HOH:O	2.18	0.42
2:H:104:DG:H2''	2:H:105:DC:C5'	2.49	0.42
3:A:822:PRO:HA	4:A:1106:HOH:O	2.18	0.42
3:D:804:HIS:O	3:D:808:ILE:HG13	2.20	0.42
2:L:107:DG:H2''	2:L:108:DT:O5'	2.20	0.42
3:D:732:THR:HG22	3:D:745:LEU:HB2	1.99	0.42
3:C:449:ARG:HA	3:C:450:PRO:HD2	1.88	0.42
3:A:126:PRO:HB3	3:A:224:PRO:HB2	2.00	0.42
3:D:65:MET:O	3:D:65:MET:HG3	2.19	0.42
3:B:229:ARG:O	3:B:233:ILE:HG13	2.20	0.42
3:A:485:HIS:C	3:A:487:GLY:H	2.21	0.42
3:A:197:LEU:HD23	3:A:197:LEU:C	2.39	0.42
3:B:494:ARG:O	3:B:498:ILE:HG12	2.19	0.42
3:C:153:ASN:HB2	3:C:192:ASP:O	2.18	0.42
1:E:2:DG:OP2	3:A:361:PRO:HD2	2.19	0.42
1:E:5:DT:C6	1:E:6:DT:H72	2.54	0.42
3:C:162:TRP:HB3	3:C:188:TYR:CE1	2.55	0.42
3:D:191:PHE:CZ	3:D:200:GLU:HG2	2.55	0.42
3:A:422:GLN:HE21	3:A:422:GLN:HB2	1.70	0.42
2:L:113:DA:H4'	3:D:728:MET:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:DT:H2''	1:G:9:DG:H5'	2.00	0.42
3:D:119:SER:OG	3:D:124:PRO:HD3	2.20	0.42
3:C:40:HIS:HE1	3:C:51:ASP:OD2	2.03	0.42
1:I:15:DC:P	4:I:440:HOH:O	2.78	0.42
3:B:653:LYS:HG3	3:B:657:GLU:OE2	2.19	0.42
3:B:856:ASP:HA	3:B:859:LYS:HB2	2.02	0.42
1:I:6:DT:H2''	1:I:7:DA:C5'	2.50	0.42
3:A:426:SER:OG	3:A:427:PRO:HD2	2.19	0.42
2:L:103:DG:H2''	2:L:104:DG:C8	2.55	0.41
2:L:105:DC:H2'	2:L:106:DT:C7	2.50	0.41
3:C:500:LYS:HE3	3:C:542:LEU:HD11	2.02	0.41
3:A:352:LYS:NZ	4:A:1069:HOH:O	2.53	0.41
3:A:803:PHE:CZ	3:A:845:CYS:HB3	2.55	0.41
3:D:440:HIS:HA	3:D:443:ILE:HD12	2.02	0.41
3:D:142:ILE:HG13	3:D:143:ASP:OD1	2.20	0.41
3:D:664:ASP:OD1	3:D:668:ARG:HD2	2.21	0.41
3:A:741:VAL:HG12	3:A:745:LEU:HD22	2.02	0.41
3:D:216:TRP:CD1	3:D:290:LEU:HB2	2.54	0.41
3:C:179:PRO:O	3:C:183:ILE:HG12	2.20	0.41
3:B:159:VAL:HG13	3:B:313:ARG:NH1	2.35	0.41
3:D:430:ILE:HG13	3:D:430:ILE:H	1.55	0.41
3:B:37:LEU:HD12	3:B:37:LEU:HA	1.79	0.41
3:C:633:ILE:HA	3:C:633:ILE:HD13	1.87	0.41
3:B:891:TYR:CD2	3:B:892:GLU:HG3	2.55	0.41
3:D:241:ARG:HB3	4:D:929:HOH:O	2.19	0.41
3:B:739:LYS:HA	3:B:739:LYS:HD3	1.87	0.41
3:D:74:ARG:O	3:D:78:ILE:HG13	2.21	0.41
3:B:436:VAL:HG12	4:B:1021:HOH:O	2.20	0.41
3:C:524:ASP:HA	3:C:527:LYS:HE3	2.00	0.41
3:A:486:LYS:HG2	3:A:486:LYS:O	2.19	0.41
3:D:878:LYS:HB3	3:D:879:PRO:HD3	2.01	0.41
3:D:15:ILE:HD13	3:D:15:ILE:O	2.20	0.41
3:B:125:GLU:HA	3:B:126:PRO:HD3	1.94	0.41
3:A:273:TYR:OH	3:A:335:ASP:HA	2.20	0.41
3:D:491:ALA:HA	3:D:521:ASP:OD1	2.20	0.41
3:A:162:TRP:HB3	3:A:188:TYR:CE1	2.55	0.41
3:A:558:ASN:O	3:A:562:LEU:HD13	2.20	0.41
3:B:562:LEU:HA	3:B:562:LEU:HD12	1.88	0.41
3:B:499:ILE:HD12	3:B:530:ILE:HG13	2.03	0.41
3:C:326:ILE:HD11	4:C:1076:HOH:O	2.20	0.41
3:D:398:GLU:CD	3:D:705:LYS:HE3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:812:ASN:CA	3:D:815:ILE:HG12	2.50	0.41
3:A:292:TYR:HB2	4:A:1131:HOH:O	2.20	0.41
1:E:16:DG:H2"	1:E:17:DC:C6	2.56	0.41
3:D:796:PHE:HB3	3:D:797:PRO:HD2	2.03	0.41
