Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 06:40 PM EDT

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.; Doublie, 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

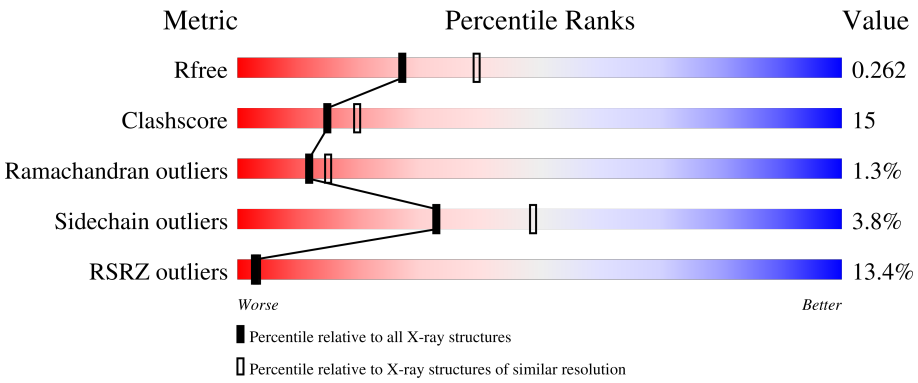
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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 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	E	18	6%; 11%, 83%, 6%
1	G	18	6%; 28%, 50%, 17%, 6%
1	I	18	6%; 39%, 44%, 11%, 6%
1	K	18	17%; 28%, 67%, 6%
2	F	15	7%; 13%, 87%

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Mol	Chain	Length	Quality of chain
2	H	15	13% 13% 80% 7%
2	J	15	20% 40% 27% 13%
2	L	15	27% 100%
3	A	896	6% 74% 24% •
3	B	896	17% 72% 26% •
3	C	896	3% 76% 21% •
3	D	896	28% 57% 39% • •

2 Entry composition (i)

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*CP*AP*GP*CP*CP*GP*CP*G)-3'.

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

- 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
			Total	C	N	O	P			
2	F	15	308	147	60	87	14	0	0	0
2	H	15	308	147	60	87	14	0	0	0
2	J	15	308	147	60	87	14	0	0	0
2	L	15	308	147	60	87	14	0	0	0

- Molecule 3 is a protein called DNA polymerase.

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

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

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087

- Molecule 4 is water.

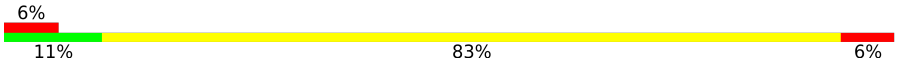
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	9	9	9	0	0
			Total	O		
4	F	10	10	10	0	0
			Total	O		
4	G	15	15	15	0	0
			Total	O		
4	H	8	8	8	0	0
			Total	O		
4	I	31	31	31	0	0
			Total	O		
4	J	18	18	18	0	0
			Total	O		
4	K	10	10	10	0	0
			Total	O		
4	A	251	251	251	0	0
			Total	O		
4	B	195	195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

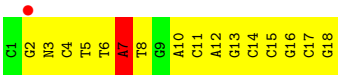
3 Residue-property plots (i)

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

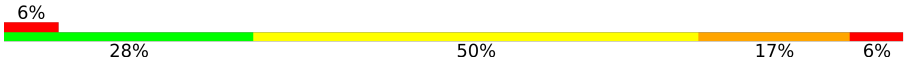
Chain E:

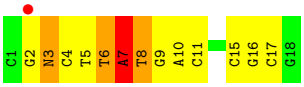




• Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

Chain G:



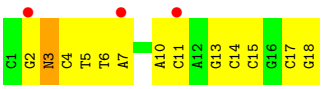


• Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

Chain I:

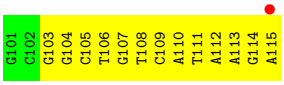
• Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

Chain K:



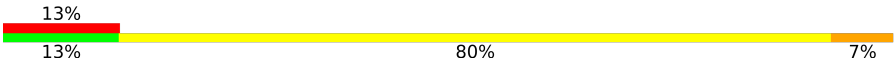
• Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

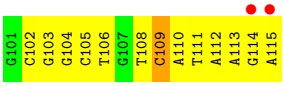
Chain F:



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

Chain H:



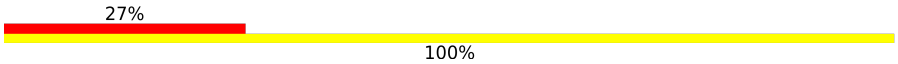


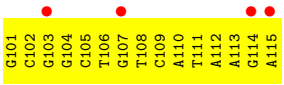
• Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

Chain J:

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

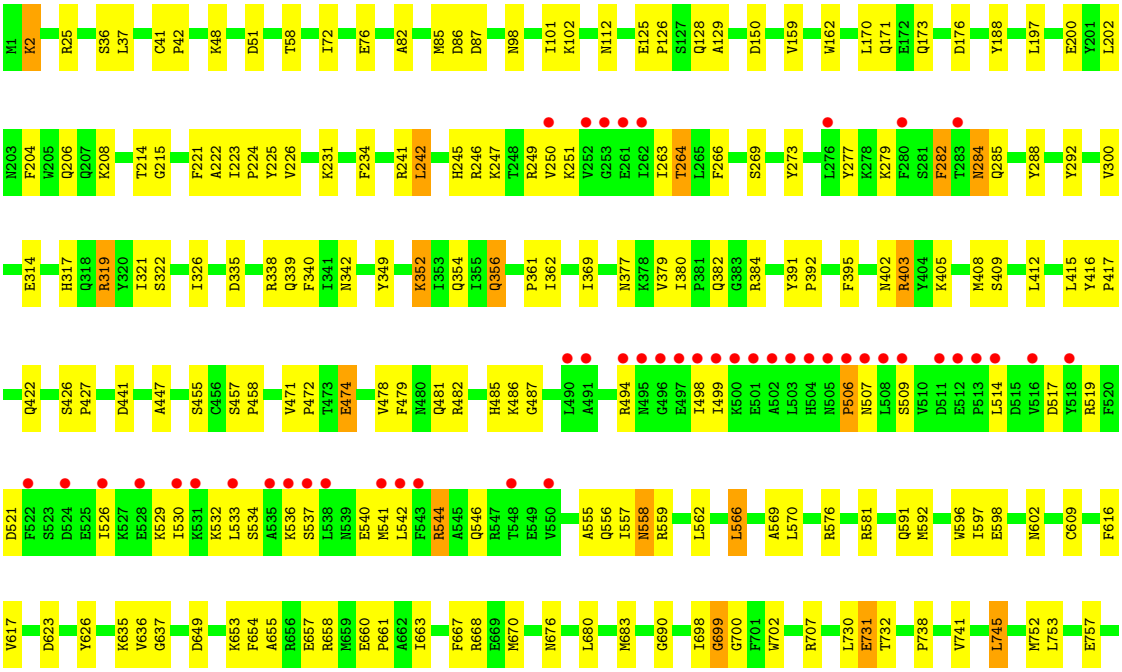
Chain L:





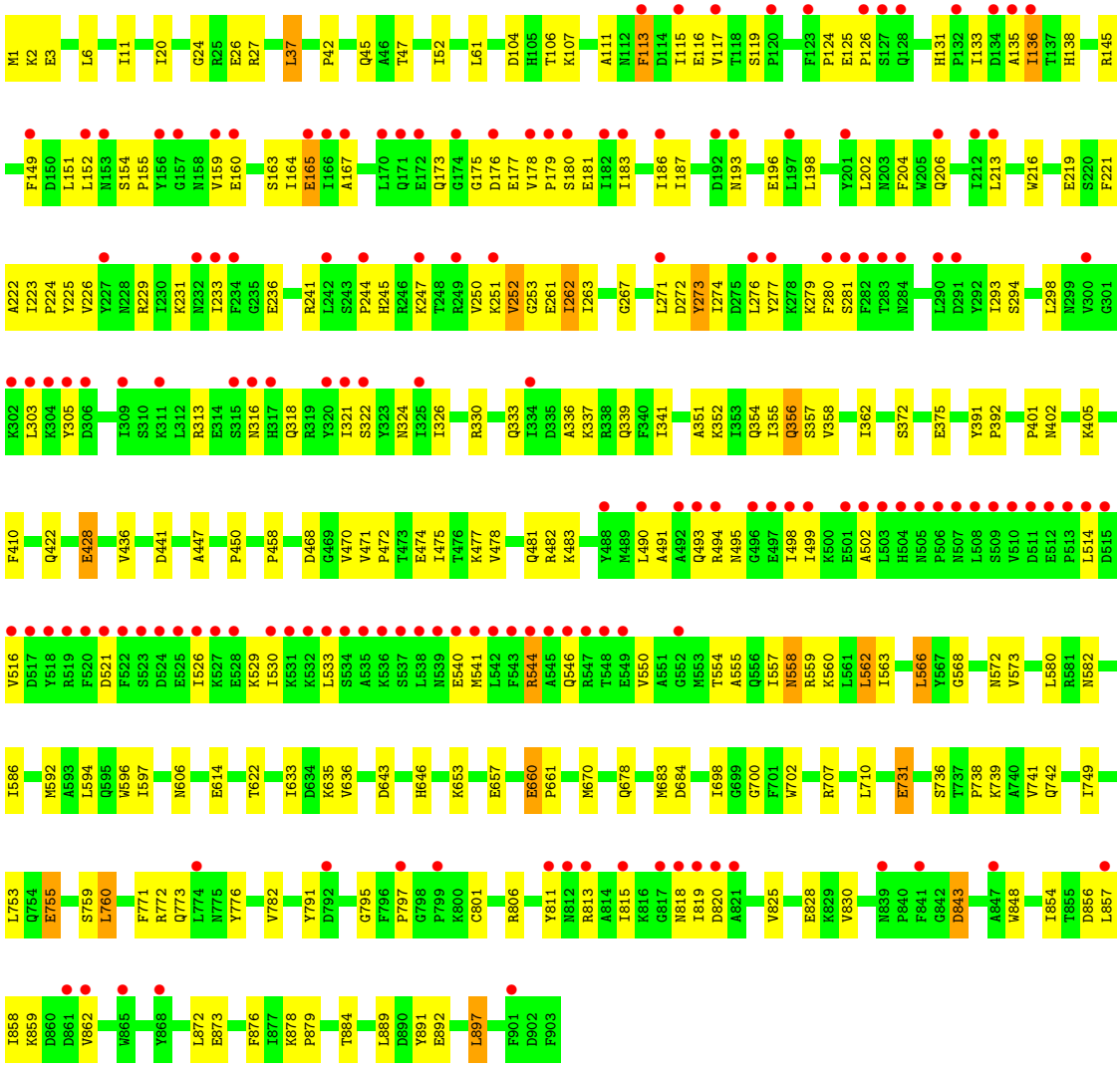
• Molecule 3: DNA polymerase

Chain A:



