



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID : 3U60  
Title : Structure of T4 Bacteriophage Clamp Loader Bound To Open Clamp, DNA and ATP Analog  
Authors : Kelch, B.A.; Makino, D.L.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2011-10-11  
Resolution : 3.34 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

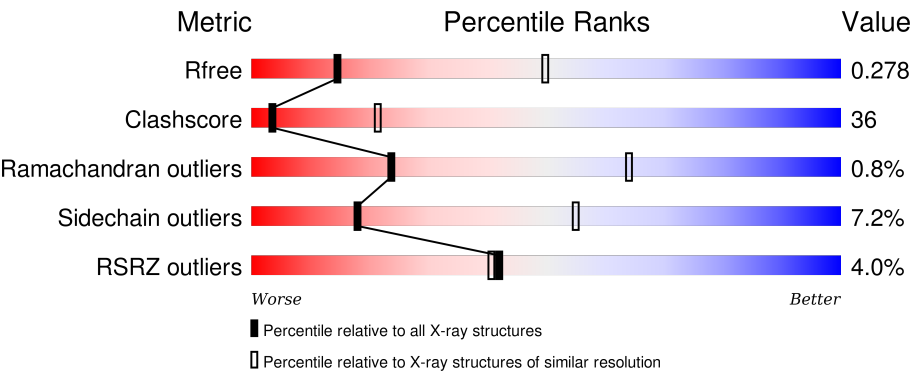
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.34 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.



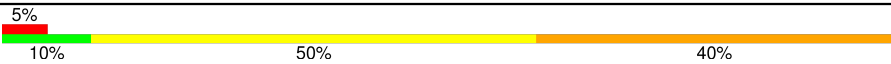


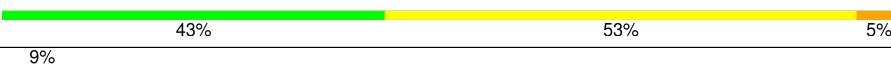
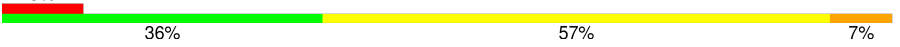
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B	324	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>60%33%5%•</div></div>
1	C	324	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>54%40%••</div></div>
1	D	324	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>58%36%••</div></div>
1	E	324	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>3%51%38%5%6%</div></div>
2	I	30	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>10%30%47%20%</div></div>

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Mol	Chain	Length	Quality of chain
3	J	20	
4	A	195	
5	F	228	
5	G	228	
5	H	228	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	B	800	-	-	-	X
7	MG	C	800	-	-	-	X
7	MG	D	800	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17695 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase accessory protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	319	Total	C	N	O	S	0	0	0
			2509	1587	431	474	17			
1	C	320	Total	C	N	O	S	0	0	0
			2515	1590	432	476	17			
1	D	319	Total	C	N	O	S	0	0	0
			2503	1584	428	474	17			
1	E	305	Total	C	N	O	S	0	0	0
			2409	1527	413	453	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP P04526
B	-3	PRO	-	EXPRESSION TAG	UNP P04526
B	-2	GLY	-	EXPRESSION TAG	UNP P04526
B	-1	GLY	-	EXPRESSION TAG	UNP P04526
B	0	SER	-	EXPRESSION TAG	UNP P04526
C	-4	GLY	-	EXPRESSION TAG	UNP P04526
C	-3	PRO	-	EXPRESSION TAG	UNP P04526
C	-2	GLY	-	EXPRESSION TAG	UNP P04526
C	-1	GLY	-	EXPRESSION TAG	UNP P04526
C	0	SER	-	EXPRESSION TAG	UNP P04526
D	-4	GLY	-	EXPRESSION TAG	UNP P04526
D	-3	PRO	-	EXPRESSION TAG	UNP P04526
D	-2	GLY	-	EXPRESSION TAG	UNP P04526
D	-1	GLY	-	EXPRESSION TAG	UNP P04526
D	0	SER	-	EXPRESSION TAG	UNP P04526
E	-4	GLY	-	EXPRESSION TAG	UNP P04526
E	-3	PRO	-	EXPRESSION TAG	UNP P04526
E	-2	GLY	-	EXPRESSION TAG	UNP P04526
E	-1	GLY	-	EXPRESSION TAG	UNP P04526
E	0	SER	-	EXPRESSION TAG	UNP P04526

- Molecule 2 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			

- Molecule 3 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	20	Total	C	N	O	P	0	0	0
			408	195	81	113	19			

- Molecule 4 is a protein called DNA polymerase accessory protein 62.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	186	Total	C	N	O	S	0	0	0
			1488	959	244	279	6			

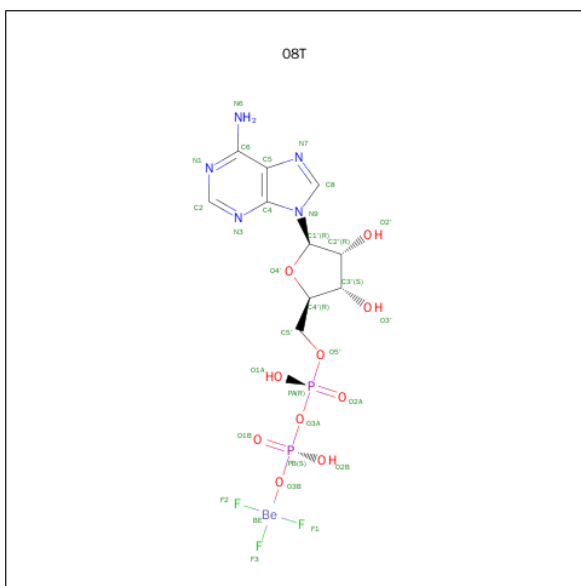
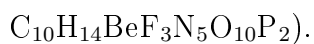
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	EXPRESSION TAG	UNP P04527
A	189	LEU	-	EXPRESSION TAG	UNP P04527
A	190	GLU	-	EXPRESSION TAG	UNP P04527
A	191	HIS	-	EXPRESSION TAG	UNP P04527
A	192	HIS	-	EXPRESSION TAG	UNP P04527
A	193	HIS	-	EXPRESSION TAG	UNP P04527
A	194	HIS	-	EXPRESSION TAG	UNP P04527
A	195	HIS	-	EXPRESSION TAG	UNP P04527
A	196	HIS	-	EXPRESSION TAG	UNP P04527

- Molecule 5 is a protein called DNA polymerase processivity component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
5	H	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
5	F	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			

- Molecule 6 is [|(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-BIS(OXIDANYL)OXOLAN-2-YL|METHOXY-OXIDANYL-PHOSPHORYL|OXY-OXIDANYL-PHOSPHORYL|OXY-TRIS(FLUORANYL)BERYLLIUM (three-letter code: 08T) (formula:

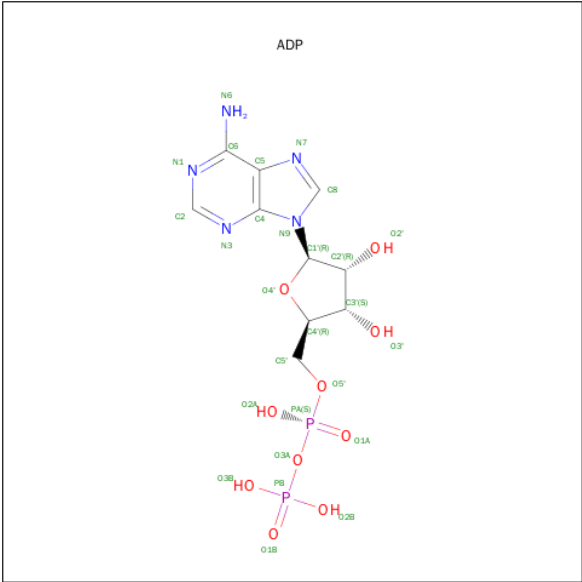


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total 31	Be 1	C 10	F 3	N 5	O 10	P 2	0	0
6	C	1	Total 31	Be 1	C 10	F 3	N 5	O 10	P 2	0	0
6	D	1	Total 31	Be 1	C 10	F 3	N 5	O 10	P 2	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	E	1	Total Mg 1 1	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).

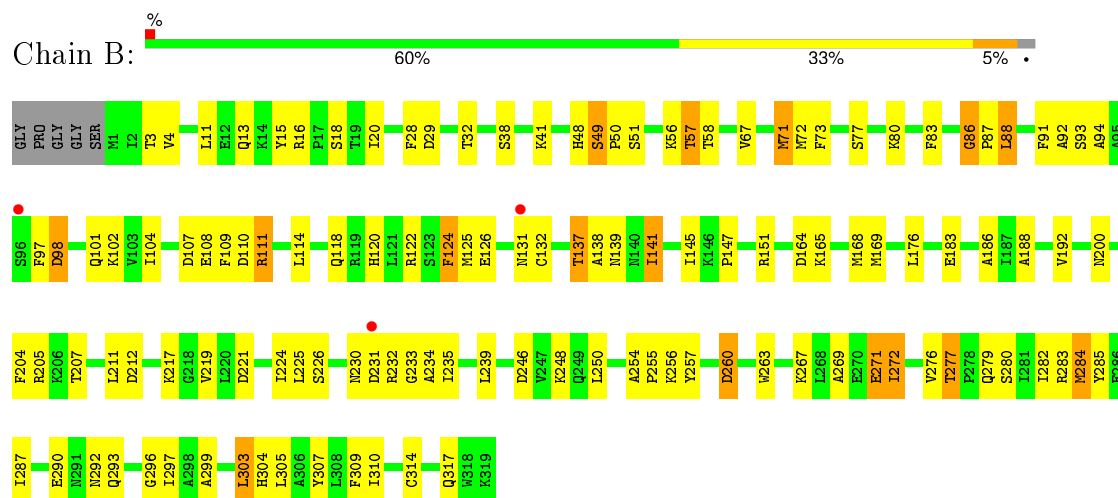


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

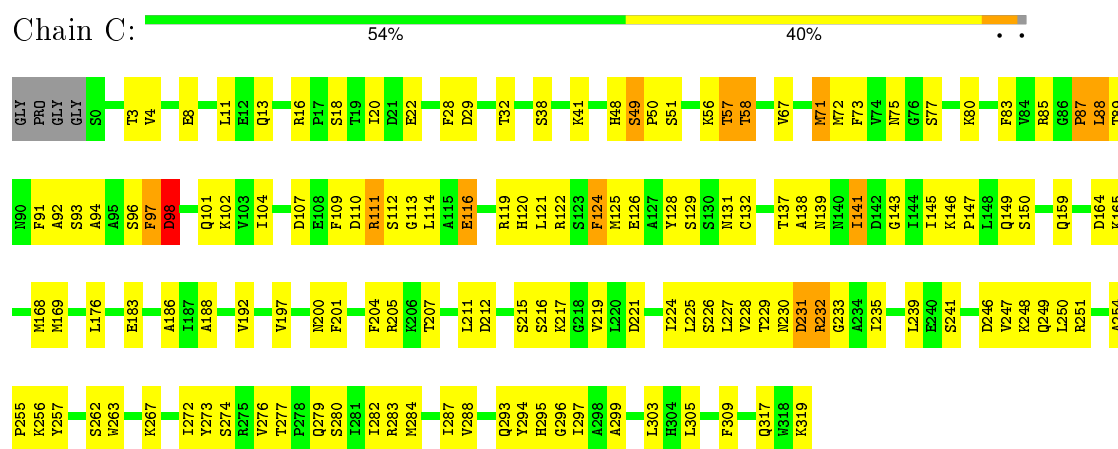
### 3 Residue-property plots

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.

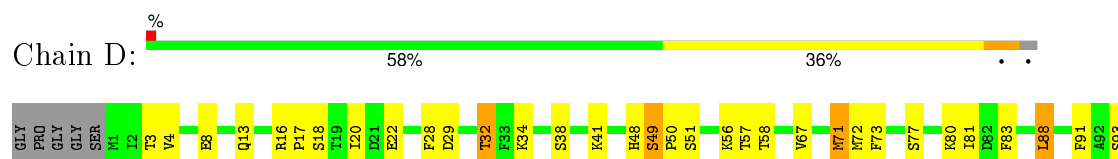
#### • Molecule 1: DNA polymerase accessory protein 44



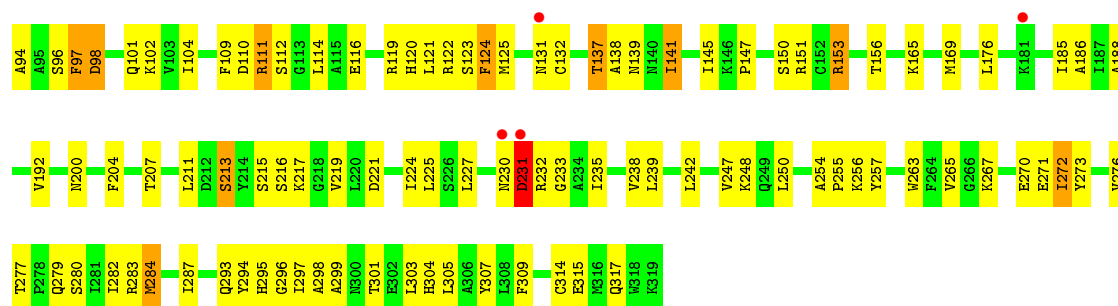
#### • Molecule 1: DNA polymerase accessory protein 44



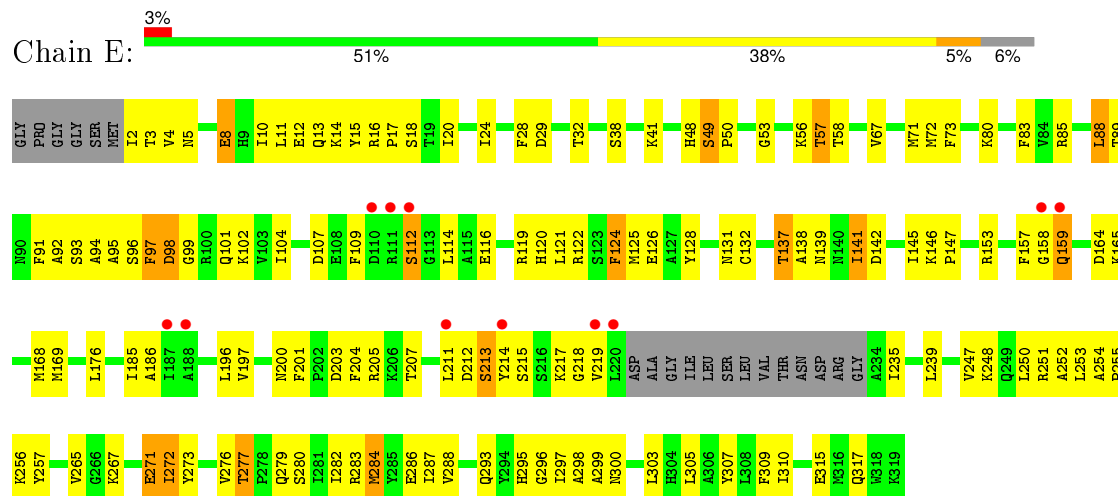
#### • Molecule 1: DNA polymerase accessory protein 44



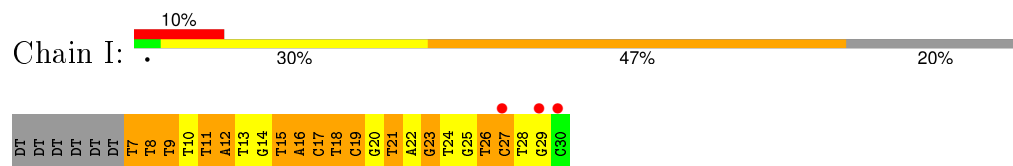




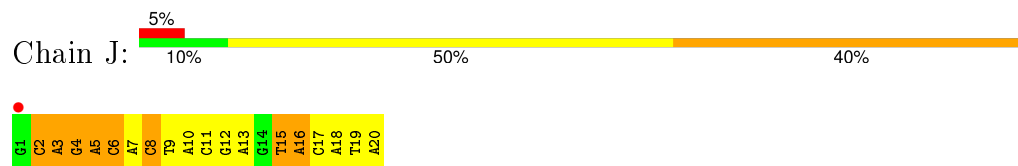
• Molecule 1: DNA polymerase accessory protein 44



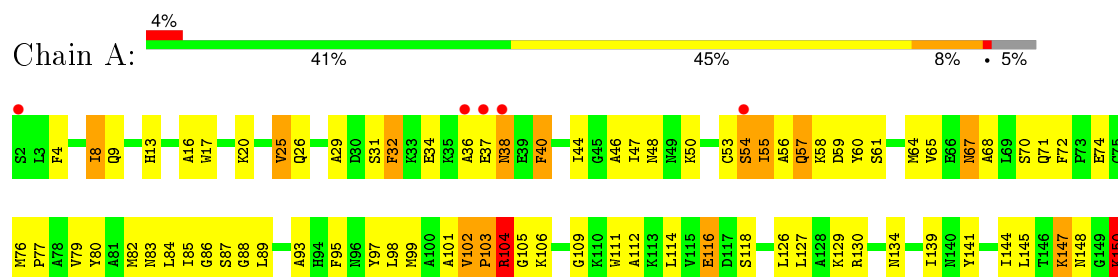
• Molecule 2: Template DNA strand



• Molecule 3: Primer DNA strand



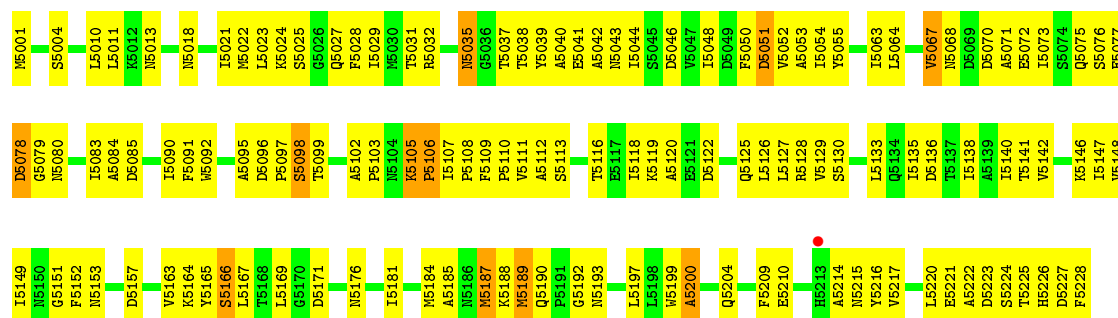
• Molecule 4: DNA polymerase accessory protein 62