3:D:475:ILE:HD11	3:D:563:ILE:HG23	2.01	0.41
3:B:355:ILE:HD13	3:B:355:ILE:HA	1.80	0.41
3:D:183:ILE:HG23	3:D:184:ASP:N	2.36	0.41
3:C:10:GLN:HG3	3:C:65:MET:HE1	2.01	0.41
3:D:9:GLU:O	3:D:15:ILE:HG12	2.21	0.41
3:D:382:GLN:HG2	3:D:383:GLY:N	2.35	0.41
3:D:770:GLU:O	3:D:774:LEU:HG	2.20	0.41
3:A:499:ILE:CG2	3:A:541:MET:HB3	2.50	0.41
3:C:897:LEU:HD13	4:C:1114:HOH:O	2.20	0.41
3:A:854:ILE:CD1	3:A:862:VAL:HG11	2.49	0.41
3:C:228:ASN:HD22	3:C:228:ASN:HA	1.64	0.41
1:I:4:DC:H2'	1:I:5:DT:H72	2.03	0.41
3:D:64:ASN:O	3:D:65:MET:HB2	2.19	0.41
3:B:873:GLU:O	3:B:878:LYS:HB2	2.20	0.41
3:D:846:ILE:HG12	3:D:847:ALA:N	2.36	0.41
3:A:356:GLN:HE21	3:A:356:GLN:H	1.69	0.41
3:C:182:ILE:O	3:C:186:ILE:HG13	2.21	0.41
3:B:731:GLU:HG3	3:B:879:PRO:HB2	2.03	0.41
3:C:16:PHE:HB3	3:C:245:HIS:CE1	2.55	0.41
3:A:457:SER:HA	3:A:458:PRO:HD3	1.92	0.41
3:B:558:ASN:HD22	3:B:558:ASN:HA	1.57	0.41
3:B:1:MET:HG2	3:B:2:LYS:N	2.36	0.41
3:A:171:GLN:HE22	3:A:319:ARG:HH12	1.69	0.41
3:D:686:GLU:HB3	3:D:687:ALA:H	1.75	0.41
3:A:150:ASP:OD2	3:A:321:ILE:HD11	2.21	0.41
3:B:884:THR:HB	3:B:889:LEU:O	2.20	0.41
3:C:321:ILE:O	3:C:325:ILE:HG13	2.20	0.41
3:A:339:GLN:HE21	3:A:339:GLN:HB3	1.68	0.41
3:D:700:GLY:HA2	3:D:753:LEU:CD2	2.48	0.41
3:A:507:ASN:HD22	3:A:532:LYS:CA	2.34	0.41
3:B:514:LEU:HD11	3:B:529:LYS:HB3	2.03	0.41
3:D:241:ARG:HH12	3:D:246:ARG:CB	2.33	0.41
3:A:125:GLU:HA	3:A:126:PRO:HD3	1.94	0.41
3:A:663:ILE:HG21	3:A:683:MET:HB2	2.03	0.41
2:F:107:DG:C8	2:F:108:DT:H72	2.56	0.41
3:D:145:ARG:NH2	3:D:185:LYS:HG2	2.36	0.41
3:B:303:LEU:HD22	3:B:303:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:204:PHE:CE1	3:A:208:LYS:HD2	2.56	0.41
3:B:113:PHE:H	3:B:113:PHE:HD1	1.68	0.41
3:B:113:PHE:CE1	3:B:213:LEU:HD11	2.55	0.41
3:B:776:TYR:OH	3:B:854:ILE:HG22	2.20	0.41
3:B:477:LYS:O	3:B:481:GLN:HG3	2.21	0.41
2:J:113:DA:H2''	2:J:114:DG:C5'	2.51	0.41
3:B:124:PRO:HB2	3:B:225:TYR:HE1	1.86	0.41
3:B:124:PRO:HG2	3:B:221:PHE:HE2	1.86	0.41
3:D:597:ILE:HA	3:D:597:ILE:HD12	1.86	0.41
3:D:421:ARG:HD3	3:D:475:ILE:HG23	2.03	0.41
2:F:108:DT:H1'	2:F:109:DC:H5'	2.03	0.41
3:C:731:GLU:HG3	3:C:879:PRO:CB	2.51	0.41
3:C:458:PRO:CG	3:C:592:MET:SD	3.09	0.41
3:D:747:GLU:HA	3:D:747:GLU:OE2	2.21	0.41
3:B:216:TRP:HE3	4:B:1083:HOH:O	2.04	0.40
2:L:110:DA:H2''	2:L:111:DT:O5'	2.21	0.40
3:C:506:PRO:C	3:C:507:ASN:HD22	2.25	0.40
3:D:250:VAL:HG12	3:D:263:ILE:CD1	2.50	0.40
3:A:730:LEU:HD22	3:A:883:PHE:HE1	1.86	0.40
3:D:870:VAL:O	3:D:874:LYS:HG2	2.22	0.40
3:A:597:ILE:HB	3:A:667:PHE:CZ	2.56	0.40
3:C:578:TYR:C	3:C:578:TYR:CD1	2.95	0.40
3:D:43:GLU:HA	3:D:56:PRO:HG3	2.02	0.40
3:B:502:ALA:HB3	3:B:530:ILE:HG12	2.03	0.40
3:D:42:PRO:HG2	3:D:45:GLN:HG2	2.03	0.40
3:D:118:THR:HG21	3:D:313:ARG:CB	2.48	0.40
3:C:530:ILE:HG23	3:C:538:LEU:CD2	2.48	0.40
3:B:736:SER:HA	3:B:782:VAL:HB	2.03	0.40
3:A:509:SER:O	3:A:534:SER:HB3	2.21	0.40