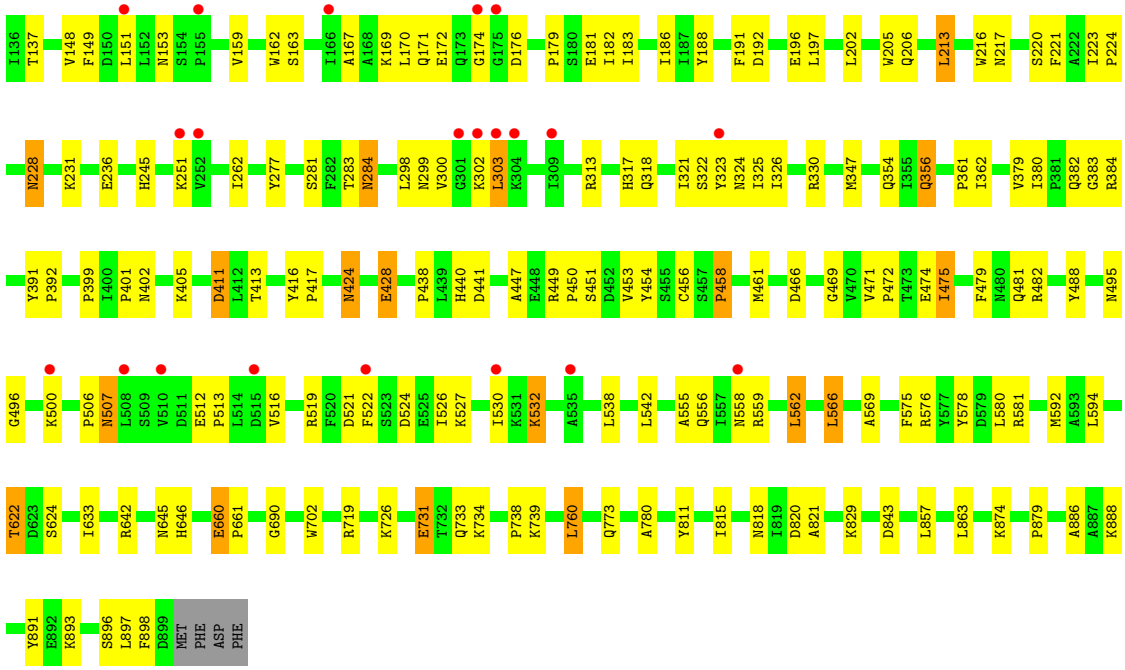
• Molecule 3: DNA polymerase

Chain B:



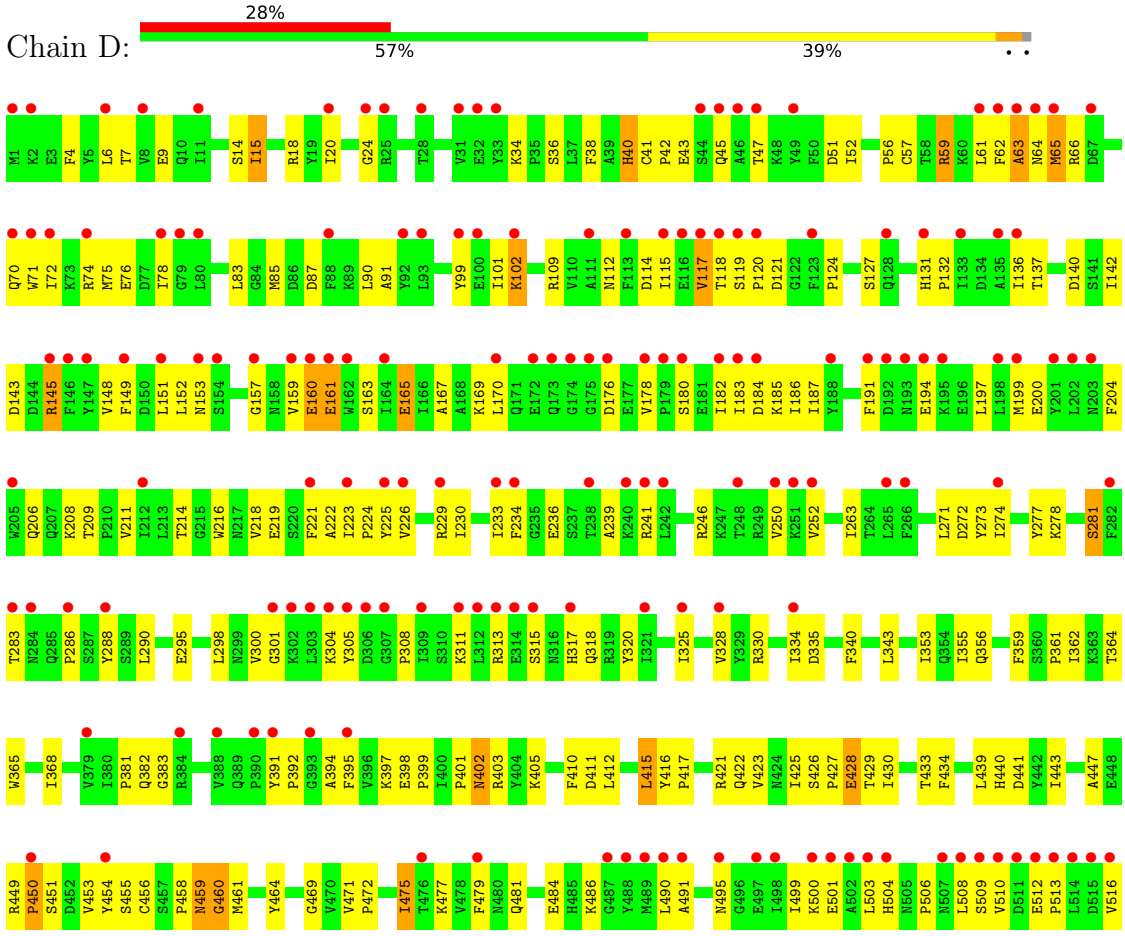
• Molecule 3: DNA polymerase

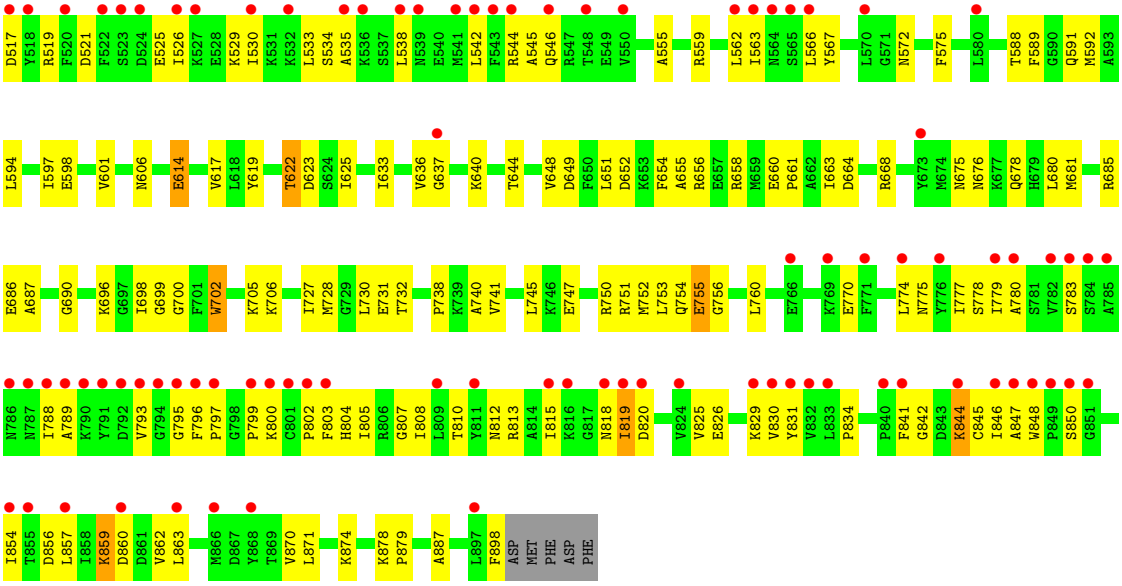
Chain C:



- Molecule 3: DNA polymerase

Chain D:




I854 T855 D856 L857 I858 K859 D860 D861 V862 L863 H866 D867 Y868 T869 V870 L871 K874 K878 P879 A887 L897 F898 ASP MET PHE ASP PHE
N786 N787 I788 A789 K790 Y791 D792 V793 G794 G795 F796 P797 G798 P799 K800 C801 P802 F803 H804 I805 R806 G807 I808 L809 T810 Y811 N812 R813 A814 I815 K816 G817 N818 I819 D820 V824 V825 E826 K829 V830 Y831 V832 L833 P834 P840 F841 G842 D843 K844 C845 I846 A847 W848 P849 S850 G851
E686 A687 G690 K696 G697 I698 G699 G700 F701 W702 K705 K706 I727 M728 G729 L730 E731 T732 P738 K739 A740 V741 L745 K746 E747 R750 R751 M752 L753 Q754 E755 G756 L760 E766 K769 E770 F771 L774 N775 Y776 I777 S778 I779 A780 S781 V782 S783 S784 A785
L594 I597 E598 V601 N606 E614 V617 L618 Y619 T622 D623 S624 I625 I633 V636 G637 K640 T644 V648 D649 F650 L651 D652 K653 F654 A655 R656 E657 R658 M659 E660 P661 A662 I663 D664 R668 Y673 M674 N675 N676 K677 Q678 H679 L680 M681 R685
D517 Y518 R519 F520 D521 F522 S523 D524 E525 I526 K527 E528 K529 I530 K531 K532 L533 S534 A535 K536 S537 L538 N539 E540 M541 L542 F543 R544 A545 Q546 R547 T548 E549 V550 A555 R559 L562 I563 N564 S565 L566 Y567 L570 G571 N572 F575 L580 T588 F589 G590 Q591 M592 A593

