



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:17 AM EDT

PDB ID : 3U60 / pdb_00003u60
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

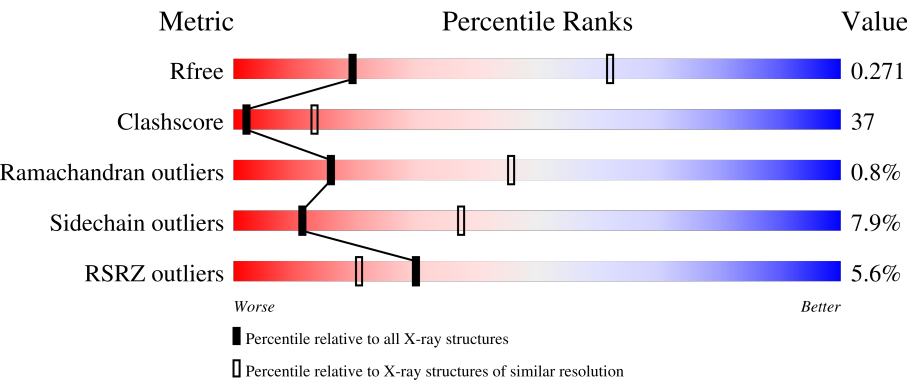
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 _{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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

Mol	Chain	Length	Quality of chain
1	B	324	5% 57% 36% 5%
1	C	324	2% 53% 39% 6%
1	D	324	4% 55% 37% 5%
1	E	324	9% 49% 37% 7% 6%
2	I	30	3% 13% 63% 20%

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Mol	Chain	Length	Quality of chain
3	J	20	35%65%
4	A	195	3% 37%44%12%5%
5	F	228	6% 39%52%9%
5	G	228	5% 39%53%7%
5	H	228	11% 32%58%9%

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			

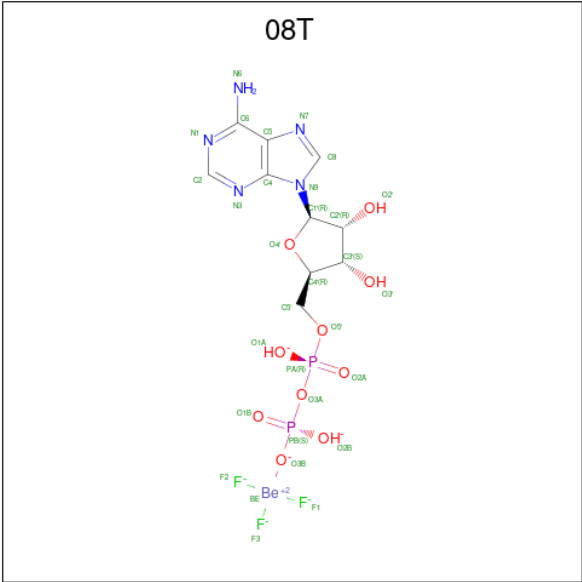
There are 9 discrepancies between the modelled and reference sequences:

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 (CCD ID: 08T) (formula: C₁₀H₁₄BeF₃N₅O₁₀P₂).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

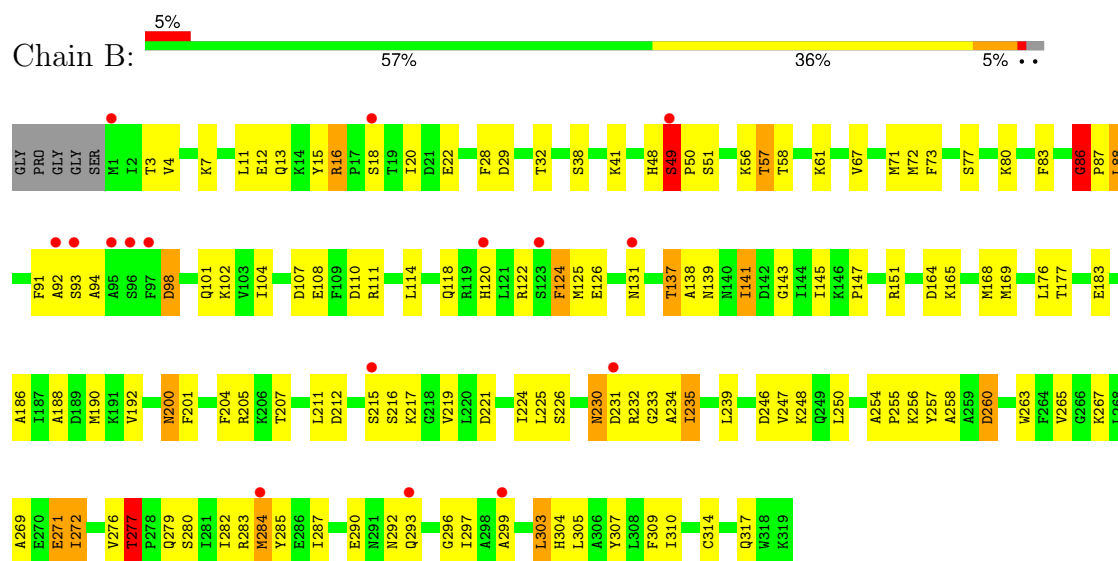


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

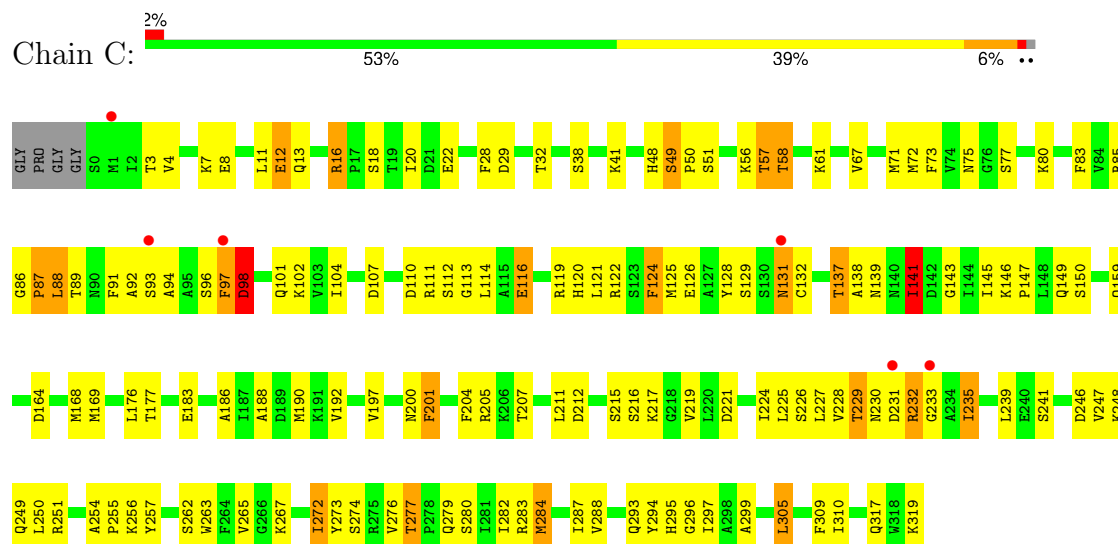
3 Residue-property plots [i](#)

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

• Molecule 1: DNA polymerase accessory protein 44

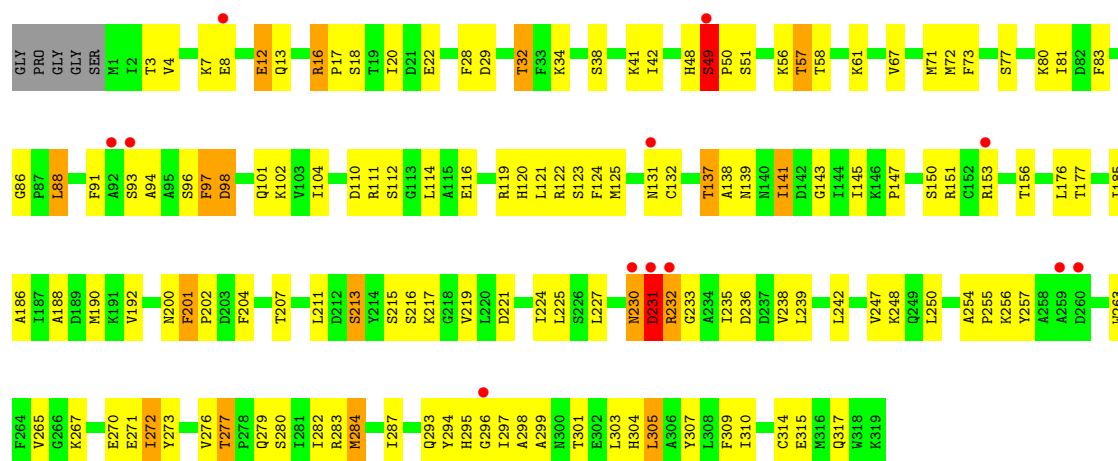


• Molecule 1: DNA polymerase accessory protein 44

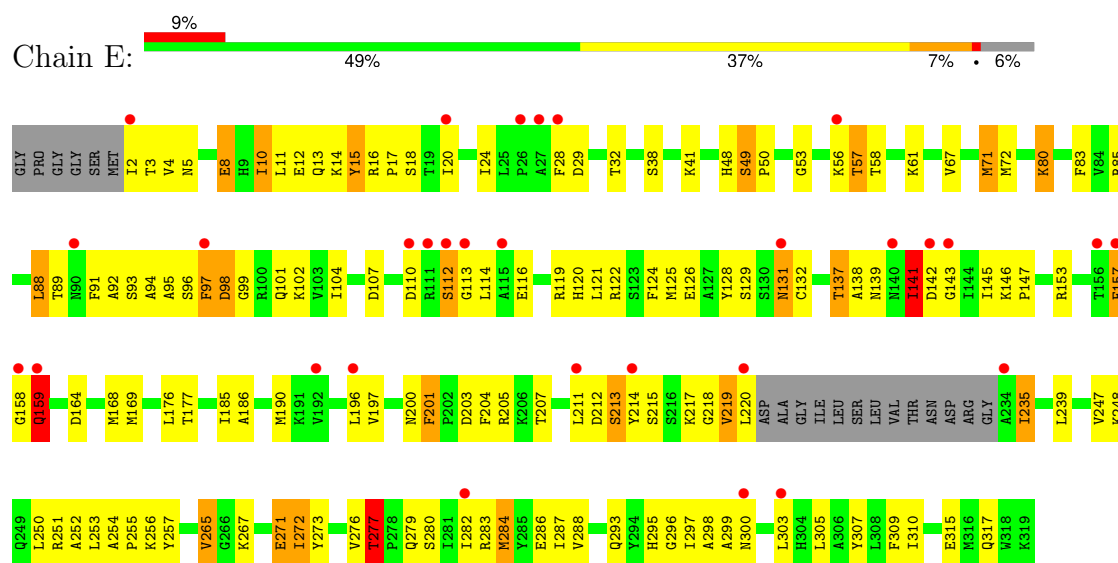


• Molecule 1: DNA polymerase accessory protein 44

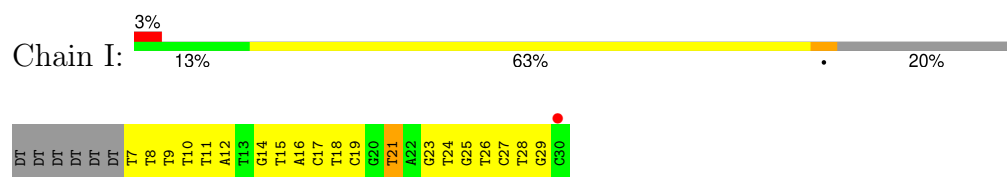




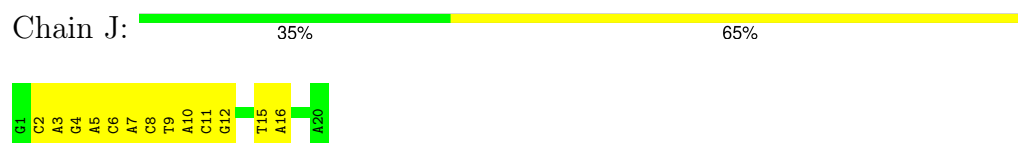
• Molecule 1: DNA polymerase accessory protein 44