3:A:478:VAL:HG13	3:A:559:ARG:HD2	2.04	0.40
3:A:822:PRO:HB2	3:A:849:PRO:HG3	2.04	0.40
3:A:530:ILE:C	3:A:532:LYS:H	2.24	0.40
3:A:839:ASN:HA	3:A:840:PRO:HD3	1.92	0.40
3:D:239:ALA:C	3:D:241:ARG:H	2.24	0.40
3:B:494:ARG:HD2	3:B:521:ASP:CG	2.42	0.40
3:C:149:PHE:HB3	3:C:197:LEU:HG	2.03	0.40
3:A:416:TYR:HB2	3:A:417:PRO:HD3	2.02	0.40
3:D:654:PHE:O	3:D:658:ARG:HB2	2.21	0.40
3:A:455:SER:OG	3:A:676:ASN:HA	2.22	0.40
1:E:10:DA:H2''	1:E:11:DC:C5'	2.51	0.40
2:J:114:DG:H2'	4:J:750:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:216:TRP:CH2	3:B:293:ILE:HG21	2.56	0.40
3:B:149:PHE:CD1	3:B:149:PHE:N	2.90	0.40
2:J:105:DC:H6	2:J:105:DC:H5''	1.85	0.40
3:A:409:SER:HB3	3:A:626:TYR:CD2	2.56	0.40
3:B:643:ASP:OD1	3:B:646:HIS:HB2	2.20	0.40
3:D:878:LYS:HB3	3:D:879:PRO:CD	2.52	0.40
2:F:111:DT:H2''	2:F:112:DA:O5'	2.21	0.40
3:C:811:TYR:O	3:C:815:ILE:HG12	2.21	0.40
2:L:106:DT:H2''	2:L:107:DG:H8	1.86	0.40
3:B:138:HIS:ND1	3:B:204:PHE:HE2	2.20	0.40
3:C:42:PRO:HD2	3:C:45:GLN:HE21	1.87	0.40
3:D:501:GLU:HA	3:D:504:HIS:HD2	1.87	0.40
3:A:738:PRO:HB3	3:A:780:ALA:O	2.22	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	
3	A	894/896 (100%)	838 (94%)	51 (6%)	5 (1%)	30	40
3	B	894/896 (100%)	815 (91%)	69 (8%)	10 (1%)	17	23
3	C	890/896 (99%)	841 (94%)	45 (5%)	4 (0%)	39	53
3	D	889/896 (99%)	746 (84%)	116 (13%)	27 (3%)	5	4
All	All	3567/3584 (100%)	3240 (91%)	281 (8%)	46 (1%)	15	19

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	65	MET
3	D	117	VAL

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Mol	Chain	Res	Type
3	D	304	LYS
3	D	450	PRO
3	D	819	ILE
3	A	699	GLY
3	B	117	VAL
3	B	160	GLU
3	B	252	VAL
3	B	356	GLN
3	D	127	SER
3	D	160	GLU
3	D	281	SER
3	D	460	GLY
3	A	284	ASN
3	A	506	PRO
3	B	136	ILE
3	B	173	GLN
3	C	622	THR
3	D	63	ALA
3	D	121	ASP
3	D	169	LYS
3	D	622	THR
3	D	818	ASN
3	D	826	GLU
3	D	415	LEU
3	D	857	LEU
3	A	282	PHE
3	B	175	GLY
3	B	262	ILE
3	C	172	GLU
3	C	458	PRO
3	D	252	VAL
3	D	315	SER
3	D	789	ALA
3	D	799	PRO
3	D	825	VAL
3	A	637	GLY
3	B	622	THR
3	D	157	GLY
3	C	12	GLY
3	D	510	VAL
3	B	819	ILE
3	D	120	PRO

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Mol	Chain	Res	Type
3	D	788	ILE
3	D	795	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	
3	A	785/793 (99%)	756 (96%)	29 (4%)	41	60
3	B	774/793 (98%)	750 (97%)	24 (3%)	47	67
3	C	781/793 (98%)	741 (95%)	40 (5%)	29	44
3	D	770/793 (97%)	746 (97%)	24 (3%)	47	67
All	All	3110/3172 (98%)	2993 (96%)	117 (4%)	40	58

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	LYS
3	A	58	THR
3	A	128	GLN
3	A	200	GLU
3	A	242	LEU
3	A	246	ARG
3	A	264	THR
3	A	314	GLU
3	A	319	ARG
3	A	342	ASN
3	A	352	LYS
3	A	356	GLN
3	A	384	ARG
3	A	403	ARG
3	A	474	GLU
3	A	479	PHE
3	A	536	LYS
3	A	544	ARG
3	A	558	ASN

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Mol	Chain	Res	Type
