



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:53 PM 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.; Doublié, S.
Deposited on : 2006-07-15
Resolution : 2.37 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

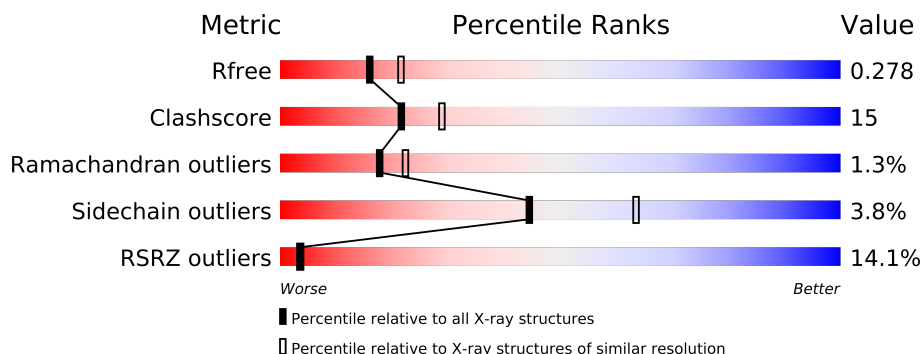
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	18	
1	G	18	
1	I	18	
1	K	18	
2	F	15	
2	H	15	
2	J	15	
2	L	15	
3	A	896	
3	B	896	
3	C	896	
3	D	896	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32454 atoms, of which 0 are hydrogen and 0 are deuterium.

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*A P*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

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.

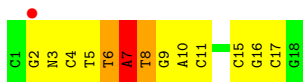
- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

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: 



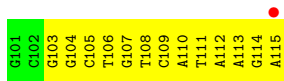
- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

Chain K: 



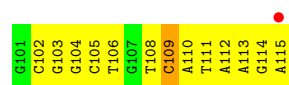
- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

Chain F: 



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

Chain H: 



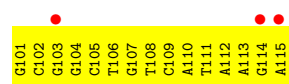
- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

Chain J: 



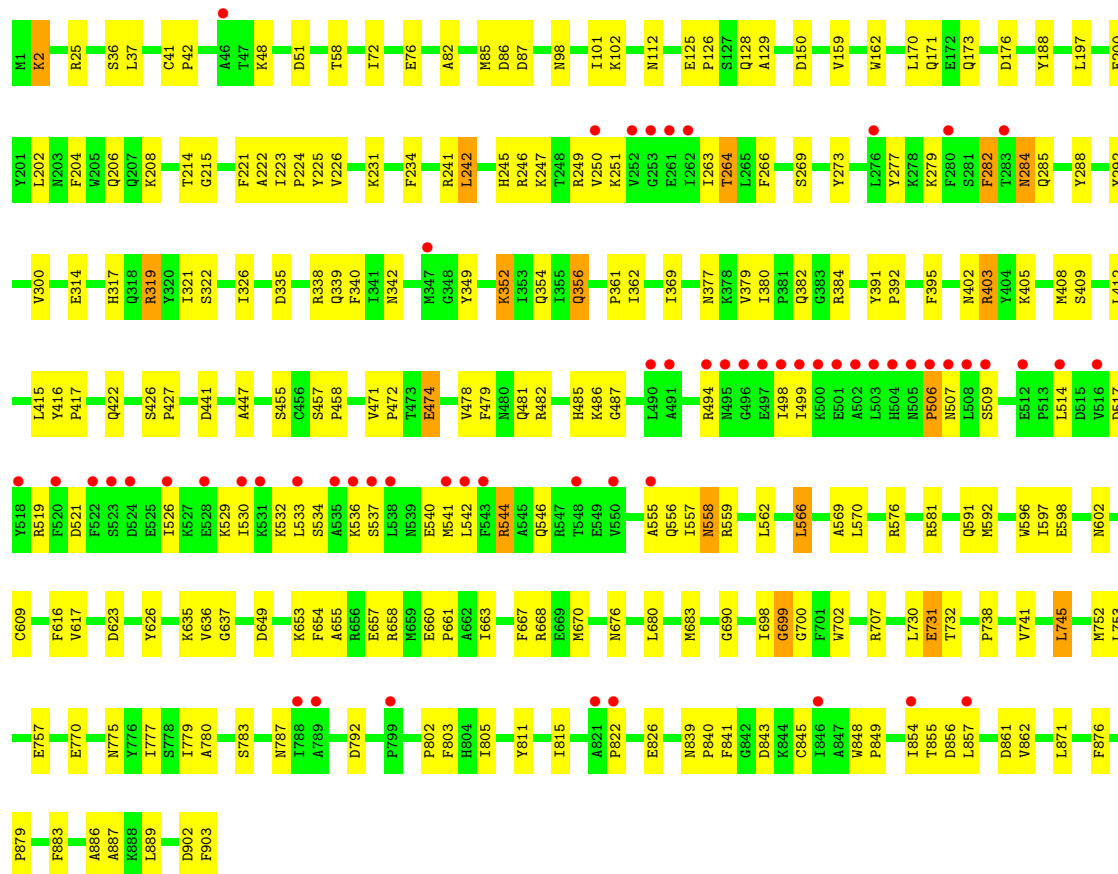
- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