• Molecule 2: Template DNA strand

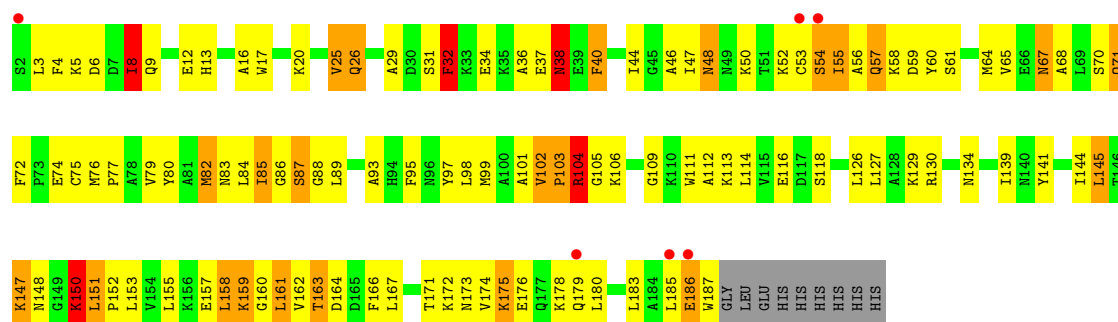


• Molecule 3: Primer DNA strand

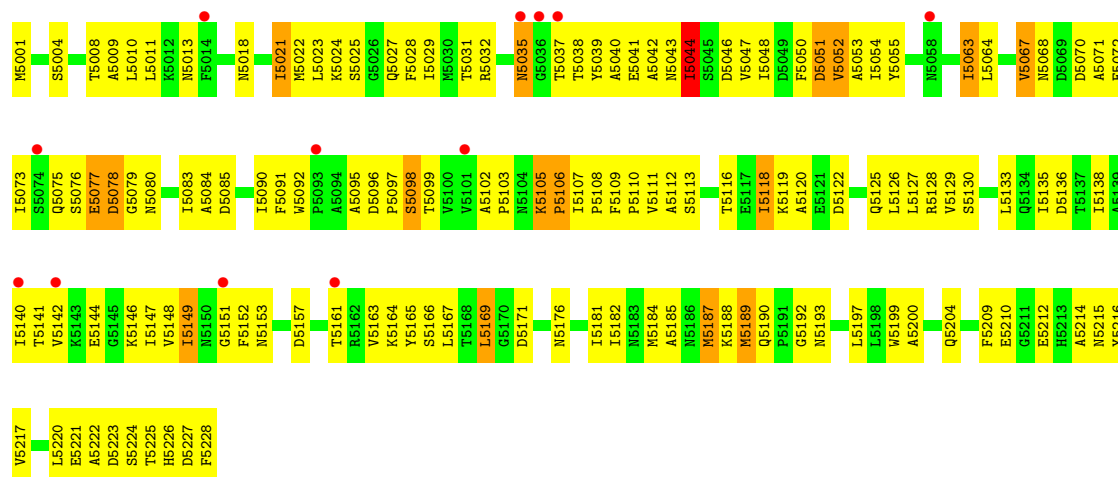


• Molecule 4: DNA polymerase accessory protein 62

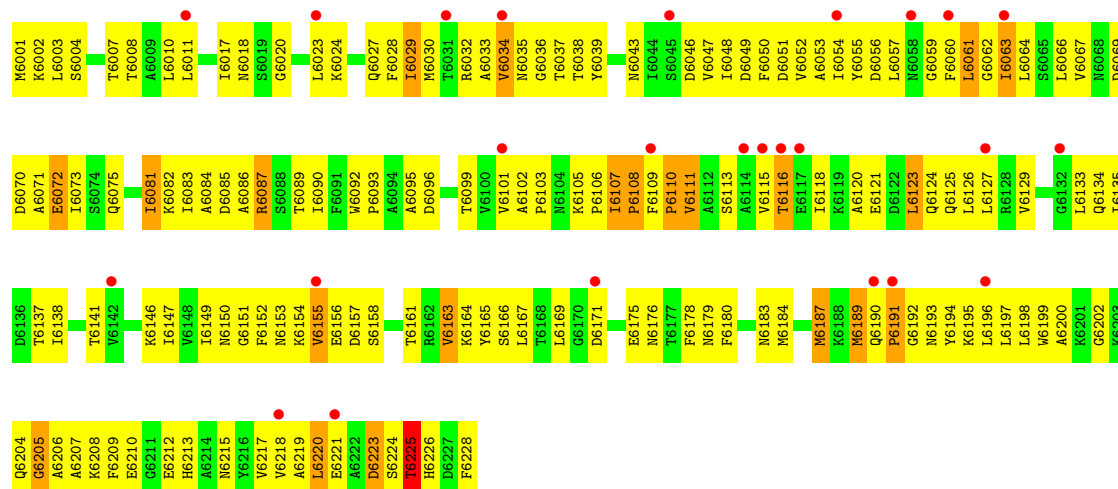




• Molecule 5: DNA polymerase processivity component



• Molecule 5: DNA polymerase processivity component



• Molecule 5: DNA polymerase processivity component



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.52Å 118.44Å 133.08Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	49.71 – 3.34 49.71 – 3.34	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.71-3.34) 93.2 (49.71-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.244 , 0.282 0.237 , 0.271	Depositor DCC
R_{free} test set	1998 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	17695	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	0/2553	1.12	18/3441 (0.5%)
1	C	0.72	1/2559 (0.0%)	1.15	19/3449 (0.6%)
1	D	0.71	0/2547	1.16	18/3434 (0.5%)
1	E	0.72	0/2452	1.16	20/3303 (0.6%)
2	I	0.47	0/544	1.22	3/838 (0.4%)
3	J	0.45	0/459	1.10	0/706
4	A	0.75	2/1516 (0.1%)	1.25	15/2042 (0.7%)
5	F	0.56	0/1774	1.26	21/2395 (0.9%)
5	G	0.54	0/1774	1.15	13/2395 (0.5%)
5	H	0.63	1/1774 (0.1%)	1.13	14/2395 (0.6%)
All	All	0.66	4/17952 (0.0%)	1.17	141/24398 (0.6%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	6	ASP	CA-C	-7.47	1.45	1.53
5	H	6206	ALA	CA-C	5.79	1.59	1.52
1	C	87	PRO	N-CD	5.46	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5	LYS	CA-CB	5.27	1.61	1.53

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	7129	VAL	N-CA-C	18.25	129.53	110.36
1	C	98	ASP	N-CA-C	-12.74	95.38	113.21
5	F	7129	VAL	CB-CA-C	-12.36	96.06	111.88
1	E	112	SER	CB-CA-C	-10.83	92.08	110.81
1	E	158	GLY	N-CA-C	10.76	131.36	115.64
1	B	12	GLU	N-CA-C	-10.53	100.55	113.50
5	F	7175	GLU	N-CA-C	10.52	124.68	107.32
1	D	12	GLU	N-CA-C	-10.37	100.24	113.72
4	A	40	PHE	N-CA-C	-9.95	101.15	113.38
1	D	49	SER	CA-C-N	9.72	131.99	119.84
1	D	49	SER	C-N-CA	9.72	131.99	119.84
5	H	6087	ARG	N-CA-C	9.70	122.74	110.61
1	D	232	ARG	N-CA-C	-9.05	99.07	113.28
1	C	277	THR	CA-C-N	8.88	128.48	119.24
1	C	277	THR	C-N-CA	8.88	128.48	119.24
1	C	12	GLU	N-CA-C	-8.84	102.23	113.72
5	G	5078	ASP	N-CA-C	-8.79	97.12	110.30
5	F	7160	LEU	N-CA-C	8.69	121.07	110.91
1	E	277	THR	CA-C-N	8.45	128.96	119.32
1	E	277	THR	C-N-CA	8.45	128.96	119.32
5	G	5169	LEU	N-CA-C	8.43	124.11	111.04
1	C	235	ILE	N-CA-C	8.41	121.15	112.83
1	E	219	VAL	N-CA-C	8.22	122.11	109.12
5	G	5035	ASN	N-CA-C	8.20	128.26	110.80
1	E	15	TYR	N-CA-C	7.95	123.96	113.30
5	G	5144	GLU	N-CA-C	7.95	122.21	111.24
1	B	277	THR	CA-C-N	7.77	128.18	119.32
1	B	277	THR	C-N-CA	7.77	128.18	119.32
1	E	110	ASP	N-CA-C	7.64	119.69	111.36
4	A	8	ILE	N-CA-C	-7.60	98.67	108.93
1	D	277	THR	CA-C-N	7.57	127.95	119.32
1	D	277	THR	C-N-CA	7.57	127.95	119.32
5	F	7117	GLU	N-CA-CB	-7.42	99.84	111.56
1	B	7	LYS	N-CA-C	-7.40	103.85	113.17
5	F	7027	GLN	N-CA-C	-7.29	104.34	112.57
1	B	230	ASN	CA-C-N	-7.17	113.01	123.05
1	B	230	ASN	C-N-CA	-7.17	113.01	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	ASP	CB-CA-C	-7.07	108.43	116.63
1	C	16	ARG	CA-C-N	7.02	127.42	119.83
1	C	16	ARG	C-N-CA	7.02	127.42	119.83
5	G	5037	THR	N-CA-CB	-7.01	100.44	110.81
1	D	7	LYS	N-CA-C	-6.86	104.94	113.38
5	F	7107	ILE	CA-C-N	6.84	130.52	120.46
5	F	7107	ILE	C-N-CA	6.84	130.52	120.46
5	H	6111	VAL	N-CA-C	-6.76	95.27	109.34
1	D	16	ARG	CA-C-N	6.76	127.13	119.83
1	D	16	ARG	C-N-CA	6.76	127.13	119.83
4	A	103	PRO	N-CA-C	6.76	126.40	112.47
5	H	6081	ILE	N-CA-C	6.66	119.52	109.20
5	G	5044	ILE	N-CA-C	6.63	119.89	108.95
1	E	113	GLY	N-CA-C	-6.62	105.51	113.99
4	A	87	SER	N-CA-C	-6.61	100.38	110.30
5	F	7092	TRP	CA-C-N	6.54	128.02	119.84
5	F	7092	TRP	C-N-CA	6.54	128.02	119.84
5	H	6102	ALA	CA-C-N	6.51	127.98	119.84
5	H	6102	ALA	C-N-CA	6.51	127.98	119.84
5	H	6220	LEU	CB-CA-C	6.44	121.15	109.62
1	B	86	GLY	N-CA-C	6.41	125.41	112.34
4	A	172	LYS	N-CA-C	6.36	121.83	113.30
5	G	5077	GLU	N-CA-C	-6.35	103.49	111.11
1	C	86	GLY	N-CA-C	6.35	125.29	112.34
4	A	159	LYS	N-CA-C	-6.34	104.10	112.34
5	F	7173	ASP	N-CA-C	6.32	118.17	111.28
5	H	6206	ALA	N-CA-C	6.31	117.73	108.14
1	C	7	LYS	N-CA-C	-6.29	105.64	113.38
1	E	49	SER	CA-C-N	6.25	142.01	127.00
1	E	49	SER	C-N-CA	6.25	142.01	127.00
2	I	10	DT	N1-C1'-C2'	6.24	122.86	113.50
1	C	201	PHE	CA-C-N	-6.23	112.42	119.28
1	C	201	PHE	C-N-CA	-6.23	112.42	119.28
1	E	49	SER	N-CA-C	6.15	123.39	109.81
5	G	5189	MSE	N-CA-C	6.10	118.47	108.52
5	F	7135	ILE	CB-CA-C	-6.07	101.43	111.32
5	F	7136	ASP	N-CA-CB	-6.06	104.52	111.79
5	F	7003	LEU	N-CA-C	6.05	119.34	109.24
1	E	141	ILE	CB-CA-C	-6.03	104.00	112.14
1	C	49	SER	CA-C-N	6.02	141.45	127.00
1	C	49	SER	C-N-CA	6.02	141.45	127.00
1	B	86	GLY	CA-C-N	5.99	125.38	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	GLY	C-N-CA	5.99	125.38	118.85
4	A	113	LYS	N-CA-C	-5.98	100.06	109.50
4	A	71	GLN	N-CA-C	5.98	117.48	110.97
5	G	5078	ASP	CB-CA-C	5.93	118.30	110.06
4	A	38	ASN	N-CA-C	5.92	123.42	110.80
1	B	16	ARG	CA-C-N	5.87	126.17	119.83
1	B	16	ARG	C-N-CA	5.87	126.17	119.83
1	B	49	SER	N-CA-C	5.86	122.75	109.81
5	F	7130	SER	N-CA-C	5.84	123.24	110.80
5	F	7133	LEU	CB-CA-C	-5.83	99.98	110.37
1	E	49	SER	C-N-CD	-5.81	107.81	120.60
5	F	7045	SER	N-CA-C	5.81	118.11	111.02
1	D	230	ASN	N-CA-C	5.81	118.88	110.28
5	F	7130	SER	N-CA-CB	-5.80	100.69	110.49
4	A	32	PHE	N-CA-C	5.80	120.05	112.92
4	A	85	ILE	N-CA-C	5.80	119.21	111.44
1	B	201	PHE	CA-C-N	-5.79	112.91	119.28
1	B	201	PHE	C-N-CA	-5.79	112.91	119.28
5	H	6205	GLY	N-CA-C	5.77	119.17	110.75
5	H	6069	ASP	N-CA-C	5.75	120.41	113.17
1	B	201	PHE	N-CA-C	5.74	122.50	109.81
1	B	258	ALA	N-CA-C	-5.72	105.56	112.54
5	H	6223	ASP	N-CA-C	5.72	120.25	113.16
2	I	10	DT	C2'-C3'-O3'	5.71	120.06	111.50
5	H	6225	THR	N-CA-C	5.67	117.88	108.13
1	D	49	SER	N-CA-C	5.66	122.32	109.81
1	C	49	SER	N-CA-C	5.65	122.30	109.81
2	I	21	DT	O4'-C1'-N1	5.65	116.88	108.40
1	E	159	GLN	CA-C-N	5.63	125.56	119.76
1	E	159	GLN	C-N-CA	5.63	125.56	119.76
5	G	5047	VAL	N-CA-C	5.61	115.95	107.75
1	D	201	PHE	CA-C-N	-5.61	113.11	119.28
1	D	201	PHE	C-N-CA	-5.61	113.11	119.28
1	D	42	ILE	N-CA-C	5.60	114.11	107.73
5	G	5052	VAL	N-CA-C	5.60	115.22	108.06
1	C	201	PHE	N-CA-CB	5.56	116.98	110.42
5	H	6123	LEU	N-CA-C	-5.55	105.14	111.14
1	D	86	GLY	N-CA-C	5.54	123.65	112.34
1	E	157	PHE	N-CA-C	5.50	117.62	110.53
1	D	231	ASP	N-CA-C	5.48	117.34	108.08
1	E	201	PHE	CA-C-N	-5.45	113.29	119.28
1	E	201	PHE	C-N-CA	-5.45	113.29	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	48	ASN	N-CA-C	5.39	117.02	111.03
5	H	6106	PRO	N-CA-C	-5.35	105.25	112.48
5	F	7081	ILE	N-CA-C	5.33	115.45	107.51
1	C	229	THR	N-CA-C	-5.32	106.77	113.20
1	D	236	ASP	N-CA-C	5.30	117.47	111.11
5	H	6155	VAL	N-CA-C	5.28	115.39	110.42
1	C	131	ASN	CB-CA-C	-5.28	102.77	110.95
4	A	104	ARG	N-CA-C	-5.27	101.69	109.86
5	F	7175	GLU	CB-CA-C	-5.27	104.80	111.70
1	C	49	SER	C-N-CD	-5.23	109.09	120.60
1	B	231	ASP	N-CA-C	5.18	116.97	108.52
5	G	5161	THR	N-CA-C	5.18	117.01	111.36
4	A	82	MET	N-CA-C	-5.17	106.94	113.20
1	E	131	ASN	CB-CA-C	-5.17	102.94	110.95
5	F	7171	ASP	N-CA-C	5.15	116.58	110.19
4	A	175	LYS	N-CA-C	-5.13	105.19	111.75
1	B	200	ASN	N-CA-C	5.08	119.63	112.72
1	E	129	SER	N-CA-C	-5.05	106.96	113.23
1	C	141	ILE	N-CA-C	5.02	115.74	110.62
5	G	5212	GLU	N-CA-C	-5.02	107.29	113.41