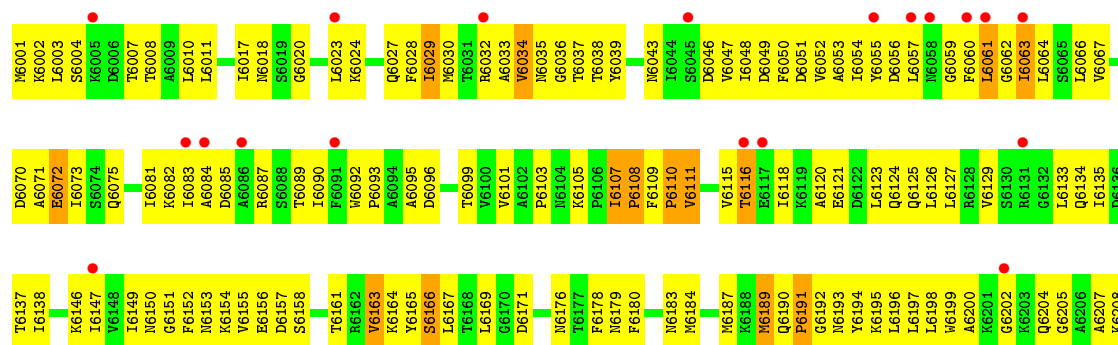
• Molecule 5: DNA polymerase processivity component

Chain G: 43% 53% 5%



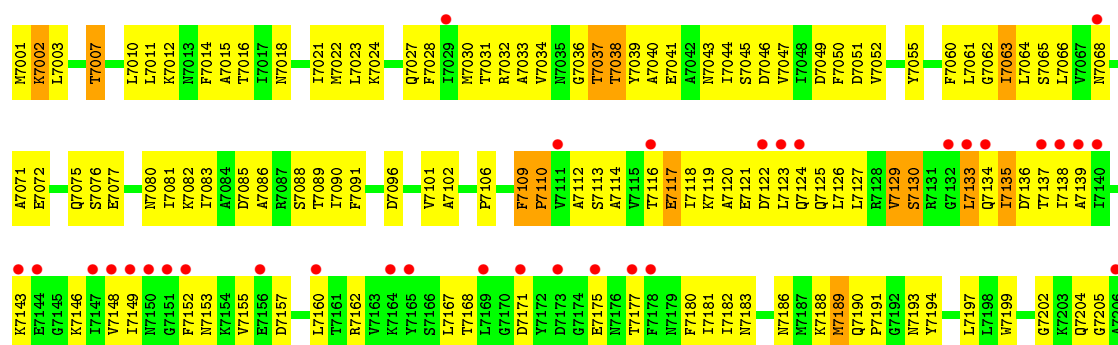
• Molecule 5: DNA polymerase processivity component

Chain H: 9% 36% 57% 7%



• Molecule 5: DNA polymerase processivity component

Chain F: 15% 42% 52% 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.52Å 118.44Å 133.08Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	49.71 – 3.34 49.71 – 3.11	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.71-3.34) 89.0 (49.71-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.244 , 0.282 0.243 , 0.278	Depositor DCC
$R_{free}$ test set	1648 reflections (4.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 50000 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	17695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 08T

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	B	0.56	0/2553	0.76	3/3441 (0.1%)
1	C	0.55	1/2559 (0.0%)	0.75	5/3449 (0.1%)
1	D	0.57	0/2547	0.74	4/3434 (0.1%)
1	E	0.58	0/2452	0.76	3/3303 (0.1%)
2	I	1.01	0/544	2.02	26/838 (3.1%)
3	J	1.03	0/459	1.82	17/706 (2.4%)
4	A	0.58	0/1516	0.86	1/2042 (0.0%)
5	F	0.43	0/1774	0.78	7/2395 (0.3%)
5	G	0.43	0/1774	0.76	4/2395 (0.2%)
5	H	0.45	0/1774	0.73	2/2395 (0.1%)
All	All	0.57	1/17952 (0.0%)	0.88	72/24398 (0.3%)

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	B	0	3
1	C	0	2
1	D	0	3
1	E	0	2
4	A	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	PRO	N-CD	5.39	1.55	1.47

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	21	DT	O4'-C1'-N1	12.68	116.88	108.00
3	J	20	DA	O4'-C1'-N9	10.43	115.30	108.00
2	I	19	DC	O4'-C1'-N1	-10.11	100.93	108.00
2	I	16	DA	O4'-C1'-N9	9.96	114.97	108.00
1	E	112	SER	CB-CA-C	-9.49	92.08	110.10
2	I	10	DT	O4'-C1'-N1	-9.03	101.68	108.00
2	I	17	DC	O4'-C1'-N1	8.30	113.81	108.00
3	J	13	DA	O4'-C1'-N9	-8.15	102.30	108.00
5	F	7129	VAL	CB-CA-C	-8.07	96.06	111.40
2	I	9	DT	C4-C5-C7	7.54	123.52	119.00
2	I	15	DT	C1'-O4'-C4'	-7.51	102.59	110.10
2	I	11	DT	N3-C4-O4	7.42	124.36	119.90
2	I	27	DC	O4'-C1'-N1	7.38	113.16	108.00
1	E	158	GLY	N-CA-C	7.30	131.36	113.10
2	I	9	DT	C6-C5-C7	-7.29	118.53	122.90
5	F	7129	VAL	N-CA-C	6.86	129.53	111.00
1	C	111	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	I	18	DT	N3-C4-O4	6.67	123.90	119.90
2	I	22	DA	O4'-C1'-N9	6.55	112.59	108.00
2	I	7	DT	O4'-C1'-N1	6.55	112.59	108.00
5	F	7130	SER	N-CA-CB	-6.54	100.69	110.50
2	I	15	DT	O4'-C1'-C2'	-6.40	100.78	105.90
5	G	5035	ASN	N-CA-C	6.39	128.26	111.00
2	I	13	DT	C5-C4-O4	-6.37	120.44	124.90
3	J	16	DA	C1'-O4'-C4'	-6.32	103.78	110.10
3	J	15	DT	N3-C2-O2	-6.32	118.51	122.30
1	D	111	ARG	NE-CZ-NH2	-6.17	117.22	120.30
3	J	8	DC	O4'-C1'-N1	6.03	112.22	108.00
5	F	7117	GLU	N-CA-CB	-5.98	99.84	110.60
3	J	5	DA	O4'-C1'-N9	5.93	112.15	108.00
3	J	18	DA	O4'-C1'-N9	5.88	112.11	108.00
3	J	4	DG	O4'-C1'-N9	5.85	112.10	108.00
5	H	6111	VAL	N-CA-C	-5.83	95.27	111.00
3	J	3	DA	N9-C4-C5	-5.82	103.47	105.80
1	E	49	SER	C-N-CD	-5.81	107.81	120.60
1	C	111	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	C	98	ASP	N-CA-C	-5.79	95.38	111.00
3	J	6	DC	O4'-C1'-N1	5.78	112.04	108.00
5	H	6220	LEU	CB-CA-C	5.76	121.15	110.20
3	J	3	DA	C5-C6-N6	-5.71	119.14	123.70
2	I	18	DT	C5-C4-O4	-5.69	120.92	124.90
2	I	16	DA	C4'-C3'-C2'	-5.67	98.00	103.10
1	D	111	ARG	NE-CZ-NH1	5.62	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	4	DG	C8-N9-C4	-5.62	104.15	106.40
2	I	10	DT	N3-C4-O4	5.55	123.23	119.90
3	J	19	DT	O4'-C1'-N1	5.54	111.88	108.00
2	I	8	DT	C4-C5-C7	5.54	122.32	119.00
3	J	17	DC	N3-C4-N4	-5.51	114.14	118.00
4	A	103	PRO	N-CA-C	5.50	126.40	112.10
3	J	15	DT	N1-C2-O2	5.49	127.49	123.10
2	I	26	DT	O4'-C1'-N1	5.46	111.82	108.00
2	I	10	DT	N1-C1'-C2'	5.40	122.86	112.60
1	B	111	ARG	NE-CZ-NH1	5.40	123.00	120.30
5	F	7133	LEU	CB-CA-C	-5.38	99.98	110.20
1	D	153	ARG	NE-CZ-NH1	-5.37	117.62	120.30
3	J	16	DA	O4'-C4'-C3'	-5.34	102.36	104.50
2	I	12	DA	C4'-C3'-C2'	-5.32	98.31	103.10
3	J	2	DC	O4'-C1'-N1	5.29	111.70	108.00
1	C	49	SER	C-N-CD	-5.23	109.09	120.60
1	D	231	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	231	ASP	CB-CG-OD2	5.22	123.00	118.30
5	G	5037	THR	N-CA-CB	-5.19	100.44	110.30
2	I	20	DG	N1-C6-O6	5.15	122.99	119.90
5	G	5200	ALA	CB-CA-C	5.14	117.81	110.10
5	G	5078	ASP	N-CA-C	-5.14	97.12	111.00
1	C	231	ASP	CB-CG-OD2	5.14	122.92	118.30
5	F	7135	ILE	CB-CA-C	-5.08	101.43	111.60
2	I	8	DT	C6-C5-C7	-5.08	119.85	122.90
5	F	7175	GLU	N-CA-C	5.07	124.68	111.00
2	I	11	DT	C5-C4-O4	-5.05	121.37	124.90
2	I	23	DG	O4'-C1'-N9	5.04	111.53	108.00
1	B	111	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	104	ARG	Peptide
1	B	296	GLY	Peptide
1	B	49	SER	Peptide
1	B	86	GLY	Mainchain
1	C	229	THR	Peptide
1	C	296	GLY	Peptide
1	D	231	ASP	Peptide
1	D	296	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	D	49	SER	Peptide
1	E	128	TYR	Mainchain
1	E	296	GLY	Peptide

## 5.2 Too-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 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	B	2509	0	2538	168	0
1	C	2515	0	2543	194	2
1	D	2503	0	2527	201	0
1	E	2409	0	2433	192	1
2	I	489	0	277	46	0
3	J	408	0	225	27	0
4	A	1488	0	1509	165	0
5	F	1750	0	1752	173	0
5	G	1750	0	1752	142	0
5	H	1750	0	1752	188	1
6	B	31	0	13	3	0
6	C	31	0	13	2	0
6	D	31	0	13	4	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	E	27	0	12	8	0
All	All	17695	0	17359	1260	3

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 36.