Chain L: 



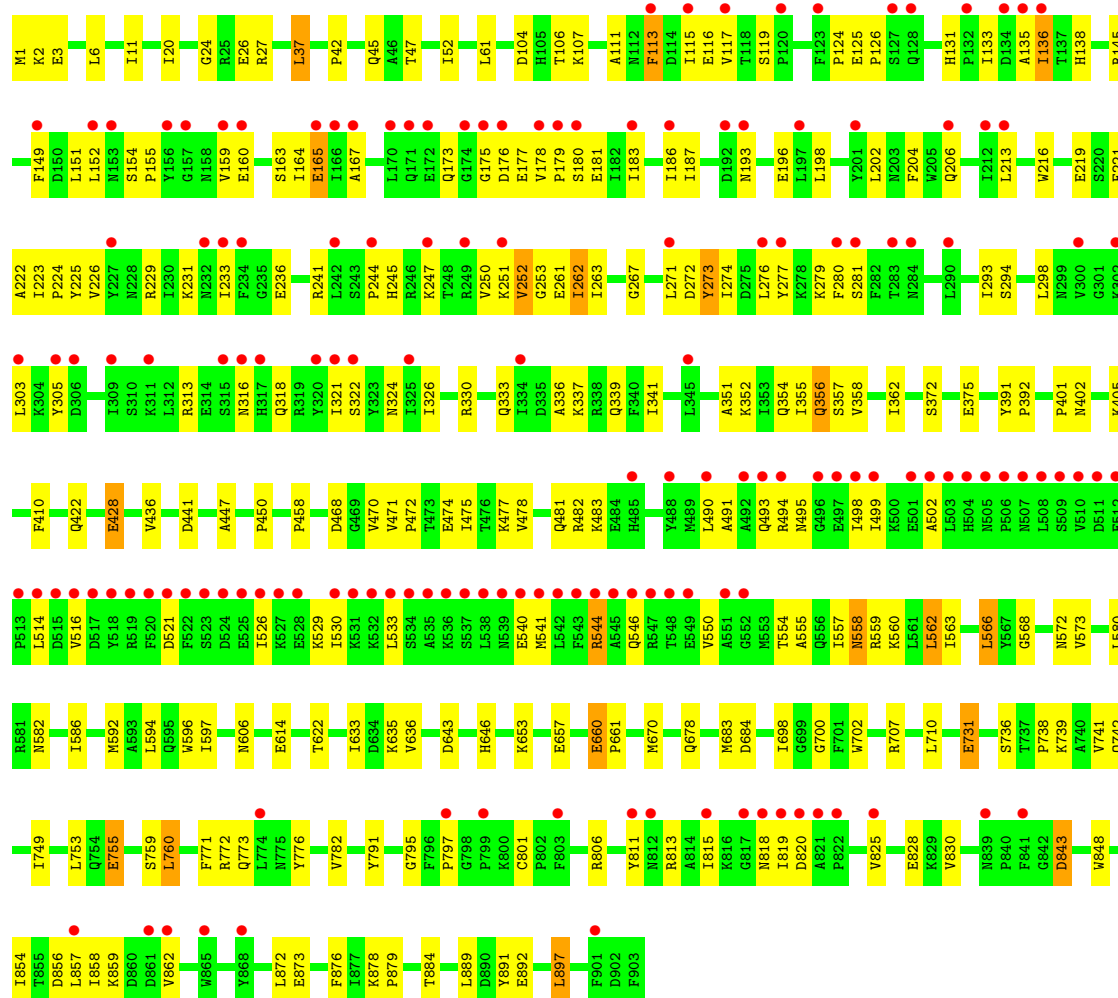
- Molecule 3: DNA polymerase

Chain A: 



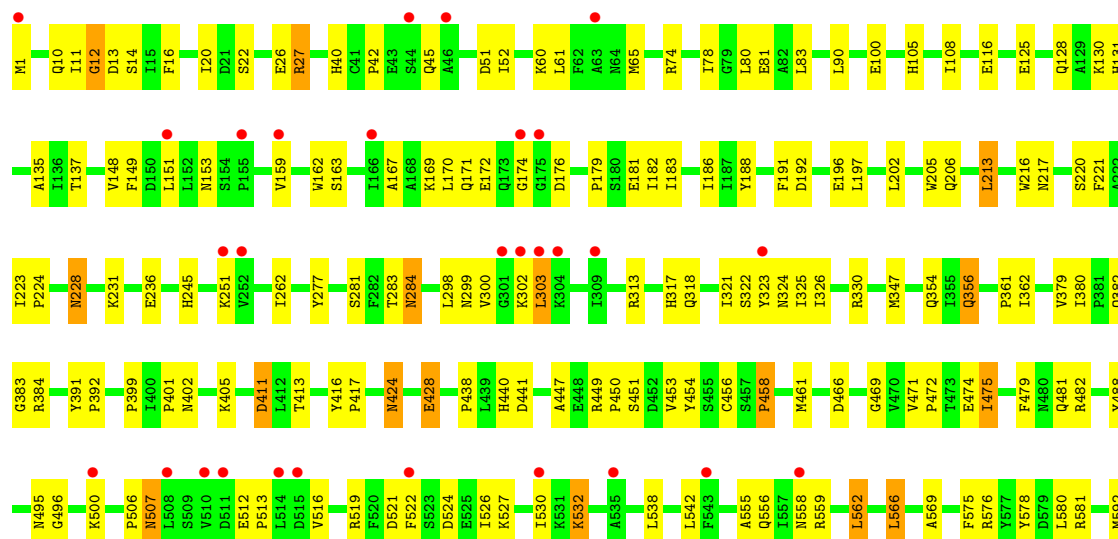
- Molecule 3: DNA polymerase

Chain B: 



- Molecule 3: DNA polymerase

Chain C:





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 0.235 , 0.278	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 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	355	0	200	18	0
2	F	308	0	170	17	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (930) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
3:D:500:LYS:HA	3:D:503:LEU:HD12	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	894/896 (100%)	838 (94%)	51 (6%)	5 (1%)	33	46
3	B	894/896 (100%)	815 (91%)	69 (8%)	10 (1%)	21	27
3	C	890/896 (99%)	841 (94%)	45 (5%)	4 (0%)	43	59
3	D	889/896 (99%)	746 (84%)	116 (13%)	27 (3%)	7	5
All	All	3567/3584 (100%)	3240 (91%)	281 (8%)	46 (1%)	18	22

All (46) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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%)	45	65
3	B	774/793 (98%)	750 (97%)	24 (3%)	52	72
3	C	781/793 (98%)	741 (95%)	40 (5%)	33	48
3	D	770/793 (97%)	746 (97%)	24 (3%)	52	72
All	All	3110/3172 (98%)	2993 (96%)	117 (4%)	44	63

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	9,11,12	0.83	1 (11%)	11,14,17	1.37	1 (9%)
1	3DR	G	3	1	9,11,12	0.83	1 (11%)	11,14,17	1.51	1 (9%)
1	3DR	I	3	1	9,11,12	0.85	1 (11%)	11,14,17	1.41	1 (9%)
1	3DR	K	3	1	9,11,12	0.83	1 (11%)	11,14,17	1.34	1 (9%)