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
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	174	0
1	C	2515	0	2543	200	2
1	D	2503	0	2527	207	0
1	E	2409	0	2433	195	1
2	I	489	0	277	45	0
3	J	408	0	225	26	0
4	A	1488	0	1509	171	0
5	F	1750	0	1752	180	0
5	G	1750	0	1752	151	0
5	H	1750	0	1752	197	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	1305	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 37.

All (1305) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:205:ARG:NH2	8:E:700:ADP:O3B	1.85	1.10
5:F:7109:PHE:HD1	5:F:7110:PRO:HD2	1.11	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:CG	1.82	1.02
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:77:SER:HB2	1:E:120:HIS:ND1	1.76	1.00
1:D:256:LYS:HG3	1:E:159:GLN:HE22	1.22	1.00
1:D:232:ARG:CB	1:D:263:TRP:CZ2	2.45	0.99
5:G:5128:ARG:HG2	5:F:7066:LEU:HD13	1.01	0.99
5:F:7007:THR:HG23	5:F:7044:ILE:HG12	1.41	0.99
5:F:7109:PHE:CD1	5:F:7110:PRO:HD2	1.97	0.99
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:CD1	1:C:97:PHE:N	2.30	0.96
5:H:6038:THR:HG23	5:H:6038:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:125:MET:HE2	1:B:151:ARG:HG2	1.49	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:226:SER:O	1:C:230:ASN:HA	1.68	0.92
1:C:231:ASP:O	1:C:233:GLY:N	2.02	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
4:A:148:ASN:O	4:A:150:LYS:N	2.03	0.90
5:H:6037:THR:HG23	5:H:6038:THR:HB	1.52	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
1:B:285:TYR:CE1	4:A:93:ALA:HB1	2.08	0.89
5:G:5210:GLU:HA	5:G:5215:ASN:ND2	1.86	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
4:A:148:ASN:C	4:A:150:LYS:H	1.76	0.88
1:D:192:VAL:CG2	1:D:225:LEU:HB2	2.04	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:97:PHE:N	1:C:97:PHE:HD1	1.70	0.84
2:I:9:DT:H72	4:A:38:ASN:ND2	1.91	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
1:D:256:LYS:HG3	1:E:159:GLN:CD	2.03	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
1:D:204:PHE:HA	1:D:207:THR:HG22	1.59	0.83
2:I:28:DT:N3	3:J:3:DA:N6	2.11	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:HD12	5:F:7023:LEU:O	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
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
5:H:6120:ALA:HB2	5:H:6192:GLY:C	2.05	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:232:ARG:CB	1:D:263:TRP:CH2	2.64	0.80
1:D:297:ILE:HD13	1:E:297:ILE:CD1	2.07	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:7085:ASP:CG	5:F:7086:ALA:H	1.88	0.80
4:A:46:ALA:O	4:A:99:MET:HE1	1.81	0.79
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:B:204:PHE:HA	1:B:207:THR:HG22	1.65	0.79
1:B:307:TYR:HE2	1:C:293:GLN:NE2	1.80	0.79
1:B:272:ILE:HB	1:B:284:MET:HE1	1.66	0.78
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:D:217:LYS:HE2	1:D:224:ILE:HD11	1.63	0.78
1:E:57:THR:HG23	8:E:700:ADP:O1B	1.84	0.78
5:H:6027:GLN:O	5:H:6043:ASN:OD1	2.00	0.78
1:B:48:HIS:CD2	1:B:141:ILE:HD11	2.18	0.78
1:C:217:LYS:HE2	1:C:224:ILE:HD11	1.66	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: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:7122:ASP:HB3	5:F:7167:LEU:HD21	1.67	0.77
1:C:71:MET:HE2	1:C:73:PHE:HB2	1.66	0.77
1:C:77:SER:HB2	1:D:120:HIS:ND1	1.99	0.77
5:G:5001:MSE:N	5:G:5072:GLU:OE2	2.18	0.77
5:G:5140:ILE:HG13	5:G:5148:VAL:O	1.84	0.77
5:F:7118:ILE:HG12	5:F:7119:LYS:N	1.98	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
5:H:6054:ILE:HG21	5:H:6056:ASP:O	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:150:LYS:C	4:A:152:PRO:HD2	2.11	0.76
1:E:307:TYR:CD2	4:A:80:TYR:CD1	2.74	0.75
2:I:26:DT:H2"	2:I:27:DC:OP2	1.86	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
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:B:217:LYS:HE2	1:B:224:ILE:HD11	1.66	0.74
1:D:97:PHE:CD1	1:D:97:PHE:N	2.55	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
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:H:6003:LEU:HD22	5:H:6007:THR:HG21	1.70	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:B:125:MET:HE2	1:B:151:ARG:CG	2.17	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:C:235:ILE:HG22	1:C:239:LEU:HG	1.70	0.73
1:D:119:ARG:HB3	1:D:122:ARG:NH1	2.02	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
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
1:C:231:ASP:O	1:C:232:ARG:C	2.32	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
1:C:119:ARG:O	1:C:122:ARG:HG2	1.89	0.72
4:A:82:MET:HE3	4:A:97:TYR:CD2	2.24	0.72
5:F:7133:LEU:O	5:F:7134:GLN:HB2	1.88	0.72
1:C:88:LEU:HD21	1:C:104:ILE:HG21	1.71	0.72
5:F:7202:GLY:C	5:F:7204:GLN:H	1.97	0.72
1:B:260:ASP:OD1	1:B:263:TRP:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:TYR:CE1	1:E:286:GLU:HA	2.24	0.72
1:E:93:SER:O	5:H:6221:GLU:OE1	2.06	0.72
1:B:299:ALA:HB1	1:C:262:SER:HB3	1.72	0.72
1:B:307:TYR:CE2	1:C:293:GLN:NE2	2.58	0.72
4:A:53:CYS:SG	4:A:95:PHE:CZ	2.83	0.72
5:G:5011:LEU:H	5:G:5011:LEU:HD12	1.55	0.72
5:G:5040:ALA:HB2	5:G:5216:TYR:CD1	2.25	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
1:E:93:SER:C	5:H:6221:GLU:OE1	2.34	0.71
2:I:29:DG:N2	3:J:3:DA:C2	2.59	0.71
1:C:49:SER:CB	1:C:51:SER:O	2.39	0.71
1:C:233:GLY:CA	1:C:263:TRP:CZ2	2.73	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
1:C:91:PHE:HD2	5:G:5035:ASN:O	1.73	0.70
4:A:82:MET:HE3	4:A:97:TYR:CG	2.25	0.70
5:G:5077:GLU:HG2	5:G:5078:ASP:N	2.03	0.70
1:B:71:MET:HE2	1:B:73:PHE:HB2	1.73	0.70
1:D:71:MET:HE2	1:D:73:PHE:HB2	1.73	0.70
1:B:98:ASP:OD1	1:B:98:ASP:N	2.21	0.70
5:F:7033:ALA:HB2	5:F:7038:THR:CG2	2.21	0.70
1:B:277:THR:HG22	1:B:317:GLN:O	1.92	0.70
4:A:145:LEU:HB3	4:A:151:LEU:CD2	2.21	0.70
5:F:7109:PHE:CD2	5:F:7208:LYS:HB3	2.27	0.70
5:F:7148:VAL:HG12	5:F:7168:THR:HA	1.73	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:O	4:A:34:GLU:HG2	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:95:ALA:HB3	5:H:6220:LEU:O	1.93	0.69
1:E:212:ASP:O	1:E:215:SER:CB	2.41	0.69
1:B:120:HIS:CE1	4:A:17:TRP:CH2	2.81	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:E:307:TYR:CD2	4:A:80:TYR:CE1	2.80	0.69
1:B:28:PHE:O	1:B:32:THR:HG22	1.93	0.69
1:B:204:PHE:HA	1:B:207:THR:CG2	2.21	0.69
5:G:5064:LEU:CD2	5:G:5083:ILE:HD13	2.22	0.69
1:B:267:LYS:HE2	1:B:271:GLU:CD	2.15	0.69
1:C:28:PHE:O	1:C:32:THR:HG22	1.93	0.69
1:C:116:GLU:OE2	1:C:119:ARG:NH1	2.26	0.69
1:D:192:VAL:HG22	1:D:225:LEU:CB	2.21	0.69
1:D:299:ALA:CB	1:E:295:HIS:CD2	2.53	0.69
1:B:80:LYS:NZ	1:C:85:ARG:NH2	2.41	0.68
5:G:5210:GLU:HG3	5:G:5215:ASN:HD21	1.58	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
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:700:08T:O1B	1.92	0.68
1:B:83:PHE:O	1:B:87:PRO:HD2	1.93	0.68
1:D:49:SER:HB3	1:D:56:LYS:NZ	2.09	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:B:314:CYS:SG	1:C:282:ILE:HD11	2.34	0.67