All (1260) 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)
5:F:7028:PHE:CZ	5:F:7030:MSE:HE2	1.22	1.68
5:F:7028:PHE:CZ	5:F:7030:MSE:CE	1.93	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:167:LEU:CD1	4:A:180:LEU:HD21	1.51	1.40
4:A:167:LEU:HD11	4:A:180:LEU:CD2	1.55	1.36
5:F:7028:PHE:CE2	5:F:7030:MSE:CE	2.10	1.33
5:F:7028:PHE:CE2	5:F:7030:MSE:HE3	1.64	1.32
1:B:267:LYS:HE2	1:B:271:GLU:OE1	1.20	1.27
5:F:7068:ASN:ND2	5:F:7086:ALA:HB2	1.44	1.27
1:B:293:GLN:NE2	4:A:85:ILE:HA	1.53	1.23
1:D:299:ALA:HB2	1:E:295:HIS:CD2	1.72	1.22
2:I:28:DT:H3	3:J:3:DA:N6	1.36	1.22
4:A:173:ASN:O	4:A:176:GLU:HG2	1.39	1.20
5:G:5128:ARG:HG2	5:F:7066:LEU:CD1	1.73	1.18
1:E:97:PHE:HB3	5:H:6205:GLY:O	1.44	1.15
1:D:297:ILE:HD13	1:E:297:ILE:HD11	1.20	1.15
1:B:267:LYS:CE	1:B:271:GLU:OE1	1.96	1.13
1:C:251:ARG:NH2	1:D:270:GLU:HA	1.62	1.13
5:F:7030:MSE:HE1	5:F:7106:PRO:HB3	1.18	1.13
1:B:226:SER:O	1:B:230:ASN:HB2	1.46	1.12
1:D:299:ALA:CB	1:E:295:HIS:HD2	1.64	1.11
1:D:256:LYS:CG	1:E:159:GLN:HE22	1.63	1.10
1:B:293:GLN:HE22	4:A:85:ILE:HA	0.99	1.10
1:D:256:LYS:HG3	1:E:159:GLN:NE2	1.64	1.10
5:F:7109:PHE:HD1	5:F:7110:PRO:HD2	1.11	1.10
1:E:205:ARG:NH2	8:E:700:ADP:O3B	1.85	1.10
5:F:7007:THR:O	5:F:7011:LEU:HD13	1.50	1.09
1:C:251:ARG:HH22	1:D:270:GLU:HA	1.05	1.08
1:D:256:LYS:CG	1:E:159:GLN:NE2	2.17	1.07
4:A:37:GLU:O	4:A:38:ASN:HB2	1.49	1.07
1:C:299:ALA:HB2	1:D:295:HIS:HD2	1.09	1.06
5:G:5010:LEU:HD12	5:G:5190:GLN:OE1	1.55	1.06
5:G:5128:ARG:CG	5:F:7066:LEU:HD13	1.85	1.05
5:F:7028:PHE:HZ	5:F:7030:MSE:CE	1.46	1.04
1:C:233:GLY:HA3	1:C:263:TRP:HZ2	1.20	1.03
2:I:9:DT:H72	4:A:38:ASN:CB	1.89	1.02
5:G:5076:SER:HB3	5:G:5078:ASP:O	1.60	1.01
1:D:256:LYS:HG3	1:E:159:GLN:HE22	1.22	1.00
1:D:77:SER:HB2	1:E:120:HIS:ND1	1.76	1.00
5:G:5128:ARG:HG2	5:F:7066:LEU:HD13	1.01	0.99
1:D:232:ARG:CB	1:D:263:TRP:CZ2	2.45	0.99
2:I:9:DT:H72	4:A:38:ASN:CG	1.82	0.99
5:F:7109:PHE:CD1	5:F:7110:PRO:HD2	1.97	0.99
5:F:7007:THR:HG23	5:F:7044:ILE:HG12	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:7135:ILE:HG23	5:F:7152:PHE:O	1.63	0.98
4:A:55:ILE:HG23	4:A:56:ALA:N	1.75	0.98
1:B:57:THR:HG22	1:B:137:THR:HG21	1.47	0.97
5:H:6146:LYS:HA	5:H:6171:ASP:HA	1.45	0.97
1:D:8:GLU:OE1	1:D:13:GLN:HB3	1.64	0.97
1:E:213:SER:HA	4:A:147:LYS:HE3	1.43	0.96
1:C:97:PHE:N	1:C:97:PHE:CD1	2.30	0.96
5:H:6038:THR:O	5:H:6038:THR:HG23	1.66	0.95
5:G:5041:GLU:O	5:G:5214:ALA:HB1	1.67	0.95
1:D:299:ALA:HB2	1:E:295:HIS:HD2	0.79	0.95
1:C:299:ALA:HB2	1:D:295:HIS:CD2	2.01	0.94
5:G:5077:GLU:HG2	5:G:5078:ASP:H	1.32	0.94
1:E:212:ASP:O	1:E:215:SER:HB3	1.67	0.94
1:C:57:THR:HG22	1:C:137:THR:HG21	1.49	0.94
1:C:8:GLU:OE1	1:C:13:GLN:HB3	1.67	0.94
5:F:7068:ASN:ND2	5:F:7086:ALA:CB	2.31	0.94
4:A:155:LEU:HB3	4:A:183:LEU:HD11	1.50	0.93
1:C:297:ILE:HD13	1:D:297:ILE:HD11	1.48	0.93
5:G:5105:LYS:HB3	5:G:5106:PRO:HD2	1.49	0.93
1:E:277:THR:HG22	1:E:317:GLN:O	1.68	0.92
1:C:231:ASP:O	1:C:233:GLY:N	2.02	0.92
1:C:226:SER:O	1:C:230:ASN:HA	1.68	0.92
5:H:6196:LEU:HD13	5:H:6209:PHE:CE1	2.03	0.92
1:C:233:GLY:HA3	1:C:263:TRP:CZ2	2.03	0.92
1:E:3:THR:HG21	1:E:18:SER:HB2	1.51	0.92
5:H:6115:VAL:HG13	5:H:6197:LEU:HD23	1.49	0.91
5:F:7068:ASN:HD21	5:F:7086:ALA:HB2	1.30	0.91
5:H:6037:THR:HG23	5:H:6038:THR:HB	1.52	0.90
4:A:148:ASN:O	4:A:150:LYS:N	2.03	0.90
1:D:57:THR:HG22	1:D:137:THR:HG21	1.53	0.90
1:D:97:PHE:HD2	5:G:5079:GLY:N	1.69	0.90
1:D:97:PHE:HD2	5:G:5079:GLY:H	1.15	0.89
5:H:6011:LEU:HB3	5:H:6061:LEU:HD11	1.52	0.89
4:A:164:ASP:HA	4:A:167:LEU:HD12	1.54	0.89
5:G:5210:GLU:HA	5:G:5215:ASN:ND2	1.86	0.89
1:B:285:TYR:CE1	4:A:93:ALA:HB1	2.08	0.89
1:E:186:ALA:HB3	1:E:219:VAL:HG22	1.55	0.89
1:D:256:LYS:CD	1:E:159:GLN:NE2	2.36	0.88
5:G:5128:ARG:HD3	5:F:7066:LEU:HD22	1.53	0.88
5:G:5210:GLU:HA	5:G:5215:ASN:HD22	1.36	0.88
1:D:192:VAL:CG2	1:D:225:LEU:HB2	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:HG2	1:C:273:TYR:OH	1.73	0.88
5:H:6178:PHE:CD2	5:H:6180:PHE:HE2	1.93	0.87
1:B:307:TYR:HE2	1:C:293:GLN:HE22	1.19	0.87
5:F:7068:ASN:HD22	5:F:7086:ALA:HB2	1.39	0.86
4:A:55:ILE:HG23	4:A:56:ALA:H	1.39	0.86
5:F:7028:PHE:HE2	5:F:7030:MSE:HE3	1.10	0.86
1:C:119:ARG:HB3	1:C:122:ARG:NH1	1.90	0.86
1:D:186:ALA:HB3	1:D:219:VAL:HG22	1.58	0.85
5:F:7033:ALA:HB2	5:F:7038:THR:HG23	1.56	0.85
1:C:299:ALA:CB	1:D:295:HIS:HD2	1.89	0.85
1:E:204:PHE:HA	1:E:207:THR:HG22	1.56	0.85
2:I:11:DT:H2"	2:I:12:DA:H5'	1.59	0.85
1:E:303:LEU:HD11	4:A:79:VAL:HG11	1.57	0.85
2:I:15:DT:H2"	2:I:16:DA:H5'	1.58	0.85
4:A:61:SER:HB3	4:A:64:MET:HB2	1.57	0.85
1:C:57:THR:HG23	6:C:700:08T:O1B	1.77	0.85
1:B:125:MET:HE2	1:B:151:ARG:HG2	1.56	0.85
1:C:192:VAL:CG2	1:C:225:LEU:HB2	2.08	0.84
2:I:9:DT:H72	4:A:38:ASN:HB3	1.58	0.84
5:F:7125:GLN:O	5:F:7129:VAL:HG23	1.77	0.84
1:E:57:THR:HG22	1:E:137:THR:HG21	1.59	0.84
2:I:9:DT:H72	4:A:38:ASN:ND2	1.91	0.84
1:C:97:PHE:N	1:C:97:PHE:HD1	1.70	0.84
2:I:28:DT:H3	3:J:3:DA:H61	0.92	0.84
4:A:36:ALA:O	4:A:37:GLU:HG2	1.77	0.84
5:H:6023:LEU:HD13	5:H:6048:ILE:HD13	1.58	0.84
5:H:6054:ILE:CG2	5:H:6056:ASP:O	2.25	0.84
5:F:7030:MSE:CE	5:F:7106:PRO:HB3	2.05	0.84
1:B:226:SER:O	1:B:230:ASN:CB	2.25	0.83
4:A:173:ASN:O	4:A:176:GLU:CG	2.24	0.83
4:A:148:ASN:C	4:A:150:LYS:H	1.76	0.83
2:I:28:DT:N3	3:J:3:DA:N6	2.11	0.83
1:D:204:PHE:HA	1:D:207:THR:HG22	1.59	0.83
2:I:9:DT:C7	4:A:38:ASN:HB3	2.09	0.83
4:A:145:LEU:HB3	4:A:151:LEU:HD23	1.60	0.83
5:H:6178:PHE:CD2	5:H:6180:PHE:CE2	2.67	0.82
5:F:7023:LEU:O	5:F:7023:LEU:HD12	1.80	0.82
5:H:6017:ILE:HG23	5:H:6038:THR:HG21	1.61	0.82
5:G:5010:LEU:CD1	5:G:5190:GLN:OE1	2.26	0.82
5:F:7146:LYS:HG2	5:F:7171:ASP:HB3	1.62	0.82
1:C:48:HIS:CD2	1:C:141:ILE:HD11	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASP:HB3	1:D:153:ARG:CZ	2.10	0.81
5:F:7030:MSE:HE1	5:F:7106:PRO:CB	2.08	0.81
1:C:227:LEU:HA	1:C:230:ASN:HB3	1.61	0.81
2:I:29:DG:O6	3:J:2:DC:N4	2.14	0.81
1:C:204:PHE:HA	1:C:207:THR:HG22	1.62	0.81
1:B:192:VAL:CG2	1:B:225:LEU:HB2	2.11	0.80
1:D:256:LYS:CB	1:E:159:GLN:HE22	1.94	0.80
1:D:297:ILE:HD13	1:E:297:ILE:CD1	2.07	0.80
1:D:232:ARG:CB	1:D:263:TRP:CH2	2.64	0.80
5:F:7153:ASN:O	5:F:7157:ASP:HB3	1.82	0.80
1:E:119:ARG:HB3	1:E:122:ARG:NH1	1.96	0.80
4:A:167:LEU:HD21	4:A:180:LEU:HD23	1.64	0.80
4:A:48:ASN:OD1	4:A:104:ARG:NH2	2.14	0.80
1:D:97:PHE:CZ	5:G:5080:ASN:ND2	2.51	0.79
5:H:6115:VAL:HG13	5:H:6197:LEU:CD2	2.12	0.79
1:D:256:LYS:HG3	1:E:159:GLN:CD	2.03	0.79
1:B:307:TYR:HE2	1:C:293:GLN:NE2	1.80	0.79
1:B:204:PHE:HA	1:B:207:THR:HG22	1.65	0.79
5:F:7109:PHE:HD1	5:F:7110:PRO:CD	1.94	0.78
5:F:7068:ASN:HD21	5:F:7086:ALA:CB	1.93	0.78
1:E:57:THR:HG23	8:E:700:ADP:O1B	1.84	0.78
1:D:217:LYS:HE2	1:D:224:ILE:HD11	1.63	0.78
5:H:6027:GLN:O	5:H:6043:ASN:OD1	2.00	0.78
3:J:6:DC:H2"	3:J:7:DA:C8	2.17	0.78
4:A:54:SER:O	4:A:55:ILE:HG22	1.83	0.78
1:C:217:LYS:HE2	1:C:224:ILE:HD11	1.66	0.78
1:B:48:HIS:CD2	1:B:141:ILE:HD11	2.18	0.78
1:B:186:ALA:HB3	1:B:219:VAL:HG22	1.66	0.78
1:E:204:PHE:HA	1:E:207:THR:CG2	2.13	0.77
1:C:186:ALA:HB3	1:C:219:VAL:HG22	1.65	0.77
1:E:88:LEU:HD21	1:E:104:ILE:HG21	1.66	0.77
5:F:7118:ILE:HG12	5:F:7119:LYS:N	1.98	0.77
5:F:7122:ASP:HB3	5:F:7167:LEU:HD21	1.67	0.77
1:C:77:SER:HB2	1:D:120:HIS:ND1	1.99	0.77
5:G:5140:ILE:HG13	5:G:5148:VAL:O	1.84	0.77
5:G:5001:MSE:N	5:G:5072:GLU:OE2	2.18	0.77
1:D:204:PHE:HA	1:D:207:THR:CG2	2.13	0.77
5:G:5105:LYS:HB3	5:G:5106:PRO:CD	2.15	0.76
5:G:5153:ASN:O	5:G:5157:ASP:HB2	1.85	0.76
1:E:277:THR:CG2	1:E:317:GLN:HB2	2.15	0.76
1:C:226:SER:O	1:C:230:ASN:CA	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6054:ILE:HG21	5:H:6056:ASP:O	1.84	0.76
5:H:6120:ALA:HB2	5:H:6192:GLY:C	2.05	0.76
1:E:213:SER:HA	4:A:147:LYS:CE	2.16	0.76
5:H:6198:LEU:HD23	5:H:6207:ALA:CB	2.16	0.76
1:D:256:LYS:HD2	1:E:159:GLN:NE2	2.01	0.76
5:G:5041:GLU:O	5:G:5214:ALA:CB	2.33	0.76
4:A:118:SER:HB2	4:A:179:GLN:NE2	2.01	0.76
2:I:26:DT:H2"	2:I:27:DC:OP2	1.86	0.75
1:E:307:TYR:CD2	4:A:80:TYR:CD1	2.74	0.75
1:B:293:GLN:HE22	4:A:85:ILE:CA	1.91	0.75
1:E:98:ASP:O	5:H:6204:GLN:NE2	2.18	0.75
1:C:204:PHE:HA	1:C:207:THR:CG2	2.16	0.75
5:F:7085:ASP:CG	5:F:7086:ALA:H	1.88	0.75
1:D:97:PHE:CD2	5:G:5079:GLY:N	2.54	0.75
1:D:28:PHE:O	1:D:32:THR:HG22	1.86	0.74
1:D:97:PHE:N	1:D:97:PHE:CD1	2.55	0.74
1:B:217:LYS:HE2	1:B:224:ILE:HD11	1.66	0.74
5:H:6129:VAL:HG11	5:H:6165:TYR:CD2	2.22	0.74
5:H:6038:THR:O	5:H:6038:THR:CG2	2.34	0.74
4:A:118:SER:HB2	4:A:179:GLN:HE22	1.52	0.74
1:C:226:SER:O	1:C:230:ASN:CB	2.35	0.74
5:H:6003:LEU:HD22	5:H:6007:THR:HG21	1.70	0.74
1:D:276:VAL:HG23	1:D:317:GLN:O	1.88	0.74
1:E:93:SER:HB2	5:H:6221:GLU:OE1	1.87	0.74
5:F:7112:ALA:HB1	5:F:7114:ALA:O	1.88	0.74
1:D:48:HIS:CD2	1:D:141:ILE:HD11	2.22	0.74
1:C:294:TYR:CD2	1:D:293:GLN:OE1	2.41	0.74
3:J:2:DC:H2"	3:J:3:DA:OP2	1.88	0.73
1:C:227:LEU:CA	1:C:230:ASN:HB3	2.17	0.73
1:D:119:ARG:O	1:D:122:ARG:HG2	1.88	0.73
1:D:119:ARG:HB3	1:D:122:ARG:NH1	2.02	0.73
1:C:235:ILE:HG22	1:C:239:LEU:HG	1.70	0.73
1:D:192:VAL:HG22	1:D:225:LEU:HB2	1.70	0.73
5:G:5149:ILE:O	5:G:5166:SER:HA	1.88	0.73
5:F:7226:HIS:HB2	5:F:7228:PHE:CD1	2.24	0.73
1:B:192:VAL:HG22	1:B:225:LEU:HD13	1.70	0.73
5:F:7133:LEU:O	5:F:7134:GLN:HB2	1.88	0.73
1:B:120:HIS:NE2	4:A:17:TRP:CH2	2.57	0.73
1:B:88:LEU:HD21	1:B:104:ILE:HG21	1.70	0.72
5:F:7061:LEU:HA	5:F:7064:LEU:HD12	1.70	0.72
1:B:235:ILE:HG22	1:B:239:LEU:HG	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ARG:O	1:C:122:ARG:HG2	1.89	0.72
1:C:88:LEU:HD21	1:C:104:ILE:HG21	1.71	0.72
1:B:260:ASP:OD1	1:B:263:TRP:HB3	1.89	0.72
1:E:93:SER:O	5:H:6221:GLU:OE1	2.06	0.72
1:D:307:TYR:CE1	1:E:286:GLU:HA	2.24	0.72
1:B:307:TYR:CE2	1:C:293:GLN:NE2	2.58	0.72
1:B:299:ALA:HB1	1:C:262:SER:HB3	1.72	0.72
4:A:53:CYS:SG	4:A:95:PHE:CZ	2.83	0.72
5:G:5040:ALA:HB2	5:G:5216:TYR:CD1	2.25	0.72
5:G:5011:LEU:HD12	5:G:5011:LEU:H	1.55	0.72
1:D:93:SER:O	5:G:5096:ASP:HB3	1.90	0.71
1:D:110:ASP:OD1	1:E:122:ARG:NH2	2.23	0.71
1:E:8:GLU:HG2	1:E:13:GLN:HB3	1.71	0.71
1:D:295:HIS:HE1	1:E:142:ASP:OD2	1.74	0.71
5:G:5023:LEU:HD12	5:G:5023:LEU:O	1.90	0.71
5:H:6030:MSE:HE3	5:H:6103:PRO:HG2	1.73	0.71
2:I:29:DG:N2	3:J:3:DA:C2	2.59	0.71
4:A:150:LYS:C	4:A:152:PRO:HD2	2.11	0.71
1:C:233:GLY:CA	1:C:263:TRP:CZ2	2.73	0.71
1:C:49:SER:CB	1:C:51:SER:O	2.39	0.71
1:E:28:PHE:O	1:E:32:THR:HG22	1.91	0.71
5:F:7134:GLN:HB3	5:F:7153:ASN:ND2	2.06	0.71
5:G:5077:GLU:HG2	5:G:5078:ASP:N	2.03	0.70
1:C:91:PHE:HD2	5:G:5035:ASN:O	1.73	0.70
5:F:7033:ALA:HB2	5:F:7038:THR:CG2	2.21	0.70
1:B:98:ASP:N	1:B:98:ASP:OD1	2.21	0.70
5:F:7109:PHE:CD2	5:F:7208:LYS:HB3	2.27	0.70
4:A:145:LEU:HB3	4:A:151:LEU:CD2	2.21	0.70
5:F:7148:VAL:HG12	5:F:7168:THR:HA	1.73	0.70
1:B:277:THR:HG22	1:B:317:GLN:O	1.92	0.70
1:B:13:GLN:HE22	1:C:126:GLU:CB	2.05	0.70
1:B:122:ARG:HG3	4:A:32:PHE:CE2	2.25	0.70
4:A:80:TYR:CZ	4:A:84:LEU:HD11	2.26	0.70
3:J:6:DC:H2"	3:J:7:DA:H8	1.55	0.70
1:B:122:ARG:CG	4:A:32:PHE:CE2	2.74	0.69
5:G:5024:LYS:HG2	5:G:5051:ASP:HB3	1.74	0.69
1:C:192:VAL:HG22	1:C:225:LEU:HD13	1.74	0.69
5:G:5133:LEU:HD22	5:G:5164:LYS:HD3	1.73	0.69
4:A:34:GLU:HG2	4:A:34:GLU:O	1.92	0.69
1:B:80:LYS:NZ	2:I:19:DC:OP1	2.25	0.69
1:E:253:LEU:HD23	4:A:114:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:ASP:O	1:E:215:SER:CB	2.41	0.69
1:E:95:ALA:HB3	5:H:6220:LEU:O	1.93	0.69
1:D:297:ILE:CD1	1:E:297:ILE:HD11	2.12	0.69
5:F:7109:PHE:CE2	5:F:7208:LYS:HB3	2.27	0.69
1:B:120:HIS:CE1	4:A:17:TRP:CH2	2.81	0.69
1:E:307:TYR:CD2	4:A:80:TYR:CE1	2.80	0.69
1:B:204:PHE:HA	1:B:207:THR:CG2	2.21	0.69
1:B:28:PHE:O	1:B:32:THR:HG22	1.93	0.69
5:G:5064:LEU:CD2	5:G:5083:ILE:HD13	2.22	0.69
1:D:299:ALA:CB	1:E:295:HIS:CD2	2.53	0.69
4:A:148:ASN:C	4:A:150:LYS:N	2.46	0.69
1:D:192:VAL:HG22	1:D:225:LEU:CB	2.21	0.69
1:C:116:GLU:OE2	1:C:119:ARG:NH1	2.26	0.69
1:C:28:PHE:O	1:C:32:THR:HG22	1.93	0.69
5:G:5210:GLU:HG3	5:G:5215:ASN:HD21	1.58	0.68
1:B:80:LYS:NZ	1:C:85:ARG:NH2	2.41	0.68
1:C:110:ASP:OD1	1:D:122:ARG:NH2	2.26	0.68
5:H:6138:ILE:HG12	5:H:6184:MSE:HE3	1.76	0.68
5:G:5010:LEU:O	5:G:5013:ASN:HB3	1.94	0.68
5:F:7136:ASP:OD2	5:F:7155:VAL:HG23	1.94	0.68
5:H:6180:PHE:HB3	5:H:6220:LEU:HD22	1.75	0.68
5:F:7022:MSE:HE2	5:F:7024:LYS:HG3	1.75	0.68
1:C:231:ASP:O	1:C:232:ARG:C	2.32	0.68
5:F:7202:GLY:C	5:F:7204:GLN:H	1.97	0.68
5:H:6085:ASP:OD2	5:H:6087:ARG:N	2.22	0.68
4:A:167:LEU:CD1	4:A:180:LEU:CD2	2.38	0.68
5:F:7085:ASP:OD1	5:F:7086:ALA:N	2.25	0.68
1:B:57:THR:HG23	6:B:700:O8T:O1B	1.92	0.68
1:D:49:SER:HB3	1:D:56:LYS:NZ	2.09	0.68
1:B:83:PHE:O	1:B:87:PRO:HD2	1.93	0.68
1:D:279:GLN:N	1:D:279:GLN:OE1	2.26	0.67
5:H:6023:LEU:CD1	5:H:6048:ILE:HG21	2.24	0.67
5:F:7210:GLU:HG2	5:F:7215:ASN:OD1	1.94	0.67
1:E:98:ASP:OD1	1:E:98:ASP:N	2.27	0.67
5:H:6135:ILE:HG23	5:H:6152:PHE:O	1.93	0.67
1:B:314:CYS:SG	1:C:282:ILE:HD11	2.34	0.67
1:E:235:ILE:HG22	1:E:239:LEU:HG	1.76	0.67
5:H:6011:LEU:O	5:H:6057:LEU:HD21	1.95	0.67
1:B:125:MET:CE	1:B:151:ARG:HG2	2.25	0.67
5:G:5050:PHE:CD2	5:G:5075:GLN:HB2	2.28	0.67
4:A:167:LEU:HD11	4:A:180:LEU:HD21	0.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:7146:LYS:HA	5:F:7171:ASP:HA	1.77	0.67
5:F:7039:TYR:OH	5:F:7041:GLU:OE1	2.07	0.67
3:J:4:DG:H2"	3:J:5:DA:OP2	1.95	0.67
1:D:49:SER:HB3	1:D:56:LYS:HZ2	1.60	0.67
1:C:72:MET:HE1	5:G:5035:ASN:HB2	1.76	0.67
5:H:6210:GLU:HG3	5:H:6215:ASN:HD21	1.60	0.67
3:J:15:DT:H2"	3:J:16:DA:O5'	1.95	0.67
5:F:7152:PHE:CD2	5:F:7160:LEU:HD22	2.31	0.66
5:H:6001:MSE:HG2	5:H:6073:ILE:O	1.94	0.66
1:D:232:ARG:CB	1:D:263:TRP:CE2	2.79	0.66
5:H:6056:ASP:OD2	5:H:6059:GLY:HA3	1.95	0.66
1:E:93:SER:C	5:H:6221:GLU:OE1	2.34	0.66
1:B:205:ARG:NH1	1:C:150:SER:OG	2.27	0.66
1:B:92:ALA:O	1:B:131:ASN:ND2	2.26	0.66
1:C:98:ASP:OD1	1:C:98:ASP:N	2.27	0.66
1:D:303:LEU:HD21	1:E:288:VAL:HG12	1.77	0.66
5:H:6178:PHE:HD2	5:H:6180:PHE:CE2	2.11	0.66
1:C:251:ARG:NH1	1:D:273:TYR:CD2	2.64	0.66
1:E:299:ALA:HB2	4:A:87:SER:HB3	1.77	0.66
1:B:49:SER:HB3	1:B:56:LYS:NZ	2.11	0.66
1:B:125:MET:HE2	1:B:151:ARG:CG	2.25	0.66
1:C:192:VAL:HG22	1:C:225:LEU:HB2	1.76	0.66
4:A:37:GLU:O	4:A:38:ASN:CB	2.33	0.66
1:E:303:LEU:HD21	4:A:79:VAL:HG12	1.77	0.66
1:E:204:PHE:CA	1:E:207:THR:HG22	2.24	0.65
4:A:55:ILE:CG2	4:A:56:ALA:H	2.08	0.65
1:C:49:SER:HB2	1:C:51:SER:O	1.97	0.65