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.92 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.268 0.218 , 0.262	Depositor DCC
R_{free} test set	37523 reflections (9.47%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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:H	3:A:2:LYS:HD2	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:O	3:A:698:ILE:HG13	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:HD22	3:C:303:LEU:H	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:H	3:C:356:GLN:NE2	1.79	0.80
3:D:295:GLU:HG2	3:D:301:GLY:HA2	1.64	0.79
3:B:2:LYS:HD3	4:B:1077:HOH:O	1.82	0.78
3:C:167:ALA:HA	3:C:176:ASP:HB2	1.66	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:HA	3:C:302:LYS:HE2	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:B:897:LEU:H	3:B:897:LEU:HD23	1.51	0.76
3:C:495:ASN:HD21	3:C:522:PHE:H	1.33	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:A:206:GLN:NE2	3:A:241:ARG:HE	1.86	0.73
3:C:482:ARG:HE	3:C:556:GLN:HE21	1.36	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:C:411:ASP:OD1	3:C:624:SER:HB3	1.91	0.70
3:D:308:PRO:HG2	3:D:311:LYS:HB2	1.74	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:471:VAL:HB	3:A:472:PRO:HD3	1.75	0.69
3:A:649:ASP:O	3:A:653:LYS:HG2	1.92	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:A:775:ASN:OD1	3:A:777:ILE:HG22	1.94	0.68
3:D:530:ILE:HG13	3:D:533:LEU:HD22	1.74	0.68
3:A:540:GLU:O	3:A:544:ARG:HD3	1.93	0.68
1:K:15:DC:H5"	4:K:457:HOH:O	1.94	0.67
3:A:85:MET:HE2	3:A:87:ASP:N	2.03	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
4:F:120:HOH:O	3:A:783:SER:HA	1.95	0.67
3:D:598:GLU:HG3	3:D:617:VAL:HG11	1.76	0.67
3:A:354:GLN:HB3	3:A:356:GLN:HE22	1.59	0.67
3:C:526:ILE:HD12	4:C:1045:HOH:O	1.94	0.67
3:D:516:VAL:HG11	3:D:526:ILE:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:860:ASP:H	3:D:863:LEU:HD23	1.60	0.67
3:A:602:ASN:ND2	3:A:616:PHE:H	1.92	0.66
3:C:148:VAL:HG13	4:C:1125:HOH:O	1.96	0.66
3:D:830:VAL:HA	3:D:850:SER:HB3	1.78	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:B:738:PRO:HG2	3:B:741:VAL:HB	1.77	0.65
3:D:738:PRO:HG2	3:D:741:VAL:HB	1.77	0.65
1:G:6:DT:H5"	1:G:6:DT:H6	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:118:THR:HG21	3:D:313:ARG:HB3	1.79	0.65
3:D:700:GLY:HA2	3:D:753:LEU:HD22	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:A:848:TRP:HB2	3:A:849:PRO:HD2	1.80	0.64
3:D:512:GLU:HG3	3:D:513:PRO:HD2	1.78	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:422:GLN:NE2	3:A:680:LEU:H	1.96	0.63
3:A:653:LYS:O	3:A:657:GLU:HG2	1.98	0.63
3:A:514:LEU:HD12	3:A:530:ILE:HG12	1.80	0.63
2:F:110:DA:H2"	2:F:111:DT:C5'	2.28	0.63
2:J:112:DA:H2'	4:J:405:HOH:O	1.98	0.63
3:A:2:LYS:H	3:A:2:LYS:CD	2.06	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
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