3	A	566	LEU
3	A	668	ARG
3	A	702	TRP
3	A	731	GLU
3	A	745	LEU
3	A	770	GLU
3	A	787	ASN
3	A	826	GLU
3	A	843	ASP
3	A	861	ASP
3	B	37	LEU
3	B	61	LEU
3	B	113	PHE
3	B	165	GLU
3	B	176	ASP
3	B	181	GLU
3	B	273	TYR
3	B	305	TYR
3	B	324	ASN
3	B	428	GLU
3	B	544	ARG
3	B	558	ASN
3	B	562	LEU
3	B	566	LEU
3	B	580	LEU
3	B	660	GLU
3	B	702	TRP
3	B	731	GLU
3	B	755	GLU
3	B	760	LEU
3	B	773	GLN
3	B	820	ASP
3	B	843	ASP
3	B	897	LEU
3	C	14	SER
3	C	27	ARG
3	C	90	LEU
3	C	100	GLU
3	C	128	GLN
3	C	151	LEU
3	C	213	LEU
3	C	220	SER

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Mol	Chain	Res	Type
3	C	228	ASN
3	C	284	ASN
3	C	303	LEU
3	C	356	GLN
3	C	384	ARG
3	C	399	PRO
3	C	411	ASP
3	C	413	THR
3	C	424	ASN
3	C	428	GLU
3	C	440	HIS
3	C	466	ASP
3	C	474	GLU
3	C	475	ILE
3	C	479	PHE
3	C	507	ASN
3	C	532	LYS
3	C	562	LEU
3	C	566	LEU
3	C	580	LEU
3	C	660	GLU
3	C	702	TRP
3	C	731	GLU
3	C	733	GLN
3	C	739	LYS
3	C	760	LEU
3	C	773	GLN
3	C	820	ASP
3	C	843	ASP
3	C	863	LEU
3	C	896	SER
3	C	898	PHE
3	D	15	ILE
3	D	40	HIS
3	D	59	ARG
3	D	99	TYR
3	D	102	LYS
3	D	145	ARG
3	D	161	GLU
3	D	165	GLU
3	D	176	ASP
3	D	199	MET

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Mol	Chain	Res	Type
3	D	305	TYR
3	D	402	ASN
3	D	428	GLU
3	D	459	ASN
3	D	475	ILE
3	D	479	PHE
3	D	614	GLU
3	D	649	ASP
3	D	702	TRP
3	D	755	GLU
3	D	760	LEU
3	D	844	LYS
3	D	848	TRP
3	D	859	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	98	ASN
3	A	173	GLN
3	A	206	GLN
3	A	245	HIS
3	A	339	GLN
3	A	342	ASN
3	A	356	GLN
3	A	371	ASN
3	A	377	ASN
3	A	422	GLN
3	A	481	GLN
3	A	495	ASN
3	A	507	ASN
3	A	546	GLN
3	A	556	GLN
3	A	558	ASN
3	A	602	ASN
3	A	678	GLN
3	A	786	ASN
3	A	812	ASN
3	A	839	ASN
3	B	40	HIS
3	B	112	ASN
3	B	153	ASN

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Mol	Chain	Res	Type
3	B	203	ASN
3	B	206	GLN
3	B	228	ASN
3	B	285	GLN
3	B	299	ASN
3	B	316	ASN
3	B	318	GLN
3	B	324	ASN
3	B	339	GLN
3	B	354	GLN
3	B	481	GLN
3	B	495	ASN
3	B	546	GLN
3	B	558	ASN
3	B	591	GLN
3	B	606	ASN
3	B	773	GLN
3	B	812	ASN
3	B	818	ASN
3	C	45	GLN
3	C	173	GLN
3	C	203	ASN
3	C	228	ASN
3	C	232	ASN
3	C	245	HIS
3	C	284	ASN
3	C	299	ASN
3	C	317	HIS
3	C	318	GLN
3	C	324	ASN
3	C	356	GLN
3	C	377	ASN
3	C	424	ASN
3	C	481	GLN
3	C	495	ASN
3	C	507	ASN
3	C	546	GLN
3	C	556	GLN
3	C	558	ASN
3	C	591	GLN
3	C	645	ASN
3	C	818	ASN

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Mol	Chain	Res	Type
3	C	864	HIS
3	D	45	GLN
3	D	70	GLN
3	D	131	HIS
3	D	173	GLN
3	D	206	GLN
3	D	207	GLN
3	D	232	ASN
3	D	284	ASN
3	D	285	GLN
3	D	318	GLN
3	D	324	ASN
3	D	339	GLN
3	D	342	ASN
3	D	389	GLN
3	D	402	ASN
3	D	422	GLN
3	D	444	ASN
3	D	459	ASN
3	D	504	HIS
3	D	505	ASN
3	D	546	GLN
3	D	558	ASN
3	D	564	ASN
3	D	572	ASN
3	D	591	GLN
3	D	606	ASN
3	D	676	ASN
3	D	679	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	$\# Z > 2$