1:E:98:ASP:OD1	1:E:98:ASP:N	2.27	0.67
1:E:235:ILE:HG22	1:E:239:LEU:HG	1.76	0.67
5:H:6135:ILE:HG23	5:H:6152:PHE:O	1.93	0.67
5:G:5050:PHE:CD2	5:G:5075:GLN:HB2	2.28	0.67
5:H:6011:LEU:O	5:H:6057:LEU:HD21	1.95	0.67
4:A:167:LEU:HD11	4:A:180:LEU:HD21	0.75	0.67
5:F:7039:TYR:OH	5:F:7041:GLU:OE1	2.07	0.67
5:F:7146:LYS:HA	5:F:7171:ASP:HA	1.77	0.67
1:C:227:LEU:C	1:C:230:ASN:HB3	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ASP:C	1:D:233:GLY:H	2.02	0.67
3:J:4:DG:H2''	3:J:5:DA:OP2	1.95	0.67
3:J:15:DT:H2''	3:J:16:DA:O5'	1.95	0.67
5:H:6210:GLU:HG3	5:H:6215:ASN:HD21	1.60	0.67
5:H:6001:MSE:HG2	5:H:6073:ILE:O	1.94	0.66
5:F:7152:PHE:CD2	5:F:7160:LEU:HD22	2.31	0.66
1:C:231:ASP:C	1:C:233:GLY:N	2.53	0.66
1:E:61:LYS:HG2	1:E:71:MET:HE1	1.76	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: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:C:192:VAL:HG22	1:C:225:LEU:HB2	1.76	0.66
1:E:24:ILE:HG22	1:E:168:MET:HE3	1.77	0.66
1:E:303:LEU:HD21	4:A:79:VAL:HG12	1.77	0.66
4:A:37:GLU:O	4:A:38:ASN:CB	2.33	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:C:49:SER:N	1:C:56:LYS:HD3	2.12	0.65
1:E:119:ARG:O	1:E:122:ARG:HG2	1.96	0.65
2:I:9:DT:C7	4:A:38:ASN:CG	2.65	0.65
5:F:7226:HIS:HB2	5:F:7228:PHE:CE1	2.32	0.65
1:B:269:ALA:HA	1:B:284:MET:HE2	1.79	0.65
4:A:102:VAL:O	4:A:102:VAL:HG22	1.97	0.65
5:H:6024:LYS:HB3	5:H:6051:ASP:OD1	1.97	0.65
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:G:5128:ARG:CD	5:F:7066:LEU:HD22	2.26	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
5:F:7068:ASN:CG	5:F:7085:ASP:OD1	2.40	0.64
1:C:192:VAL:HG22	1:C:225:LEU:CB	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:SER:HB3	1:D:111:ARG:HH11	1.61	0.64
4:A:167:LEU:HD13	4:A:180:LEU:HD21	1.71	0.64
5:F:7050:PHE:CD2	5:F:7075:GLN:HB2	2.32	0.64
1:C:279:GLN:N	1:C:279:GLN:OE1	2.29	0.64
1:D:297:ILE:HG21	1:E:297:ILE:HG13	1.80	0.64
1:B:269:ALA:HA	1:B:284:MET:CE	2.28	0.64
1:C:88:LEU:HD23	1:C:104:ILE:HD13	1.78	0.64
1:E:95:ALA:CB	5:H:6220:LEU:O	2.45	0.64
5:G:5024:LYS:HG2	5:G:5051:ASP:CB	2.27	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:C:251:ARG:HH22	1:D:270:GLU:CA	1.97	0.64
1:B:192:VAL:HG22	1:B:225:LEU:HB2	1.80	0.64
1:D:235:ILE:HG22	1:D:239:LEU:HG	1.80	0.64
1:D:314:CYS:SG	1:E:282:ILE:HD11	2.38	0.64
1:E:303:LEU:CD2	4:A:79:VAL:HG12	2.28	0.64
3:J:3:DA:H1'	3:J:4:DG:H5'	1.79	0.64
1:B:125:MET:CE	1:B:151:ARG:HG2	2.25	0.64
1:C:231:ASP:O	1:C:263:TRP:CZ2	2.51	0.64
1:D:97:PHE:N	1:D:97:PHE:HD1	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:700:08T:O2A	2.31	0.63
5:H:6059:GLY:C	5:H:6092:TRP:CH2	2.76	0.63
1:B:234:ALA:O	1:B:235:ILE:HD13	1.97	0.63
1:C:274:SER:O	1:C:319:LYS:HE2	1.99	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:E:80:LYS:HB3	2:I:14:DG:OP1	1.99	0.63
1:D:204:PHE:CA	1:D:207:THR:HG22	2.28	0.63
5:G:5120:ALA:HB2	5:G:5192:GLY:C	2.23	0.63
5:G:5122:ASP:HB3	5:G:5167:LEU:HD21	1.81	0.63
5:H:6023:LEU:HD13	5:H:6048:ILE:HG21	1.80	0.63
1:B:77:SER:HB3	1:B:111:ARG:HH11	1.64	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
5:H:6002:LYS:HG2	5:H:6070:ASP:O	1.99	0.63
1:D:88:LEU:HD21	1:D:104:ILE:HG21	1.80	0.63
1:E:10:ILE:HG12	4:A:145:LEU:HD11	1.79	0.63
4:A:158:LEU:C	4:A:160:GLY:N	2.53	0.63
5:H:6063:ILE:HG21	5:H:6090:ILE:HG21	1.81	0.63
4:A:72:PHE:HB3	4:A:74:GLU:OE1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:F:7034:VAL:HG13	5:F:7101:VAL:HG21	1.81	0.62
5:F:7134:GLN:HB3	5:F:7153:ASN:HD21	1.62	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
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
1:C:230:ASN:OD1	1:C:230:ASN:O	2.18	0.62
5:F:7109:PHE:HD2	5:F:7208:LYS:HD3	1.63	0.62
1:C:177:THR:OG1	1:C:190:MET:HE1	1.99	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:277:THR:O	1:C:280:SER:HB2	2.00	0.61
1:E:177:THR:OG1	1:E:190:MET:HE1	2.00	0.61
3:J:3:DA:H2"	3:J:4:DG:OP2	2.01	0.61
5:G:5146:LYS:HA	5:G:5171:ASP:HA	1.82	0.61
5:H:6027:GLN:NE2	5:H:6047:VAL:HB	2.15	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:D:307:TYR:HE1	1:E:286:GLU:HA	1.65	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
5:F:7136:ASP:O	5:F:7137:THR:OG1	2.16	0.61
1:B:111:ARG:HE	1:C:116:GLU:CD	2.08	0.61
1:B:277:THR:CG2	1:B:317:GLN:O	2.48	0.61
5:F:7085:ASP:CG	5:F:7086:ALA:N	2.57	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:H:6133:LEU:C	5:H:6134:GLN:HG2	2.26	0.61
2:I:8:DT:O2	4:A:109:GLY:HA2	2.01	0.61
5:G:5129:VAL:CG1	5:G:5133:LEU:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:277:THR:HG21	1:E:317:GLN:HB2	1.81	0.60
4:A:164:ASP:CA	4:A:167:LEU:HD12	2.30	0.60
5:H:6023:LEU:HB3	5:H:6029:ILE:HG22	1.84	0.60
5:H:6210:GLU:HA	5:H:6215:ASN:ND2	2.16	0.60
1:B:272:ILE:HB	1:B:284:MET:CE	2.32	0.60
5:G:5064:LEU:HD21	5:G:5083:ILE:HD13	1.82	0.60
5:G:5200:ALA:HB1	5:G:5226:HIS:NE2	2.16	0.60
5:F:7118:ILE:CG1	5:F:7119:LYS:N	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: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
4:A:148:ASN:C	4:A:150:LYS:N	2.46	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
1:E:72:MET:HE1	1:E:91:PHE:HB2	1.84	0.59
1:E:49:SER:N	1:E:56:LYS:HD3	2.17	0.59
5:F:7133:LEU:O	5:F:7134:GLN:CB	2.50	0.59
5:F:7022:MSE:HB3	5:F:7102:ALA:HB2	1.84	0.59
5:H:6199:TRP:CD1	5:H:6200:ALA:N	2.71	0.59
1:D:94:ALA:HA	5:G:5095:ALA:HA	1.83	0.59
5:F:7041:GLU:O	5:F:7214:ALA:HB1	2.02	0.59
5:F:7130:SER:HA	5:F:7135:ILE:HD12	1.83	0.59
5:G:5040:ALA:HB2	5:G:5216:TYR:CE1	2.37	0.58
1:C:48:HIS:NE2	1:C:141:ILE:HD11	2.18	0.58
1:D:111:ARG:HB2	1:D:114:LEU:HD13	1.83	0.58
4:A:129:LYS:HD3	4:A:161:LEU:HD11	1.84	0.58
4:A:151:LEU:HD13	4:A:155:LEU:HG	1.84	0.58
5:F:7027:GLN:CG	5:F:7047:VAL:HG12	2.33	0.58
1:B:233:GLY:HA3	1:C:159:GLN:CD	2.29	0.58
1:B:61:LYS:HG2	1:B:71:MET:HE1	1.84	0.58
1:D:83:PHE:HZ	5:H:6155:VAL:HG21	1.69	0.58
5:H:6120:ALA:HB2	5:H:6193:ASN:N	2.17	0.58
1:B:111:ARG:HB2	1:B:114:LEU:HD13	1.86	0.58
1:D:61:LYS:HG2	1:D:71:MET:HE1	1.86	0.58
1:D:83:PHE:CZ	5:H:6155:VAL:HG21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:5127:LEU:HD23	5:G:5184:MSE:HE1	1.85	0.58
5:F:7003:LEU:HA	5:F:7046:ASP:OD2	2.04	0.58
1:C:72:MET:CE	5:G:5035:ASN:CB	2.80	0.58
1:E:5:ASN:O	1:E:14:LYS:HB2	2.03	0.58
5:G:5135:ILE:HA	5:G:5152:PHE:O	2.04	0.58
5:H:6010:LEU:HD11	5:H:6213:HIS:O	2.02	0.58
5:F:7022:MSE:HB3	5:F:7102:ALA:CB	2.33	0.58
1:D:13:GLN:HE22	1:E:126:GLU:CA	2.17	0.58
3:J:9:DT:H1'	3:J:10:DA:H5'	1.85	0.58
5:H:6138:ILE:HG22	5:H:6151:GLY:HA2	1.86	0.58
5:H:6198:LEU:HD23	5:H:6207:ALA:HB1	1.84	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:7109:PHE:CD2	5:F:7208:LYS:HD3	2.37	0.58
4:A:25:VAL:HG12	4:A:26:GLN:N	2.18	0.58
5:F:7134:GLN:CB	5:F:7153:ASN:ND2	2.67	0.58
1:B:177:THR:OG1	1:B:190:MET:HE1	2.04	0.57
1:C:72:MET:HE1	1:C:91:PHE:HB2	1.85	0.57
1:D:72:MET:HE2	5:H:6156:GLU:HA	1.86	0.57