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	-	0/4/15/16	0/1/1/1
1	3DR	G	3	1	-	0/4/15/16	0/1/1/1
1	3DR	I	3	1	-	0/4/15/16	0/1/1/1
1	3DR	K	3	1	-	0/4/15/16	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	3	3DR	P-OP1	2.23	1.49	1.46
1	E	3	3DR	P-OP1	2.16	1.49	1.46
1	K	3	3DR	P-OP1	2.12	1.49	1.46
1	G	3	3DR	P-OP1	2.12	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	3	3DR	O3'-C3'-C2'	3.76	121.23	111.78
1	I	3	3DR	O3'-C3'-C2'	3.50	120.58	111.78
1	K	3	3DR	O3'-C3'-C2'	3.27	120.00	111.78
1	E	3	3DR	O3'-C3'-C2'	3.26	119.98	111.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	18/18 (100%)	0.30	2 (11%) 6 7	54, 87, 144, 146	0
1	G	18/18 (100%)	0.12	1 (5%) 24 26	45, 64, 140, 148	0
1	I	18/18 (100%)	0.04	1 (5%) 24 26	35, 46, 107, 115	0
1	K	18/18 (100%)	0.97	2 (11%) 6 7	45, 128, 168, 169	0
2	F	15/15 (100%)	0.40	1 (6%) 17 19	68, 99, 128, 141	0
2	H	15/15 (100%)	0.28	1 (6%) 17 19	56, 71, 126, 153	0
2	J	15/15 (100%)	0.06	0 100 100	38, 57, 91, 96	0
2	L	15/15 (100%)	1.15	3 (20%) 2 1	126, 131, 153, 157	0
3	A	896/896 (100%)	0.52	59 (6%) 18 19	30, 47, 125, 149	0
3	B	896/896 (100%)	1.06	154 (17%) 2 2	28, 62, 154, 165	0
3	C	892/896 (99%)	0.42	30 (3%) 43 45	23, 48, 83, 106	0
3	D	891/896 (99%)	1.57	267 (29%) 1 1	53, 117, 153, 160	0
All	All	3707/3716 (99%)	0.88	521 (14%) 3 4	23, 62, 148, 169	0

All (521) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	514	LEU	13.7
3	A	530	ILE	12.2
3	B	508	LEU	11.8
3	D	117	VAL	11.4
3	B	514	LEU	10.6
3	B	516	VAL	10.6
3	A	542	LEU	9.5
3	B	507	ASN	9.0
3	B	511	ASP	9.0
3	D	64	ASN	8.9
3	D	99	TYR	8.8