1	3DR	E	3	1	7,11,12	0.45	0	8,14,17	1.63	1 (12%)
1	3DR	G	3	1	7,11,12	0.47	0	8,14,17	1.84	1 (12%)
1	3DR	I	3	1	7,11,12	0.44	0	8,14,17	1.71	1 (12%)
1	3DR	K	3	1	7,11,12	0.47	0	8,14,17	1.61	1 (12%)

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
1	3DR	E	3	1	-	0/3/15/16	0/1/1/1
1	3DR	G	3	1	-	0/3/15/16	0/1/1/1
1	3DR	I	3	1	-	0/3/15/16	0/1/1/1
1	3DR	K	3	1	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	3DR	O3'-C3'-C2'	3.62	119.98	111.71
1	K	3	3DR	O3'-C3'-C2'	3.62	120.00	111.71
1	I	3	3DR	O3'-C3'-C2'	3.88	120.58	111.71
1	G	3	3DR	O3'-C3'-C2'	4.17	121.23	111.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	3	3DR	2	0
1	I	3	3DR	1	0
1	K	3	3DR	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	E	17/18 (94%)	0.28	1 (5%) 26 30	54, 75, 126, 146	0
1	G	17/18 (94%)	0.20	1 (5%) 26 30	45, 57, 133, 148	0
1	I	17/18 (94%)	0.14	1 (5%) 26 30	35, 42, 101, 115	0
1	K	17/18 (94%)	1.24	3 (17%) 2 2	45, 123, 161, 169	0
2	F	15/15 (100%)	0.66	1 (6%) 21 24	68, 99, 128, 141	0
2	H	15/15 (100%)	0.44	2 (13%) 4 5	56, 71, 126, 153	0
2	J	15/15 (100%)	0.14	0 100 100	38, 57, 91, 96	0
2	L	15/15 (100%)	1.57	5 (33%) 0 0	126, 131, 153, 157	0
3	A	896/896 (100%)	0.54	61 (6%) 20 23	30, 47, 125, 149	0
3	B	896/896 (100%)	1.09	165 (18%) 2 2	28, 62, 154, 165	0
3	C	892/896 (99%)	0.43	26 (2%) 55 58	23, 48, 83, 106	0
3	D	891/896 (99%)	1.60	268 (30%) 1 0	53, 117, 153, 160	0
All	All	3703/3716 (99%)	0.91	534 (14%) 3 4	23, 62, 148, 169	0

All (534) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	516	VAL	13.7
3	A	530	ILE	13.5
3	D	514	LEU	13.0
3	B	508	LEU	11.5
3	D	117	VAL	11.2
3	D	157	GLY	10.9
3	B	511	ASP	10.4
3	B	507	ASN	9.8
3	A	542	LEU	9.7
3	D	99	TYR	9.2
3	B	514	LEU	8.6

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Mol	Chain	Res	Type	RSRZ
3	D	64	ASN	8.5
3	B	510	VAL	8.4
3	B	538	LEU	8.2
3	B	509	SER	8.2
3	B	819	ILE	8.2
3	B	502	ALA	8.0
3	B	541	MET	7.7
3	D	809	LEU	7.6
3	D	831	TYR	7.6
3	B	503	LEU	7.4
3	D	538	LEU	7.4
3	B	178	VAL	7.4
3	D	539	ASN	7.3
3	B	134	ASP	7.3
3	D	535	ALA	7.0
3	D	788	ILE	7.0
3	B	498	ILE	6.8
3	D	173	GLN	6.7
3	D	65	MET	6.7
3	B	303	LEU	6.6
3	B	156	TYR	6.6
3	D	799	PRO	6.6
3	B	535	ALA	6.6
3	B	545	ALA	6.6
3	B	530	ILE	6.6
3	D	393	GLY	6.5
3	D	120	PRO	6.5
3	D	282	PHE	6.5
3	B	528	GLU	6.4
3	B	522	PHE	6.4
3	B	542	LEU	6.3
3	B	183	ILE	6.2
3	A	522	PHE	6.2
3	B	518	TYR	6.2
3	D	160	GLU	6.1
3	D	796	PHE	6.1
3	A	503	LEU	6.1
3	B	820	ASP	6.1
3	B	277	TYR	6.1
3	D	548	THR	6.0
3	A	498	ILE	6.0
3	D	794	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
3	D	159	VAL	6.0
3	D	498	ILE	6.0
3	D	849	PRO	5.9
3	B	520	PHE	5.9
3	B	527	LYS	5.9
3	A	504	HIS	5.9
3	B	504	HIS	5.9
3	D	504	HIS	5.9
3	B	490	LEU	5.8
3	A	252	VAL	5.8
3	C	303	LEU	5.7
3	A	507	ASN	5.7
3	B	309	ILE	5.7
3	B	513	PRO	5.7
3	B	519	ARG	5.6