1:E:88:LEU:CD2	1:E:104:ILE:HG21	2.34	0.57
1:E:186:ALA:CB	1:E:219:VAL:HG22	2.32	0.57
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:D:49:SER:HB3	1:D:56:LYS:HZ2	1.70	0.57
1:E:3:THR:CG2	1:E:18:SER:HB2	2.30	0.57
1:E:10:ILE:HD12	4:A:141:TYR:CD2	2.39	0.57
5:H:6037:THR:HG23	5:H:6038:THR:CB	2.29	0.57
1:B:176:LEU:HD22	1:B:211:LEU:HD22	1.86	0.57
5:F:7068:ASN:O	5:F:7071:ALA:N	2.38	0.57
1:E:279:GLN:OE1	1:E:279:GLN:N	2.35	0.57
5:G:5129:VAL:HG13	5:G:5133:LEU:HD12	1.86	0.57
1:C:3:THR:HG21	1:C:18:SER:HB2	1.85	0.57
4:A:174:VAL:HG12	4:A:174:VAL:O	2.04	0.57
5:H:6028:PHE:CE2	5:H:6043:ASN:ND2	2.73	0.57
1:B:260:ASP:OD1	1:B:260:ASP:O	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:57:THR:HG23	6:D:700:08T:O1B	2.03	0.57
1:C:88:LEU:HD23	1:C:104:ILE:CD1	2.35	0.57
1:D:8:GLU:OE1	1:D:13:GLN:CB	2.47	0.57
1:C:50:PRO:HA	1:C:139:ASN:O	2.05	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
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
5:H:6123:LEU:CD2	5:H:6191:PRO:HA	2.34	0.57
5:H:6133:LEU:O	5:H:6134:GLN:HG3	2.05	0.57
1:B:13:GLN:HE22	1:C:126:GLU:HB3	1.70	0.56
1:B:248:LYS:HG2	1:C:273:TYR:HH	1.70	0.56
1:D:298:ALA:HB2	1:E:293:GLN:HA	1.87	0.56
5:H:6071:ALA:HA	5:H:6084:ALA:O	2.05	0.56
5:H:6109:PHE:CZ	5:H:6199:TRP:HB3	2.40	0.56
5:H:6129:VAL:HG21	5:H:6165:TYR:CE2	2.40	0.56
1:C:256:LYS:HE2	1:C:257:TYR:CZ	2.40	0.56
1:D:177:THR:OG1	1:D:190:MET:HE1	2.05	0.56
1:D:283:ARG:NE	1:D:315:GLU:OE1	2.38	0.56
1:E:88:LEU:HD23	1:E:104:ILE:HD13	1.87	0.56
4:A:67:ASN:O	4:A:70:SER:HB3	2.06	0.56
5:G:5010:LEU:O	5:G:5013:ASN:N	2.36	0.56
5:H:6082:LYS:HE3	5:H:6089:THR:HG21	1.87	0.56
5:H:6092:TRP:HD1	5:H:6093:PRO:O	1.88	0.56
5:F:7039:TYR:CD1	5:F:7040:ALA:N	2.74	0.56
5:G:5076:SER:C	5:G:5078:ASP:O	2.48	0.56
5:H:6066:LEU:HD12	5:H:6067:VAL:N	2.20	0.56
1:B:49:SER:HB3	1:B:56:LYS:HZ2	1.70	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
1:E:254:ALA:N	1:E:255:PRO:HD2	2.21	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:D:88:LEU:HD23	1:D:104:ILE:HD13	1.87	0.56
1:D:97:PHE:HD1	1:D:97:PHE:H	1.51	0.56
1:C:97:PHE:O	5:G:5204:GLN:HB3	2.05	0.56
1:C:212:ASP:CG	1:D:153:ARG:NH1	2.64	0.56
1:E:92:ALA:O	1:E:131:ASN:ND2	2.31	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
5:F:7089:THR:HG22	5:F:7091:PHE:HE1	1.71	0.56
1:B:13:GLN:HE22	1:C:126:GLU:CA	2.19	0.56
1:C:72:MET:HE1	1:C:91:PHE:CB	2.36	0.56
1:C:205:ARG:HD3	1:D:151:ARG:HA	1.87	0.55
5:F:7189:MSE:HB2	5:F:7216:TYR:CE1	2.41	0.55
1:E:95:ALA:O	5:H:6219:ALA:HB1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ALA:HA	4:A:84:LEU:HA	1.86	0.55
1:B:277:THR:HG21	1:B:317:GLN:HG2	1.88	0.55
4:A:53:CYS:SG	4:A:95:PHE:HZ	2.29	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
1:D:213:SER:HB3	1:E:153:ARG:NE	2.22	0.55
1:E:50:PRO:HA	1:E:139:ASN:O	2.07	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
5:F:7202:GLY:C	5:F:7204:GLN:N	2.60	0.55
5:H:6033:ALA:C	5:H:6035:ASN:H	2.14	0.55
1:B:110:ASP:OD1	1:C:122:ARG:NH2	2.39	0.55
1:D:272:ILE:CG2	1:D:284:MET:HE3	2.37	0.55
1:C:188:ALA:HB3	1:C:221:ASP:HA	1.89	0.54
1:E:107:ASP:OD1	1:E:137:THR:HG21	2.07	0.54
2:I:25:DG:H1	3:J:6:DC:N4	2.05	0.54
5:H:6017:ILE:CG2	5:H:6038:THR:CG2	2.84	0.54
5:H:6133:LEU:C	5:H:6134:GLN:CG	2.80	0.54
1:B:192:VAL:HG22	1:B:225:LEU:CD1	2.36	0.54
1:C:61:LYS:HG2	1:C:71:MET:HE1	1.89	0.54
1:D:303:LEU:HD13	1:E:265:VAL:HG13	1.90	0.54
1:E:204:PHE:C	1:E:207:THR:HG22	2.31	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
5:G:5118:ILE:O	5:G:5118:ILE:HG13	2.07	0.54
5:H:6195:LYS:HD3	5:H:6197:LEU:HD21	1.88	0.54
5:F:7028:PHE:CZ	5:F:7030:MSE:HE1	2.26	0.54
1:D:50:PRO:HA	1:D:139:ASN:O	2.07	0.54
1:B:72:MET:HE1	1:B:91:PHE:HB2	1.88	0.54
1:D:217:LYS:CE	1:D:224:ILE:HD11	2.37	0.54
4:A:158:LEU:C	4:A:160:GLY:H	2.15	0.54
5:H:6011:LEU:C	5:H:6061:LEU:HD11	2.32	0.54
5:H:6063:ILE:CG2	5:H:6090:ILE:HG21	2.38	0.54
5:F:7134:GLN:O	5:F:7153:ASN:ND2	2.40	0.54
1:C:77:SER:HB3	1:C:111:ARG:HH11	1.71	0.54
1:B:49:SER:OG	1:B:50:PRO:C	2.51	0.54
1:B:139:ASN:ND2	1:C:147:PRO:HG3	2.22	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
5:F:7121:GLU:O	5:F:7125:GLN:N	2.25	0.54
1:D:111:ARG:NE	1:E:116:GLU:HG3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:5210:GLU:HG3	5:G:5215:ASN:ND2	2.22	0.54
5:H:6081:ILE:HG22	5:H:6082:LYS:N	2.23	0.54
5:F:7130:SER:CA	5:F:7135:ILE:HB	2.38	0.54
5:F:7226:HIS:HB2	5:F:7228:PHE:HD1	1.71	0.54
1:C:72:MET:CE	1:C:91:PHE:CG	2.91	0.54
1:C:247:VAL:O	1:C:248:LYS:C	2.50	0.54
1:D:256:LYS:HG3	1:E:159:GLN:OE1	2.08	0.54
4:A:116:GLU:O	4:A:116:GLU:HG2	2.06	0.54
5:F:7068:ASN:CB	5:F:7085:ASP:OD1	2.56	0.54
1:B:122:ARG:HG2	4:A:32:PHE:CD2	2.43	0.54
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
1:E:303:LEU:CD1	4:A:79:VAL:HG11	2.33	0.54
2:I:27:DC:H2"	2:I:28:DT:H71	1.90	0.54
5:F:7116:THR:C	5:F:7117:GLU:HG3	2.33	0.54
1:B:188:ALA:HB3	1:B:221:ASP:HA	1.89	0.53
5:G:5064:LEU:HD23	5:G:5083:ILE:HD13	1.90	0.53
5:H:6189:MSE:H	5:H:6189:MSE:SE	2.41	0.53
5:F:7122:ASP:CB	5:F:7167:LEU:HD21	2.37	0.53
1:B:88:LEU:HD23	1:B:104:ILE:CD1	2.37	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: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
1:C:88:LEU:CD2	1:C:104:ILE:HG21	2.39	0.53
1:E:164:ASP:O	1:E:168:MET:HG3	2.09	0.53
5:G:5063:ILE:HG12	5:G:5092:TRP:HZ3	1.74	0.53
5:G:5077:GLU:CG	5:G:5078:ASP:H	2.15	0.53
5:F:7089:THR:CG2	5:F:7091:PHE:HE1	2.22	0.53
5:F:7162:ARG:HG3	5:F:7162:ARG:HH11	1.73	0.53
5:F:7205:GLY:HA3	5:F:7220:LEU:HD12	1.90	0.53
1:C:111:ARG:HB2	1:C:114:LEU:HD13	1.90	0.53
1:D:13:GLN:HE22	1:E:126:GLU:CB	2.22	0.53
2:I:25:DG:H2"	2:I:26:DT:H71	1.90	0.53
4:A:76:MET:N	4:A:77:PRO:HD2	2.23	0.53
5:G:5220:LEU:N	5:G:5220:LEU:HD23	2.24	0.53
1:C:124:PHE:CD1	1:C:124:PHE:C	2.87	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
1:D:227:LEU:HA	1:D:230:ASN:HB3	1.91	0.53
5:G:5189:MSE:HB2	5:G:5216:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:7123:LEU:O	5:F:7127:LEU:HG	2.09	0.53
1:B:277:THR:O	1:B:280:SER:HB2	2.08	0.53
1:D:256:LYS:HE2	1:D:257:TYR:CZ	2.44	0.53
5:G:5126:LEU:HD13	5:G:5165:TYR:CE2	2.43	0.53
5:G:5189:MSE:HE2	5:G:5209:PHE:CG	2.44	0.53
5:H:6032:ARG:HB3	5:H:6039:TYR:HD1	1.73	0.53
1:E:93:SER:CB	5:H:6221:GLU:OE1	2.56	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
5:H:6126:LEU:HD12	5:H:6126:LEU:O	2.09	0.53
1:C:8:GLU:OE1	1:C:13:GLN:CB	2.50	0.53
1:C:72:MET:HE2	5:G:5035:ASN:CB	2.38	0.53
1:D:213:SER:HB3	1:E:153:ARG:HE	1.74	0.53
4:A:118:SER:OG	4:A:175:LYS:HE2	2.09	0.53
5:G:5021:ILE:HG12	5:G:5022:MSE:N	2.23	0.53
1:D:276:VAL:HG22	1:D:280:SER:CB	2.39	0.52
1:E:124:PHE:CD1	1:E:124:PHE:C	2.87	0.52
5:G:5032:ARG:HB2	5:G:5039:TYR:HB2	1.91	0.52
5:H:6062:GLY:C	5:H:6064:LEU:H	2.17	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:7010:LEU:O	5:F:7014:PHE:HD1	1.92	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