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Mol	Chain	Res	Type	RSRZ
3	D	157	GLY	8.8
3	B	819	ILE	8.6
3	D	799	PRO	8.5
3	B	538	LEU	8.4
3	D	538	LEU	7.9
3	B	178	VAL	7.8
3	B	503	LEU	7.8
3	A	503	LEU	7.7
3	D	831	TYR	7.7
3	B	509	SER	7.7
3	B	510	VAL	7.7
3	B	502	ALA	7.6
3	D	809	LEU	7.5
3	B	541	MET	7.5
3	B	520	PHE	7.5
3	D	510	VAL	7.4
3	D	535	ALA	7.3
3	B	528	GLU	7.3
3	B	542	LEU	7.2
3	D	833	LEU	7.2
3	B	545	ALA	7.1
3	D	393	GLY	6.9
3	B	820	ASP	6.9
3	A	522	PHE	6.8
3	D	65	MET	6.7
3	D	788	ILE	6.7
3	B	522	PHE	6.7
3	B	156	TYR	6.7
3	B	498	ILE	6.6
3	B	277	TYR	6.6
3	D	801	CYS	6.5
3	B	309	ILE	6.5
3	B	530	ILE	6.4
3	B	170	LEU	6.3
3	B	504	HIS	6.3
3	B	857	LEU	6.2
3	A	504	HIS	6.1
3	B	527	LYS	6.1
3	B	496	GLY	6.1
3	D	539	ASN	6.0
3	B	303	LEU	6.0
3	B	518	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
3	B	535	ALA	6.0
3	A	498	ILE	5.9
3	D	512	GLU	5.8
3	D	160	GLU	5.8
3	A	508	LEU	5.8
3	D	173	GLN	5.8
3	B	134	ASP	5.8
3	A	252	VAL	5.7
3	D	802	PRO	5.6
3	D	498	ILE	5.6
3	B	505	ASN	5.6
3	B	519	ARG	5.5
3	B	539	ASN	5.5
3	D	251	LYS	5.5
3	A	507	ASN	5.5
3	C	46	ALA	5.5
3	D	846	ILE	5.5
3	D	530	ILE	5.4
3	D	796	PHE	5.3
3	D	282	PHE	5.3
3	D	174	GLY	5.3
3	B	513	PRO	5.2
3	B	490	LEU	5.2
3	D	779	ILE	5.2
3	B	525	GLU	5.2
3	A	501	GLU	5.2
3	D	847	ALA	5.2
3	D	159	VAL	5.1
3	D	265	LEU	5.1
3	C	530	ILE	5.1
3	B	179	PRO	5.1
3	B	153	ASN	5.1
3	C	303	LEU	5.1
3	B	183	ILE	5.1
3	C	508	LEU	5.1
3	B	506	PRO	5.0
3	D	516	VAL	4.9
3	A	514	LEU	4.9
3	D	526	ILE	4.9
3	D	503	LEU	4.9
3	D	811	TYR	4.8
3	B	523	SER	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	252	VAL	4.8
3	B	176	ASP	4.8
3	B	166	ILE	4.8
3	D	541	MET	4.8
3	A	541	MET	4.7
3	B	524	ASP	4.7
3	D	504	HIS	4.7
3	B	172	GLU	4.7
3	B	821	ALA	4.7
3	D	234	PHE	4.7
3	D	522	PHE	4.7
3	D	790	LYS	4.7
3	A	535	ALA	4.6
3	D	548	THR	4.6
3	A	497	GLU	4.6
3	B	492	ALA	4.6
3	D	120	PRO	4.6
3	B	117	VAL	4.6
3	D	849	PRO	4.6
3	B	818	ASN	4.6
3	D	252	VAL	4.6
3	B	861	ASP	4.6
3	D	250	VAL	4.5
3	D	520	PHE	4.5
3	D	61	LEU	4.5
3	D	178	VAL	4.5
3	B	115	ILE	4.5
3	D	47	THR	4.4
3	D	523	SER	4.4
3	B	526	ILE	4.4
3	B	543	PHE	4.3
3	D	147	TYR	4.3
3	D	71	TRP	4.3
3	D	8	VAL	4.3
3	D	803	PHE	4.3
3	D	544	ARG	4.2
3	D	194	GLU	4.2
3	D	192	ASP	4.2
3	D	20	ILE	4.1
3	D	145	ARG	4.1
3	B	306	ASP	4.1
3	D	508	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
3	A	509	SER	4.1