3	D	801	CYS	5.6
3	D	178	VAL	5.6
3	B	492	ALA	5.6
3	D	510	VAL	5.6
1	K	2	DG	5.5
3	A	541	MET	5.5
3	B	539	ASN	5.5
3	D	541	MET	5.5
3	D	833	LEU	5.5
3	B	857	LEU	5.4
3	D	520	PHE	5.4
3	B	505	ASN	5.4
3	B	496	GLY	5.3
3	D	544	ARG	5.3
3	B	525	GLU	5.3
3	D	811	TYR	5.3
3	D	147	TYR	5.2
3	D	503	LEU	5.2
3	B	523	SER	5.1
3	B	172	GLU	5.1
3	D	512	GLU	5.1
3	B	506	PRO	5.1
3	D	8	VAL	5.1
3	D	47	THR	5.1
3	A	508	LEU	5.1
3	A	501	GLU	5.0
3	D	530	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
3	C	46	ALA	5.0
3	D	846	ILE	5.0
3	B	524	ASP	5.0
3	D	192	ASP	4.9
3	B	170	LEU	4.9
3	B	176	ASP	4.9
3	D	523	SER	4.8
3	D	802	PRO	4.8
3	B	179	PRO	4.8
3	D	145	ARG	4.8
3	D	20	ILE	4.8
3	D	516	VAL	4.8
3	D	265	LEU	4.8
3	B	818	ASN	4.8
3	B	166	ILE	4.7
3	B	515	ASP	4.7
3	B	160	GLU	4.7
3	D	44	SER	4.7
3	D	119	SER	4.7
3	C	508	LEU	4.6
3	D	508	LEU	4.6
3	A	535	ALA	4.5
3	D	786	ASN	4.5
3	A	497	GLU	4.5
3	B	497	GLU	4.5
3	D	252	VAL	4.5
3	D	175	GLY	4.5
3	D	857	LEU	4.5
3	A	854	ILE	4.4
3	B	861	ASP	4.4
3	D	779	ILE	4.4
3	B	157	GLY	4.4
3	D	118	THR	4.4
3	A	509	SER	4.4
3	D	855	THR	4.4
3	B	115	ILE	4.4
3	D	526	ILE	4.4
3	D	251	LYS	4.4
3	D	847	ALA	4.3
3	C	252	VAL	4.3
3	D	793	VAL	4.3
3	D	234	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	250	VAL	4.3
3	D	194	GLU	4.3
3	B	135	ALA	4.3
3	C	304	LYS	4.3
3	B	512	GLU	4.2
3	D	513	PRO	4.2
3	C	530	ILE	4.2
3	A	536	LYS	4.2
3	D	71	TRP	4.2
3	A	499	ILE	4.2
3	A	821	ALA	4.2
3	B	526	ILE	4.2
3	B	532	LYS	4.2
3	D	174	GLY	4.2
3	B	127	SER	4.2
3	B	817	GLY	4.2
3	A	506	PRO	4.2
3	B	153	ASN	4.2
3	B	117	VAL	4.1
3	B	501	GLU	4.1
3	B	493	GLN	4.1
3	D	61	LEU	4.1
3	A	537	SER	4.0
3	D	198	LEU	4.0
3	D	790	LYS	4.0
3	A	514	LEU	4.0
3	B	821	ALA	4.0
3	D	28	THR	4.0
3	D	201	TYR	4.0
3	B	494	ARG	3.9
3	D	522	PHE	3.9
3	B	549	GLU	3.9
3	D	524	ASP	3.9
3	B	865	TRP	3.9
3	D	182	ILE	3.9
3	A	528	GLU	3.9
1	E	2	DG	3.9
3	B	540	GLU	3.9
3	D	32	GLU	3.9
1	G	2	DG	3.8
3	D	303	LEU	3.8
3	B	552	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
3	D	830	VAL	3.8
3	B	547	ARG	3.8
3	C	166	ILE	3.8
3	D	72	ILE	3.8
3	C	302	LYS	3.7
3	D	771	PHE	3.7
3	B	321	ILE	3.7
3	D	789	ALA	3.7
3	D	792	ASP	3.7
3	D	24	GLY	3.7
3	D	820	ASP	3.7
3	B	306	ASP	3.7
3	D	153	ASN	3.7
3	A	857	LEU	3.7
3	D	863	LEU	3.7
3	B	233	ILE	3.7
3	D	131	HIS	3.7
3	D	491	ALA	3.7
3	A	490	LEU	3.7
3	D	183	ILE	3.7
3	B	537	SER	3.6
3	D	832	VAL	3.6
3	D	517	ASP	3.6
2	H	115	DA	3.6
3	D	46	ALA	3.6
3	B	533	LEU	3.6
3	D	776	TYR	3.6
3	B	325	ILE	3.6
3	B	315	SER	3.6
3	D	78	ILE	3.5
3	A	538	LEU	3.5
3	D	191	PHE	3.5
3	D	490	LEU	3.5
3	B	815	ILE	3.5
3	D	164	ILE	3.5
3	A	253	GLY	3.5
3	D	113	PHE	3.5
3	D	488	TYR	3.5
3	B	302	LYS	3.5
3	D	304	LYS	3.5
3	D	305	TYR	3.5
3	D	176	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	A	502	ALA	3.5
3	B	171	GLN	3.4
3	A	505	ASN	3.4
3	B	543	PHE	3.4
3	B	797	PRO	3.4
3	D	546	GLN	3.4
3	D	866	MET	3.4