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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:2:LYS:HG2	3:A:102:LYS:HE3	1.81	0.62
3:A:395:PHE:HB2	3:A:591:GLN:CG	2.25	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:1:MET:HG2	3:C:22:SER:O	2.00	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
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: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:151:LEU:HD11	3:D:194:GLU:HA	1.83	0.61
3:D:812:ASN:HA	3:D:815:ILE:HG12	1.83	0.61
3:B:514:LEU:HG	3:B:533:LEU:HD21	1.82	0.61
3:D:859:LYS:HD3	3:D:860:ASP:HB2	1.81	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
1:K:17:DC:H2"	1:K:18:DG:OP1	2.01	0.60
3:B:606:ASN:HD21	3:B:614:GLU:N	1.97	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:B:202:LEU:O	3:B:206:GLN:HG2	2.01	0.60
3:D:401:PRO:HA	3:D:702:TRP:O	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:C:424:ASN:HD21	3:C:469:GLY:H	1.48	0.60
3:D:535:ALA:HA	3:D:538:LEU:HB2	1.84	0.60
3:B:154:SER:HB2	3:B:155:PRO:HD2	1.82	0.60
3:A:176:ASP:HA	3:A:319:ARG:NH2	2.16	0.60
3:B:582:ASN:O	3:B:586:ILE:HG13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:140:ASP:HB3	3:D:143:ASP:HB2	1.84	0.60
3:D:271:LEU:HD21	3:D:356:GLN:HA	1.84	0.60
3:B:825:VAL:HB	3:B:828:GLU:HG3	1.84	0.60
3:D:87:ASP:OD1	3:D:90:LEU:HD13	2.01	0.60
2:J:101:DG:H2'	2:J:102:DC:C5	2.36	0.60
2:J:110:DA:C2'	2:J:111:DT:H5"	2.32	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:C:52:ILE:HD12	3:C:428:GLU:HG3	1.82	0.59
3:D:434:PHE:CE1	3:D:460:GLY:HA2	2.37	0.59
3:D:449:ARG:HH21	3:D:675:ASN:HB2	1.65	0.59
3:A:556:GLN:HE22	3:A:557:ILE:HD13	1.67	0.59
3:B:261:GLU:HG3	3:B:262:ILE:N	2.17	0.59
3:D:131:HIS:HB3	3:D:132:PRO:HD2	1.85	0.59
3:D:698:ILE:HG12	3:D:752:MET:O	2.02	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:B:136:ILE:HG23	3:B:149:PHE:HB2	1.84	0.58
3:C:60:LYS:C	4:C:1100:HOH:O	2.41	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:A:41:CYS:HB2	3:A:42:PRO:HD2	1.84	0.58
3:D:503:LEU:O	3:D:506:PRO:HD3	2.04	0.58
3:A:354:GLN:HB3	3:A:356:GLN:NE2	2.17	0.58
3:A:403:ARG:HD2	3:A:887:ALA:O	2.04	0.58
3:A:839:ASN:HD22	3:A:841:PHE:HB2	1.69	0.58
3:B:797:PRO:HG3	3:B:806:ARG:NH1	2.19	0.58
3:D:395:PHE:HB2	3:D:591:GLN:HG2	1.86	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:B:760:LEU:HD13	3:B:891:TYR:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ILE:CG1	3:C:80:LEU:HD23	2.34	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
2:J:101:DG:H2'	2:J:102:DC:C6	2.41	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:D:405:LYS:O	3:D:699:GLY:HA3	2.05	0.56
3:D:698:ILE:O	3:D:753:LEU:HA	2.05	0.56
3:C:302:LYS:HG2	3:C:330:ARG:HH12	1.71	0.56
1:E:18:DG:OP1	1:E:18:DG:H3'	2.06	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:I:7:DA:H2'	1:I:8:DT:H72	1.88	0.56
3:A:402:ASN:HA	3:A:886:ALA:O	2.06	0.56
3:D:545:ALA:HB1	4:D:923:HOH:O	2.04	0.56
2:J:111:DT:H2"	2:J:112:DA:H8	1.71	0.56
3:A:51:ASP:HA	3:A:379:VAL:HG22	1.87	0.56
3:A:362:ILE:HD11	3:A:569:ALA:HA	1.88	0.56
4:K:596:HOH:O	3:D:800:LYS:HG3	2.06	0.56
3:C:481:GLN:HE21	3:C:559:ARG:HE	1.53	0.56
3:C:507:ASN:N	3:C:507:ASN:HD22	2.04	0.56
3:A:112:ASN:HB3	4:A:1119:HOH:O	2.05	0.55
3:D:597:ILE:O	3:D:601:VAL:HG23	2.06	0.55
3:D:856:ASP:HA	3:D:859:LYS:HG2	1.88	0.55
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.42	0.55
3:A:249:ARG:HB3	3:A:264:THR:HG23	1.89	0.55
3:B:326:ILE:O	3:B:330:ARG:HG2	2.06	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
2:H:109:DC:H2"	2:H:110:DA:H5'	1.89	0.55
3:A:202:LEU:CD1	3:A:242:LEU:HD13	2.36	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:61:LEU:N	4:C:1100:HOH:O	2.39	0.55
3:C:303:LEU:HB2	3:C:323:TYR:OH	2.07	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:A:654:PHE:O	3:A:658:ARG:HB2	2.07	0.55
3:D:206:GLN:HE22	3:D:241:ARG:HE	1.55	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:223:ILE:HB	3:A:224:PRO:HD3	1.89	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
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:A:25:ARG:HD2	4:A:926:HOH:O	2.08	0.54
3:B:2:LYS:HA	4:B:1077:HOH:O	2.07	0.54
3:B:47:THR:HB	4:B:1059:HOH:O	2.08	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
1:G:15:DC:H5"	4:G:515:HOH:O	2.08	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
3:D:229:ARG:NE	3:D:233:ILE:HD11	2.22	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: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:B:516:VAL:HG11	3:B:526:ILE:HD13	1.89	0.54
1:K:2:DG:C3'	1:K:3:3DR:H5'	2.38	0.54
3:A:98:ASN:HB3	4:A:1126:HOH:O	2.07	0.54
3:A:222:ALA:O	3:A:226:VAL:HG23	2.08	0.54
3:C:469:GLY:C	3:C:472:PRO:HD2	2.29	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
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:C:354:GLN:HB3	3:C:356:GLN:NE2	2.23	0.53
3:D:241:ARG:CZ	3:D:241:ARG:HA	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: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:475:ILE:CG1	3:C:566:LEU:HD12	2.38	0.52
3:D:397:LYS:O	3:D:399:PRO:HD3	2.09	0.52
3:D:422:GLN:NE2	3:D:681:MET:HG2	2.18	0.52
3:B:250:VAL:HA	3:B:263:ILE:HG22	1.90	0.52
3:C:27:ARG:HH11	3:C:27:ARG:HB3	1.74	0.52
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.91	0.52
3:C:516:VAL:CG1	3:C:526:ILE:HD13	2.39	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:333:GLN:O	3:B:337:LYS:HG2	2.08	0.52
3:A:101:ILE:HD11	3:A:349:TYR:O	2.09	0.52
3:A:338:ARG:HB3	3:A:340:PHE:CE1	2.44	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:245:HIS:HE1	4:A:938:HOH:O	1.92	0.52
3:A:285:GLN:HB3	3:A:292:TYR:HE2	1.75	0.52
3:B:145:ARG:HD2	3:B:187:ILE:HD11	1.91	0.52
3:B:294:SER:O	3:B:298:LEU:HB2	2.10	0.52
3:C:874:LYS:HB2	4:C:1151:HOH:O	2.07	0.52
3:D:271:LEU:HD11	3:D:355:ILE:HG22	1.90	0.52
3:C:738:PRO:HB3	3:C:780:ALA:O	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:A:609:CYS:HA	3:A:635:LYS:HE3	1.91	0.52
3:B:755:GLU:HB3	3:B:759:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:642:ARG:HH11	3:C:646:HIS:CD2	2.27	0.52
3:B:491:ALA:HA	3:B:494:ARG:HH11	1.73	0.52
3:C:81:GLU:HG2	3:C:83:LEU:HD11	1.91	0.52
3:D:36:SER:HB3	3:D:59:ARG:HD3	1.92	0.52
3:D:594:LEU:O	3:D:597:ILE:HG22	2.09	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:A:566:LEU:O	3:A:570:LEU:HD23	2.10	0.51
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.91	0.51
3:D:148:VAL:HG21	3:D:325:ILE:HD11	1.93	0.51
3:D:403:ARG:HD2	3:D:887:ALA:O	2.10	0.51
1:E:15:DC:H2"	1:E:16:DG:O5'	2.09	0.51
3:B:316:ASN:C	3:B:318:GLN:H	2.14	0.51
3:D:793:VAL:HG22	3:D:796:PHE:O	2.10	0.51
3:D:863:LEU:HD22	3:D:863:LEU:H	1.74	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:A:556:GLN:NE2	3:A:557:ILE:HD13	2.26	0.51
3:D:109:ARG:NH1	3:D:142:ILE:HD11	2.25	0.51
2:H:114:DG:H2"	2:H:115:DA:C8	2.46	0.51
2:J:113:DA:H2"	2:J:114:DG:H5"	1.93	0.51
3:A:356:GLN:NE2	3:A:356:GLN:H	2.08	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:D:802:PRO:HD2	3:D:805:ILE:HG13	1.92	0.51
3:C:284:ASN:HD21	3:C:829:LYS:NZ	2.07	0.51
3:D:475:ILE:HD13	3:D:475:ILE:O	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:179:PRO:HB3	3:C:181:GLU:OE1	2.10	0.50
3:C:555:ALA:O	3:C:559:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:273:TYR:OH	3:D:335:ASP:HA	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:277:TYR:O	3:D:281:SER:HB2	2.12	0.50
3:D:637:GLY:O	3:D:640:LYS:HB2	2.11	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: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
3:D:197:LEU:HD23	3:D:197:LEU:O	2.12	0.50
3:D:439:LEU:O	3:D:443:ILE:HG13	2.12	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
2:H:102:DC:H2"	2:H:103:DG:C8	2.46	0.50
3:A:517:ASP:OD2	3:A:519:ARG:HB2	2.11	0.50
3:C:171:GLN:HE22	3:C:303:LEU:HB3	1.77	0.50
3:D:863:LEU:HD22	3:D:863:LEU:N	2.27	0.50
2:F:108:DT:H2"	2:F:109:DC:O5'	2.12	0.50
1:K:11:DC:H4'	3:D:803:PHE:HB2	1.94	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
3:D:109:ARG:HD2	3:D:209:THR:O	2.12	0.50
3:D:330:ARG:O	3:D:334:ILE:HG13	2.12	0.50
3:D:458:PRO:HG3	3:D:592:MET:SD	2.51	0.50
3:A:48:LYS:HZ1	3:A:377:ASN:ND2	2.10	0.50
3:B:356:GLN:C	3:B:358:VAL:H	2.14	0.50
3:C:302:LYS:HD2	3:C:326:ILE:HD13	1.93	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:C:191:PHE:CD2	3:C:196:GLU:HG3	2.46	0.49
3:D:422:GLN:HG3	3:D:678:GLN:O	2.13	0.49
2:H:112:DA:C2'	2:H:113:DA:H5'	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:483:LYS:NZ	3:B:483:LYS:HB3	2.27	0.49
3:B:555:ALA:O	3:B:559:ARG:HG2	2.13	0.49
3:C:300:VAL:O	3:C:300:VAL:HG13	2.11	0.49
3:C:322:SER:O	3:C:326:ILE:HG23	2.12	0.49
3:C:362:ILE:HD13	3:C:569:ALA:HB1	1.95	0.49
3:A:481:GLN:HE21	3:A:559:ARG:NE	2.07	0.49
3:D:145:ARG:HG2	3:D:187:ILE:HD11	1.93	0.49
3:D:831:TYR:CD1	3:D:850:SER:HA	2.48	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:D:469:GLY:C	3:D:472:PRO:HD2	2.33	0.49
3:A:101:ILE:HG12	4:A:1047:HOH:O	2.12	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:633:ILE:HG13	3:D:651:LEU:HD21	1.94	0.49
1:E:12:DA:H2"	1:E:13:DG:O5'	2.13	0.49
3:A:731:GLU:HG3	3:A:879:PRO:CB	2.43	0.49
3:D:191:PHE:HB2	3:D:197:LEU:HD12	1.94	0.49
3:A:856:ASP:O	3:A:857:LEU:HB2	2.13	0.49
3:B:405:LYS:HA	3:B:698:ILE:O	2.12	0.49
3:C:488:TYR:CD1	3:C:519:ARG:HB3	2.48	0.49
3:B:303:LEU:H	3:B:303:LEU:HD22	1.78	0.48
3:B:458:PRO:HG3	3:B:592:MET:SD	2.52	0.48
3:D:204:PHE:HE1	3:D:208:LYS:HD2	1.78	0.48
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:509:SER:HA	3:D:534:SER:CB	2.43	0.48
3:D:727:ILE:HG23	3:D:730:LEU:HD12	1.95	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
1:G:2:DG:H5'	1:G:3:3DR:H5'	1.95	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
2:F:115:DA:H62	3:A:282:PHE:HE2	1.62	0.48
1:G:3:3DR:H2"	1:G:4:DC:O4'	2.13	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
1:G:10:DA:H1'	1:G:11:DC:H5'	1.94	0.48
2:L:102:DC:H2"	2:L:103:DG:C8	2.49	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:B:355:ILE:C	3:B:356:GLN:O	2.51	0.48
3:D:102:LYS:O	3:D:102:LYS:HD3	2.14	0.48
3:A:902:ASP:O	3:A:903:PHE:HB2	2.14	0.48
3:D:219:GLU:O	3:D:219:GLU:HG2	2.14	0.48
3:D:300:VAL:O	3:D:300:VAL:HG13	2.14	0.48
3:B:124:PRO:HB2	3:B:225:TYR:CE1	2.47	0.48
3:B:554:THR:O	3:B:557:ILE:HG22	2.14	0.48
3:C:52:ILE:HB	3:C:428:GLU:HG2	1.95	0.48
3:D:450:PRO:HB2	3:D:456:CYS:SG	2.53	0.48
3:B:45:GLN:O	3:B:45:GLN:HG3	2.14	0.48
3:B:401:PRO:O	3:B:402:ASN:HB2	2.13	0.48
3:C:12:GLY:O	3:C:13:ASP:HB2	2.13	0.48
3:D:750:ARG:HG3	3:D:754:GLN:NE2	2.29	0.48
2:H:108:DT:H5"	4:H:575:HOH:O	2.13	0.47
1:K:13:DG:H2"	1:K:14:DC:C6	2.48	0.47
3:C:382:GLN:HG2	3:C:383:GLY:N	2.28	0.47
3:C:495:ASN:HD21	3:C:522:PHE:N	2.04	0.47
3:D:402:ASN:ND2	3:D:403:ARG:N	2.59	0.47
3:D:503:LEU:HG	3:D:538:LEU:HB3	1.95	0.47
1:E:4:DC:H2'	1:E:5:DT:H71	1.96	0.47
4:K:745:HOH:O	3:D:361:PRO:HD2	2.14	0.47
3:B:354:GLN:HG3	4:B:907:HOH:O	2.14	0.47
3:D:38:PHE:CZ	3:D:59:ARG:HG2	2.48	0.47
3:D:41:CYS:CB	3:D:45:GLN:HG3	2.43	0.47
3:D:61:LEU:HD23	3:D:62:PHE:N	2.29	0.47
3:D:481:GLN:HB3	3:D:559:ARG:HE	1.79	0.47
2:H:110:DA:H2'	2:H:111:DT:H71	1.96	0.47