3	D	201	TYR	4.1
3	D	44	SER	4.1
1	K	2	DG	4.1
3	D	305	TYR	4.1
3	D	303	LEU	4.0
3	A	499	ILE	4.0
3	D	517	ASP	4.0
3	A	506	PRO	4.0
3	A	526	ILE	4.0
3	D	72	ILE	4.0
3	D	797	PRO	4.0
3	D	857	LEU	4.0
3	D	175	GLY	3.9
3	D	118	THR	3.9
3	D	848	TRP	3.9
3	D	113	PHE	3.9
3	D	513	PRO	3.9
3	D	866	MET	3.9
3	D	794	GLY	3.9
3	D	863	LEU	3.9
3	B	512	GLU	3.9
3	D	304	LYS	3.9
3	B	160	GLU	3.9
3	B	540	GLU	3.9
3	D	78	ILE	3.8
3	B	497	GLU	3.8
3	B	549	GLU	3.8
3	B	499	ILE	3.8
3	A	821	ALA	3.8
3	D	868	TYR	3.8
3	D	63	ALA	3.8
3	B	532	LYS	3.8
3	D	830	VAL	3.8
3	D	840	PRO	3.8
3	D	28	THR	3.7
3	D	855	THR	3.7
3	B	515	ASP	3.7
3	B	501	GLU	3.7
3	D	182	ILE	3.7
3	B	533	LEU	3.7
3	D	771	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
3	A	854	ILE	3.7
3	D	786	ASN	3.7
1	E	3	3DR	3.7
3	D	198	LEU	3.7
3	D	543	PHE	3.7
3	B	797	PRO	3.6
3	D	46	ALA	3.6
3	D	524	ASP	3.6
3	D	832	VAL	3.6
3	A	857	LEU	3.6
3	B	817	GLY	3.6
3	D	391	TYR	3.6
3	D	515	ASP	3.6
3	B	157	GLY	3.6
3	B	494	ARG	3.5
3	B	547	ARG	3.5
3	D	32	GLU	3.5
3	B	865	TRP	3.5
3	D	191	PHE	3.4
3	B	521	ASP	3.4
3	C	510	VAL	3.4
2	H	115	DA	3.4
3	A	490	LEU	3.4
3	B	201	TYR	3.4
3	D	562	LEU	3.4
3	D	313	ARG	3.4
3	A	491	ALA	3.4
3	B	315	SER	3.4
3	A	528	GLU	3.4
3	B	233	ILE	3.4
3	B	552	GLY	3.3
3	B	135	ALA	3.3
3	C	166	ILE	3.3
3	A	261	GLU	3.3
3	B	493	GLN	3.3
3	D	776	TYR	3.3
3	A	536	LYS	3.3
3	B	862	VAL	3.3
3	C	304	LYS	3.3
3	B	171	GLN	3.3
1	G	2	DG	3.2
3	D	199	MET	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	25	ARG	3.2
3	D	392	PRO	3.2
3	D	793	VAL	3.2
3	D	509	SER	3.2
3	D	164	ILE	3.2
3	A	518	TYR	3.2
3	D	851	GLY	3.2
3	A	496	GLY	3.2
3	D	288	TYR	3.2
3	D	479	PHE	3.2
3	B	325	ILE	3.2
3	B	305	TYR	3.2
3	D	223	ILE	3.1
3	C	302	LYS	3.1
3	D	314	GLU	3.1
3	D	850	SER	3.1
3	A	253	GLY	3.1
3	D	226	VAL	3.1
3	B	136	ILE	3.1
3	B	192	ASP	3.1
3	A	505	ASN	3.1
3	D	79	GLY	3.1
3	D	532	LYS	3.1
3	B	322	SER	3.1
3	A	799	PRO	3.1
3	D	791	TYR	3.1
3	B	186	ILE	3.1
3	C	174	GLY	3.1
3	D	546	GLN	3.1
3	A	500	LYS	3.1
3	D	119	SER	3.1
3	D	128	GLN	3.1
3	A	543	PHE	3.1
3	B	815	ILE	3.1
3	D	820	ASP	3.1
3	B	841	PHE	3.0
3	D	62	PHE	3.0
3	D	153	ASN	3.0
3	D	202	LEU	3.0
3	D	80	LEU	3.0
3	D	566	LEU	3.0
3	D	309	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	B	317	HIS	3.0
3	D	92	TYR	3.0
3	B	247	LYS	3.0
3	A	280	PHE	3.0
3	D	183	ILE	3.0
3	B	127	SER	3.0
3	C	522	PHE	3.0
3	D	162	TRP	3.0