5:H:6135:ILE:HD13	5:H:6151:GLY:HA3	1.76	0.65
1:B:192:VAL:HG22	1:B:225:LEU:CB	2.27	0.65
1:E:119:ARG:O	1:E:122:ARG:HG2	1.96	0.65
1:C:49:SER:N	1:C:56:LYS:HD3	2.12	0.65
5:F:7226:HIS:HB2	5:F:7228:PHE:CE1	2.32	0.65
5:H:6024:LYS:HB3	5:H:6051:ASP:OD1	1.97	0.65
4:A:102:VAL:O	4:A:102:VAL:HG22	1.97	0.65
5:G:5128:ARG:CD	5:F:7066:LEU:HD22	2.26	0.64
1:D:97:PHE:HE2	5:G:5078:ASP:HB3	1.62	0.64
1:D:192:VAL:HG22	1:D:225:LEU:HD13	1.78	0.64
5:H:6202:GLY:O	5:H:6226:HIS:CE1	2.50	0.64
5:G:5136:ASP:O	5:G:5184:MSE:HB2	1.97	0.64
4:A:167:LEU:HD13	4:A:180:LEU:HD21	1.71	0.64
1:D:77:SER:HB3	1:D:111:ARG:HH11	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:VAL:HG22	1:C:225:LEU:CB	2.26	0.64
5:F:7050:PHE:CD2	5:F:7075:GLN:HB2	2.32	0.64
1:D:297:ILE:HG21	1:E:297:ILE:HG13	1.80	0.64
1:C:279:GLN:N	1:C:279:GLN:OE1	2.29	0.64
1:E:95:ALA:CB	5:H:6220:LEU:O	2.45	0.64
1:C:88:LEU:HD23	1:C:104:ILE:HD13	1.78	0.64
5:G:5024:LYS:HG2	5:G:5051:ASP:CB	2.27	0.64
1:B:269:ALA:HA	1:B:284:MET:CE	2.28	0.64
5:H:6121:GLU:O	5:H:6124:GLN:HB3	1.97	0.64
5:H:6179:ASN:HB3	5:H:6225:THR:HG23	1.80	0.64
1:B:267:LYS:HE2	1:B:271:GLU:CD	2.15	0.64
1:C:251:ARG:HH22	1:D:270:GLU:CA	1.97	0.64
3:J:3:DA:H1'	3:J:4:DG:H5'	1.79	0.64
1:E:303:LEU:CD2	4:A:79:VAL:HG12	2.28	0.64
1:B:192:VAL:HG22	1:B:225:LEU:HB2	1.80	0.64
1:D:314:CYS:SG	1:E:282:ILE:HD11	2.38	0.64
1:D:235:ILE:HG22	1:D:239:LEU:HG	1.80	0.64
1:C:231:ASP:O	1:C:263:TRP:CZ2	2.51	0.64
1:D:97:PHE:HD1	1:D:97:PHE:N	1.96	0.64
5:F:7148:VAL:HG12	5:F:7168:THR:HG23	1.79	0.64
1:D:16:ARG:NH2	6:D:700:O8T:O2A	2.31	0.63
1:B:234:ALA:O	1:B:235:ILE:HD13	1.97	0.63
1:E:10:ILE:HG12	4:A:145:LEU:CD1	2.29	0.63
1:E:196:LEU:HD11	1:E:214:TYR:CE2	2.33	0.63
1:C:274:SER:O	1:C:319:LYS:HE2	1.99	0.63
1:E:80:LYS:HB3	2:I:14:DG:OP1	1.99	0.63
5:H:6023:LEU:HD13	5:H:6048:ILE:HG21	1.80	0.63
1:D:204:PHE:CA	1:D:207:THR:HG22	2.28	0.63
5:G:5122:ASP:HB3	5:G:5167:LEU:HD21	1.81	0.63
1:B:77:SER:HB3	1:B:111:ARG:HH11	1.64	0.63
5:H:6002:LYS:HG2	5:H:6070:ASP:O	1.99	0.63
1:B:126:GLU:OE1	4:A:13:HIS:CE1	2.52	0.63
1:E:267:LYS:HE3	1:E:271:GLU:OE1	1.97	0.63
1:E:10:ILE:HG12	4:A:145:LEU:HD11	1.79	0.63
5:H:6063:ILE:HG21	5:H:6090:ILE:HG21	1.81	0.63
1:D:88:LEU:HD21	1:D:104:ILE:HG21	1.80	0.63
5:G:5076:SER:CB	5:G:5078:ASP:O	2.43	0.63
5:G:5116:THR:HB	5:G:5147:ILE:HD12	1.79	0.63
4:A:72:PHE:HB3	4:A:74:GLU:OE1	1.99	0.63
1:D:80:LYS:HE2	1:E:85:ARG:NH2	2.14	0.62
1:E:48:HIS:CD2	1:E:141:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:7134:GLN:HB3	5:F:7153:ASN:HD21	1.62	0.62
5:F:7034:VAL:HG13	5:F:7101:VAL:HG21	1.81	0.62
1:B:290:GLU:HB2	4:A:85:ILE:HD11	1.81	0.62
1:D:297:ILE:CG2	1:E:297:ILE:HG13	2.29	0.62
1:D:231:ASP:C	1:D:233:GLY:H	2.02	0.62
5:H:6054:ILE:HG22	5:H:6056:ASP:O	1.99	0.62
1:B:235:ILE:HG12	1:B:267:LYS:HG2	1.80	0.62
1:B:293:GLN:OE1	1:E:297:ILE:CG2	2.47	0.62
5:F:7109:PHE:HD2	5:F:7208:LYS:HD3	1.63	0.62
1:C:230:ASN:OD1	1:C:230:ASN:O	2.18	0.62
5:G:5010:LEU:HD23	5:G:5029:ILE:HD11	1.82	0.62
5:H:6208:LYS:HA	5:H:6217:VAL:HG22	1.82	0.62
1:B:88:LEU:HD23	1:B:104:ILE:HD13	1.82	0.62
5:F:7089:THR:HG22	5:F:7091:PHE:CE1	2.35	0.62
1:C:231:ASP:C	1:C:233:GLY:N	2.53	0.62
1:C:72:MET:HE1	5:G:5035:ASN:CB	2.30	0.62
3:J:3:DA:H2"	3:J:4:DG:OP2	2.01	0.61
5:H:6027:GLN:NE2	5:H:6047:VAL:HB	2.15	0.61
5:G:5146:LYS:HA	5:G:5171:ASP:HA	1.82	0.61
1:C:277:THR:O	1:C:280:SER:HB2	2.00	0.61
1:B:49:SER:HB3	1:B:56:LYS:HZ2	1.65	0.61
1:C:227:LEU:C	1:C:230:ASN:HB3	2.20	0.61
5:F:7120:ALA:N	5:F:7193:ASN:OD1	2.33	0.61
5:G:5029:ILE:HG13	5:G:5042:ALA:HB3	1.81	0.61
5:H:6027:GLN:HG2	5:H:6047:VAL:HA	1.82	0.61
1:B:256:LYS:HE2	1:B:257:TYR:CZ	2.34	0.61
1:E:205:ARG:HH22	8:E:700:ADP:PB	2.17	0.61
4:A:55:ILE:CG2	4:A:56:ALA:N	2.48	0.61
5:F:7112:ALA:HB2	5:F:7197:LEU:HD22	1.83	0.61
1:D:307:TYR:HE1	1:E:286:GLU:HA	1.65	0.61
5:F:7136:ASP:O	5:F:7137:THR:OG1	2.16	0.61
1:B:277:THR:CG2	1:B:317:GLN:O	2.48	0.61
1:B:125:MET:CE	1:B:151:ARG:CG	2.78	0.61
1:B:279:GLN:N	1:B:279:GLN:OE1	2.32	0.61
4:A:105:GLY:O	4:A:106:LYS:HE2	1.99	0.61
5:G:5129:VAL:CG1	5:G:5133:LEU:HD12	2.30	0.61
2:I:8:DT:O2	4:A:109:GLY:HA2	2.01	0.61
1:B:120:HIS:NE2	4:A:17:TRP:HH2	1.97	0.61
1:C:92:ALA:O	1:C:131:ASN:ND2	2.32	0.61
4:A:164:ASP:CA	4:A:167:LEU:HD12	2.30	0.60
1:E:277:THR:HG21	1:E:317:GLN:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ILE:HB	1:D:284:MET:HE1	1.83	0.60
1:C:71:MET:HE2	1:C:73:PHE:HB2	1.82	0.60
5:H:6210:GLU:HA	5:H:6215:ASN:ND2	2.16	0.60
5:H:6023:LEU:HB3	5:H:6029:ILE:HG22	1.84	0.60
1:E:71:MET:HE3	1:E:73:PHE:HB2	1.84	0.60
5:F:7118:ILE:CG1	5:F:7119:LYS:N	2.65	0.60
5:G:5064:LEU:HD21	5:G:5083:ILE:HD13	1.82	0.60
1:B:272:ILE:HB	1:B:284:MET:CE	2.32	0.60
5:G:5200:ALA:HB1	5:G:5226:HIS:NE2	2.16	0.60
2:I:9:DT:C7	4:A:38:ASN:CG	2.65	0.60
1:D:80:LYS:HB3	2:I:16:DA:OP1	2.02	0.60
5:H:6028:PHE:CD2	5:H:6043:ASN:ND2	2.70	0.60
5:F:7060:PHE:CE2	5:F:7064:LEU:HD11	2.37	0.60
1:C:72:MET:CE	5:G:5035:ASN:HB2	2.32	0.60
5:F:7068:ASN:CG	5:F:7085:ASP:OD1	2.40	0.60
5:G:5128:ARG:HD3	5:F:7066:LEU:CD2	2.27	0.60
1:D:98:ASP:OD1	1:D:98:ASP:N	2.33	0.59
4:A:68:ALA:O	4:A:71:GLN:HG2	2.02	0.59
1:B:77:SER:HB2	1:C:120:HIS:ND1	2.18	0.59
5:G:5053:ALA:HB3	5:G:5095:ALA:O	2.01	0.59
5:F:7133:LEU:O	5:F:7134:GLN:CB	2.50	0.59
1:E:49:SER:N	1:E:56:LYS:HD3	2.17	0.59
5:F:7022:MSE:HB3	5:F:7102:ALA:HB2	1.84	0.59
5:H:6059:GLY:C	5:H:6092:TRP:CH2	2.76	0.59
5:H:6199:TRP:CD1	5:H:6200:ALA:N	2.71	0.59
5:F:7130:SER:HA	5:F:7135:ILE:HD12	1.83	0.59
5:F:7041:GLU:O	5:F:7214:ALA:HB1	2.02	0.59
1:D:94:ALA:HA	5:G:5095:ALA:HA	1.83	0.59
5:G:5040:ALA:HB2	5:G:5216:TYR:CE1	2.37	0.58
5:F:7027:GLN:CG	5:F:7047:VAL:HG12	2.33	0.58
1:D:111:ARG:HB2	1:D:114:LEU:HD13	1.83	0.58
4:A:151:LEU:HD13	4:A:155:LEU:HG	1.84	0.58
1:C:48:HIS:NE2	1:C:141:ILE:HD11	2.18	0.58
4:A:129:LYS:HD3	4:A:161:LEU:HD11	1.84	0.58
5:H:6120:ALA:HB2	5:H:6193:ASN:N	2.17	0.58
4:A:158:LEU:C	4:A:160:GLY:N	2.53	0.58
1:D:83:PHE:HZ	5:H:6155:VAL:HG21	1.69	0.58
1:B:111:ARG:HB2	1:B:114:LEU:HD13	1.86	0.58
5:G:5127:LEU:HD23	5:G:5184:MSE:HE1	1.85	0.58
1:D:83:PHE:CZ	5:H:6155:VAL:HG21	2.39	0.58
5:F:7003:LEU:HA	5:F:7046:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:5120:ALA:HB2	5:G:5192:GLY:C	2.23	0.58
5:F:7022:MSE:HB3	5:F:7102:ALA:CB	2.33	0.58
1:E:5:ASN:O	1:E:14:LYS:HB2	2.03	0.58
1:C:72:MET:CE	5:G:5035:ASN:CB	2.80	0.58
5:H:6010:LEU:HD11	5:H:6213:HIS:O	2.02	0.58
5:G:5135:ILE:HA	5:G:5152:PHE:O	2.04	0.58
3:J:9:DT:H1'	3:J:10:DA:H5'	1.85	0.58
1:D:13:GLN:HE22	1:E:126:GLU:CA	2.17	0.58
5:H:6198:LEU:HD23	5:H:6207:ALA:HB1	1.84	0.58
5:H:6138:ILE:HG22	5:H:6151:GLY:HA2	1.86	0.58
5:F:7109:PHE:CD2	5:F:7208:LYS:HD3	2.37	0.58
1:C:204:PHE:CA	1:C:207:THR:HG22	2.32	0.58
4:A:47:ILE:O	4:A:50:LYS:NZ	2.37	0.58
5:F:7134:GLN:CB	5:F:7153:ASN:ND2	2.67	0.58
1:D:71:MET:HE2	1:D:73:PHE:HB2	1.85	0.58
4:A:25:VAL:HG12	4:A:26:GLN:N	2.18	0.58
1:E:213:SER:CA	4:A:147:LYS:HE3	2.26	0.57
5:H:6017:ILE:HG23	5:H:6038:THR:CG2	2.33	0.57
1:E:186:ALA:CB	1:E:219:VAL:HG22	2.32	0.57
1:E:88:LEU:CD2	1:E:104:ILE:HG21	2.34	0.57
5:H:6037:THR:HG23	5:H:6038:THR:CB	2.29	0.57
1:E:10:ILE:HD12	4:A:141:TYR:CD2	2.39	0.57
1:E:3:THR:CG2	1:E:18:SER:HB2	2.30	0.57
4:A:174:VAL:O	4:A:174:VAL:HG12	2.04	0.57
5:F:7068:ASN:O	5:F:7071:ALA:N	2.38	0.57
1:B:176:LEU:HD22	1:B:211:LEU:HD22	1.86	0.57
5:G:5129:VAL:HG13	5:G:5133:LEU:HD12	1.86	0.57
1:E:279:GLN:N	1:E:279:GLN:OE1	2.35	0.57
5:H:6028:PHE:CE2	5:H:6043:ASN:ND2	2.73	0.57
1:C:3:THR:HG21	1:C:18:SER:HB2	1.85	0.57
1:D:57:THR:HG23	6:D:700:08T:O1B	2.03	0.57
1:B:260:ASP:O	1:B:260:ASP:OD1	2.23	0.57
1:C:91:PHE:CD2	5:G:5035:ASN:O	2.55	0.57
1:C:205:ARG:NH1	1:D:150:SER:OG	2.33	0.57
1:D:8:GLU:OE1	1:D:13:GLN:CB	2.47	0.57
1:C:88:LEU:HD23	1:C:104:ILE:CD1	2.35	0.57
5:F:7085:ASP:CG	5:F:7086:ALA:N	2.57	0.57
1:E:97:PHE:CB	5:H:6205:GLY:O	2.36	0.57
1:E:277:THR:CG2	1:E:317:GLN:O	2.48	0.57
1:C:50:PRO:HA	1:C:139:ASN:O	2.05	0.57
5:H:6123:LEU:CD2	5:H:6191:PRO:HA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:TYR:CD2	1:E:293:GLN:NE2	2.73	0.57
5:H:6133:LEU:O	5:H:6134:GLN:HG3	2.05	0.57
1:B:248:LYS:HG2	1:C:273:TYR:HH	1.70	0.56
5:H:6129:VAL:HG21	5:H:6165:TYR:CE2	2.40	0.56
5:H:6071:ALA:HA	5:H:6084:ALA:O	2.05	0.56
1:B:13:GLN:HE22	1:C:126:GLU:HB3	1.70	0.56
5:H:6109:PHE:CZ	5:H:6199:TRP:HB3	2.40	0.56
1:D:298:ALA:HB2	1:E:293:GLN:HA	1.87	0.56
5:G:5010:LEU:O	5:G:5013:ASN:N	2.36	0.56
1:B:111:ARG:HE	1:C:116:GLU:CD	2.08	0.56
5:H:6092:TRP:HD1	5:H:6093:PRO:O	1.88	0.56
1:E:88:LEU:HD23	1:E:104:ILE:HD13	1.87	0.56
5:F:7039:TYR:CD1	5:F:7040:ALA:N	2.74	0.56
1:C:256:LYS:HE2	1:C:257:TYR:CZ	2.40	0.56
1:D:283:ARG:NE	1:D:315:GLU:OE1	2.38	0.56
4:A:67:ASN:O	4:A:70:SER:HB3	2.06	0.56
5:H:6082:LYS:HE3	5:H:6089:THR:HG21	1.87	0.56
5:H:6066:LEU:HD12	5:H:6067:VAL:N	2.20	0.56
5:H:6133:LEU:C	5:H:6134:GLN:HG2	2.26	0.56
1:B:94:ALA:O	1:B:102:LYS:HE3	2.05	0.56
5:H:6049:ASP:O	5:H:6050:PHE:HB3	2.05	0.56
2:I:9:DT:H71	4:A:38:ASN:HB3	1.87	0.56
5:H:6017:ILE:CG2	5:H:6038:THR:HG21	2.33	0.56
1:E:254:ALA:N	1:E:255:PRO:HD2	2.21	0.56
1:D:97:PHE:HD1	1:D:97:PHE:H	1.51	0.56
1:D:88:LEU:HD23	1:D:104:ILE:HD13	1.87	0.56
1:C:97:PHE:O	5:G:5204:GLN:HB3	2.05	0.56
5:F:7089:THR:HG22	5:F:7091:PHE:HE1	1.71	0.56
4:A:163:THR:O	4:A:166:PHE:N	2.36	0.56
5:H:6133:LEU:O	5:H:6134:GLN:CG	2.53	0.56
1:E:92:ALA:O	1:E:131:ASN:ND2	2.31	0.56
1:B:13:GLN:HE22	1:C:126:GLU:CA	2.19	0.56
5:F:7189:MSE:HB2	5:F:7216:TYR:CE1	2.41	0.55
1:C:205:ARG:HD3	1:D:151:ARG:HA	1.87	0.55
1:E:95:ALA:O	5:H:6219:ALA:HB1	2.05	0.55
1:E:298:ALA:HA	4:A:84:LEU:HA	1.86	0.55
4:A:53:CYS:SG	4:A:95:PHE:HZ	2.29	0.55
1:C:72:MET:HE1	1:C:91:PHE:HB2	1.87	0.55
1:B:277:THR:HG21	1:B:317:GLN:HG2	1.88	0.55
1:C:247:VAL:HG12	1:C:251:ARG:HG3	1.88	0.55
1:C:276:VAL:HG22	1:C:280:SER:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:PRO:HA	1:E:139:ASN:O	2.07	0.55
1:D:213:SER:HB3	1:E:153:ARG:NE	2.22	0.55
1:D:3:THR:HG21	1:D:18:SER:HB2	1.88	0.55
1:B:204:PHE:CA	1:B:207:THR:HG22	2.33	0.55
1:B:110:ASP:OD1	1:C:122:ARG:NH2	2.39	0.55
2:I:25:DG:H1	3:J:6:DC:N4	2.05	0.54
1:E:107:ASP:OD1	1:E:137:THR:HG21	2.07	0.54
5:H:6017:ILE:CG2	5:H:6038:THR:CG2	2.84	0.54
5:F:7202:GLY:C	5:F:7204:GLN:N	2.60	0.54
1:C:188:ALA:HB3	1:C:221:ASP:HA	1.89	0.54
5:F:7028:PHE:CZ	5:F:7030:MSE:HE1	2.26	0.54
5:H:6195:LYS:HD3	5:H:6197:LEU:HD21	1.88	0.54
1:B:192:VAL:HG22	1:B:225:LEU:CD1	2.36	0.54
1:D:303:LEU:HD13	1:E:265:VAL:HG13	1.90	0.54
5:G:5118:ILE:HG13	5:G:5118:ILE:O	2.07	0.54
1:E:217:LYS:O	1:E:217:LYS:HG3	2.06	0.54
5:G:5071:ALA:HB1	5:G:5084:ALA:O	2.06	0.54
1:D:50:PRO:HA	1:D:139:ASN:O	2.07	0.54
4:A:116:GLU:HG2	4:A:116:GLU:O	2.06	0.54
5:F:7134:GLN:O	5:F:7153:ASN:ND2	2.40	0.54
1:D:217:LYS:CE	1:D:224:ILE:HD11	2.37	0.54
5:H:6063:ILE:CG2	5:H:6090:ILE:HG21	2.38	0.54
1:C:77:SER:HB3	1:C:111:ARG:HH11	1.71	0.54
1:B:139:ASN:ND2	1:C:147:PRO:HG3	2.22	0.54
5:F:7121:GLU:O	5:F:7125:GLN:N	2.25	0.54
2:I:8:DT:O4'	4:A:109:GLY:HA3	2.07	0.54
5:G:5118:ILE:HG22	5:G:5169:LEU:HD13	1.89	0.54
1:D:111:ARG:NE	1:E:116:GLU:HG3	2.22	0.54
5:F:7130:SER:CA	5:F:7135:ILE:HB	2.38	0.54
5:G:5210:GLU:HG3	5:G:5215:ASN:ND2	2.22	0.54
5:F:7226:HIS:HB2	5:F:7228:PHE:HD1	1.71	0.54
1:B:272:ILE:HB	1:B:284:MET:HE1	1.88	0.54
5:H:6081:ILE:HG22	5:H:6082:LYS:N	2.23	0.54
5:F:7068:ASN:CB	5:F:7085:ASP:OD1	2.56	0.54
1:D:256:LYS:HG3	1:E:159:GLN:OE1	2.08	0.54
1:C:72:MET:CE	1:C:91:PHE:CG	2.91	0.54
1:E:72:MET:HE1	1:E:91:PHE:HB2	1.89	0.54
1:B:233:GLY:HA3	1:C:159:GLN:CD	2.29	0.54
2:I:27:DC:H2"	2:I:28:DT:H71	1.90	0.54
1:E:303:LEU:CD1	4:A:79:VAL:HG11	2.33	0.54
1:B:122:ARG:HG2	4:A:32:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LEU:O	1:D:125:MET:HG3	2.08	0.54
1:D:188:ALA:HB3	1:D:221:ASP:HA	1.90	0.54
5:F:7122:ASP:CB	5:F:7167:LEU:HD21	2.37	0.53
5:G:5064:LEU:HD23	5:G:5083:ILE:HD13	1.90	0.53
1:B:188:ALA:HB3	1:B:221:ASP:HA	1.89	0.53
5:H:6189:MSE:H	5:H:6189:MSE:SE	2.41	0.53
4:A:151:LEU:N	4:A:152:PRO:HD2	2.22	0.53
5:H:6194:TYR:HA	5:H:6210:GLU:O	2.08	0.53
1:B:88:LEU:HD23	1:B:104:ILE:CD1	2.37	0.53
5:G:5021:ILE:HG12	5:G:5022:MSE:N	2.23	0.53
1:D:256:LYS:HD2	1:E:159:GLN:HE21	1.72	0.53
5:F:7109:PHE:CD1	5:F:7110:PRO:CD	2.79	0.53
5:G:5077:GLU:CG	5:G:5078:ASP:H	2.15	0.53
1:C:88:LEU:CD2	1:C:104:ILE:HG21	2.39	0.53
5:F:7089:THR:CG2	5:F:7091:PHE:HE1	2.22	0.53
1:E:164:ASP:O	1:E:168:MET:HG3	2.09	0.53
5:F:7162:ARG:HH11	5:F:7162:ARG:HG3	1.73	0.53
5:G:5063:ILE:HG12	5:G:5092:TRP:HZ3	1.74	0.53
5:F:7205:GLY:HA3	5:F:7220:LEU:HD12	1.90	0.53
2:I:25:DG:H2"	2:I:26:DT:H71	1.90	0.53
1:D:13:GLN:HE22	1:E:126:GLU:CB	2.22	0.53
1:C:111:ARG:HB2	1:C:114:LEU:HD13	1.90	0.53
4:A:76:MET:N	4:A:77:PRO:HD2	2.23	0.53
5:G:5220:LEU:HD23	5:G:5220:LEU:N	2.24	0.53
1:C:192:VAL:HG22	1:C:225:LEU:CD1	2.38	0.53
1:E:256:LYS:HE2	1:E:257:TYR:CZ	2.43	0.53
5:G:5189:MSE:HB2	5:G:5216:TYR:CE2	2.43	0.53
1:D:227:LEU:HA	1:D:230:ASN:HB3	1.91	0.53
5:F:7123:LEU:O	5:F:7127:LEU:HG	2.09	0.53
1:D:256:LYS:HE2	1:D:257:TYR:CZ	2.44	0.53
5:G:5189:MSE:HE2	5:G:5209:PHE:CG	2.44	0.53
1:B:277:THR:O	1:B:280:SER:HB2	2.08	0.53
5:H:6032:ARG:HB3	5:H:6039:TYR:HD1	1.73	0.53
5:G:5126:LEU:HD13	5:G:5165:TYR:CE2	2.43	0.53
2:I:9:DT:C7	4:A:38:ASN:CB	2.69	0.53
4:A:155:LEU:HD13	4:A:183:LEU:HD13	1.91	0.53
5:H:6071:ALA:O	5:H:6073:ILE:HG13	2.09	0.53
5:H:6072:GLU:HB3	5:H:6084:ALA:HB3	1.89	0.53
1:E:93:SER:CB	5:H:6221:GLU:OE1	2.56	0.53
4:A:46:ALA:O	4:A:99:MET:HE1	2.08	0.53
5:H:6126:LEU:HD12	5:H:6126:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:118:SER:OG	4:A:175:LYS:HE2	2.09	0.53
1:C:8:GLU:OE1	1:C:13:GLN:CB	2.50	0.53
1:D:213:SER:HB3	1:E:153:ARG:HE	1.74	0.53
1:D:276:VAL:HG22	1:D:280:SER:CB	2.39	0.52
5:G:5032:ARG:HB2	5:G:5039:TYR:HB2	1.91	0.52
5:H:6163:VAL:O	5:H:6163:VAL:CG2	2.57	0.52
1:B:145:ILE:HG13	1:B:147:PRO:HD2	1.92	0.52
4:A:4:PHE:CZ	5:F:7032:ARG:HD2	2.44	0.52
2:I:23:DG:N2	3:J:8:DC:O2	2.36	0.52
5:F:7027:GLN:HG3	5:F:7047:VAL:HG12	1.91	0.52
5:F:7064:LEU:HD23	5:F:7083:ILE:HD13	1.91	0.52
5:F:7010:LEU:O	5:F:7014:PHE:HD1	1.92	0.52
5:H:6180:PHE:HB3	5:H:6220:LEU:CD2	2.38	0.52
5:H:6110:PRO:HG3	5:H:6199:TRP:CD2	2.45	0.52
1:B:254:ALA:N	1:B:255:PRO:HD2	2.24	0.52
5:F:7012:LYS:O	5:F:7015:ALA:HB3	2.09	0.52
5:G:5141:THR:OG1	5:G:5142:VAL:N	2.43	0.52