3:B:164:ILE:HG23	3:B:165:GLU:OE1	2.14	0.47
3:B:277:TYR:O	3:B:281:SER:HB2	2.15	0.47
3:B:660:GLU:CB	3:B:661:PRO:HD3	2.44	0.47
3:A:369:ILE:HG12	3:A:474:GLU:HG2	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:52:ILE:HD12	3:D:428:GLU:HG3	1.96	0.47
3:D:484:GLU:HG2	4:D:927:HOH:O	2.15	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:A:415:LEU:HD22	3:A:623:ASP:HB3	1.95	0.47
3:C:27:ARG:HB3	3:C:27:ARG:NH1	2.30	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:B:529:LYS:O	3:B:533:LEU:HG	2.15	0.47
3:C:20:ILE:HD13	3:C:26:GLU:HA	1.97	0.47
3:C:137:THR:OG1	3:C:324:ASN:ND2	2.48	0.47
3:C:362:ILE:HD12	3:C:575:PHE:HB2	1.96	0.47
3:C:402:ASN:HA	3:C:886:ALA:O	2.14	0.47
3:D:362:ILE:HD11	3:D:572:ASN:ND2	2.29	0.47
3:D:423:VAL:HB	3:D:425:ILE:HG13	1.96	0.47
1:K:10:DA:OP1	3:D:878:LYS:HG2	2.14	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:455:SER:OG	3:D:676:ASN:HA	2.13	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:D:819:ILE:HG22	3:D:820:ASP:N	2.23	0.47
3:B:596:TRP:CE2	3:B:670:MET:HB2	2.50	0.47
1:G:4:DC:H2'	1:G:5:DT:C6	2.50	0.47
3:B:351:ALA:O	3:B:352:LYS:HB2	2.14	0.47
3:D:38:PHE:CE2	3:D:59:ARG:HG2	2.49	0.47
3:D:180:SER:O	3:D:183:ILE:HG22	2.14	0.47
3:D:459:ASN:N	3:D:459:ASN:HD22	2.13	0.47
3:D:834:PRO:HD2	3:D:871:LEU:HD13	1.97	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:C:731:GLU:HA	3:C:734:LYS:HG3	1.98	0.46
3:D:810:THR:HG23	3:D:813:ARG:HH21	1.81	0.46
3:D:52:ILE:HG12	4:D:912:HOH:O	2.15	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:C:660:GLU:CB	3:C:661:PRO:HD3	2.45	0.46
3:D:458:PRO:HG2	3:D:589:PHE:HA	1.96	0.46
3:D:775:ASN:OD1	3:D:777:ILE:HG13	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:362:ILE:HD11	3:B:572:ASN:HB3	1.98	0.46
3:C:303:LEU:H	3:C:303:LEU:CD2	2.23	0.46
3:D:159:VAL:HB	3:D:317:HIS:CD2	2.51	0.46
3:D:281:SER:OG	3:D:283:THR:HG22	2.14	0.46
3:D:412:LEU:HD13	3:D:415:LEU:HD13	1.98	0.46
3:A:247:LYS:HG3	3:A:266:PHE:CD1	2.50	0.46
3:A:263:ILE:HD12	3:A:263:ILE:N	2.31	0.46
3:A:494:ARG:HD2	3:A:521:ASP:OD1	2.16	0.46
3:B:633:ILE:O	3:B:636:VAL:HG22	2.15	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:D:191:PHE:HZ	3:D:200:GLU:HG2	1.81	0.46
3:A:241:ARG:NE	4:A:1105:HOH:O	2.49	0.46
3:A:566:LEU:HD13	3:A:570:LEU:HD23	1.98	0.46
3:B:514:LEU:HB2	3:B:541:MET:HE3	1.97	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:C:594:LEU:HD22	3:C:622:THR:O	2.16	0.46
3:D:391:TYR:HB2	3:D:392:PRO:HD2	1.97	0.46
3:D:512:GLU:CG	3:D:513:PRO:HD2	2.44	0.46
3:A:206:GLN:HE21	3:A:241:ARG:HE	1.63	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
3:D:41:CYS:SG	3:D:45:GLN:HG3	2.56	0.46
1:K:13:DG:H2"	1:K:14:DC:H6	1.81	0.46
3:A:129:ALA:HA	3:A:225:TYR:CE1	2.51	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:206:GLN:NE2	3:D:241:ARG:HE	2.13	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
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:A:86:ASP:OD1	3:A:86:ASP:N	2.49	0.45
3:A:636:VAL:HG12	3:A:636:VAL:O	2.16	0.45
3:D:544:ARG:HH11	3:D:544:ARG:HG3	1.81	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:34:LYS:HG3	3:D:64:ASN:HA	1.98	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:516:VAL:HG11	3:D:526:ILE:CG2	2.46	0.45
3:D:625:ILE:O	3:D:625:ILE:HG13	2.16	0.45
3:B:180:SER:O	3:B:183:ILE:HG22	2.16	0.45
3:B:231:LYS:HG3	3:B:236:GLU:CA	2.43	0.45
3:B:471:VAL:N	3:B:472:PRO:HD2	2.31	0.45
3:D:398:GLU:HA	3:D:705:LYS:HE2	1.98	0.45
3:D:644:THR:O	3:D:648:VAL:HG23	2.17	0.45
3:A:533:LEU:HB3	3:A:537:SER:OG	2.16	0.45
3:B:494:ARG:HG3	3:B:495:ASN:ND2	2.32	0.45
3:C:149:PHE:CD1	3:C:149:PHE:N	2.84	0.45
3:C:558:ASN:HD22	3:C:558:ASN:HA	1.66	0.45
3:D:295:GLU:CG	3:D:301:GLY:HA2	2.42	0.45
3:D:422:GLN:NE2	3:D:680:LEU:H	2.13	0.45
3:D:451:SER:HB3	3:D:456:CYS:SG	2.56	0.45
2:F:104:DG:H2"	2:F:105:DC:O5'	2.15	0.45
1:G:6:DT:C2'	1:G:7:DA:C5'	2.80	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:O	2.17	0.45
3:D:738:PRO:HB3	3:D:780:ALA:C	2.36	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:85:MET:HG2	3:D:91:ALA:HB2	1.99	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:D:433:THR:CG2	3:D:461:MET:HE1	2.47	0.45
3:D:800:LYS:HD2	3:D:800:LYS:N	2.32	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:B:273:TYR:HE2	3:B:341:ILE:HG12	1.82	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:830:VAL:HG22	3:D:831:TYR:N	2.31	0.45
2:L:111:DT:H2"	2:L:112:DA:C8	2.52	0.44
3:B:104:ASP:OD1	3:B:106:THR:OG1	2.31	0.44
3:B:119:SER:HB2	3:B:124:PRO:HB3	1.99	0.44
3:B:339:GLN:HB2	4:B:1092:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:472:PRO:HA	3:B:475:ILE:HG22	1.99	0.44
3:B:546:GLN:O	3:B:550:VAL:HG23	2.16	0.44
3:C:302:LYS:CG	3:C:330:ARG:HH12	2.28	0.44
3:D:112:ASN:HB3	3:D:214:THR:CG2	2.38	0.44
3:D:655:ALA:O	3:D:660:GLU:HG3	2.17	0.44
2:H:113:DA:H5'	4:H:758:HOH:O	2.15	0.44
1:K:13:DG:H2"	1:K:14:DC:O5'	2.15	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
3:A:653:LYS:HD3	4:A:1043:HOH:O	2.17	0.44
3:D:4:PHE:HB3	3:D:101:ILE:CG2	2.48	0.44
1:I:7:DA:H2"	1:I:8:DT:C6	2.53	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
3:B:3:GLU:HG3	3:B:20:ILE:O	2.18	0.44
3:C:130:LYS:HG3	3:C:131:HIS:N	2.31	0.44
3:D:20:ILE:HD11	3:D:24:GLY:HA2	1.99	0.44
3:D:486:LYS:O	3:D:490:LEU:HG	2.18	0.44
2:F:105:DC:H2'	2:F:106:DT:H72	1.99	0.44
3:A:745:LEU:HD12	3:A:745:LEU:HA	1.83	0.44
3:D:6:LEU:HB2	3:D:18:ARG:O	2.17	0.44
3:D:109:ARG:HH12	3:D:142:ILE:HD11	1.83	0.44
3:D:779:ILE:O	3:D:871:LEU:HD21	2.17	0.44
2:L:101:DG:H2"	2:L:102:DC:C6	2.53	0.44
3:A:506:PRO:HG3	4:A:1153:HOH:O	2.16	0.44
3:A:698:ILE:HG12	3:A:752:MET:O	2.17	0.44
3:B:6:LEU:CD1	3:B:26:GLU:HG3	2.48	0.44
3:C:125:GLU:HG3	4:C:1142:HOH:O	2.17	0.44
3:D:163:SER:HB3	3:D:165:GLU:OE1	2.17	0.44
3:D:566:LEU:HD13	3:D:566:LEU:C	2.37	0.44
3:D:652:ASP:OD1	3:D:656:ARG:NH1	2.46	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:C:818:ASN:ND2	3:C:857:LEU:HD11	2.32	0.44
3:D:841:PHE:CZ	3:D:862:VAL:HG22	2.52	0.44
2:L:115:DA:H2"	3:D:567:TYR:HD2	1.82	0.44
3:A:101:ILE:HD12	3:A:349:TYR:HD1	1.83	0.44
3:A:277:TYR:C	3:A:279:LYS:H	2.20	0.44
3:B:326:ILE:HG23	3:B:330:ARG:HE	1.81	0.44
3:C:197:LEU:HD23	3:C:197:LEU:C	2.38	0.44
3:A:322:SER:O	3:A:326:ILE:HG12	2.16	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:C:512:GLU:HB3	3:C:513:PRO:HD2	1.99	0.44
3:D:40:HIS:ND1	3:D:83:LEU:HD11	2.32	0.44
3:D:731:GLU:HG3	3:D:879:PRO:CB	2.46	0.44
3:D:844:LYS:HD3	3:D:844:LYS:N	2.33	0.44
1:E:14:DC:H2'	1:E:15:DC:C5	2.53	0.44
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.99	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:D:63:ALA:HB3	3:D:66:ARG:HG2	1.99	0.44
3:D:525:GLU:O	3:D:529:LYS:HG3	2.17	0.44
3:D:783:SER:O	3:D:829:LYS:HB3	2.17	0.44
1:E:8:DT:H4'	3:A:707:ARG:CD	2.47	0.43
1:G:7:DA:H2'	1:G:8:DT:C7	2.48	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:A:48:LYS:NZ	3:A:377:ASN:CG	2.71	0.43
3:B:858:ILE:O	3:B:862:VAL:HG23	2.17	0.43
3:D:178:VAL:HG11	3:D:186:ILE:HD11	1.99	0.43
3:A:36:SER:O	3:A:37:LEU:HD23	2.18	0.43
3:A:85:MET:HE3	3:A:576:ARG:NH2	2.33	0.43
3:B:42:PRO:HG2	3:B:45:GLN:HG2	2.00	0.43
3:C:10:GLN:HG3	3:C:65:MET:CE	2.48	0.43
3:C:186:ILE:HG23	4:C:1125:HOH:O	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:14:SER:HA	3:D:65:MET:HG2	1.99	0.43
3:D:495:ASN:O	3:D:499:ILE:HG13	2.18	0.43
3:D:530:ILE:O	3:D:533:LEU:HB2	2.18	0.43
3:D:597:ILE:HD11	3:D:663:ILE:HG23	2.00	0.43
3:B:245:HIS:O	3:B:247:LYS:HG2	2.18	0.43
3:D:72:ILE:O	3:D:76:GLU:HG3	2.18	0.43
3:D:114:ASP:HB3	3:D:328:VAL:HG13	2.00	0.43
3:D:143:ASP:OD2	3:D:208:LYS:HE2	2.16	0.43
3:D:151:LEU:HD23	3:D:153:ASN:H	1.82	0.43
3:D:459:ASN:HD22	3:D:459:ASN:H	1.66	0.43
2:J:111:DT:H2"	2:J:112:DA:C8	2.51	0.43
3:A:730:LEU:HB3	3:A:883:PHE:CZ	2.53	0.43
3:C:81:GLU:HG2	3:C:83:LEU:HD12	1.99	0.43
3:D:117:VAL:HG13	3:D:124:PRO:HG3	2.00	0.43
3:D:221:PHE:O	3:D:225:TYR:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:410:PHE:CD2	3:D:685:ARG:HA	2.54	0.43
1:E:8:DT:H4'	3:A:707:ARG:HD2	2.00	0.43
3:A:300:VAL:O	3:A:300:VAL:HG23	2.18	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
2:H:113:DA:H2"	2:H:114:DG:O5'	2.18	0.43
3:A:249:ARG:HG2	3:A:250:VAL:N	2.33	0.43
3:D:878:LYS:N	3:D:879:PRO:HD2	2.33	0.43
3:B:111:ALA:HB1	3:B:138:HIS:NE2	2.33	0.43
3:C:205:TRP:HH2	3:C:213:LEU:HD11	1.84	0.43
3:C:461:MET:CE	3:C:581:ARG:HD2	2.49	0.43
3:D:555:ALA:O	3:D:559:ARG:HG2	2.18	0.43
2:H:113:DA:H3'	4:H:758:HOH:O	2.18	0.43
3:B:271:LEU:HB3	3:B:276:LEU:HD11	2.01	0.43
3:B:279:LYS:HE3	3:B:280:PHE:CE2	2.54	0.43
3:C:105:HIS:HA	3:C:108:ILE:HD12	2.01	0.43
3:C:416:TYR:HB2	3:C:417:PRO:HD3	2.00	0.43
3:D:477:LYS:O	3:D:481:GLN:HG3	2.18	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:A:700:GLY:HA2	3:A:753:LEU:HD22	2.00	0.43
3:B:131:HIS:HB2	3:B:225:TYR:OH	2.19	0.43
3:C:495:ASN:HD21	3:C:521:ASP:HA	1.83	0.43
3:C:532:LYS:HD2	3:C:532:LYS:N	2.34	0.43
3:D:458:PRO:HB2	3:D:588:THR:CG2	2.42	0.43
3:A:214:THR:OG1	3:A:215:GLY:N	2.51	0.43
3:A:405:LYS:HA	4:A:998:HOH:O	2.19	0.43
3:A:494:ARG:O	3:A:498:ILE:HG12	2.19	0.43
3:B:356:GLN:O	3:B:358:VAL:N	2.52	0.43
3:B:830:VAL:HB	3:B:848:TRP:O	2.18	0.43
3:C:262:ILE:HG13	3:C:262:ILE:O	2.19	0.43
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.99	0.43
3:D:559:ARG:O	3:D:563:ILE:HG13	2.19	0.43
3:A:482:ARG:HG2	3:A:482:ARG:NH1	2.34	0.42
3:B:244:PRO:HG2	3:B:267:GLY:HA3	2.01	0.42
3:B:251:LYS:C	3:B:253:GLY:H	2.22	0.42
3:C:284:ASN:ND2	3:C:829:LYS:NZ	2.66	0.42
3:D:15:ILE:HD13	3:D:15:ILE:C	2.40	0.42
3:D:340:PHE:HD1	3:D:343:LEU:HD12	1.84	0.42
3:D:381:PRO:HG3	4:D:912:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:394:ALA:HB1	3:D:622:THR:HA	2.01	0.42
3:D:456:CYS:HA	3:D:461:MET:O	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
4:K:745:HOH:O	3:D:362:ILE:HG13	2.18	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:A:221:PHE:C	3:A:224:PRO:HD2	2.39	0.42
3:B:202:LEU:HD23	3:B:241:ARG:HH21	1.83	0.42
3:B:313:ARG:HG2	3:B:313:ARG:NH1	2.33	0.42
3:B:422:GLN:HG3	3:B:678:GLN:O	2.20	0.42
3:B:468:ASP:HB2	4:B:957:HOH:O	2.20	0.42
3:A:170:LEU:HB2	3:A:173:GLN:HE21	1.84	0.42
3:A:380:ILE:HD12	3:A:576:ARG:CZ	2.49	0.42
3:B:186:ILE:HG22	4:B:1053:HOH:O	2.18	0.42
3:B:806:ARG:HD3	3:B:843:ASP:OD1	2.20	0.42
3:D:102:LYS:HB2	3:D:102:LYS:HZ3	1.83	0.42
3:D:230:ILE:HG23	3:D:234:PHE:CD2	2.51	0.42
3:D:500:LYS:O	3:D:503:LEU:HB2	2.19	0.42
2:H:104:DG:H2"	2:H:105:DC:C5'	2.49	0.42
2:L:107:DG:H2"	2:L:108:DT:O5'	2.20	0.42
3:A:822:PRO:HA	4:A:1106:HOH:O	2.18	0.42
3:C:449:ARG:HA	3:C:450:PRO:HD2	1.88	0.42
3:D:732:THR:HG22	3:D:745:LEU:HB2	1.99	0.42
3:D:804:HIS:O	3:D:808:ILE:HG13	2.20	0.42
3:A:126:PRO:HB3	3:A:224:PRO:HB2	2.00	0.42
3:A:197:LEU:HD23	3:A:197:LEU:C	2.39	0.42
3:A:485:HIS:C	3:A:487:GLY:H	2.21	0.42
3:B:229:ARG:O	3:B:233:ILE:HG13	2.20	0.42
3:D:65:MET:O	3:D:65:MET:HG3	2.19	0.42
1:E:2:DG:OP2	3:A:361:PRO:HD2	2.19	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:5:DT:C6	1:E:6:DT:H72	2.54	0.42
2:L:113:DA:H4'	3:D:728:MET:HE2	2.02	0.42
3:A:422:GLN:HE21	3:A:422:GLN:HB2	1.70	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