3	B	322	SER	3.4
2	L	114	DG	3.4
3	D	515	ASP	3.4
3	D	543	PHE	3.4
3	A	526	ILE	3.4
3	D	288	TYR	3.4
3	A	261	GLU	3.4
3	D	226	VAL	3.3
3	B	544	ARG	3.3
3	B	234	PHE	3.3
3	D	309	ILE	3.3
3	B	201	TYR	3.3
3	D	223	ILE	3.3
3	D	45	GLN	3.3
3	B	159	VAL	3.3
3	D	854	ILE	3.3
3	D	784	SER	3.2
3	D	848	TRP	3.2
3	D	170	LEU	3.2
3	D	868	TYR	3.2
3	D	199	MET	3.2
3	C	510	VAL	3.2
3	D	395	PHE	3.2
3	A	491	ALA	3.2
3	D	100	GLU	3.2
3	B	517	ASP	3.2
3	D	63	ALA	3.2
3	D	518	TYR	3.2
3	D	495	ASN	3.2
3	B	186	ILE	3.2
3	D	797	PRO	3.2
3	D	509	SER	3.1
3	D	391	TYR	3.1
3	B	521	ASP	3.1
3	A	533	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	566	LEU	3.1
3	D	205	TRP	3.1
3	D	202	LEU	3.1
3	D	829	LYS	3.1
3	D	390	PRO	3.1
3	D	840	PRO	3.1
3	A	518	TYR	3.1
3	A	543	PHE	3.1
3	D	111	ALA	3.0
3	B	232	ASN	3.0
3	C	522	PHE	3.0
3	B	247	LYS	3.0
3	B	499	ILE	3.0
3	D	562	LEU	3.0
3	D	501	GLU	3.0
3	B	317	HIS	3.0
2	F	115	DA	3.0
3	D	489	MET	3.0
3	B	536	LYS	3.0
3	D	317	HIS	3.0
3	B	812	ASN	3.0
3	C	174	GLY	3.0
3	C	309	ILE	3.0
3	D	80	LEU	3.0
3	A	496	GLY	2.9
3	B	534	SER	2.9
3	D	850	SER	2.9
3	A	280	PHE	2.9
3	D	803	PHE	2.9
3	C	301	GLY	2.9
3	B	120	PRO	2.9
3	D	248	THR	2.9
3	D	476	THR	2.9
3	D	479	PHE	2.9
3	B	271	LEU	2.9
3	D	769	LYS	2.9
3	D	313	ARG	2.9
3	D	172	GLU	2.9
3	B	152	LEU	2.9
3	D	816	LYS	2.9
3	B	862	VAL	2.9
3	D	497	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	128	GLN	2.9
3	D	135	ALA	2.8
3	D	379	VAL	2.8
3	D	550	VAL	2.8
3	D	92	TYR	2.8
3	D	115	ILE	2.8
3	B	291	ASP	2.8
3	D	193	ASN	2.8
3	B	305	TYR	2.8
3	C	323	TYR	2.8
3	D	507	ASN	2.8
3	A	494	ARG	2.8
3	D	532	LYS	2.8
3	A	788	ILE	2.8
3	D	570	LEU	2.8
3	A	512	GLU	2.8
3	D	162	TRP	2.8
3	B	244	PRO	2.8
3	D	2	LYS	2.8
3	D	782	VAL	2.8
2	L	115	DA	2.8
3	D	70	GLN	2.8
3	A	262	ILE	2.8
3	B	841	PHE	2.8
3	D	25	ARG	2.8
3	A	789	ALA	2.8
3	B	192	ASP	2.7
3	B	249	ARG	2.7
3	B	197	LEU	2.7
3	B	320	TYR	2.7
3	D	88	PHE	2.7
3	A	511	ASP	2.7
3	C	44	SER	2.7
3	D	180	SER	2.7
3	D	487	GLY	2.7
3	B	206	GLN	2.7
3	D	151	LEU	2.7
3	C	500	LYS	2.7
3	B	868	TYR	2.7
3	A	500	LYS	2.7
3	D	203	ASN	2.7
3	D	844	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	B	774	LEU	2.7
3	B	136	ILE	2.7
3	D	274	ILE	2.7
3	B	123	PHE	2.7
3	B	149	PHE	2.7
3	B	283	THR	2.7
3	B	792	ASP	2.7
3	D	511	ASP	2.7
3	D	233	ILE	2.6
3	D	67	ASP	2.6
3	A	531	LYS	2.6
3	D	240	LYS	2.6
3	B	316	ASN	2.6
3	A	250	VAL	2.6
3	B	242	LEU	2.6
3	D	563	ILE	2.6
1	I	2	DG	2.6
3	A	495	ASN	2.6
3	C	175	GLY	2.6
3	B	167	ALA	2.6
3	D	242	LEU	2.6
3	B	311	LYS	2.6
3	D	212	ILE	2.6
3	A	548	THR	2.6
3	D	238	THR	2.6
3	D	33	TYR	2.6
3	B	180	SER	2.6
3	B	174	GLY	2.6
3	D	93	LEU	2.6
3	D	542	LEU	2.6
3	D	62	PHE	2.6
3	D	266	PHE	2.6
3	D	315	SER	2.6
3	B	213	LEU	2.6
3	D	325	ILE	2.6
3	D	815	ILE	2.6
3	B	165	GLU	2.5
3	A	799	PRO	2.5
3	D	637	GLY	2.5
3	B	488	TYR	2.5
3	D	225	TYR	2.5
3	D	851	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	811	TYR	2.5