1:B:254:ALA:N	1:B:255:PRO:HD2	2.24	0.52
1:E:98:ASP:C	5:H:6204:GLN:NE2	2.67	0.52
5:H:6110:PRO:HG3	5:H:6199:TRP:CD2	2.45	0.52
5:H:6180:PHE:HB3	5:H:6220:LEU:CD2	2.38	0.52
5:F:7012:LYS:O	5:F:7015:ALA:HB3	2.09	0.52
1:D:72:MET:HE1	1:D:91:PHE:HB2	1.92	0.52
4:A:82:MET:O	4:A:86:GLY:HA3	2.10	0.52
5:G:5141:THR:OG1	5:G:5142:VAL:N	2.43	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:D:277:THR:O	1:D:280:SER:HB2	2.10	0.52
1:E:307:TYR:CE2	4:A:80:TYR:CE1	2.97	0.52
5:H:6054:ILE:HG22	5:H:6056:ASP:C	2.34	0.52
1:C:72:MET:CE	5:G:5035:ASN:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ASP:CA	1:D:233:GLY:H	2.23	0.52
1:E:12:GLU:OE1	1:E:205:ARG:HG3	2.10	0.52
1:E:276:VAL:HG22	1:E:280:SER:CB	2.40	0.52
5:H:6099:THR:HG22	5:H:6099:THR:O	2.09	0.52
1:C:113:GLY:O	2:I:17:DC:H4'	2.09	0.52
1:E:72:MET:CE	1:E:91:PHE:CD2	2.93	0.52
5:G:5128:ARG:CD	5:F:7066:LEU:HD13	2.39	0.52
5:F:7028:PHE:HE2	5:F:7030:MSE:CE	1.81	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:HB2	5:F:7082:LYS:HB2	1.91	0.52
1:B:50:PRO:HA	1:B:139:ASN:O	2.10	0.51
1:C:72:MET:HE2	5:G:5035:ASN:HB2	1.91	0.51
1:D:41:LYS:HD2	1:D:101:GLN:OE1	2.10	0.51
1:D:49:SER:HB2	1:D:51:SER:O	2.10	0.51
4:A:187:TRP:HE3	4:A:187:TRP:C	2.18	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
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
1:C:254:ALA:N	1:C:255:PRO:HD2	2.24	0.51
5:H:6034:VAL:HG13	5:H:6101:VAL:HG21	1.91	0.51
5:F:7138:ILE:HD12	5:F:7149:ILE:HG21	1.90	0.51
1:E:88:LEU:HD23	1:E:104:ILE:CD1	2.40	0.51
4:A:187:TRP:C	4:A:187:TRP:CE3	2.88	0.51
5:H:6004:SER:N	5:H:6046:ASP:OD2	2.43	0.51
5:H:6149:ILE:HD12	5:H:6167:LEU:HD23	1.93	0.51
5:F:7076:SER:OG	5:F:7077:GLU:N	2.42	0.51
1:B:41:LYS:HD2	1:B:101:GLN:OE1	2.11	0.51
1:E:17:PRO:HG2	8:E:700:ADP:C2	2.46	0.51
1:E:277:THR:O	1:E:280:SER:HB2	2.10	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
5:F:7027:GLN:HB3	5:F:7044:ILE:O	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:72:MET:HE1	1:B:91:PHE:CB	2.41	0.51
1:C:94:ALA:O	1:C:102:LYS:HE3	2.10	0.51
1:D:276:VAL:HG22	1:D:280:SER:HB2	1.93	0.51
1:E:16:ARG:O	1:E:17:PRO:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:GLY:N	5:H:6204:GLN:HB3	2.26	0.51
4:A:60:TYR:CE2	4:A:95:PHE:HB2	2.46	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:C:283:ARG:O	1:C:287:ILE:HG13	2.11	0.51
1:D:72:MET:HE1	1:D:91:PHE:CB	2.41	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: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
5:H:6123:LEU:CD2	5:H:6127:LEU:HD11	2.41	0.51
5:H:6146:LYS:CA	5:H:6171:ASP:HA	2.31	0.51
1:B:48:HIS:NE2	1:B:141:ILE:HD11	2.25	0.50
1:C:49:SER:OG	1:C:50:PRO:C	2.55	0.50
1:C:121:LEU:O	1:C:125:MET:HG3	2.11	0.50
1:D:94:ALA:O	1:D:102:LYS:HE3	2.12	0.50
2:I:11:DT:H2''	2:I:12:DA:C5'	2.38	0.50
2:I:25:DG:H1	3:J:6:DC:H42	1.58	0.50
5:F:7177:THR:O	5:F:7227:ASP:HB2	2.11	0.50
1:B:80:LYS:NZ	2:I:19:DC:P	2.85	0.50
1:C:299:ALA:CB	1:D:295:HIS:CD2	2.79	0.50
1:D:192:VAL:HG22	1:D:225:LEU:CD1	2.41	0.50
1:D:297:ILE:O	1:E:295:HIS:O	2.29	0.50
4:A:157:GLU:CG	5:H:6096:ASP:OD2	2.59	0.50
5:G:5028:PHE:HA	5:G:5042:ALA:O	2.11	0.50
1:C:176:LEU:HD22	1:C:211:LEU:HD22	1.92	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:3:THR:OG1	1:C:22:GLU:OE1	2.27	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
5:F:7126:LEU:HD12	5:F:7126:LEU:C	2.37	0.50
1:B:13:GLN:NE2	1:C:126:GLU:HB3	2.25	0.50
1:C:231:ASP:O	1:C:263:TRP:CE2	2.64	0.50
4:A:20:LYS:HE2	5:F:7055:TYR:CZ	2.47	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
1:B:111:ARG:CZ	1:C:116:GLU:HG3	2.42	0.50
1:C:58:THR:HB	6:C:700:08T:O1A	2.12	0.50
1:D:283:ARG:CZ	1:D:315:GLU:OE1	2.60	0.50
4:A:53:CYS:SG	4:A:54:SER:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:2:ILE:CG2	1:E:3:THR:N	2.75	0.49
1:E:8:GLU:HG2	1:E:13:GLN:CB	2.42	0.49
1:E:8:GLU:HB3	1:E:14:LYS:HB3	1.93	0.49
2:I:27:DC:H2''	2:I:28:DT:C7	2.42	0.49
5:H:6123:LEU:HD22	5:H:6191:PRO:HA	1.94	0.49
1:B:3:THR:HG21	1:B:18:SER:HB2	1.94	0.49
1:C:139:ASN:ND2	1:D:147:PRO:CG	2.75	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
5:G:5092:TRP:CD1	5:G:5092:TRP:C	2.89	0.49
1:C:13:GLN:HG3	1:C:16:ARG:HH21	1.77	0.49
1:D:215:SER:O	1:D:216:SER:C	2.55	0.49
5:H:6052:VAL:HG21	5:H:6081:ILE:HD11	1.95	0.49
1:D:231:ASP:C	1:D:233:GLY:N	2.67	0.49
1:D:304:HIS:CE1	1:E:293:GLN:HG3	2.47	0.49
3:J:7:DA:H2''	3:J:8:DC:OP2	2.13	0.49
5:G:5189:MSE:HE2	5:G:5209:PHE:CD2	2.48	0.49
5:H:6011:LEU:HD22	5:H:6057:LEU:HD11	1.95	0.49
5:F:7130:SER:HA	5:F:7135:ILE:HB	1.93	0.49
1:C:48:HIS:HA	1:C:138:ALA:O	2.13	0.49
1:D:204:PHE:C	1:D:207:THR:HG22	2.37	0.49
5:H:6092:TRP:CD1	5:H:6093:PRO:O	2.65	0.49
5:H:6178:PHE:HD2	5:H:6180:PHE:CD2	2.30	0.49
5:H:6198:LEU:CD2	5:H:6207:ALA:CB	2.89	0.49
5:F:7022:MSE:HE3	5:F:7023:LEU:O	2.11	0.49
5:F:7044:ILE:HG13	5:F:7045:SER:H	1.77	0.49
5:F:7065:SER:C	5:F:7066:LEU:HD23	2.36	0.49
1:E:72:MET:HE1	1:E:91:PHE:CB	2.43	0.49
5:G:5110:PRO:O	5:G:5111:VAL:C	2.54	0.49
5:H:6176:ASN:CG	5:H:6228:PHE:CE1	2.91	0.49
5:F:7028:PHE:HZ	5:F:7030:MSE:HE2	0.73	0.49
1:C:276:VAL:HG22	1:C:280:SER:HB2	1.95	0.49
1:D:254:ALA:N	1:D:255:PRO:HD2	2.28	0.49
1:E:24:ILE:CG2	1:E:168:MET:HG2	2.43	0.49
4:A:130:ARG:CB	4:A:158:LEU:HD11	2.43	0.49
1:B:139:ASN:ND2	1:C:147:PRO:CG	2.76	0.49
1:B:276:VAL:HG22	1:B:280:SER:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:ND2	1:D:147:PRO:HG3	2.27	0.49
1:D:124:PHE:CD1	1:D:124:PHE:C	2.91	0.49
1:D:301:THR:OG1	1:E:142:ASP:OD2	2.15	0.49
4:A:161:LEU:HB3	5:H:6055:TYR:CD1	2.48	0.49
1:B:49:SER:N	1:B:56:LYS:HD3	2.28	0.49
1:B:217:LYS:CE	1:B:224:ILE:HD11	2.38	0.49
1:C:75:ASN:CG	1:D:123:SER:HB3	2.38	0.49
1:E:300:ASN:N	4:A:83:ASN:OD1	2.30	0.49
4:A:44:ILE:HD11	4:A:65:VAL:HA	1.94	0.49
4:A:55:ILE:HG12	4:A:56:ALA:H	1.76	0.49
4:A:167:LEU:CD2	4:A:180:LEU:HD23	2.40	0.49
5:F:7023:LEU:HD11	5:F:7052:VAL:HG13	1.94	0.49
1:D:88:LEU:HD23	1:D:104:ILE:CD1	2.43	0.49
1:D:256:LYS:HE3	1:E:159:GLN:CD	2.38	0.49
4:A:68:ALA:O	4:A:71:GLN:CG	2.61	0.49
5:G:5078:ASP:C	5:G:5080:ASN:H	2.21	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:E:247:VAL:O	1:E:248:LYS:C	2.55	0.48
5:F:7068:ASN:H	5:F:7085:ASP:CG	2.21	0.48
5:F:7109:PHE:CD2	5:F:7208:LYS:CB	2.96	0.48
1:E:94:ALA:O	1:E:102:LYS:HE3	2.12	0.48
1:E:252:ALA:HB2	4:A:112:ALA:HB1	1.95	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: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:7007:THR:O	5:F:7011:LEU:CD1	2.42	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
1:E:276:VAL:HG23	1:E:317:GLN:O	2.14	0.48
5:G:5120:ALA:HB2	5:G:5193:ASN:N	2.29	0.48
5:F:7044:ILE:HG13	5:F:7045:SER:N	2.28	0.48
5:G:5097:PRO:O	5:G:5098:SER:C	2.56	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
2:I:23:DG:H2''	2:I:24:DT:H71	1.94	0.48
1:C:212:ASP:CG	1:D:153:ARG:HH12	2.22	0.48
1:D:231:ASP:O	1:D:232:ARG:CB	2.61	0.48