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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
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
3:C:40:HIS:HE1	3:C:51:ASP:OD2	2.03	0.42
3:D:119:SER:OG	3:D:124:PRO:HD3	2.20	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: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:C:500:LYS:HE3	3:C:542:LEU:HD11	2.02	0.41
3:A:741:VAL:HG12	3:A:745:LEU:HD22	2.02	0.41
3:B:37:LEU:HD12	3:B:37:LEU:HA	1.79	0.41
3:B:159:VAL:HG13	3:B:313:ARG:NH1	2.35	0.41
3:C:179:PRO:O	3:C:183:ILE:HG12	2.20	0.41
3:C:633:ILE:HD13	3:C:633:ILE:HA	1.87	0.41
3:D:142:ILE:HG13	3:D:143:ASP:OD1	2.20	0.41
3:D:216:TRP:CD1	3:D:290:LEU:HB2	2.54	0.41
3:D:430:ILE:H	3:D:430:ILE:HG13	1.55	0.41
3:D:440:HIS:HA	3:D:443:ILE:HD12	2.02	0.41
3:D:664:ASP:OD1	3:D:668:ARG:HD2	2.21	0.41
3:A:486:LYS:O	3:A:486:LYS:HG2	2.19	0.41
3:B:436:VAL:HG12	4:B:1021:HOH:O	2.20	0.41
3:B:739:LYS:HD3	3:B:739:LYS:HA	1.87	0.41
3:B:891:TYR:CD2	3:B:892:GLU:HG3	2.55	0.41
3:C:524:ASP:HA	3:C:527:LYS:HE3	2.00	0.41
3:D:74:ARG:O	3:D:78:ILE:HG13	2.21	0.41
3:D:241:ARG:HB3	4:D:929:HOH:O	2.19	0.41
3:A:162:TRP:HB3	3:A:188:TYR:CE1	2.55	0.41
3:A:273:TYR:OH	3:A:335:ASP:HA	2.20	0.41
3:A:558:ASN:O	3:A:562:LEU:HD13	2.20	0.41
3:B:125:GLU:HA	3:B:126:PRO:HD3	1.94	0.41
3:B:562:LEU:HD12	3:B:562:LEU:HA	1.88	0.41
3:D:15:ILE:HD13	3:D:15:ILE:O	2.20	0.41
3:D:491:ALA:HA	3:D:521:ASP:OD1	2.20	0.41
3:D:878:LYS:HB3	3:D:879:PRO:HD3	2.01	0.41
1:E:16:DG:H2"	1:E:17:DC:C6	2.56	0.41
3:A:292:TYR:HB2	4:A:1131:HOH:O	2.20	0.41
3:A:499:ILE:CG2	3:A:541:MET:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:854:ILE:CD1	3:A:862:VAL:HG11	2.49	0.41
3:B:355:ILE:HD13	3:B:355:ILE:HA	1.80	0.41
3:B:499:ILE:HD12	3:B:530:ILE:HG13	2.03	0.41
3:C:10:GLN:HG3	3:C:65:MET:HE1	2.01	0.41
3:C:228:ASN:HD22	3:C:228:ASN:HA	1.64	0.41
3:C:326:ILE:HD11	4:C:1076:HOH:O	2.20	0.41
3:C:897:LEU:HD13	4:C:1114:HOH:O	2.20	0.41
3:D:9:GLU:O	3:D:15:ILE:HG12	2.21	0.41
3:D:183:ILE:HG23	3:D:184:ASP:N	2.36	0.41
3:D:382:GLN:HG2	3:D:383:GLY:N	2.35	0.41
3:D:398:GLU:CD	3:D:705:LYS:HE3	2.40	0.41
3:D:475:ILE:HD11	3:D:563:ILE:HG23	2.01	0.41
3:D:770:GLU:O	3:D:774:LEU:HG	2.20	0.41
3:D:796:PHE:HB3	3:D:797:PRO:HD2	2.03	0.41
3:D:812:ASN:CA	3:D:815:ILE:HG12	2.50	0.41
1:I:4:DC:H2'	1:I:5:DT:H72	2.03	0.41
3:B:873:GLU:O	3:B:878:LYS:HB2	2.20	0.41
3:D:64:ASN:O	3:D:65:MET:HB2	2.19	0.41
3:D:846:ILE:HG12	3:D:847:ALA:N	2.36	0.41
3:A:356:GLN:H	3:A:356:GLN:HE21	1.69	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: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:C:182:ILE:O	3:C:186:ILE:HG13	2.21	0.41
3:A:150:ASP:OD2	3:A:321:ILE:HD11	2.21	0.41
3:A:171:GLN:HE22	3:A:319:ARG:HH12	1.69	0.41
3:A:339:GLN:HE21	3:A:339:GLN:HB3	1.68	0.41
3:B:1:MET:HG2	3:B:2:LYS:N	2.36	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:D:686:GLU:HB3	3:D:687:ALA:H	1.75	0.41
2:F:107:DG:C8	2:F:108:DT:H72	2.56	0.41
3:A:125:GLU:HA	3:A:126:PRO:HD3	1.94	0.41
3:A:204:PHE:CE1	3:A:208:LYS:HD2	2.56	0.41
3:A:507:ASN:HD22	3:A:532:LYS:CA	2.34	0.41
3:A:663:ILE:HG21	3:A:683:MET:HB2	2.03	0.41
3:B:113:PHE:CE1	3:B:213:LEU:HD11	2.55	0.41
3:B:113:PHE:H	3:B:113:PHE:HD1	1.68	0.41
3:B:303:LEU:HD22	3:B:303:LEU:N	2.35	0.41
3:B:514:LEU:HD11	3:B:529:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:776:TYR:OH	3:B:854:ILE:HG22	2.20	0.41
3:D:145:ARG:NH2	3:D:185:LYS:HG2	2.36	0.41
3:D:241:ARG:HH12	3:D:246:ARG:CB	2.33	0.41
3:D:700:GLY:HA2	3:D:753:LEU:CD2	2.48	0.41
2:F:108:DT:H1'	2:F:109:DC:H5'	2.03	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:B:477:LYS:O	3:B:481:GLN:HG3	2.21	0.41
3:C:458:PRO:CG	3:C:592:MET:SD	3.09	0.41
3:C:731:GLU:HG3	3:C:879:PRO:CB	2.51	0.41
3:D:421:ARG:HD3	3:D:475:ILE:HG23	2.03	0.41
3:D:597:ILE:HA	3:D:597:ILE:HD12	1.86	0.41
3:D:747:GLU:OE2	3:D:747:GLU:HA	2.21	0.41
2:L:110:DA:H2"	2:L:111:DT:O5'	2.21	0.40
3:A:597:ILE:HB	3:A:667:PHE:CZ	2.56	0.40
3:A:730:LEU:HD22	3:A:883:PHE:HE1	1.86	0.40
3:B:216:TRP:HE3	4:B:1083:HOH:O	2.04	0.40
3:C:506:PRO:C	3:C:507:ASN:HD22	2.25	0.40
3:C:578:TYR:CD1	3:C:578:TYR:C	2.95	0.40
3:D:43:GLU:HA	3:D:56:PRO:HG3	2.02	0.40
3:D:250:VAL:HG12	3:D:263:ILE:CD1	2.50	0.40
3:D:870:VAL:O	3:D:874:LYS:HG2	2.22	0.40
3:A:509:SER:O	3:A:534:SER:HB3	2.21	0.40
3:B:502:ALA:HB3	3:B:530:ILE:HG12	2.03	0.40
3:B:736:SER:HA	3:B:782:VAL:HB	2.03	0.40
3:C:530:ILE:HG23	3:C:538:LEU:CD2	2.48	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
1:E:10:DA:H2"	1:E:11:DC:C5'	2.51	0.40
3:A:416:TYR:HB2	3:A:417:PRO:HD3	2.02	0.40
3:A:455:SER:OG	3:A:676:ASN:HA	2.22	0.40
3:A:478:VAL:HG13	3:A:559:ARG:HD2	2.04	0.40
3:A:530:ILE:C	3:A:532:LYS:H	2.24	0.40
3:A:822:PRO:HB2	3:A:849:PRO:HG3	2.04	0.40
3:A:839:ASN:HA	3:A:840:PRO:HD3	1.92	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:D:239:ALA:C	3:D:241:ARG:H	2.24	0.40
3:D:654:PHE:O	3:D:658:ARG:HB2	2.21	0.40
2:J:105:DC:H5"	2:J:105:DC:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:114:DG:H2'	4:J:750:HOH:O	2.21	0.40
3:A:409:SER:HB3	3:A:626:TYR:CD2	2.56	0.40
3:B:149:PHE:N	3:B:149:PHE:CD1	2.90	0.40
3:B:216:TRP:CH2	3:B:293:ILE:HG21	2.56	0.40
3:B:643:ASP:OD1	3:B:646:HIS:HB2	2.20	0.40
2:F:111:DT:H2"	2:F:112:DA:O5'	2.21	0.40
2:L:106:DT:H2"	2:L:107:DG:H8	1.86	0.40
3:A:738:PRO:HB3	3:A:780:ALA:O	2.22	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:C:811:TYR:O	3:C:815:ILE:HG12	2.21	0.40
3:D:501:GLU:HA	3:D:504:HIS:HD2	1.87	0.40
3:D:878:LYS:HB3	3:D:879:PRO:CD	2.52	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%)	25 34
3	B	894/896 (100%)	815 (91%)	69 (8%)	10 (1%)	14 18
3	C	890/896 (99%)	841 (94%)	45 (5%)	4 (0%)	34 46
3	D	889/896 (99%)	746 (84%)	116 (13%)	27 (3%)	4 3
All	All	3567/3584 (100%)	3240 (91%)	281 (8%)	46 (1%)	12 15