4:A:82:MET:O	4:A:86:GLY:HA3	2.10	0.52
1:B:285:TYR:HE1	4:A:93:ALA:HB1	1.70	0.52
5:G:5055:TYR:HB2	5:G:5095:ALA:HB2	1.92	0.52
1:E:307:TYR:CE2	4:A:80:TYR:CE1	2.97	0.52
1:D:277:THR:O	1:D:280:SER:HB2	2.10	0.52
1:E:12:GLU:OE1	1:E:205:ARG:HG3	2.10	0.52
1:D:231:ASP:CA	1:D:233:GLY:H	2.23	0.52
1:E:276:VAL:HG22	1:E:280:SER:CB	2.40	0.52
1:C:72:MET:CE	5:G:5035:ASN:HB3	2.40	0.52
5:H:6099:THR:O	5:H:6099:THR:HG22	2.09	0.52
5:F:7028:PHE:HE2	5:F:7030:MSE:CE	1.81	0.52
5:G:5128:ARG:CD	5:F:7066:LEU:HD13	2.39	0.52
1:E:72:MET:CE	1:E:91:PHE:CD2	2.93	0.52
1:C:113:GLY:O	2:I:17:DC:H4'	2.09	0.52
4:A:164:ASP:HA	4:A:167:LEU:CD1	2.35	0.52
5:H:6002:LYS:HE2	5:H:6072:GLU:OE1	2.10	0.52
5:F:7076:SER:OG	5:F:7077:GLU:N	2.42	0.52
5:F:7076:SER:HB2	5:F:7082:LYS:HB2	1.91	0.52
5:G:5076:SER:C	5:G:5078:ASP:O	2.48	0.51
1:B:50:PRO:HA	1:B:139:ASN:O	2.10	0.51
1:D:49:SER:HB2	1:D:51:SER:O	2.10	0.51
5:H:6129:VAL:HG21	5:H:6165:TYR:HE2	1.74	0.51
5:H:6149:ILE:HD11	5:H:6169:LEU:HD11	1.92	0.51
1:D:41:LYS:HD2	1:D:101:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6116:THR:HG21	5:H:6147:ILE:HD11	1.90	0.51
5:F:7116:THR:HG23	5:F:7117:GLU:N	2.25	0.51
1:B:304:HIS:HE1	1:C:293:GLN:HG3	1.75	0.51
5:F:7138:ILE:HD12	5:F:7149:ILE:HG21	1.90	0.51
5:H:6034:VAL:HG13	5:H:6101:VAL:HG21	1.91	0.51
1:C:254:ALA:N	1:C:255:PRO:HD2	2.24	0.51
1:E:88:LEU:HD23	1:E:104:ILE:CD1	2.40	0.51
5:H:6149:ILE:HD12	5:H:6167:LEU:HD23	1.93	0.51
5:H:6004:SER:N	5:H:6046:ASP:OD2	2.43	0.51
1:E:17:PRO:HG2	8:E:700:ADP:C2	2.46	0.51
5:F:7027:GLN:HB3	5:F:7044:ILE:O	2.11	0.51
1:E:277:THR:O	1:E:280:SER:HB2	2.10	0.51
1:C:212:ASP:CG	1:D:153:ARG:NH1	2.64	0.51
5:G:5072:GLU:HG3	5:G:5073:ILE:N	2.25	0.51
5:F:7001:MSE:HB3	5:F:7049:ASP:OD2	2.11	0.51
1:B:165:LYS:HG2	1:B:169:MET:HE2	1.93	0.51
1:B:41:LYS:HD2	1:B:101:GLN:OE1	2.11	0.51
5:G:5040:ALA:CB	5:G:5216:TYR:CE1	2.93	0.51
5:F:7189:MSE:HE2	5:F:7209:PHE:CD2	2.46	0.51
1:B:269:ALA:HA	1:B:284:MET:HE2	1.93	0.51
1:E:272:ILE:HB	1:E:284:MET:HE1	1.93	0.51
1:C:94:ALA:O	1:C:102:LYS:HE3	2.10	0.51
4:A:60:TYR:CE2	4:A:95:PHE:HB2	2.46	0.51
1:E:99:GLY:N	5:H:6204:GLN:HB3	2.26	0.51
1:D:276:VAL:HG22	1:D:280:SER:HB2	1.93	0.51
5:H:6157:ASP:OD2	5:H:6161:THR:N	2.44	0.51
1:C:97:PHE:O	5:G:5204:GLN:CB	2.59	0.51
1:E:196:LEU:HD21	1:E:214:TYR:HE2	1.74	0.51
5:H:6055:TYR:HD1	5:H:6099:THR:HG22	1.75	0.51
1:C:283:ARG:O	1:C:287:ILE:HG13	2.11	0.51
5:H:6146:LYS:CA	5:H:6171:ASP:HA	2.31	0.51
1:C:72:MET:CE	1:C:91:PHE:CD2	2.94	0.51
5:H:6066:LEU:HD12	5:H:6067:VAL:H	1.76	0.51
1:D:72:MET:HE3	1:D:91:PHE:CG	2.46	0.51
5:H:6123:LEU:CD2	5:H:6127:LEU:HD11	2.41	0.51
2:I:25:DG:H1	3:J:6:DC:H42	1.58	0.50
2:I:11:DT:H2"	2:I:12:DA:C5'	2.38	0.50
1:B:48:HIS:NE2	1:B:141:ILE:HD11	2.25	0.50
1:D:94:ALA:O	1:D:102:LYS:HE3	2.12	0.50
1:C:121:LEU:O	1:C:125:MET:HG3	2.11	0.50
5:F:7177:THR:O	5:F:7227:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ILE:O	1:E:295:HIS:O	2.29	0.50
1:C:299:ALA:CB	1:D:295:HIS:CD2	2.79	0.50
5:G:5028:PHE:HA	5:G:5042:ALA:O	2.11	0.50
1:D:192:VAL:HG22	1:D:225:LEU:CD1	2.41	0.50
1:B:80:LYS:NZ	2:I:19:DC:P	2.85	0.50
4:A:157:GLU:CG	5:H:6096:ASP:OD2	2.59	0.50
5:H:6033:ALA:C	5:H:6035:ASN:H	2.14	0.50
1:C:212:ASP:HB3	1:D:153:ARG:NH1	2.27	0.50
4:A:4:PHE:CE2	5:F:7032:ARG:HD2	2.47	0.50
1:C:176:LEU:HD22	1:C:211:LEU:HD22	1.92	0.50
5:H:6195:LYS:N	5:H:6210:GLU:O	2.44	0.50
5:F:7089:THR:CG2	5:F:7091:PHE:CE1	2.95	0.50
1:C:3:THR:OG1	1:C:22:GLU:OE1	2.27	0.50
1:B:71:MET:HE2	1:B:73:PHE:HB2	1.92	0.50
1:C:231:ASP:O	1:C:263:TRP:CE2	2.64	0.50
4:A:53:CYS:SG	4:A:54:SER:N	2.84	0.50
4:A:20:LYS:HE2	5:F:7055:TYR:CZ	2.47	0.50
1:B:13:GLN:NE2	1:C:126:GLU:HB3	2.25	0.50
1:C:226:SER:O	1:C:230:ASN:HB3	2.12	0.50
1:E:49:SER:HA	1:E:157:PHE:HB2	1.94	0.50
5:H:6133:LEU:C	5:H:6134:GLN:CG	2.80	0.50
1:C:58:THR:HB	6:C:700:08T:O1A	2.12	0.50
1:B:111:ARG:CZ	1:C:116:GLU:HG3	2.42	0.50
1:D:283:ARG:CZ	1:D:315:GLU:OE1	2.60	0.50
1:E:204:PHE:C	1:E:207:THR:HG22	2.31	0.50
4:A:17:TRP:O	4:A:20:LYS:HG3	2.12	0.50
4:A:161:LEU:O	4:A:161:LEU:HG	2.12	0.50
5:H:6050:PHE:CE2	5:H:6075:GLN:HB3	2.47	0.50
1:B:233:GLY:O	1:B:234:ALA:HB3	2.12	0.49
2:I:27:DC:H2"	2:I:28:DT:C7	2.42	0.49
1:E:2:ILE:CG2	1:E:3:THR:N	2.75	0.49
5:H:6011:LEU:C	5:H:6061:LEU:HD11	2.32	0.49
1:E:8:GLU:HB3	1:E:14:LYS:HB3	1.93	0.49
1:E:8:GLU:HG2	1:E:13:GLN:CB	2.42	0.49
5:H:6123:LEU:HD22	5:H:6191:PRO:HA	1.94	0.49
2:I:15:DT:H2"	2:I:16:DA:C5'	2.35	0.49
4:A:20:LYS:HE2	5:F:7055:TYR:CE1	2.47	0.49
1:C:139:ASN:ND2	1:D:147:PRO:CG	2.75	0.49
1:B:3:THR:HG21	1:B:18:SER:HB2	1.94	0.49
1:C:13:GLN:HG3	1:C:16:ARG:HH21	1.77	0.49
5:H:6052:VAL:HG21	5:H:6081:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:7:DA:H2"	3:J:8:DC:OP2	2.13	0.49
5:F:7130:SER:HA	5:F:7135:ILE:HB	1.93	0.49
1:B:49:SER:OG	1:B:50:PRO:C	2.51	0.49
5:H:6011:LEU:HD22	5:H:6057:LEU:HD11	1.95	0.49
5:G:5189:MSE:HE2	5:G:5209:PHE:CD2	2.48	0.49
1:D:304:HIS:CE1	1:E:293:GLN:HG3	2.47	0.49
5:F:7044:ILE:HG13	5:F:7045:SER:H	1.77	0.49
5:H:6198:LEU:CD2	5:H:6207:ALA:CB	2.89	0.49
5:H:6178:PHE:HD2	5:H:6180:PHE:CD2	2.30	0.49
5:H:6092:TRP:CD1	5:H:6093:PRO:O	2.65	0.49
5:F:7022:MSE:HE3	5:F:7023:LEU:O	2.11	0.49
1:C:48:HIS:HA	1:C:138:ALA:O	2.13	0.49
5:F:7028:PHE:HZ	5:F:7030:MSE:HE2	0.73	0.49
1:C:247:VAL:O	1:C:248:LYS:C	2.50	0.49
1:C:276:VAL:HG22	1:C:280:SER:HB2	1.95	0.49
4:A:130:ARG:CB	4:A:158:LEU:HD11	2.43	0.49
4:A:158:LEU:C	4:A:160:GLY:H	2.15	0.49
1:E:24:ILE:CG2	1:E:168:MET:HG2	2.43	0.49
1:D:254:ALA:N	1:D:255:PRO:HD2	2.28	0.49
1:D:301:THR:OG1	1:E:142:ASP:OD2	2.15	0.49
1:B:139:ASN:ND2	1:C:147:PRO:CG	2.76	0.49
1:C:139:ASN:ND2	1:D:147:PRO:HG3	2.27	0.49
1:B:276:VAL:HG22	1:B:280:SER:CB	2.43	0.49
4:A:161:LEU:HB3	5:H:6055:TYR:CD1	2.48	0.49
5:F:7116:THR:C	5:F:7117:GLU:HG3	2.33	0.49
4:A:167:LEU:CD2	4:A:180:LEU:HD23	2.40	0.49
4:A:55:ILE:HG12	4:A:56:ALA:H	1.76	0.49
1:B:49:SER:N	1:B:56:LYS:HD3	2.28	0.49
5:F:7023:LEU:HD11	5:F:7052:VAL:HG13	1.94	0.49
1:B:217:LYS:CE	1:B:224:ILE:HD11	2.38	0.49
4:A:44:ILE:HD11	4:A:65:VAL:HA	1.94	0.49
1:E:300:ASN:N	4:A:83:ASN:OD1	2.30	0.49
5:F:7068:ASN:HB2	5:F:7085:ASP:OD1	2.12	0.49
5:F:7190:GLN:O	5:F:7194:TYR:OH	2.18	0.49
1:D:88:LEU:HD23	1:D:104:ILE:CD1	2.43	0.49
4:A:68:ALA:O	4:A:71:GLN:CG	2.61	0.49
5:F:7109:PHE:CD2	5:F:7208:LYS:CB	2.96	0.48
1:B:72:MET:HE1	1:B:91:PHE:HB2	1.94	0.48
5:G:5128:ARG:CG	5:F:7066:LEU:CD1	2.64	0.48
5:H:6063:ILE:HG22	5:H:6063:ILE:O	2.13	0.48
1:E:94:ALA:O	1:E:102:LYS:HE3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ALA:HB2	4:A:112:ALA:HB1	1.95	0.48
5:F:7007:THR:O	5:F:7011:LEU:CD1	2.42	0.48
1:B:13:GLN:HE22	1:C:126:GLU:HA	1.78	0.48
1:C:131:ASN:HD21	5:G:5222:ALA:HB2	1.78	0.48
5:F:7044:ILE:HG13	5:F:7045:SER:N	2.28	0.48
1:E:276:VAL:HG23	1:E:317:GLN:O	2.14	0.48
1:B:285:TYR:CD1	4:A:89:LEU:HD21	2.49	0.48
1:C:212:ASP:CB	1:D:153:ARG:CZ	2.88	0.48
5:G:5120:ALA:HB2	5:G:5193:ASN:N	2.29	0.48
1:C:124:PHE:C	1:C:124:PHE:CD1	2.87	0.48
2:I:23:DG:H2''	2:I:24:DT:H71	1.94	0.48
1:C:77:SER:OG	1:C:111:ARG:HD3	2.13	0.48
1:C:235:ILE:CG2	1:C:235:ILE:O	2.61	0.48
2:I:8:DT:H1'	4:A:109:GLY:HA2	1.95	0.48
1:D:231:ASP:O	1:D:232:ARG:CB	2.61	0.48
5:H:6198:LEU:HD23	5:H:6207:ALA:HB2	1.92	0.48
1:E:307:TYR:CE2	4:A:80:TYR:CZ	3.02	0.48
4:A:71:GLN:HB2	4:A:72:PHE:CD1	2.49	0.48
1:E:169:MET:HG2	1:E:197:VAL:CG1	2.44	0.48
5:G:5167:LEU:CD1	5:F:7088:SER:HB3	2.44	0.48
1:E:72:MET:CE	1:E:91:PHE:CG	2.96	0.48
1:B:72:MET:HE3	1:B:91:PHE:CG	2.49	0.48
1:B:283:ARG:O	1:B:287:ILE:HG13	2.14	0.48
1:B:48:HIS:CG	1:B:141:ILE:HD11	2.48	0.48
5:F:7001:MSE:N	5:F:7072:GLU:HG3	2.29	0.48
5:H:6062:GLY:C	5:H:6064:LEU:H	2.17	0.48
5:G:5029:ILE:CG1	5:G:5042:ALA:HB3	2.44	0.48
1:C:131:ASN:OD1	5:G:5222:ALA:HB1	2.14	0.48
1:C:71:MET:CE	1:C:73:PHE:HB2	2.44	0.48
1:E:124:PHE:CD1	1:E:124:PHE:C	2.87	0.48
1:D:235:ILE:HG22	1:D:235:ILE:O	2.13	0.47
1:D:88:LEU:CD2	1:D:104:ILE:HG21	2.44	0.47
5:G:5181:ILE:HB	5:G:5221:GLU:HB2	1.95	0.47
1:E:176:LEU:HD22	1:E:211:LEU:HD22	1.96	0.47
1:D:13:GLN:HE22	1:E:126:GLU:HB3	1.79	0.47
1:E:276:VAL:HG22	1:E:280:SER:HB2	1.95	0.47
5:H:6195:LYS:HB3	5:H:6210:GLU:HB3	1.96	0.47
1:E:98:ASP:C	5:H:6204:GLN:NE2	2.67	0.47
5:G:5223:ASP:N	5:G:5223:ASP:OD1	2.39	0.47
1:D:231:ASP:HB3	1:D:233:GLY:H	1.80	0.47
5:H:6149:ILE:O	5:H:6166:SER:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:5109:PHE:HA	5:G:5110:PRO:HD2	1.69	0.47
4:A:171:THR:HG23	4:A:176:GLU:HB3	1.96	0.47
5:F:7007:THR:CG2	5:F:7044:ILE:HG21	2.44	0.47
5:F:7118:ILE:HG12	5:F:7119:LYS:H	1.77	0.47
4:A:161:LEU:O	4:A:161:LEU:CG	2.62	0.47
5:G:5097:PRO:O	5:G:5099:THR:N	2.48	0.47
1:E:205:ARG:NH2	8:E:700:ADP:PB	2.82	0.47
1:B:122:ARG:CG	4:A:32:PHE:CD2	2.97	0.47
1:B:49:SER:HB2	1:B:51:SER:O	2.14	0.47
1:B:56:LYS:N	6:B:700:08T:O2B	2.47	0.47
1:D:49:SER:N	1:D:56:LYS:HD3	2.29	0.47
5:F:7113:SER:HB3	5:F:7228:PHE:CE2	2.49	0.47
5:H:6156:GLU:OE1	5:H:6164:LYS:NZ	2.47	0.47
5:F:7018:ASN:HB2	5:F:7032:ARG:O	2.14	0.47
1:D:256:LYS:HB2	1:E:159:GLN:HE22	1.76	0.47
5:G:5076:SER:O	5:G:5078:ASP:O	2.32	0.47
4:A:151:LEU:HD22	4:A:151:LEU:HA	1.68	0.47
1:C:116:GLU:OE2	1:C:116:GLU:HA	2.15	0.47
5:H:6054:ILE:HG22	5:H:6056:ASP:C	2.34	0.47
5:F:7118:ILE:CG1	5:F:7119:LYS:H	2.27	0.47
5:G:5125:GLN:O	5:G:5129:VAL:HG23	2.15	0.47
5:H:6202:GLY:O	5:H:6226:HIS:NE2	2.47	0.47
4:A:16:ALA:HB1	4:A:25:VAL:HA	1.97	0.47
5:G:5223:ASP:O	5:G:5225:THR:HG23	2.15	0.47
1:E:41:LYS:HD2	1:E:101:GLN:OE1	2.15	0.47
5:F:7139:ALA:HA	5:F:7180:PHE:O	2.14	0.47
5:G:5018:ASN:HB3	5:G:5031:THR:OG1	2.14	0.47
5:H:6187:MSE:HB3	5:H:6187:MSE:HE3	1.78	0.47
1:B:151:ARG:HG3	1:B:151:ARG:O	2.14	0.47
1:C:72:MET:HE1	1:C:91:PHE:CB	2.45	0.47
4:A:187:TRP:HE3	4:A:187:TRP:C	2.18	0.47
5:G:5068:ASN:HB2	5:G:5070:ASP:OD1	2.15	0.47
2:I:25:DG:N2	3:J:6:DC:N3	2.61	0.47
1:D:80:LYS:CE	1:E:85:ARG:CZ	2.92	0.47
1:C:217:LYS:CE	1:C:224:ILE:HD11	2.42	0.47
1:D:3:THR:OG1	1:D:22:GLU:OE1	2.32	0.47
1:C:11:LEU:O	1:C:11:LEU:HG	2.14	0.47
1:C:41:LYS:HD2	1:C:101:GLN:OE1	2.15	0.47
5:H:6053:ALA:HB3	5:H:6095:ALA:O	2.14	0.47
5:G:5176:ASN:ND2	5:G:5227:ASP:OD1	2.39	0.47
5:G:5128:ARG:HG2	5:F:7066:LEU:HD11	1.86	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:DT:C7	4:A:38:ASN:ND2	2.72	0.46
1:B:108:GLU:HB3	1:C:122:ARG:CZ	2.45	0.46
5:G:5133:LEU:HD11	5:F:7090:ILE:HG23	1.97	0.46
1:E:49:SER:H	1:E:56:LYS:HD3	1.80	0.46
2:I:17:DC:C6	2:I:18:DT:H72	2.50	0.46
4:A:187:TRP:CE3	4:A:187:TRP:C	2.88	0.46
1:D:248:LYS:HG2	1:E:273:TYR:OH	2.15	0.46
1:C:145:ILE:HG13	1:C:147:PRO:HD2	1.98	0.46
5:H:6118:ILE:O	5:H:6118:ILE:HG23	2.14	0.46
1:D:116:GLU:HG2	2:I:16:DA:H4'	1.98	0.46
1:B:80:LYS:NZ	1:C:85:ARG:HH22	2.13	0.46
1:D:83:PHE:HZ	5:H:6155:VAL:CG2	2.28	0.46
5:H:6123:LEU:HD21	5:H:6127:LEU:HD11	1.97	0.46
1:B:72:MET:CE	1:B:91:PHE:CD2	2.98	0.46
4:A:29:ALA:O	4:A:31:SER:N	2.49	0.46
1:B:124:PHE:HB2	4:A:17:TRP:CZ2	2.50	0.46
1:D:71:MET:CE	1:D:73:PHE:HB2	2.46	0.46
1:E:283:ARG:O	1:E:287:ILE:HG13	2.15	0.46
4:A:55:ILE:CD1	4:A:60:TYR:CD2	2.98	0.46
5:H:6067:VAL:HG13	5:H:6085:ASP:HB2	1.97	0.46
1:D:304:HIS:HE1	1:E:293:GLN:HG3	1.79	0.46
5:F:7181:ILE:HB	5:F:7221:GLU:HB2	1.97	0.46
1:E:16:ARG:O	1:E:17:PRO:C	2.52	0.46
1:E:53:GLY:HA3	1:E:203:ASP:OD1	2.15	0.46
1:C:235:ILE:O	1:C:235:ILE:HG22	2.15	0.46
1:B:13:GLN:HG3	1:B:16:ARG:NH1	2.30	0.46
1:C:294:TYR:HB3	1:D:293:GLN:HG2	1.97	0.46
5:G:5011:LEU:HD12	5:G:5011:LEU:N	2.27	0.46
1:B:80:LYS:HZ1	1:C:85:ARG:NH2	2.12	0.46
4:A:50:LYS:HA	4:A:99:MET:CE	2.46	0.46
5:H:6081:ILE:CG2	5:H:6082:LYS:N	2.78	0.46
5:F:7014:PHE:HD2	5:F:7031:THR:HG22	1.81	0.46
3:J:11:DC:H2"	3:J:12:DG:C8	2.50	0.46
1:C:75:ASN:ND2	1:D:123:SER:HB3	2.31	0.46
5:F:7037:THR:CB	5:F:7186:ASN:HD21	2.28	0.46
5:F:7016:THR:O	5:F:7188:LYS:NZ	2.45	0.46
3:J:4:DG:H2"	3:J:5:DA:C8	2.51	0.46
5:H:6008:THR:O	5:H:6011:LEU:HB2	2.16	0.46
4:A:158:LEU:O	4:A:160:GLY:N	2.47	0.46
1:B:72:MET:CE	1:B:91:PHE:CG	2.99	0.46
1:B:293:GLN:NE2	4:A:85:ILE:CA	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:54:SER:O	4:A:55:ILE:CG2	2.61	0.46
1:B:192:VAL:CG2	1:B:225:LEU:CB	2.86	0.46
1:D:176:LEU:HD22	1:D:211:LEU:HD22	1.97	0.46
1:B:11:LEU:HD22	1:B:212:ASP:HB2	1.97	0.46
5:H:6116:THR:O	5:H:6196:LEU:HB3	2.16	0.46
1:D:29:ASP:HA	1:D:32:THR:CG2	2.45	0.46
1:B:269:ALA:HA	1:B:284:MET:HE1	1.97	0.46
5:G:5226:HIS:CE1	5:G:5228:PHE:HB2	2.51	0.46
5:H:6154:LYS:O	5:H:6158:SER:HA	2.16	0.46
1:C:250:LEU:HD13	1:C:309:PHE:HB3	1.98	0.46
1:B:48:HIS:HA	1:B:138:ALA:O	2.16	0.46
5:H:6183:ASN:HB2	5:H:6221:GLU:HG3	1.98	0.46
1:D:122:ARG:HG2	1:D:122:ARG:HH11	1.81	0.46
1:B:88:LEU:CD2	1:B:104:ILE:HG21	2.41	0.46
5:G:5038:THR:HA	5:G:5217:VAL:O	2.16	0.46
5:G:5027:GLN:O	5:G:5043:ASN:HA	2.16	0.46
5:F:7076:SER:HB3	5:F:7080:ASN:O	2.15	0.45
1:B:15:TYR:OH	1:B:183:GLU:OE1	2.27	0.45
1:C:49:SER:OG	1:C:50:PRO:C	2.55	0.45
5:H:6138:ILE:HD12	5:H:6149:ILE:CG2	2.46	0.45
5:H:6055:TYR:CD1	5:H:6099:THR:HG22	2.51	0.45
1:D:283:ARG:NH2	1:D:315:GLU:OE1	2.49	0.45
5:F:7126:LEU:C	5:F:7126:LEU:HD12	2.37	0.45
1:B:305:LEU:HA	1:B:305:LEU:HD12	1.77	0.45
5:F:7036:GLY:O	5:F:7038:THR:N	2.49	0.45
5:H:6054:ILE:HG22	5:H:6056:ASP:N	2.31	0.45
1:D:276:VAL:CG2	1:D:317:GLN:O	2.60	0.45
5:G:5127:LEU:CD2	5:G:5184:MSE:HE1	2.47	0.45
4:A:159:LYS:HD3	4:A:187:TRP:HE1	1.81	0.45
1:E:17:PRO:CG	8:E:700:ADP:C2	2.99	0.45
4:A:55:ILE:CG1	4:A:56:ALA:H	2.28	0.45
1:C:305:LEU:HD12	1:C:305:LEU:HA	1.80	0.45
1:B:57:THR:CG2	1:B:137:THR:HG21	2.33	0.45
1:D:13:GLN:HE22	1:E:126:GLU:HA	1.80	0.45
1:B:111:ARG:NE	1:C:116:GLU:HG3	2.31	0.45
1:E:8:GLU:HB3	1:E:14:LYS:CB	2.46	0.45
1:E:48:HIS:CE1	1:E:141:ILE:HG13	2.52	0.45
1:D:77:SER:OG	1:D:111:ARG:HD3	2.16	0.45
1:D:72:MET:CE	1:D:91:PHE:CG	3.00	0.45
1:C:227:LEU:HA	1:C:230:ASN:CB	2.39	0.45
5:G:5011:LEU:CD1	5:G:5011:LEU:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:VAL:HG22	1:B:280:SER:HB2	1.98	0.45
1:D:235:ILE:CG2	1:D:235:ILE:O	2.64	0.45
5:G:5044:ILE:HD13	5:G:5046:ASP:O	2.16	0.45
5:F:7007:THR:HG23	5:F:7044:ILE:CG1	2.30	0.45
5:H:6196:LEU:HD11	5:H:6198:LEU:HD21	1.99	0.45
1:D:192:VAL:HG22	1:D:225:LEU:CA	2.47	0.45
5:H:6138:ILE:CG1	5:H:6184:MSE:HE3	2.45	0.45
1:D:72:MET:HE1	1:D:91:PHE:HB2	1.98	0.45
1:E:72:MET:HB2	1:E:72:MET:HE2	1.85	0.45
1:C:297:ILE:HD13	1:D:297:ILE:CD1	2.34	0.45