1:E:169:MET:HG2	1:E:197:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:H:6198:LEU:HD23	5:H:6207:ALA:HB2	1.92	0.48
1:B:124:PHE:CD1	1:B:124:PHE:C	2.92	0.48
1:B:283:ARG:O	1:B:287:ILE:HG13	2.14	0.48
1:E:72:MET:CE	1:E:91:PHE:CG	2.96	0.48
5:G:5167:LEU:CD1	5:F:7088:SER:HB3	2.44	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
1:C:131:ASN:OD1	5:G:5222:ALA:HB1	2.14	0.48
5:G:5029:ILE:CG1	5:G:5042:ALA:HB3	2.44	0.48
1:D:88:LEU:CD2	1:D:104:ILE:HG21	2.44	0.47
1:D:235:ILE:HG22	1:D:235:ILE:O	2.13	0.47
1:E:176:LEU:HD22	1:E:211:LEU:HD22	1.96	0.47
5:G:5181:ILE:HB	5:G:5221:GLU:HB2	1.95	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:G:5223:ASP:OD1	5:G:5223:ASP:N	2.39	0.47
5:H:6195:LYS:HB3	5:H:6210:GLU:HB3	1.96	0.47
1:D:231:ASP:HB3	1:D:233:GLY:H	1.80	0.47
1:E:272:ILE:CG2	1:E:284:MET:HE3	2.43	0.47
5:G:5109:PHE:HA	5:G:5110:PRO:HD2	1.69	0.47
5:H:6149:ILE:O	5:H:6166:SER:HA	2.14	0.47
4:A:161:LEU:O	4:A:161:LEU:CG	2.62	0.47
4:A:171:THR:HG23	4:A:176:GLU:HB3	1.96	0.47
5:G:5097:PRO:O	5:G:5099:THR:N	2.48	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
1:B:122:ARG:CG	4:A:32:PHE:CD2	2.97	0.47
1:E:205:ARG:NH2	8:E:700:ADP:PB	2.82	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:C:72:MET:HE1	5:G:5035:ASN:HB2	1.96	0.47
1:D:49:SER:N	1:D:56:LYS:HD3	2.29	0.47
1:D:247:VAL:O	1:D:248:LYS:C	2.56	0.47
1:E:11:LEU:HD12	1:E:212:ASP:CG	2.40	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
5:F:7113:SER:HB3	5:F:7228:PHE:CE2	2.49	0.47
1:B:204:PHE:C	1:B:207:THR:HG22	2.39	0.47
1:C:116:GLU:OE2	1:C:116:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:PHE:C	1:C:207:THR:HG22	2.40	0.47
1:D:256:LYS:HB2	1:E:159:GLN:HE22	1.76	0.47
1:D:284:MET:HE2	1:D:284:MET:HB2	1.62	0.47
1:E:41:LYS:HD2	1:E:101:GLN:OE1	2.15	0.47
4:A:16:ALA:HB1	4:A:25:VAL:HA	1.97	0.47
4:A:151:LEU:HD22	4:A:151:LEU:HA	1.68	0.47
5:G:5018:ASN:HB3	5:G:5031:THR:OG1	2.14	0.47
5:G:5076:SER:O	5:G:5078:ASP:O	2.32	0.47
5:G:5125:GLN:O	5:G:5129:VAL:HG23	2.15	0.47
5:G:5223:ASP:O	5:G:5225:THR:HG23	2.15	0.47
5:H:6187:MSE:HE3	5:H:6187:MSE:HB3	1.78	0.47
5:H:6202:GLY:O	5:H:6226:HIS:NE2	2.47	0.47
5:F:7118:ILE:CG1	5:F:7119:LYS:H	2.27	0.47
5:F:7139:ALA:HA	5:F:7180:PHE:O	2.14	0.47
1:B:151:ARG:O	1:B:151:ARG:HG3	2.14	0.47
5:G:5068:ASN:HB2	5:G:5070:ASP:OD1	2.15	0.47
5:F:7134:GLN:O	5:F:7153:ASN:CG	2.57	0.47
1:C:11:LEU:O	1:C:11:LEU:HG	2.14	0.47
1:C:217:LYS:CE	1:C:224:ILE:HD11	2.42	0.47
1:D:80:LYS:CE	1:E:85:ARG:CZ	2.92	0.47
2:I:25:DG:N2	3:J:6:DC:N3	2.61	0.47
1:C:41:LYS:HD2	1:C:101:GLN:OE1	2.15	0.47
5:G:5176:ASN:ND2	5:G:5227:ASP:OD1	2.39	0.47
5:H:6053:ALA:HB3	5:H:6095:ALA:O	2.14	0.47
1:B:108:GLU:HB3	1:C:122:ARG:CZ	2.45	0.46
1:D:248:LYS:HG2	1:E:273:TYR:OH	2.15	0.46
1:E:49:SER:H	1:E:56:LYS:HD3	1.80	0.46
2:I:9:DT:C7	4:A:38:ASN:ND2	2.72	0.46
2:I:17:DC:C6	2:I:18:DT:H72	2.50	0.46
5:G:5128:ARG:HG2	5:F:7066:LEU:HD11	1.86	0.46
5:G:5133:LEU:HD11	5:F:7090:ILE:HG23	1.97	0.46
1:B:72:MET:CE	1:B:91:PHE:CD2	2.98	0.46
1:B:80:LYS:NZ	1:C:85:ARG:HH22	2.13	0.46
1:C:145:ILE:HG13	1:C:147:PRO:HD2	1.98	0.46
1:D:83:PHE:HZ	5:H:6155:VAL:CG2	2.28	0.46
1:D:116:GLU:HG2	2:I:16:DA:H4'	1.98	0.46
4:A:29:ALA:O	4:A:31:SER:N	2.49	0.46
5:H:6118:ILE:HG23	5:H:6118:ILE:O	2.14	0.46
5:H:6123:LEU:HD21	5:H:6127:LEU:HD11	1.97	0.46
1:B:124:PHE:HB2	4:A:17:TRP:CZ2	2.50	0.46
1:E:283:ARG:O	1:E:287:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:SER:O	1:C:216:SER:C	2.58	0.46
1:D:304:HIS:HE1	1:E:293:GLN:HG3	1.79	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
5:F:7181:ILE:HB	5:F:7221:GLU:HB2	1.97	0.46
1:B:13:GLN:HG3	1:B:16:ARG:NH1	2.30	0.46
1:C:235:ILE:HG22	1:C:235:ILE:O	2.15	0.46
1:E:53:GLY:HA3	1:E:203:ASP:OD1	2.15	0.46
4:A:8:ILE:O	4:A:9:GLN:C	2.58	0.46
1:C:75:ASN:ND2	1:D:123:SER:HB3	2.31	0.46
1:C:294:TYR:HB3	1:D:293:GLN:HG2	1.97	0.46
3:J:11:DC:H2"	3:J:12:DG:C8	2.50	0.46
4:A:50:LYS:HA	4:A:99:MET:CE	2.46	0.46
5:G:5011:LEU:HD12	5:G:5011:LEU:N	2.27	0.46
5:H:6060:PHE:C	5:H:6062:GLY:H	2.23	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
5:F:7016:THR:O	5:F:7188:LYS:NZ	2.45	0.46
5:F:7037:THR:CB	5:F:7186:ASN:HD21	2.28	0.46
1:B:72:MET:CE	1:B:91:PHE:CG	2.99	0.46
3:J:4:DG:H2"	3:J:5:DA:C8	2.51	0.46
4:A:158:LEU:O	4:A:160:GLY:N	2.47	0.46
5:H:6008:THR:O	5:H:6011:LEU:HB2	2.16	0.46
1:B:11:LEU:HD22	1:B:212:ASP:HB2	1.97	0.46
1:B:192:VAL:CG2	1:B:225:LEU:CB	2.86	0.46
1:B:293:GLN:NE2	4:A:85:ILE:CA	2.48	0.46
1:D:176:LEU:HD22	1:D:211:LEU:HD22	1.97	0.46
4:A:54:SER:O	4:A:55:ILE:CG2	2.61	0.46
1:C:250:LEU:HD13	1:C:309:PHE:HB3	1.98	0.46
1:D:29:ASP:HA	1:D:32:THR:CG2	2.45	0.46
5:G:5226:HIS:CE1	5:G:5228:PHE:HB2	2.51	0.46
5:H:6116:THR:O	5:H:6196:LEU:HB3	2.16	0.46
5:H:6120:ALA:CB	5:H:6192:GLY:C	2.83	0.46
5:H:6154:LYS:O	5:H:6158:SER:HA	2.16	0.46
1:B:48:HIS:HA	1:B:138:ALA:O	2.16	0.46
1:B:88:LEU:CD2	1:B:104:ILE:HG21	2.41	0.46
1:D:122:ARG:HG2	1:D:122:ARG:HH11	1.81	0.46
5:G:5027:GLN:O	5:G:5043:ASN:HA	2.16	0.46
5:G:5038:THR:HA	5:G:5217:VAL:O	2.16	0.46
5:H:6183:ASN:HB2	5:H:6221:GLU:HG3	1.98	0.46
1:B:15:TYR:OH	1:B:183:GLU:OE1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ILE:HG21	1:D:284:MET:HE3	1.98	0.45
1:E:112:SER:C	1:E:114:LEU:H	2.24	0.45
5:H:6108:PRO:O	5:H:6109:PHE:C	2.59	0.45
5:F:7076:SER:HB3	5:F:7080:ASN:O	2.15	0.45
1:B:305:LEU:HD12	1:B:305:LEU:HA	1.77	0.45
1:D:283:ARG:NH2	1:D:315:GLU:OE1	2.49	0.45
5:H:6033:ALA:C	5:H:6035:ASN:N	2.74	0.45
5:H:6055:TYR:CD1	5:H:6099:THR:HG22	2.51	0.45
5:H:6138:ILE:HD12	5:H:6149:ILE:CG2	2.46	0.45
1:C:246:ASP:OD1	1:C:246:ASP:C	2.60	0.45
1:D:276:VAL:CG2	1:D:317:GLN:O	2.60	0.45
4:A:159:LYS:HD3	4:A:187:TRP:HE1	1.81	0.45
5:G:5127:LEU:CD2	5:G:5184:MSE:HE1	2.47	0.45
5:H:6054:ILE:HG22	5:H:6056:ASP:N	2.31	0.45
5:F:7036:GLY:O	5:F:7038:THR:N	2.49	0.45
5:F:7178:PHE:CD1	5:F:7178:PHE:C	2.95	0.45
1:C:305:LEU:HD12	1:C:305:LEU:HA	1.80	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
5:H:6141:THR:OG1	5:H:6178:PHE:O	2.32	0.45
1:B:57:THR:CG2	1:B:137:THR:HG21	2.33	0.45
1:B:111:ARG:NE	1:C:116:GLU:HG3	2.31	0.45
1:D:13:GLN:HE22	1:E:126:GLU:HA	1.80	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:72:MET:CE	1:D:91:PHE:CG	3.00	0.45
1:D:77:SER:OG	1:D:111:ARG:HD3	2.16	0.45
1:B:276:VAL:HG22	1:B:280:SER:HB2	1.98	0.45
1:C:227:LEU:HA	1:C:230:ASN:CB	2.39	0.45
1:D:3:THR:OG1	1:D:22:GLU:OE1	2.32	0.45
1:D:235:ILE:O	1:D:235:ILE:CG2	2.64	0.45
5:G:5011:LEU:H	5:G:5011:LEU:CD1	2.28	0.45
5:G:5044:ILE:HD13	5:G:5046:ASP:O	2.16	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
5:H:6196:LEU:HD11	5:H:6198:LEU:HD21	1.99	0.45
5:F:7007:THR:HG23	5:F:7044:ILE:CG1	2.30	0.45
1:B:80:LYS:HZ1	1:C:85:ARG:NH2	2.13	0.45
1:B:107:ASP:OD1	1:B:137:THR:HG21	2.17	0.45
1:C:297:ILE:HD13	1:D:297:ILE:CD1	2.34	0.45