3	D	238	THR	3.0
3	A	502	ALA	3.0
3	D	135	ALA	3.0
3	D	490	LEU	3.0
3	A	550	VAL	2.9
3	B	213	LEU	2.9
3	B	536	LYS	2.9
3	D	225	TYR	2.9
3	D	476	THR	2.9
3	D	70	GLN	2.9
1	K	3	3DR	2.9
3	B	537	SER	2.9
3	D	507	ASN	2.9
3	C	309	ILE	2.9
3	D	16	PHE	2.9
3	D	317	HIS	2.9
3	D	511	ASP	2.9
3	D	93	LEU	2.9
3	B	113	PHE	2.9
3	D	2	LYS	2.9
3	D	789	ALA	2.9
3	B	271	LEU	2.9
3	D	151	LEU	2.9
3	B	546	GLN	2.9
3	C	155	PRO	2.9
3	D	497	GLU	2.9
3	A	495	ASN	2.9
3	D	111	ALA	2.9
3	D	829	LYS	2.9
3	C	515	ASP	2.8
3	D	550	VAL	2.8
3	D	488	TYR	2.8
3	D	306	ASP	2.8
3	B	488	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	2	DG	2.8
3	D	176	ASP	2.8
3	C	251	LYS	2.8
3	D	131	HIS	2.8
3	D	311	LYS	2.8
3	D	379	VAL	2.8
3	D	253	GLY	2.8
3	D	205	TRP	2.8
3	B	316	ASN	2.8
3	D	800	LYS	2.8
3	C	44	SER	2.8
2	F	115	DA	2.8
3	D	570	LEU	2.8
3	B	283	THR	2.8
3	D	395	PHE	2.7
3	B	321	ILE	2.7
3	D	563	ILE	2.7
3	B	280	PHE	2.7
3	B	244	PRO	2.7
3	B	300	VAL	2.7
3	B	242	LEU	2.7
3	B	320	TYR	2.7
3	A	250	VAL	2.7
3	A	262	ILE	2.7
3	B	868	TYR	2.7
3	B	206	GLN	2.7
3	D	45	GLN	2.7
3	D	286	PRO	2.7
3	D	819	ILE	2.7
3	D	221	PHE	2.7
3	D	637	GLY	2.7
3	B	811	TYR	2.7
2	L	115	DA	2.7
3	B	132	PRO	2.7
3	D	290	LEU	2.6
3	D	388	VAL	2.6
3	A	548	THR	2.6
3	C	500	LYS	2.6
3	B	159	VAL	2.6
3	B	197	LEU	2.6
3	D	307	GLY	2.6
3	D	792	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	B	149	PHE	2.6
3	C	535	ALA	2.6
3	D	489	MET	2.6
3	D	785	ALA	2.6
3	A	846	ILE	2.6
3	D	325	ILE	2.6
3	D	129	ALA	2.6
3	D	88	PHE	2.6
3	D	161	GLU	2.6
3	B	251	LYS	2.6
3	B	534	SER	2.6
3	A	533	LEU	2.6
3	B	120	PRO	2.6
3	D	501	GLU	2.6
3	D	156	TYR	2.6
3	D	495	ASN	2.6
3	B	249	ARG	2.6
3	D	390	PRO	2.5
3	D	133	ILE	2.5
3	D	854	ILE	2.5
3	C	323	TYR	2.5
3	D	33	TYR	2.5
3	D	784	SER	2.5
3	D	312	LEU	2.5
3	D	818	ASN	2.5
3	D	24	GLY	2.5
3	B	551	ALA	2.5
3	A	494	ARG	2.5
3	B	123	PHE	2.5
3	B	152	LEU	2.5
3	B	302	LYS	2.5
3	B	531	LYS	2.5
3	D	115	ILE	2.5
3	D	274	ILE	2.5
3	D	321	ILE	2.5
3	D	102	LYS	2.5
3	D	213	LEU	2.5
3	B	544	ARG	2.5
3	D	844	LYS	2.5
3	A	524	ASP	2.5
2	L	114	DG	2.5
3	B	517	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	283	THR	2.5
3	A	516	VAL	2.5
3	D	212	ILE	2.5
3	B	234	PHE	2.4
3	D	536	LYS	2.4
3	D	824	VAL	2.4
3	D	136	ILE	2.4
3	B	901	PHE	2.4
3	D	100	GLU	2.4
3	B	822	PRO	2.4
3	D	179	PRO	2.4
3	B	165	GLU	2.4
3	D	302	LYS	2.4
3	A	789	ALA	2.4
3	D	262	ILE	2.4
3	B	227	TYR	2.4