1:B:107:ASP:OD1	1:B:137:THR:HG21	2.17	0.45
5:H:6001:MSE:HE2	5:H:6003:LEU:HG	1.98	0.45
5:G:5092:TRP:CD1	5:G:5092:TRP:C	2.89	0.45
5:H:6032:ARG:NH1	5:H:6036:GLY:HA2	2.31	0.45
1:C:165:LYS:HG2	1:C:169:MET:HE2	1.99	0.45
1:D:215:SER:O	1:D:216:SER:C	2.55	0.45
5:F:7062:GLY:O	5:F:7065:SER:OG	2.26	0.45
1:D:231:ASP:C	1:D:233:GLY:N	2.67	0.45
1:B:49:SER:OG	1:B:50:PRO:CA	2.65	0.45
1:D:204:PHE:C	1:D:207:THR:HG22	2.37	0.45
1:B:48:HIS:CE1	1:B:141:ILE:HG13	2.51	0.45
1:D:48:HIS:HA	1:D:138:ALA:O	2.17	0.45
1:D:72:MET:CE	1:D:91:PHE:CD2	3.00	0.45
1:D:185:ILE:HD13	1:D:215:SER:HB2	1.97	0.45
5:H:6176:ASN:CB	5:H:6228:PHE:CE1	3.00	0.45
5:F:7065:SER:C	5:F:7066:LEU:HD23	2.36	0.44
5:H:6115:VAL:CG1	5:H:6197:LEU:CD2	2.89	0.44
5:F:7167:LEU:HD12	5:F:7168:THR:H	1.82	0.44
5:F:7194:TYR:HA	5:F:7210:GLU:O	2.16	0.44
1:E:48:HIS:HA	1:E:138:ALA:O	2.17	0.44
1:E:72:MET:HE3	1:E:91:PHE:CG	2.52	0.44
5:F:7001:MSE:N	5:F:7072:GLU:CG	2.80	0.44
1:B:50:PRO:HG3	4:A:57:GLN:HG3	1.99	0.44
5:H:6195:LYS:HG2	5:H:6197:LEU:HD21	1.98	0.44
5:G:5110:PRO:O	5:G:5111:VAL:C	2.54	0.44
5:H:6176:ASN:CG	5:H:6228:PHE:CE1	2.91	0.44
1:B:164:ASP:O	1:B:168:MET:HG3	2.16	0.44
4:A:162:VAL:O	4:A:162:VAL:HG12	2.18	0.44
5:G:5107:ILE:HG23	5:G:5108:PRO:HD2	1.98	0.44
1:D:124:PHE:C	1:D:124:PHE:CD1	2.91	0.44
5:G:5050:PHE:CE2	5:G:5075:GLN:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6049:ASP:OD1	5:H:6050:PHE:HD1	2.00	0.44
1:C:75:ASN:CG	1:D:123:SER:HB3	2.38	0.44
3:J:4:DG:H1'	3:J:5:DA:O4'	2.18	0.44
1:D:256:LYS:HE3	1:E:159:GLN:CD	2.38	0.44
5:G:5078:ASP:C	5:G:5080:ASN:H	2.21	0.44
2:I:16:DA:C2	3:J:16:DA:C2	3.06	0.44
1:C:72:MET:HE3	1:C:91:PHE:CG	2.53	0.44
5:H:6066:LEU:HD11	5:H:6090:ILE:CD1	2.47	0.44
5:F:7189:MSE:HA	5:F:7216:TYR:CE2	2.52	0.44
1:E:196:LEU:HD21	1:E:214:TYR:CE2	2.52	0.44
5:G:5067:VAL:HB	5:G:5085:ASP:OD2	2.17	0.44
1:C:29:ASP:HA	1:C:32:THR:HG22	1.99	0.44
4:A:159:LYS:HE2	4:A:187:TRP:CZ2	2.53	0.44
2:I:7:DT:O5'	2:I:7:DT:H6	2.00	0.44
5:F:7068:ASN:H	5:F:7085:ASP:CG	2.21	0.44
6:B:700:08T:O1B	6:B:700:08T:F1	2.26	0.44
1:D:56:LYS:N	6:D:700:08T:O2B	2.51	0.44
1:D:272:ILE:HG21	1:D:284:MET:HE3	2.00	0.44
5:F:7002:LYS:O	5:F:7003:LEU:HD23	2.18	0.44
1:E:185:ILE:HG23	1:E:218:GLY:O	2.17	0.44
1:E:247:VAL:O	1:E:248:LYS:C	2.55	0.44
1:C:57:THR:CG2	1:C:107:ASP:OD1	2.66	0.44
5:H:6011:LEU:CB	5:H:6061:LEU:HD21	2.48	0.44
5:H:6125:GLN:O	5:H:6129:VAL:HG23	2.17	0.44
1:C:235:ILE:HG12	1:C:267:LYS:HG2	2.00	0.44
4:A:106:LYS:HE2	4:A:106:LYS:HB2	1.71	0.44
4:A:174:VAL:O	4:A:174:VAL:CG1	2.66	0.44
5:H:6018:ASN:HD22	5:H:6020:GLY:H	1.66	0.44
4:A:38:ASN:OD1	4:A:40:PHE:CD2	2.71	0.43
4:A:155:LEU:HD13	4:A:183:LEU:CD1	2.48	0.43
5:H:6135:ILE:HD13	5:H:6151:GLY:CA	2.47	0.43
5:G:5063:ILE:HG12	5:G:5092:TRP:CZ3	2.53	0.43
5:G:5220:LEU:HB3	5:G:5224:SER:OG	2.18	0.43
1:C:164:ASP:O	1:C:168:MET:HG3	2.17	0.43
4:A:101:ALA:O	4:A:103:PRO:HD3	2.18	0.43
5:H:6118:ILE:HG22	5:H:6194:TYR:O	2.18	0.43
1:C:141:ILE:O	1:C:143:GLY:N	2.51	0.43
1:D:48:HIS:NE2	1:D:141:ILE:HD11	2.33	0.43
5:G:5097:PRO:O	5:G:5098:SER:C	2.56	0.43
4:A:55:ILE:HG12	4:A:56:ALA:N	2.33	0.43
5:H:6011:LEU:CB	5:H:6061:LEU:HD11	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:HIS:CG	1:D:141:ILE:HD11	2.52	0.43
5:F:7226:HIS:CD2	5:F:7228:PHE:HD1	2.36	0.43
5:H:6163:VAL:O	5:H:6163:VAL:HG22	2.18	0.43
5:F:7182:ILE:HG22	5:F:7183:ASN:O	2.18	0.43
4:A:55:ILE:HD11	4:A:60:TYR:CD2	2.53	0.43
1:B:77:SER:OG	1:B:111:ARG:HD3	2.18	0.43
1:C:212:ASP:CG	1:D:153:ARG:HH12	2.22	0.43
1:D:284:MET:HB2	1:D:284:MET:HE2	1.92	0.43
5:G:5004:SER:N	5:G:5046:ASP:OD2	2.47	0.43
5:G:5090:ILE:HG22	5:G:5091:PHE:N	2.34	0.43
5:G:5185:ALA:O	5:G:5188:LYS:HE3	2.18	0.43
5:G:5138:ILE:HG22	5:G:5151:GLY:HA2	1.99	0.43
1:C:201:PHE:CD1	1:C:201:PHE:O	2.72	0.43
1:E:53:GLY:N	8:E:700:ADP:O2B	2.52	0.43
1:E:204:PHE:O	1:E:207:THR:HG22	2.19	0.43
5:H:6204:GLN:HB3	5:H:6204:GLN:HE21	1.68	0.43
1:B:124:PHE:C	1:B:124:PHE:CD1	2.92	0.43
1:C:29:ASP:HA	1:C:32:THR:CG2	2.47	0.43
5:F:7190:GLN:HG2	5:F:7216:TYR:OH	2.18	0.43
1:E:169:MET:HG2	1:E:197:VAL:HG12	1.99	0.43
5:H:6210:GLU:CG	5:H:6215:ASN:HD21	2.29	0.43
1:C:87:PRO:O	5:G:5035:ASN:ND2	2.52	0.43
1:B:80:LYS:HZ3	1:C:85:ARG:NH2	2.15	0.43
1:D:96:SER:N	1:D:102:LYS:HE2	2.33	0.43
5:H:6033:ALA:O	5:H:6035:ASN:N	2.51	0.43
1:B:93:SER:O	5:F:7096:ASP:HB3	2.19	0.43
1:D:67:VAL:HG12	1:D:67:VAL:O	2.17	0.43
1:D:305:LEU:HA	1:D:305:LEU:HD12	1.84	0.43
1:B:235:ILE:O	1:B:235:ILE:CG2	2.67	0.43
5:F:7007:THR:HG23	5:F:7044:ILE:HG21	2.00	0.43
5:G:5010:LEU:O	5:G:5013:ASN:CB	2.64	0.43
5:H:6210:GLU:HA	5:H:6215:ASN:HD22	1.82	0.43
1:B:125:MET:CE	1:B:151:ARG:HG3	2.48	0.43
1:D:298:ALA:CB	1:E:293:GLN:HA	2.49	0.43
1:E:146:LYS:HB3	1:E:146:LYS:HE3	1.81	0.43
2:I:26:DT:C2'	2:I:27:DC:OP2	2.61	0.43
1:B:57:THR:HG22	1:B:137:THR:CG2	2.34	0.43
5:H:6056:ASP:OD2	5:H:6059:GLY:CA	2.63	0.43
4:A:68:ALA:HA	4:A:111:TRP:CZ2	2.53	0.43
4:A:46:ALA:O	4:A:99:MET:CE	2.67	0.43
5:F:7126:LEU:O	5:F:7126:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:185:LEU:HG	4:A:186:GLU:N	2.34	0.43
5:G:5025:SER:HA	5:G:5048:ILE:HG22	2.01	0.43
3:J:2:DC:C2'	3:J:3:DA:OP2	2.62	0.43
3:J:8:DC:H1'	3:J:9:DT:H5'	2.00	0.43
5:F:7007:THR:CG2	5:F:7044:ILE:HG12	2.30	0.43
5:F:7014:PHE:CD2	5:F:7031:THR:HG22	2.54	0.43
2:I:26:DT:H6	2:I:26:DT:H2'	1.56	0.43
3:J:4:DG:OP2	3:J:4:DG:H8	2.02	0.43
5:F:7121:GLU:HA	5:F:7124:GLN:HB3	2.01	0.43
1:D:48:HIS:CE1	1:D:141:ILE:HG13	2.53	0.43
1:B:29:ASP:HA	1:B:32:THR:CG2	2.49	0.43
1:C:276:VAL:CG2	1:C:280:SER:HB3	2.49	0.43
5:G:5112:ALA:CB	5:G:5197:LEU:HD22	2.48	0.43
1:E:121:LEU:O	1:E:125:MET:HG3	2.19	0.43
1:B:290:GLU:HB2	4:A:85:ILE:CD1	2.49	0.42
1:B:192:VAL:HG22	1:B:225:LEU:CA	2.49	0.42
1:B:48:HIS:ND1	1:B:141:ILE:CG1	2.82	0.42
5:F:7064:LEU:CD2	5:F:7083:ILE:HD13	2.49	0.42
5:H:6067:VAL:HG21	5:H:6083:ILE:HG21	2.00	0.42
5:F:7189:MSE:HB2	5:F:7216:TYR:CD1	2.53	0.42
1:E:235:ILE:HA	1:E:235:ILE:HD13	1.67	0.42
1:D:165:LYS:HG2	1:D:169:MET:HE2	2.01	0.42
5:F:7063:ILE:HA	5:F:7063:ILE:HD13	1.73	0.42
1:C:107:ASP:OD1	1:C:137:THR:HG21	2.19	0.42
5:G:5105:LYS:CB	5:G:5106:PRO:CD	2.82	0.42
1:E:83:PHE:CE2	1:E:88:LEU:CD1	3.03	0.42
5:H:6003:LEU:HD22	5:H:6007:THR:CG2	2.46	0.42
1:D:96:SER:HB3	1:D:102:LYS:HE2	2.01	0.42
4:A:127:LEU:HA	4:A:127:LEU:HD23	1.79	0.42
5:F:7110:PRO:HB2	5:F:7199:TRP:CD1	2.55	0.42
1:E:11:LEU:HD12	1:E:212:ASP:CG	2.40	0.42
4:A:61:SER:CB	4:A:64:MET:HB2	2.38	0.42
1:C:192:VAL:HG22	1:C:225:LEU:CA	2.49	0.42
1:B:86:GLY:HA3	1:B:87:PRO:HD3	1.67	0.42
1:C:276:VAL:HG22	1:C:277:THR:N	2.34	0.42
1:B:176:LEU:CD2	1:B:211:LEU:HD22	2.48	0.42
1:D:247:VAL:O	1:D:248:LYS:C	2.56	0.42
1:E:67:VAL:O	1:E:67:VAL:HG12	2.19	0.42
4:A:173:ASN:O	4:A:176:GLU:N	2.34	0.42
1:D:13:GLN:NE2	1:E:126:GLU:HB3	2.34	0.42
1:C:204:PHE:C	1:C:207:THR:HG22	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ARG:NH1	1:E:251:ARG:O	2.48	0.42
1:E:305:LEU:HA	1:E:305:LEU:HD12	1.72	0.42
4:A:173:ASN:OD1	4:A:175:LYS:HB3	2.20	0.42
1:C:212:ASP:CB	1:D:153:ARG:NH1	2.82	0.42
5:G:5189:MSE:HG2	5:G:5189:MSE:O	2.19	0.42
5:G:5112:ALA:HB2	5:G:5197:LEU:HD22	2.02	0.42
2:I:12:DA:H2'	2:I:12:DA:OP2	2.19	0.42
1:B:125:MET:HE1	1:B:151:ARG:CG	2.48	0.42
5:F:7134:GLN:O	5:F:7153:ASN:CG	2.57	0.42
1:B:204:PHE:C	1:B:207:THR:HG22	2.39	0.42
1:C:49:SER:OG	1:C:50:PRO:CA	2.67	0.42
2:I:21:DT:H2'	2:I:21:DT:O5'	2.20	0.42
1:B:122:ARG:HB3	4:A:32:PHE:CE2	2.54	0.42
1:E:56:LYS:HE2	1:E:56:LYS:HB2	1.85	0.42
5:H:6133:LEU:O	5:H:6133:LEU:HG	2.19	0.42
4:A:82:MET:HE3	4:A:97:TYR:CG	2.55	0.42
4:A:98:LEU:HA	4:A:98:LEU:HD23	1.89	0.42
5:H:6120:ALA:CB	5:H:6192:GLY:C	2.83	0.42
1:C:83:PHE:CE2	1:C:88:LEU:CD1	3.03	0.42
5:F:7189:MSE:HA	5:F:7216:TYR:CZ	2.54	0.42
5:G:5119:LYS:O	5:G:5122:ASP:HB2	2.19	0.42
5:G:5102:ALA:HA	5:G:5103:PRO:HD3	1.81	0.42
1:D:17:PRO:HG2	6:D:700:08T:C2	2.50	0.42
5:H:6198:LEU:CD2	5:H:6207:ALA:HB1	2.49	0.42
1:D:29:ASP:HA	1:D:32:THR:HG22	2.01	0.42
1:B:13:GLN:HG3	1:B:16:ARG:HH11	1.85	0.42
2:I:8:DT:C1'	4:A:109:GLY:HA2	2.50	0.42
5:G:5055:TYR:HB2	5:G:5095:ALA:CB	2.49	0.42
1:D:72:MET:HG3	5:H:6155:VAL:O	2.19	0.42
4:A:8:ILE:O	4:A:9:GLN:C	2.58	0.42
1:C:297:ILE:CG2	1:D:297:ILE:HG13	2.50	0.42
1:D:81:ILE:HG21	2:I:16:DA:H3'	2.01	0.42
1:D:279:GLN:O	1:D:282:ILE:HG22	2.19	0.42
5:G:5126:LEU:HD13	5:G:5165:TYR:HE2	1.83	0.42
4:A:159:LYS:HD3	4:A:187:TRP:NE1	2.34	0.42
1:E:201:PHE:O	1:E:201:PHE:CD1	2.72	0.42
5:F:7021:ILE:HG12	5:F:7022:MSE:N	2.35	0.41
1:D:48:HIS:NE2	1:D:156:THR:HB	2.35	0.41
5:F:7113:SER:HB3	5:F:7228:PHE:CZ	2.55	0.41
1:C:49:SER:HB3	1:C:56:LYS:HZ2	1.85	0.41
1:D:145:ILE:HG13	1:D:147:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ARG:NH1	1:D:287:ILE:CG1	2.83	0.41
1:E:283:ARG:NE	1:E:315:GLU:OE1	2.53	0.41
1:B:297:ILE:HG22	1:C:295:HIS:O	2.20	0.41
4:A:178:LYS:HB3	4:A:178:LYS:HE3	1.83	0.41
4:A:164:ASP:CB	4:A:167:LEU:HD12	2.50	0.41
2:I:27:DC:H2"	2:I:28:DT:C5	2.55	0.41
1:D:111:ARG:CZ	1:E:116:GLU:HG3	2.50	0.41
4:A:147:LYS:O	4:A:147:LYS:CG	2.68	0.41
5:F:7123:LEU:HG	5:F:7127:LEU:HD11	2.01	0.41
5:H:6032:ARG:HH11	5:H:6036:GLY:HA2	1.84	0.41
1:C:215:SER:O	1:C:216:SER:C	2.58	0.41
1:C:146:LYS:HE3	1:C:146:LYS:HB3	1.85	0.41
1:E:85:ARG:O	1:E:89:THR:HB	2.20	0.41
1:C:141:ILE:HG22	1:C:149:GLN:NE2	2.36	0.41
1:C:139:ASN:HD22	1:D:147:PRO:CG	2.33	0.41
4:A:105:GLY:O	4:A:106:LYS:HB2	2.20	0.41
1:E:250:LEU:HD13	1:E:309:PHE:HB3	2.02	0.41
1:B:250:LEU:HD13	1:B:309:PHE:HB3	2.01	0.41
1:B:108:GLU:HG3	1:C:122:ARG:HG3	2.01	0.41
5:H:6023:LEU:CB	5:H:6029:ILE:HG22	2.49	0.41
5:G:5040:ALA:HB2	5:G:5216:TYR:HD1	1.80	0.41
4:A:163:THR:HG23	5:H:6055:TYR:HD2	1.85	0.41
5:H:6153:ASN:HD22	5:H:6164:LYS:NZ	2.18	0.41
4:A:157:GLU:HA	5:H:6096:ASP:HB2	2.03	0.41
5:H:6060:PHE:C	5:H:6062:GLY:H	2.23	0.41
5:H:6018:ASN:HB3	5:H:6020:GLY:O	2.20	0.41
1:E:57:THR:CG2	1:E:107:ASP:OD1	2.68	0.41
5:F:7027:GLN:O	5:F:7043:ASN:HA	2.20	0.41
1:C:48:HIS:CG	1:C:141:ILE:HD11	2.51	0.41
1:D:131:ASN:ND2	5:G:5096:ASP:OD2	2.31	0.41
1:E:235:ILE:O	1:E:235:ILE:CG2	2.69	0.41
1:E:141:ILE:HG23	1:E:141:ILE:HD13	1.70	0.41
1:E:165:LYS:HG2	1:E:169:MET:HE2	2.02	0.41
1:E:283:ARG:CZ	1:E:315:GLU:OE1	2.68	0.41
1:E:251:ARG:HA	1:E:251:ARG:HD2	1.82	0.41
1:C:241:SER:OG	1:C:249:GLN:HG2	2.20	0.41
1:B:67:VAL:CG1	1:B:67:VAL:O	2.69	0.41
5:F:7143:LYS:HE3	5:F:7143:LYS:HB2	1.72	0.41
1:B:29:ASP:HA	1:B:32:THR:HG22	2.01	0.41
1:D:250:LEU:HD13	1:D:309:PHE:HB3	2.02	0.41
4:A:53:CYS:O	4:A:54:SER:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:7024:LYS:HG2	5:F:7051:ASP:OD2	2.19	0.41
1:D:141:ILE:HG23	1:D:141:ILE:HD13	1.77	0.41
1:B:279:GLN:O	1:B:282:ILE:HG22	2.20	0.41
5:H:6155:VAL:HG13	5:H:6156:GLU:H	1.86	0.41
5:G:5130:SER:HA	5:G:5135:ILE:HB	2.02	0.41
5:H:6190:GLN:O	5:H:6191:PRO:O	2.39	0.41
5:F:7123:LEU:HD23	5:F:7191:PRO:HA	2.01	0.41
5:G:5163:VAL:CG1	5:G:5165:TYR:O	2.69	0.41
5:G:5138:ILE:CD1	5:G:5187:MSE:HE2	2.50	0.41
5:H:6105:LYS:HB3	5:H:6107:ILE:CG1	2.50	0.41
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.71	0.41
5:F:7052:VAL:HG21	5:F:7081:ILE:HD11	2.02	0.41
5:H:6027:GLN:HE21	5:H:6047:VAL:HB	1.83	0.41
5:F:7167:LEU:HD12	5:F:7168:THR:N	2.36	0.41
1:C:72:MET:HE2	1:C:72:MET:HB2	1.84	0.41
1:E:71:MET:HG2	1:E:71:MET:O	2.20	0.41
1:D:67:VAL:CG1	1:D:67:VAL:O	2.68	0.41
1:D:34:LYS:HD2	1:D:34:LYS:HA	1.86	0.41
1:C:67:VAL:CG1	1:C:67:VAL:O	2.69	0.41
1:C:67:VAL:HG12	1:C:67:VAL:O	2.20	0.41
1:E:205:ARG:NH2	8:E:700:ADP:O2A	2.54	0.41
1:D:29:ASP:O	1:D:32:THR:HG23	2.20	0.41
5:H:6150:ASN:HA	5:H:6165:TYR:O	2.21	0.41
5:G:5125:GLN:O	5:G:5125:GLN:HG2	2.20	0.41
1:D:272:ILE:CG2	1:D:284:MET:HE3	2.51	0.41
5:H:6108:PRO:O	5:H:6109:PHE:C	2.59	0.41
1:B:254:ALA:HB3	1:B:255:PRO:CD	2.51	0.41
5:H:6033:ALA:C	5:H:6035:ASN:N	2.74	0.41
1:B:67:VAL:HG12	1:B:67:VAL:O	2.21	0.41
1:D:297:ILE:HG21	1:E:297:ILE:CG1	2.49	0.41
1:D:263:TRP:CZ2	1:D:267:LYS:HG3	2.56	0.41
5:H:6195:LYS:HB3	5:H:6210:GLU:CB	2.51	0.41
5:H:6071:ALA:O	5:H:6073:ILE:N	2.54	0.41
1:E:279:GLN:O	1:E:282:ILE:HG22	2.22	0.41
1:B:118:GLN:OE1	1:B:145:ILE:HG23	2.21	0.41
1:C:246:ASP:C	1:C:246:ASP:OD1	2.60	0.41
1:E:4:VAL:HG12	1:E:15:TYR:CE1	2.56	0.41
3:J:8:DC:H2"	3:J:9:DT:H71	2.03	0.40
1:E:96:SER:N	1:E:102:LYS:HE2	2.36	0.40
1:E:112:SER:C	1:E:114:LEU:H	2.24	0.40
1:D:13:GLN:HG3	1:D:16:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:HIS:CE1	1:C:141:ILE:HG13	2.56	0.40
5:H:6208:LYS:CA	5:H:6217:VAL:HG22	2.48	0.40
5:F:7188:LYS:HA	5:F:7188:LYS:HD3	1.95	0.40
1:C:93:SER:HB3	1:C:128:TYR:HE2	1.86	0.40
1:B:292:ASN:ND2	4:A:88:GLY:O	2.54	0.40
1:B:303:LEU:HD21	1:C:288:VAL:HG12	2.03	0.40
1:D:297:ILE:HG23	1:E:297:ILE:HG13	2.03	0.40
3:J:15:DT:H2''	3:J:16:DA:C5'	2.51	0.40
1:B:83:PHE:CD1	1:B:87:PRO:HG2	2.56	0.40
1:B:83:PHE:CE2	1:B:88:LEU:CD1	3.04	0.40
1:C:85:ARG:O	1:C:89:THR:HB	2.22	0.40
5:G:5110:PRO:HB2	5:G:5199:TRP:CD1	2.57	0.40
5:G:5113:SER:OG	5:G:5199:TRP:HA	2.21	0.40
1:B:49:SER:OG	1:B:50:PRO:HA	2.21	0.40
1:C:192:VAL:HG22	1:C:225:LEU:HA	2.03	0.40
1:C:224:ILE:O	1:C:228:VAL:HG23	2.21	0.40
1:E:29:ASP:HA	1:E:32:THR:HG22	2.03	0.40
4:A:163:THR:HG23	5:H:6055:TYR:CD2	2.57	0.40
1:C:96:SER:N	1:C:102:LYS:HE2	2.37	0.40
1:C:169:MET:HG2	1:C:197:VAL:CG1	2.52	0.40
1:E:145:ILE:HG13	1:E:147:PRO:HD2	2.03	0.40
1:E:107:ASP:HA	1:E:137:THR:HB	2.03	0.40
5:H:6198:LEU:CD2	5:H:6207:ALA:HB2	2.50	0.40
1:E:307:TYR:HD2	4:A:80:TYR:CE1	2.36	0.40
1:C:169:MET:HG2	1:C:197:VAL:HG12	2.03	0.40
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.89	0.40
1:D:238:VAL:O	1:D:242:LEU:HG	2.22	0.40
1:B:232:ARG:HD2	1:B:232:ARG:HA	1.93	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:OE1	1:C:248:LYS:NZ[2_655]	1.58	0.62
1:C:183:GLU:CD	1:C:248:LYS:NZ[2_655]	2.14	0.06
1:E:185:ILE:C	5:H:6212:GLU:OE1[2_646]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	317/324 (98%)	304 (96%)	13 (4%)	0	100	100
1	C	318/324 (98%)	305 (96%)	12 (4%)	1 (0%)	46	81
1	D	317/324 (98%)	303 (96%)	14 (4%)	0	100	100
1	E	301/324 (93%)	294 (98%)	7 (2%)	0	100	100
4	A	184/195 (94%)	161 (88%)	20 (11%)	3 (2%)	12	49
5	F	226/228 (99%)	179 (79%)	44 (20%)	3 (1%)	15	53
5	G	226/228 (99%)	183 (81%)	40 (18%)	3 (1%)	15	53
5	H	226/228 (99%)	184 (81%)	35 (16%)	7 (3%)	5	34
All	All	2115/2175 (97%)	1913 (90%)	185 (9%)	17 (1%)	24	64