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 (i)

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%)	34	50
3	B	774/793 (98%)	750 (97%)	24 (3%)	40	57
3	C	781/793 (98%)	741 (95%)	40 (5%)	24	36
3	D	770/793 (97%)	746 (97%)	24 (3%)	40	57
All	All	3110/3172 (98%)	2993 (96%)	117 (4%)	33	49

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	I	3	1	8,11,12	0.48	0	9,14,17	1.68	1 (11%)
1	3DR	K	3	1	8,11,12	0.50	0	9,14,17	1.61	1 (11%)
1	3DR	E	3	1	8,11,12	0.50	0	9,14,17	1.64	1 (11%)
1	3DR	G	3	1	8,11,12	0.53	0	9,14,17	1.81	1 (11%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	3	3DR	O3'-C3'-C2'	4.07	121.23	111.54
1	I	3	3DR	O3'-C3'-C2'	3.80	120.58	111.54
1	K	3	3DR	O3'-C3'-C2'	3.55	120.00	111.54
1	E	3	3DR	O3'-C3'-C2'	3.54	119.98	111.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	3	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.21	1 (5%)	22	24	54, 75, 126, 146	0
1	G	17/18 (94%)	0.13	1 (5%)	22	24	45, 57, 133, 148	0
1	I	17/18 (94%)	0.08	1 (5%)	22	24	35, 42, 101, 115	0
1	K	17/18 (94%)	1.15	3 (17%)	1	1	45, 123, 161, 169	0
2	F	15/15 (100%)	0.58	1 (6%)	17	19	68, 99, 128, 141	0
2	H	15/15 (100%)	0.36	2 (13%)	3	3	56, 71, 126, 152	0
2	J	15/15 (100%)	0.08	0	100	100	38, 57, 91, 96	0
2	L	15/15 (100%)	1.46	4 (26%)	0	0	126, 131, 153, 157	0
3	A	896/896 (100%)	0.47	55 (6%)	21	23	30, 47, 125, 149	0
3	B	896/896 (100%)	1.00	155 (17%)	1	1	28, 62, 154, 165	0
3	C	892/896 (99%)	0.37	23 (2%)	56	57	23, 48, 83, 106	0
3	D	891/896 (99%)	1.50	251 (28%)	0	0	53, 117, 153, 160	0
All	All	3703/3716 (99%)	0.82	497 (13%)	3	3	23, 62, 148, 169	0

All (497) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	516	VAL	13.1
3	A	530	ILE	13.0
3	D	514	LEU	12.4
3	B	508	LEU	11.4
3	D	117	VAL	11.1
3	D	157	GLY	10.6
3	B	511	ASP	10.0
3	B	507	ASN	9.4
3	A	542	LEU	9.3
3	B	514	LEU	8.9
3	D	99	TYR	8.7

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Mol	Chain	Res	Type	RSRZ
3	D	64	ASN	8.5
3	B	509	SER	8.2
3	B	538	LEU	8.1
3	B	510	VAL	8.0
3	B	819	ILE	7.9
3	B	502	ALA	7.9
3	B	541	MET	7.6
3	D	809	LEU	7.5
3	D	831	TYR	7.4
3	D	538	LEU	7.2
3	B	503	LEU	7.1
3	B	178	VAL	7.1
3	B	134	ASP	7.1
3	D	539	ASN	7.1
3	B	498	ILE	6.9
3	D	788	ILE	6.7
3	D	799	PRO	6.7
3	D	535	ALA	6.7
3	D	65	MET	6.6
3	B	530	ILE	6.5
3	B	156	TYR	6.4
3	D	393	GLY	6.4
3	B	303	LEU	6.3
3	D	173	GLN	6.3
3	D	282	PHE	6.2
3	A	503	LEU	6.2
3	B	545	ALA	6.2
3	B	522	PHE	6.2
3	B	528	GLU	6.1
3	B	277	TYR	6.1
3	B	542	LEU	6.1
3	B	535	ALA	6.1
3	B	520	PHE	6.1
3	A	522	PHE	6.0
3	A	498	ILE	5.9
3	B	820	ASP	5.9
3	B	183	ILE	5.9
3	D	120	PRO	5.8
3	D	498	ILE	5.8
3	D	160	GLU	5.8
3	D	796	PHE	5.8
3	B	518	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
3	D	801	CYS	5.7
3	B	513	PRO	5.7
3	B	504	HIS	5.7
3	B	519	ARG	5.6
3	A	504	HIS	5.6
3	D	504	HIS	5.6
3	D	178	VAL	5.6
3	D	849	PRO	5.6
3	B	527	LYS	5.6
3	C	303	LEU	5.5
3	D	159	VAL	5.5
3	B	309	ILE	5.5
3	D	548	THR	5.5
3	B	490	LEU	5.5
3	D	510	VAL	5.4
3	D	833	LEU	5.4
1	K	2	DG	5.4
3	A	541	MET	5.4
3	A	507	ASN	5.4
3	B	496	GLY	5.3
3	B	857	LEU	5.3
3	D	794	GLY	5.3
3	A	252	VAL	5.2
3	D	541	MET	5.2
3	B	505	ASN	5.2
3	B	492	ALA	5.2
3	B	539	ASN	5.2
3	D	520	PHE	5.2
3	D	811	TYR	5.2
3	D	503	LEU	5.1
3	D	147	TYR	5.1
3	D	47	THR	5.0
3	D	512	GLU	5.0
3	A	501	GLU	5.0
3	B	506	PRO	5.0
3	B	172	GLU	4.9
3	A	508	LEU	4.9
3	B	525	GLU	4.9
3	C	46	ALA	4.9
3	D	523	SER	4.9
3	D	802	PRO	4.9
3	D	544	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
3	B	170	LEU	4.8
3	D	8	VAL	4.8
3	B	523	SER	4.8
3	D	192	ASP	4.8
3	D	846	ILE	4.8
3	D	516	VAL	4.7
3	D	530	ILE	4.7
3	D	265	LEU	4.7
3	B	179	PRO	4.7
3	D	145	ARG	4.6
3	B	524	ASP	4.6
3	B	818	ASN	4.6
3	B	176	ASP	4.6
3	D	20	ILE	4.5
3	B	497	GLU	4.5
3	D	44	SER	4.5
3	D	857	LEU	4.5
3	B	166	ILE	4.5
3	A	497	GLU	4.5
3	B	515	ASP	4.4
3	B	160	GLU	4.4
3	D	118	THR	4.4
3	D	251	LYS	4.4
3	C	508	LEU	4.3
3	B	861	ASP	4.3
3	D	194	GLU	4.3
3	D	175	GLY	4.3
3	D	779	ILE	4.3
3	A	535	ALA	4.3
3	D	508	LEU	4.3
3	B	115	ILE	4.3
3	B	157	GLY	4.3
3	D	119	SER	4.3
3	A	499	ILE	4.2
3	D	786	ASN	4.2
3	C	530	ILE	4.2
3	D	847	ALA	4.2
3	C	304	LYS	4.2
3	D	526	ILE	4.2
3	B	153	ASN	4.2
3	D	855	THR	4.2
3	A	509	SER	4.2

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Mol	Chain	Res	Type	RSRZ
3	C	252	VAL	4.1
3	A	854	ILE	4.1
3	D	513	PRO	4.1
3	B	817	GLY	4.1
3	B	512	GLU	4.1
3	A	536	LYS	4.1
3	B	532	LYS	4.1
3	D	174	GLY	4.1
3	D	522	PHE	4.1
3	D	252	VAL	4.1
3	B	501	GLU	4.0
3	B	135	ALA	4.0
3	D	250	VAL	4.0
3	D	234	PHE	4.0
3	D	28	THR	4.0
3	D	71	TRP	4.0
3	B	127	SER	4.0
3	A	821	ALA	3.9
3	D	790	LYS	3.9
3	B	117	VAL	3.9
3	B	526	ILE	3.9
3	D	793	VAL	3.9
3	D	201	TYR	3.9
3	A	506	PRO	3.9
3	A	514	LEU	3.9
3	B	493	GLN	3.9
3	A	537	SER	3.9
3	D	61	LEU	3.9
3	B	821	ALA	3.8
3	A	528	GLU	3.8
3	D	198	LEU	3.8
3	D	524	ASP	3.8
1	E	2	DG	3.8
3	B	540	GLU	3.8
3	B	549	GLU	3.8
3	D	182	ILE	3.7
1	G	2	DG	3.7
3	A	857	LEU	3.7
3	D	303	LEU	3.7
3	B	494	ARG	3.7
3	B	552	GLY	3.7
3	D	72	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	32	GLU	3.7
3	B	865	TRP	3.6
3	C	166	ILE	3.6
3	D	517	ASP	3.6
3	B	547	ARG	3.6
3	C	302	LYS	3.6
3	B	321	ILE	3.6
3	B	533	LEU	3.6
2	H	115	DA	3.6
3	D	789	ALA	3.6
3	D	153	ASN	3.6
3	B	306	ASP	3.5
3	D	792	ASP	3.5
3	D	164	ILE	3.5
3	D	832	VAL	3.5
3	B	233	ILE	3.5
3	A	538	LEU	3.5
3	B	171	GLN	3.5
3	D	771	PHE	3.5
3	D	830	VAL	3.5
3	B	537	SER	3.5
3	D	863	LEU	3.5
3	A	502	ALA	3.5
3	D	131	HIS	3.5
3	A	490	LEU	3.4
3	D	78	ILE	3.4
3	B	302	LYS	3.4
3	B	325	ILE	3.4
3	D	183	ILE	3.4
3	D	820	ASP	3.4
3	D	304	LYS	3.4
3	D	305	TYR	3.4
3	D	776	TYR	3.4
3	B	797	PRO	3.4
3	D	24	GLY	3.4
3	D	113	PHE	3.4
3	D	866	MET	3.4
3	D	46	ALA	3.4
3	B	543	PHE	3.4
3	A	526	ILE	3.4
3	D	515	ASP	3.3
3	B	315	SER	3.3