3	A	538	LEU	2.4
3	D	74	ARG	2.4
3	B	284	ASN	2.4
3	B	812	ASN	2.4
3	D	263	ILE	2.4
3	D	149	PHE	2.4
3	D	841	PHE	2.4
3	C	175	GLY	2.3
3	C	63	ALA	2.3
3	B	180	SER	2.3
3	D	834	PRO	2.3
3	A	788	ILE	2.3
3	D	229	ARG	2.3
3	A	276	LEU	2.3
3	D	242	LEU	2.3
3	D	782	VAL	2.3
3	D	804	HIS	2.3
3	D	769	LYS	2.3
3	D	673	TYR	2.3
3	B	281	SER	2.3
3	A	822	PRO	2.3
3	B	128	GLN	2.3
3	D	193	ASN	2.3
3	D	518	TYR	2.3
3	D	897	LEU	2.3
3	D	815	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	315	SER	2.3
3	D	283	THR	2.3
3	B	212	ILE	2.3
3	B	232	ASN	2.3
3	C	898	PHE	2.3
3	D	123	PHE	2.3
3	C	511	ASP	2.3
3	B	276	LEU	2.3
3	D	774	LEU	2.3
3	D	1	MET	2.2
3	D	188	TYR	2.2
3	D	172	GLU	2.2
3	D	293	ILE	2.2
3	D	816	LYS	2.2
3	A	537	SER	2.2
3	D	146	PHE	2.2
3	D	589	PHE	2.2
3	B	774	LEU	2.2
3	D	730	LEU	2.2
3	D	783	SER	2.2
3	B	193	ASN	2.2
3	B	345	LEU	2.2
3	C	151	LEU	2.2
3	D	454	TYR	2.2
3	D	301	GLY	2.2
3	C	514	LEU	2.2
3	D	542	LEU	2.2
3	D	780	ALA	2.2
3	D	154	SER	2.2
3	D	475	ILE	2.2
3	C	543	PHE	2.2
3	B	167	ALA	2.2
3	A	347	MET	2.2
3	B	334	ILE	2.2
3	D	798	GLY	2.2
3	B	311	LYS	2.2
3	D	264	THR	2.2
3	B	825	VAL	2.2
3	C	159	VAL	2.2
3	D	487	GLY	2.1
3	D	6	LEU	2.1
3	C	558	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	564	ASN	2.1
3	A	512	GLU	2.1
3	A	520	PHE	2.1
3	D	266	PHE	2.1
3	D	502	ALA	2.1
3	D	574	TRP	2.1
3	B	839	ASN	2.1
3	D	292	TYR	2.1
3	D	817	GLY	2.1
3	D	276	LEU	2.1
3	D	621	ASP	2.1
3	D	500	LYS	2.1
3	B	799	PRO	2.1
3	D	49	TYR	2.1
3	D	273	TYR	2.1
3	B	485	HIS	2.1
3	D	29	ARG	2.1
3	B	548	THR	2.1
3	A	555	ALA	2.1
3	C	1	MET	2.1
3	C	301	GLY	2.1
3	D	203	ASN	2.1
3	D	227	TYR	2.1
3	D	334	ILE	2.1
3	D	248	THR	2.1
3	D	240	LYS	2.1
3	D	280	PHE	2.1
3	D	860	ASP	2.1
3	B	174	GLY	2.1
3	B	175	GLY	2.1
3	B	290	LEU	2.1
3	D	31	VAL	2.1
3	A	531	LYS	2.1
3	D	195	LYS	2.1
1	I	2	DG	2.1
3	A	46	ALA	2.1
2	L	103	DG	2.0
3	D	134	ASP	2.0
3	A	523	SER	2.0
3	D	116	GLU	2.0
3	D	328	VAL	2.0
3	D	565	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	11	ILE	2.0
3	D	166	ILE	2.0
3	D	827	GLY	2.0
3	B	803	PHE	2.0
3	D	18	ARG	2.0
3	D	27	ARG	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	3DR	E	3	11/12	0.35	1.99	138,143,147,147	0
1	3DR	K	3	11/12	0.31	0.74	165,167,169,169	0
1	3DR	G	3	11/12	0.24	0.46	132,137,146,147	0
1	3DR	I	3	11/12	0.17	-0.43	102,105,111,112	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.