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	232	ARG
4	A	38	ASN
4	A	150	LYS
5	G	5106	PRO
5	F	7037	THR
5	G	5105	LYS
5	H	6191	PRO
5	F	7110	PRO
4	A	55	ILE
5	H	6034	VAL
5	H	6061	LEU
5	H	6072	GLU
5	G	5098	SER
5	H	6063	ILE
5	F	7002	LYS
5	H	6108	PRO
5	H	6110	PRO



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	277/279 (99%)	254 (92%)	23 (8%)	14	47
1	C	278/279 (100%)	256 (92%)	22 (8%)	15	50
1	D	276/279 (99%)	255 (92%)	21 (8%)	16	52
1	E	266/279 (95%)	245 (92%)	21 (8%)	15	50
4	A	161/170 (95%)	139 (86%)	22 (14%)	4	20
5	F	189/183 (103%)	183 (97%)	6 (3%)	46	80
5	G	189/183 (103%)	182 (96%)	7 (4%)	41	76
5	H	189/183 (103%)	179 (95%)	10 (5%)	28	66
All	All	1825/1835 (100%)	1693 (93%)	132 (7%)	18	55

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	VAL
1	B	20	ILE
1	B	38	SER
1	B	57	THR
1	B	58	THR
1	B	71	MET
1	B	88	LEU
1	B	97	PHE
1	B	98	ASP
1	B	109	PHE
1	B	124	PHE
1	B	132	CYS
1	B	137	THR
1	B	141	ILE
1	B	200	ASN
1	B	246	ASP
1	B	260	ASP
1	B	271	GLU
1	B	272	ILE