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Mol	Chain	Res	Type	RSRZ
3	B	815	ILE	3.3
2	L	114	DG	3.3
3	D	176	ASP	3.3
3	B	322	SER	3.2
3	D	191	PHE	3.2
3	B	499	ILE	3.2
3	D	488	TYR	3.2
3	A	261	GLU	3.2
3	D	797	PRO	3.2
3	D	490	LEU	3.2
3	D	288	TYR	3.2
3	D	868	TYR	3.2
3	B	159	VAL	3.2
3	D	45	GLN	3.2
3	A	253	GLY	3.2
3	B	201	TYR	3.2
3	B	544	ARG	3.2
3	D	63	ALA	3.2
3	D	546	GLN	3.2
3	D	199	MET	3.2
3	D	223	ILE	3.2
3	D	848	TRP	3.1
3	D	309	ILE	3.1
3	A	505	ASN	3.1
3	D	491	ALA	3.1
3	D	226	VAL	3.1
3	D	391	TYR	3.1
3	C	510	VAL	3.1
3	D	840	PRO	3.1
3	A	491	ALA	3.1
3	D	205	TRP	3.1
3	B	234	PHE	3.1
3	D	395	PHE	3.1
3	D	543	PHE	3.1
3	B	521	ASP	3.0
3	B	186	ILE	3.0
3	D	495	ASN	3.0
3	B	247	LYS	3.0
3	B	517	ASP	3.0
3	D	854	ILE	3.0
3	C	522	PHE	3.0
3	D	518	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	566	LEU	3.0
3	D	509	SER	3.0
3	C	174	GLY	2.9
3	B	317	HIS	2.9
3	A	518	TYR	2.9
3	A	533	LEU	2.9
3	D	784	SER	2.9
3	D	111	ALA	2.9
3	D	313	ARG	2.9
3	D	202	LEU	2.9
3	C	309	ILE	2.9
3	D	100	GLU	2.9
2	F	115	DA	2.9
3	D	390	PRO	2.9
3	D	489	MET	2.9
3	D	562	LEU	2.9
3	B	862	VAL	2.9
3	D	550	VAL	2.9
3	D	497	GLU	2.9
3	D	501	GLU	2.8
3	D	803	PHE	2.8
3	D	829	LYS	2.8
3	A	543	PHE	2.8
3	A	280	PHE	2.8
3	D	479	PHE	2.8
3	A	500	LYS	2.8
3	B	536	LYS	2.8
3	D	80	LEU	2.8
3	B	232	ASN	2.8
3	D	92	TYR	2.8
3	D	128	GLN	2.8
3	B	320	TYR	2.8
3	B	120	PRO	2.8
3	D	170	LEU	2.8
3	D	769	LYS	2.8
3	D	476	THR	2.8
3	D	317	HIS	2.8
3	D	532	LYS	2.8
3	B	841	PHE	2.7
3	A	496	GLY	2.7
3	B	152	LEU	2.7
3	B	271	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	193	ASN	2.7
3	D	507	ASN	2.7
3	D	816	LYS	2.7
3	B	192	ASP	2.7
3	B	244	PRO	2.7
2	L	115	DA	2.7
3	B	868	TYR	2.7
3	C	323	TYR	2.7
3	A	789	ALA	2.7
3	D	850	SER	2.7
3	B	291	ASP	2.7
3	B	534	SER	2.7
3	D	135	ALA	2.7
3	D	25	ARG	2.7
3	A	512	GLU	2.7
3	A	788	ILE	2.7
3	A	494	ARG	2.7
3	D	151	LEU	2.7
3	C	500	LYS	2.7
3	D	172	GLU	2.7
3	D	379	VAL	2.7
3	C	44	SER	2.6
3	D	162	TRP	2.6
3	B	812	ASN	2.6
3	B	305	TYR	2.6
3	B	197	LEU	2.6
3	D	2	LYS	2.6
3	A	262	ILE	2.6
3	D	115	ILE	2.6
3	C	301	GLY	2.6
3	D	88	PHE	2.6
3	D	570	LEU	2.6
3	D	782	VAL	2.6
3	B	206	GLN	2.6
3	D	70	GLN	2.6
3	D	238	THR	2.6
3	D	248	THR	2.6
3	B	316	ASN	2.6
3	D	33	TYR	2.6
3	C	175	GLY	2.6
1	I	2	DG	2.6
3	B	792	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	511	ASP	2.6
3	A	250	VAL	2.6
3	B	136	ILE	2.6
3	B	123	PHE	2.5
3	B	488	TYR	2.5
3	B	249	ARG	2.5
3	D	274	ILE	2.5
3	B	242	LEU	2.5
3	B	149	PHE	2.5
3	D	240	LYS	2.5
3	D	844	LYS	2.5
3	D	315	SER	2.5
3	A	548	THR	2.5
3	B	283	THR	2.5
3	D	203	ASN	2.5
3	D	791	TYR	2.5
3	A	511	ASP	2.5
3	D	225	TYR	2.5
3	D	325	ILE	2.5
3	A	495	ASN	2.5
3	D	93	LEU	2.5
3	A	550	VAL	2.5
3	D	314	GLU	2.5
3	B	311	LYS	2.5
3	D	212	ILE	2.5
3	D	851	GLY	2.5
3	D	242	LEU	2.5
3	A	531	LYS	2.4
3	B	174	GLY	2.4
3	D	563	ILE	2.4
3	D	62	PHE	2.4
3	A	799	PRO	2.4
3	D	487	GLY	2.4
3	D	637	GLY	2.4
3	B	180	SER	2.4
3	B	213	LEU	2.4
3	B	774	LEU	2.4
3	B	165	GLU	2.4
3	D	527	LYS	2.4
3	D	180	SER	2.4
3	D	266	PHE	2.4
3	D	542	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	67	ASP	2.4
3	B	901	PHE	2.4
3	B	811	TYR	2.4
3	D	188	TYR	2.4
3	D	815	ILE	2.4
3	C	151	LEU	2.4
3	D	673	TYR	2.3
3	B	167	ALA	2.3
3	D	897	LEU	2.3
3	B	113	PHE	2.3
3	B	282	PHE	2.3
3	B	839	ASN	2.3
3	D	221	PHE	2.3
3	B	276	LEU	2.3
3	A	524	ASP	2.3
3	A	513	PRO	2.3
3	D	454	TYR	2.3
3	D	116	GLU	2.3
3	D	841	PHE	2.3
2	L	103	DG	2.3
3	B	813	ARG	2.3
3	D	229	ARG	2.3
3	D	136	ILE	2.3
3	B	227	TYR	2.3
3	D	49	TYR	2.3
3	C	251	LYS	2.3
3	B	128	GLN	2.3
3	D	161	GLU	2.3
2	H	114	DG	2.3
3	C	155	PRO	2.3
3	D	179	PRO	2.3
3	D	450	PRO	2.3
3	B	304	LYS	2.3
3	D	233	ILE	2.3
3	D	500	LYS	2.3
3	A	283	THR	2.3
3	D	154	SER	2.3
3	D	565	SER	2.3
3	D	774	LEU	2.3
3	B	546	GLN	2.3
3	D	800	LYS	2.3
3	D	780	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	280	PHE	2.2
3	D	795	GLY	2.2
3	C	515	ASP	2.2
3	D	860	ASP	2.2
3	D	123	PHE	2.2
3	D	286	PRO	2.2
3	D	312	LEU	2.2
3	C	558	ASN	2.2
3	D	766	GLU	2.2
3	D	241	ARG	2.2
3	B	193	ASN	2.2
3	D	321	ILE	2.2
3	D	819	ILE	2.2
3	B	251	LYS	2.2
3	A	516	VAL	2.2
3	D	824	VAL	2.2
3	D	311	LYS	2.2
3	D	283	THR	2.2
3	B	212	ILE	2.2
3	D	783	SER	2.2
3	D	564	ASN	2.1
3	D	328	VAL	2.1
3	B	548	THR	2.1
3	D	6	LEU	2.1
3	B	126	PRO	2.1
3	B	132	PRO	2.1
3	D	302	LYS	2.1
3	B	284	ASN	2.1
3	B	847	ALA	2.1
3	C	535	ALA	2.1
3	D	502	ALA	2.1
3	B	531	LYS	2.1
3	D	580	LEU	2.1
3	D	787	ASN	2.1
1	K	11	DC	2.1
3	D	146	PHE	2.1
3	D	149	PHE	2.1
3	D	79	GLY	2.1
3	D	195	LYS	2.1
3	D	284	ASN	2.1
3	B	300	VAL	2.1
3	B	182	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	334	ILE	2.1
2	L	107	DG	2.1
3	B	281	SER	2.1
3	D	31	VAL	2.1
3	D	306	ASP	2.0
3	A	846	ILE	2.0
3	B	290	LEU	2.0
3	D	536	LYS	2.0
3	D	818	ASN	2.0
3	D	307	GLY	2.0
3	B	799	PRO	2.0
3	D	184	ASP	2.0
3	D	388	VAL	2.0
3	D	74	ARG	2.0
3	D	102	LYS	2.0
3	D	334	ILE	2.0
3	D	1	MET	2.0
1	K	7	DA	2.0
3	D	785	ALA	2.0
3	A	276	LEU	2.0
3	D	11	ILE	2.0
3	D	133	ILE	2.0
3	D	301	GLY	2.0
3	D	384	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	3DR	K	3	11/12	0.72	0.37	165,167,169,169	0
1	3DR	E	3	11/12	0.75	0.35	138,143,147,147	0
1	3DR	G	3	11/12	0.76	0.27	132,137,146,147	0
1	3DR	I	3	11/12	0.81	0.19	102,105,111,112	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.