3	D	454	TYR	2.5
3	D	791	TYR	2.5
3	A	524	ASP	2.5
3	C	151	LEU	2.5
3	D	314	GLU	2.5
3	B	901	PHE	2.5
3	D	527	LYS	2.5
3	D	774	LEU	2.5
3	D	795	GLY	2.5
3	B	276	LEU	2.5
3	D	450	PRO	2.5
3	A	550	VAL	2.5
3	D	229	ARG	2.5
3	D	188	TYR	2.4
3	B	282	PHE	2.4
3	A	283	THR	2.4
3	B	839	ASN	2.4
3	D	783	SER	2.4
3	D	897	LEU	2.4
3	D	673	TYR	2.4
3	B	113	PHE	2.4
3	D	116	GLU	2.4
3	D	221	PHE	2.4
3	B	128	GLN	2.4
3	D	565	SER	2.4
3	B	548	THR	2.4
3	B	304	LYS	2.4
3	D	286	PRO	2.4
3	D	136	ILE	2.4
3	B	280	PHE	2.4
3	D	841	PHE	2.4
3	D	241	ARG	2.4
3	D	321	ILE	2.4
3	D	161	GLU	2.4
3	B	126	PRO	2.4
3	D	860	ASP	2.4
3	B	227	TYR	2.4
3	C	155	PRO	2.4
3	B	546	GLN	2.4
3	D	312	LEU	2.3
3	D	787	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	49	TYR	2.3
3	D	819	ILE	2.3
3	B	813	ARG	2.3
3	D	780	ALA	2.3
3	D	154	SER	2.3
3	A	516	VAL	2.3
3	B	300	VAL	2.3
3	D	328	VAL	2.3
3	D	824	VAL	2.3
3	D	179	PRO	2.3
3	D	766	GLU	2.3
3	D	283	THR	2.3
3	D	123	PHE	2.3
3	D	785	ALA	2.3
3	C	251	LYS	2.3
2	L	103	DG	2.3
3	A	513	PRO	2.3
3	D	302	LYS	2.3
1	K	7	DA	2.3
3	B	193	ASN	2.3
3	C	558	ASN	2.3
3	D	818	ASN	2.3
3	B	212	ILE	2.3
3	D	301	GLY	2.3
3	D	500	LYS	2.3
3	B	284	ASN	2.3
3	D	564	ASN	2.3
2	H	114	DG	2.3
3	B	847	ALA	2.3
3	D	146	PHE	2.3
3	B	531	LYS	2.3
3	D	6	LEU	2.3
3	A	819	ILE	2.2
3	D	149	PHE	2.2
3	D	580	LEU	2.2
3	B	334	ILE	2.2
3	D	502	ALA	2.2
3	D	800	LYS	2.2
2	L	107	DG	2.2
3	B	294	SER	2.2
3	B	251	LYS	2.2
3	B	290	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	515	ASP	2.2
3	C	535	ALA	2.2
3	D	158	ASN	2.2
3	A	846	ILE	2.2
3	D	31	VAL	2.2
3	D	156	TYR	2.2
3	D	184	ASP	2.2
1	K	11	DC	2.2
3	D	284	ASN	2.2
3	D	79	GLY	2.2
3	D	311	LYS	2.2
3	D	1	MET	2.2
2	L	109	DC	2.2
3	D	307	GLY	2.1
3	A	493	GLN	2.1
3	A	523	SER	2.1
3	D	536	LYS	2.1
3	D	547	ARG	2.1
3	B	182	ILE	2.1
3	D	11	ILE	2.1
3	D	827	GLY	2.1
3	B	793	VAL	2.1
3	C	159	VAL	2.1
3	B	281	SER	2.1
3	D	195	LYS	2.1
3	A	276	LEU	2.1
3	D	121	ASP	2.1
3	D	334	ILE	2.1
3	B	132	PRO	2.1
3	B	822	PRO	2.1
3	C	898	PHE	2.1
3	D	292	TYR	2.1
3	D	306	ASP	2.1
3	D	388	VAL	2.1
3	B	175	GLY	2.1
3	D	18	ARG	2.1
3	D	29	ARG	2.1
3	D	74	ARG	2.1
3	D	384	ARG	2.1
3	B	799	PRO	2.1
3	D	101	ILE	2.1
3	D	281	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	804	HIS	2.1
3	A	303	LEU	2.1
3	B	47	THR	2.1
3	D	475	ILE	2.1
3	D	148	VAL	2.1
3	D	728	MET	2.0
3	B	188	TYR	2.0
3	D	521	ASP	2.0
3	D	102	LYS	2.0
3	B	267	GLY	2.0
3	B	118	THR	2.0
3	D	737	THR	2.0
3	D	589	PHE	2.0
3	B	551	ALA	2.0
3	A	822	PRO	2.0
3	D	253	GLY	2.0
3	A	282	PHE	2.0
3	B	803	PHE	2.0
3	C	63	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	3DR	E	3	11/12	0.75	0.35	-	138,143,147,147	0
1	3DR	K	3	11/12	0.72	0.38	-	165,167,169,169	0
1	3DR	I	3	11/12	0.81	0.19	-	102,105,111,112	0
1	3DR	G	3	11/12	0.76	0.27	-	132,137,146,147	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.