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Mol	Chain	Res	Type
1	B	277	THR
1	B	284	MET
1	B	303	LEU
1	B	310	ILE
1	C	4	VAL
1	C	20	ILE
1	C	38	SER
1	C	57	THR
1	C	58	THR
1	C	71	MET
1	C	80	LYS
1	C	88	LEU
1	C	97	PHE
1	C	98	ASP
1	C	109	PHE
1	C	112	SER
1	C	116	GLU
1	C	124	PHE
1	C	129	SER
1	C	132	CYS
1	C	141	ILE
1	C	200	ASN
1	C	272	ILE
1	C	284	MET
1	C	303	LEU
1	C	317	GLN
1	D	4	VAL
1	D	20	ILE
1	D	32	THR
1	D	38	SER
1	D	58	THR
1	D	71	MET
1	D	88	LEU
1	D	97	PHE
1	D	98	ASP
1	D	109	PHE
1	D	112	SER
1	D	124	PHE
1	D	132	CYS
1	D	137	THR
1	D	141	ILE
1	D	200	ASN

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Mol	Chain	Res	Type
1	D	213	SER
1	D	265	VAL
1	D	271	GLU
1	D	272	ILE
1	D	284	MET
1	E	8	GLU
1	E	20	ILE
1	E	38	SER
1	E	57	THR
1	E	58	THR
1	E	88	LEU
1	E	97	PHE
1	E	98	ASP
1	E	109	PHE
1	E	124	PHE
1	E	132	CYS
1	E	137	THR
1	E	141	ILE
1	E	159	GLN
1	E	200	ASN
1	E	213	SER
1	E	271	GLU
1	E	272	ILE
1	E	277	THR
1	E	284	MET
1	E	310	ILE
4	A	8	ILE
4	A	25	VAL
4	A	32	PHE
4	A	40	PHE
4	A	54	SER
4	A	57	GLN
4	A	58	LYS
4	A	59	ASP
4	A	67	ASN
4	A	102	VAL
4	A	104	ARG
4	A	116	GLU
4	A	126	LEU
4	A	134	ASN
4	A	139	ILE
4	A	144	ILE

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Mol	Chain	Res	Type
4	A	147	LYS
4	A	150	LYS
4	A	151	LEU
4	A	153	LEU
4	A	161	LEU
4	A	163	THR
5	G	5051	ASP
5	G	5052	VAL
5	G	5054	ILE
5	G	5067	VAL
5	G	5166	SER
5	G	5187	MSE
5	G	5189	MSE
5	H	6029	ILE
5	H	6107	ILE
5	H	6111	VAL
5	H	6116	THR
5	H	6137	THR
5	H	6163	VAL
5	H	6166	SER
5	H	6189	MSE
5	H	6218	VAL
5	H	6225	THR
5	F	7007	THR
5	F	7038	THR
5	F	7063	ILE
5	F	7109	PHE
5	F	7189	MSE
5	F	7215	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	GLN
1	B	292	ASN
1	C	13	GLN
1	C	139	ASN
1	C	230	ASN
1	C	293	GLN
1	D	13	GLN
1	D	293	GLN
1	D	295	HIS

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Mol	Chain	Res	Type
1	E	159	GLN
1	E	295	HIS
4	A	13	HIS
4	A	179	GLN
5	G	5068	ASN
5	G	5215	ASN
5	H	6018	ASN
5	H	6027	GLN
5	H	6043	ASN
5	H	6153	ASN
5	H	6176	ASN
5	H	6204	GLN
5	H	6215	ASN
5	F	7068	ASN
5	F	7153	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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
6	08T	B	700	7	26,33,33	1.83	9 (34%)	28,52,52	2.82	7 (25%)
6	08T	C	700	7	26,33,33	1.95	10 (38%)	28,52,52	2.33	7 (25%)
6	08T	D	700	7	26,33,33	2.02	11 (42%)	28,52,52	3.07	7 (25%)
8	ADP	E	700	7	22,29,29	1.07	2 (9%)	27,45,45	1.80	7 (25%)

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
6	08T	B	700	7	-	0/12/38/38	0/3/3/3
6	08T	C	700	7	-	0/12/38/38	0/3/3/3
6	08T	D	700	7	-	0/12/38/38	0/3/3/3
8	ADP	E	700	7	-	0/12/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	700	08T	C2'-C3'	-4.30	1.41	1.53
6	C	700	08T	C2'-C3'	-4.19	1.42	1.53
6	B	700	08T	C2'-C3'	-4.04	1.42	1.53
6	D	700	08T	F2-BE	-3.33	1.45	1.54
6	B	700	08T	F2-BE	-3.29	1.45	1.54
6	C	700	08T	F2-BE	-3.26	1.45	1.54
6	D	700	08T	PB-O3A	-3.04	1.54	1.60
6	D	700	08T	O4'-C4'	-2.71	1.38	1.45
6	C	700	08T	O4'-C4'	-2.59	1.39	1.45
6	B	700	08T	O4'-C4'	-2.56	1.39	1.45
6	C	700	08T	PB-O3A	-2.24	1.55	1.60
6	D	700	08T	C3'-C4'	-2.22	1.47	1.53
6	C	700	08T	C3'-C4'	-2.22	1.47	1.53
6	B	700	08T	PB-O3A	-2.21	1.55	1.60
6	D	700	08T	O4'-C1'	-2.01	1.38	1.41
6	B	700	08T	PB-O1B	2.11	1.54	1.48
8	E	700	ADP	O4'-C1'	2.20	1.44	1.41
6	B	700	08T	PA-O2A	2.23	1.54	1.48
6	D	700	08T	PB-O2B	2.27	1.54	1.48
6	C	700	08T	PB-O2B	2.27	1.54	1.48
6	B	700	08T	PB-O2B	2.35	1.54	1.48
6	D	700	08T	PA-O2A	2.41	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	700	08T	C6-N6	2.45	1.42	1.34
6	C	700	08T	PA-O2A	2.47	1.55	1.48
6	C	700	08T	PB-O1B	2.56	1.55	1.48
6	D	700	08T	PA-O1A	2.58	1.54	1.48
6	B	700	08T	PA-O1A	2.61	1.54	1.48
6	C	700	08T	PA-O1A	2.67	1.55	1.48
6	D	700	08T	PB-O1B	2.71	1.55	1.48
6	D	700	08T	C6-N6	3.01	1.44	1.34
6	C	700	08T	C6-N6	3.10	1.44	1.34
8	E	700	ADP	C5-C4	3.21	1.47	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	700	08T	N3-C2-N1	-11.48	120.10	128.89
6	D	700	08T	N3-C2-N1	-10.08	121.18	128.89
6	C	700	08T	N3-C2-N1	-8.84	122.13	128.89
6	D	700	08T	C2'-C1'-N9	-7.74	102.46	114.29
6	D	700	08T	PB-O3A-PA	-6.52	114.84	132.99
6	B	700	08T	C2'-C1'-N9	-4.77	107.00	114.29
8	E	700	ADP	N3-C2-N1	-4.65	125.33	128.89
6	B	700	08T	PB-O3A-PA	-4.38	120.80	132.99
6	D	700	08T	O1A-PA-O2A	-3.96	106.91	118.70
6	C	700	08T	PB-O3A-PA	-3.80	122.40	132.99
6	C	700	08T	C2'-C1'-N9	-3.64	108.73	114.29
6	D	700	08T	O2B-PB-O1B	-3.42	108.50	118.70
8	E	700	ADP	PA-O3A-PB	-3.18	122.02	132.67
8	E	700	ADP	C2'-C1'-N9	-2.96	109.77	114.29
6	B	700	08T	O1A-PA-O2A	-2.95	109.91	118.70
8	E	700	ADP	C4-C5-N7	-2.93	106.79	109.48
6	B	700	08T	C4-C5-N7	-2.80	106.90	109.48
6	C	700	08T	O1A-PA-O3A	-2.50	101.98	108.79
6	C	700	08T	C4-C5-N7	-2.46	107.21	109.48
8	E	700	ADP	O3'-C3'-C4'	-2.39	103.87	111.05
6	D	700	08T	C4-C5-N7	-2.13	107.52	109.48
6	B	700	08T	O2B-PB-O1B	-2.07	112.52	118.70
6	C	700	08T	O1A-PA-O2A	-2.03	112.66	118.70
6	C	700	08T	C1'-N9-C4	2.06	130.05	126.94
6	D	700	08T	O5'-C5'-C4'	2.10	116.86	109.12
6	B	700	08T	O3A-PB-O3B	2.37	110.32	101.31
8	E	700	ADP	O3B-PB-O2B	2.44	116.66	107.38
8	E	700	ADP	C4'-O4'-C1'	2.58	112.55	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	700	08T	3	0
6	C	700	08T	2	0
6	D	700	08T	4	0
8	E	700	ADP	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	319/324 (98%)	-0.14	3 (0%) 85 86	24, 54, 94, 158	0
1	C	320/324 (98%)	-0.26	0 100 100	26, 45, 82, 131	0
1	D	319/324 (98%)	-0.17	4 (1%) 79 80	25, 48, 95, 170	0
1	E	305/324 (94%)	0.10	11 (3%) 46 45	31, 63, 110, 185	0
2	I	24/30 (80%)	0.20	3 (12%) 5 4	35, 66, 216, 261	0
3	J	20/20 (100%)	-0.12	1 (5%) 32 32	54, 92, 235, 258	0
4	A	186/195 (95%)	0.05	8 (4%) 39 37	29, 70, 122, 157	0
5	F	222/228 (97%)	1.04	35 (15%) 3 2	76, 129, 172, 202	0
5	G	222/228 (97%)	0.19	1 (0%) 91 92	54, 80, 121, 136	0
5	H	222/228 (97%)	0.64	20 (9%) 12 11	67, 99, 147, 185	0
All	All	2159/2225 (97%)	0.13	86 (3%) 42 41	24, 66, 146, 261	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	30	DC	6.7
4	A	186	GLU	4.8
1	E	158	GLY	4.7
5	F	7122	ASP	4.3
5	F	7165	TYR	4.1
4	A	37	GLU	4.1
5	F	7123	LEU	4.1
5	F	7151	GLY	3.9
5	F	7152	PHE	3.9
1	B	96	SER	3.9
5	F	7138	ILE	3.8
1	E	110	ASP	3.8
1	E	112	SER	3.7

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Mol	Chain	Res	Type	RSRZ
5	F	7144	GLU	3.7
5	F	7173	ASP	3.7
5	F	7150	ASN	3.7
5	F	7132	GLY	3.5
5	F	7140	ILE	3.4
5	H	6091	PHE	3.3
5	H	6045	SER	3.2
5	F	7177	THR	3.2
4	A	38	ASN	3.1
1	E	214	TYR	3.1
5	F	7171	ASP	3.1
5	H	6063	ILE	3.1
5	H	6058	ASN	3.1
5	H	6086	ALA	3.1
1	E	211	LEU	3.0
5	F	7143	LYS	3.0
5	F	7178	PHE	3.0
5	F	7139	ALA	3.0
5	F	7133	LEU	3.0
5	H	6202	GLY	3.0
4	A	54	SER	2.9
5	F	7149	ILE	2.9
5	H	6083	ILE	2.8
4	A	2	SER	2.8
5	H	6117	GLU	2.7
1	B	131	ASN	2.7
4	A	36	ALA	2.6
1	E	187	ILE	2.6
4	A	185	LEU	2.6
5	F	7068	ASN	2.6
5	F	7029	ILE	2.6
1	E	220	LEU	2.5
1	E	111	ARG	2.5
5	F	7134	GLN	2.5
3	J	1	DG	2.5
1	E	188	ALA	2.4
1	D	230	ASN	2.4
1	D	231	ASP	2.4
5	H	6131	ARG	2.4
5	F	7147	ILE	2.4
5	G	5213	HIS	2.4
5	F	7111	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
5	H	6057	LEU	2.4
5	H	6055	TYR	2.4
5	H	6005	LYS	2.3
1	B	231	ASP	2.3
2	I	29	DG	2.3
5	F	7169	LEU	2.3
2	I	27	DC	2.3
5	H	6084	ALA	2.3
5	F	7223	ASP	2.3
5	H	6147	ILE	2.2
5	F	7116	THR	2.2
5	F	7209	PHE	2.2
5	F	7164	LYS	2.2
1	E	159	GLN	2.2
5	F	7137	THR	2.2
5	H	6116	THR	2.2
4	A	171	THR	2.1
5	F	7175	GLU	2.1
1	D	131	ASN	2.1
5	F	7124	GLN	2.1
5	H	6060	PHE	2.1
5	F	7206	ALA	2.1
5	H	6032	ARG	2.0
1	D	181	LYS	2.0
5	H	6061	LEU	2.0
5	F	7160	LEU	2.0
5	F	7156	GLU	2.0
5	H	6215	ASN	2.0
1	E	219	VAL	2.0
5	F	7148	VAL	2.0
5	H	6023	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	C	800	1/1	0.88	0.42	9.93	47,47,47,47	0
7	MG	D	800	1/1	0.87	0.46	6.05	47,47,47,47	0
7	MG	B	800	1/1	0.98	0.37	5.59	47,47,47,47	0
6	08T	B	700	31/31	0.97	0.20	0.29	47,47,48,48	0
6	08T	C	700	31/31	0.96	0.20	0.23	47,47,48,48	0
6	08T	D	700	31/31	0.95	0.20	0.09	47,47,48,48	0
8	ADP	E	700	27/27	0.95	0.18	-1.08	47,47,48,48	0
7	MG	E	801	1/1	0.82	0.41	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.