5:H:6001:MSE:HE2	5:H:6003:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6032:ARG:NH1	5:H:6036:GLY:HA2	2.31	0.45
5:H:6060:PHE:C	5:H:6062:GLY:N	2.75	0.45
1:B:48:HIS:CE1	1:B:141:ILE:HG13	2.51	0.45
1:B:49:SER:OG	1:B:50:PRO:CA	2.65	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:7062:GLY:O	5:F:7065:SER:OG	2.26	0.45
1:B:3:THR:OG1	1:B:22:GLU:OE1	2.35	0.44
1:B:80:LYS:HZ3	1:C:85:ARG:NH2	2.13	0.44
1:C:284:MET:HB2	1:C:284:MET:HE2	1.60	0.44
1:E:48:HIS:HA	1:E:138:ALA:O	2.17	0.44
5:H:6115:VAL:CG1	5:H:6197:LEU:CD2	2.89	0.44
5:F:7001:MSE:N	5:F:7072:GLU:CG	2.80	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:B:50:PRO:HG3	4:A:57:GLN:HG3	1.99	0.44
1:B:164:ASP:O	1:B:168:MET:HG3	2.16	0.44
5:H:6195:LYS:HG2	5:H:6197:LEU:HD21	1.98	0.44
4:A:162:VAL:HG12	4:A:162:VAL:O	2.18	0.44
5:G:5077:GLU:H	5:G:5077:GLU:CD	2.26	0.44
1:B:215:SER:O	1:B:216:SER:C	2.60	0.44
4:A:158:LEU:O	4:A:159:LYS:C	2.57	0.44
5:G:5107:ILE:HG23	5:G:5108:PRO:HD2	1.98	0.44
4:A:150:LYS:C	4:A:152:PRO:CD	2.86	0.44
5:G:5050:PHE:CE2	5:G:5075:GLN:HB2	2.52	0.44
5:H:6049:ASP:OD1	5:H:6050:PHE:HD1	2.00	0.44
1:E:196:LEU:HD21	1:E:214:TYR:CE2	2.52	0.44
2:I:16:DA:C2	3:J:16:DA:C2	3.06	0.44
3:J:4:DG:H1'	3:J:5:DA:O4'	2.18	0.44
5:G:5067:VAL:HB	5:G:5085:ASP:OD2	2.17	0.44
5:H:6066:LEU:HD11	5:H:6090:ILE:CD1	2.47	0.44
5:F:7023:LEU:HD12	5:F:7023:LEU:C	2.42	0.44
5:F:7189:MSE:HA	5:F:7216:TYR:CE2	2.52	0.44
1:C:29:ASP:HA	1:C:32:THR:HG22	1.99	0.44
2:I:7:DT:O5'	2:I:7:DT:H6	2.00	0.44
4:A:159:LYS:HE2	4:A:187:TRP:CZ2	2.53	0.44
5:H:6223:ASP:O	5:H:6224:SER:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:SER:HB2	5:H:6221:GLU:CD	2.43	0.44
1:E:185:ILE:HG23	1:E:218:GLY:O	2.17	0.44
1:E:284:MET:HE2	1:E:284:MET:HB2	1.57	0.44
5:F:7002:LYS:O	5:F:7003:LEU:HD23	2.18	0.44
1:C:57:THR:CG2	1:C:107:ASP:OD1	2.66	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:6011:LEU:CB	5:H:6061:LEU:HD21	2.48	0.44
5:H:6018:ASN:HD22	5:H:6020:GLY:H	1.66	0.44
5:H:6125:GLN:O	5:H:6129:VAL:HG23	2.17	0.44
1:C:164:ASP:O	1:C:168:MET:HG3	2.17	0.43
4:A:38:ASN:OD1	4:A:40:PHE:CD2	2.71	0.43
4:A:101:ALA:O	4:A:103:PRO:HD3	2.18	0.43
4:A:155:LEU:HD13	4:A:183:LEU:CD1	2.48	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
5:H:6135:ILE:HD13	5:H:6151:GLY:CA	2.47	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
1:D:49:SER:OG	1:D:50:PRO:C	2.61	0.43
5:H:6118:ILE:HG22	5:H:6194:TYR:O	2.18	0.43
1:D:48:HIS:CG	1:D:141:ILE:HD11	2.52	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
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
5:F:7226:HIS:CD2	5:F:7228:PHE:HD1	2.36	0.43
1:B:77:SER:OG	1:B:111:ARG:HD3	2.18	0.43
1:C:201:PHE:O	1:C:201:PHE:CD1	2.72	0.43
4:A:55:ILE:HD11	4:A:60:TYR:CD2	2.53	0.43
4:A:162:VAL:O	4:A:163:THR:C	2.61	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:5138:ILE:HG22	5:G:5151:GLY:HA2	1.99	0.43
5:G:5185:ALA:O	5:G:5188:LYS:HE3	2.18	0.43
5:H:6085:ASP:CG	5:H:6086:ALA:N	2.75	0.43
1:C:29:ASP:HA	1:C:32:THR:CG2	2.47	0.43
1:E:53:GLY:N	8:E:700:ADP:O2B	2.52	0.43
1:E:169:MET:HG2	1:E:197:VAL:HG12	1.99	0.43
1:E:204:PHE:O	1:E:207:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:6204:GLN:HB3	5:H:6204:GLN:HE21	1.68	0.43
5:F:7190:GLN:HG2	5:F:7216:TYR:OH	2.18	0.43
1:B:93:SER:O	5:F:7096:ASP:HB3	2.19	0.43
1:C:87:PRO:O	5:G:5035:ASN:ND2	2.52	0.43
1:C:141:ILE:C	1:C:143:GLY:N	2.76	0.43
1:D:67:VAL:O	1:D:67:VAL:HG12	2.17	0.43
1:D:96:SER:N	1:D:102:LYS:HE2	2.33	0.43
1:D:305:LEU:HD12	1:D:305:LEU:HA	1.84	0.43
5:H:6033:ALA:O	5:H:6035:ASN:N	2.51	0.43
5:H:6210:GLU:CG	5:H:6215:ASN:HD21	2.29	0.43
1:B:125:MET:CE	1:B:151:ARG:HG3	2.48	0.43
1:B:235:ILE:O	1:B:235:ILE:CG2	2.67	0.43
1:D:298:ALA:CB	1:E:293:GLN:HA	2.49	0.43
1:E:146:LYS:HE3	1:E:146:LYS:HB3	1.81	0.43
5:G:5010:LEU:O	5:G:5013:ASN:CB	2.64	0.43
5:H:6123:LEU:O	5:H:6124:GLN:C	2.62	0.43
5:H:6210:GLU:HA	5:H:6215:ASN:HD22	1.82	0.43
5:F:7007:THR:HG23	5:F:7044:ILE:HG21	2.00	0.43
1:B:57:THR:HG22	1:B:137:THR:CG2	2.34	0.43
1:E:272:ILE:HB	1:E:284:MET:HE3	2.01	0.43
2:I:26:DT:C2'	2:I:27:DC:OP2	2.61	0.43
4:A:68:ALA:HA	4:A:111:TRP:CZ2	2.53	0.43
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
5:H:6056:ASP:OD2	5:H:6059:GLY:CA	2.63	0.43
5:F:7126:LEU:HD12	5:F:7126:LEU:O	2.18	0.43
1:B:165:LYS:HG2	1:B:169:MET:HE2	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
1:B:29:ASP:HA	1:B:32:THR:CG2	2.49	0.43
1:C:231:ASP:C	1:C:233:GLY:H	2.27	0.43
1:C:276:VAL:CG2	1:C:280:SER:HB3	2.49	0.43
1:D:48:HIS:CE1	1:D:141:ILE:HG13	2.53	0.43
1:E:121:LEU:O	1:E:125:MET:HG3	2.19	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:G:5112:ALA:CB	5:G:5197:LEU:HD22	2.48	0.43
5:G:5153:ASN:C	5:G:5157:ASP:HB2	2.42	0.43
5:F:7121:GLU:HA	5:F:7124:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:HIS:ND1	1:B:141:ILE:CG1	2.82	0.42
1:B:192:VAL:HG22	1:B:225:LEU:CA	2.49	0.42
1:B:290:GLU:HB2	4:A:85:ILE:CD1	2.49	0.42
1:E:235:ILE:HA	1:E:235:ILE:HD13	1.67	0.42
5:H:6067:VAL:HG21	5:H:6083:ILE:HG21	2.00	0.42
5:F:7033:ALA:O	5:F:7034:VAL:C	2.62	0.42
5:F:7063:ILE:HD13	5:F:7063:ILE:HA	1.73	0.42
5:F:7064:LEU:CD2	5:F:7083:ILE:HD13	2.49	0.42
5:F:7189:MSE:HB2	5:F:7216:TYR:CD1	2.53	0.42
1:C:107:ASP:OD1	1:C:137:THR:HG21	2.19	0.42
1:C:272:ILE:CG2	1:C:284:MET:HE3	2.49	0.42
1:D:96:SER:HB3	1:D:102:LYS:HE2	2.01	0.42
1:E:83:PHE:CE2	1:E:88:LEU:CD1	3.03	0.42
4:A:127:LEU:HD23	4:A:127:LEU:HA	1.79	0.42
5:G:5105:LYS:CB	5:G:5106:PRO:CD	2.82	0.42
5:H:6003:LEU:HD22	5:H:6007:THR:CG2	2.46	0.42
1:B:86:GLY:HA3	1:B:87:PRO:HD3	1.67	0.42
1:B:176:LEU:CD2	1:B:211:LEU:HD22	2.48	0.42
1:C:192:VAL:HG22	1:C:225:LEU:CA	2.49	0.42
1:C:276:VAL:HG22	1:C:277:THR:N	2.34	0.42
1:D:272:ILE:HB	1:D:284:MET:CE	2.49	0.42
1:E:67:VAL:O	1:E:67:VAL:HG12	2.19	0.42
4:A:61:SER:CB	4:A:64:MET:HB2	2.38	0.42
5:F:7110:PRO:HB2	5:F:7199:TRP:CD1	2.55	0.42
1:B:141:ILE:C	1:B:143:GLY:N	2.76	0.42
1:D:13:GLN:NE2	1:E:126:GLU:HB3	2.34	0.42
1:E:251:ARG:O	1:E:251:ARG:NH1	2.48	0.42
1:E:305:LEU:HA	1:E:305:LEU:HD12	1.72	0.42
4:A:173:ASN:O	4:A:176:GLU:N	2.34	0.42
1:C:212:ASP:CB	1:D:153:ARG:NH1	2.82	0.42
1:D:71:MET:CE	1:D:73:PHE:HB2	2.46	0.42
4:A:173:ASN:OD1	4:A:175:LYS:HB3	2.20	0.42
5:G:5112:ALA:HB2	5:G:5197:LEU:HD22	2.02	0.42
1:C:49:SER:OG	1:C:50:PRO:CA	2.67	0.42
2:I:12:DA:OP2	2:I:12:DA:H2'	2.19	0.42
2:I:21:DT:O5'	2:I:21:DT:H2'	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
4:A:98:LEU:HD23	4:A:98:LEU:HA	1.89	0.42
5:H:6133:LEU:O	5:H:6133:LEU:HG	2.19	0.42
5:F:7196:LEU:C	5:F:7196:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PHE:CE2	1:C:88:LEU:CD1	3.03	0.42
5:G:5102:ALA:HA	5:G:5103:PRO:HD3	1.81	0.42
5:G:5119:LYS:O	5:G:5122:ASP:HB2	2.19	0.42
5:F:7189:MSE:HA	5:F:7216:TYR:CZ	2.54	0.42
1:B:13:GLN:HG3	1:B:16:ARG:HH11	1.85	0.42
1:B:247:VAL:O	1:B:248:LYS:C	2.62	0.42
1:D:17:PRO:HG2	6:D:700:08T:C2	2.50	0.42
1:D:29:ASP:HA	1:D:32:THR:HG22	2.01	0.42
1:D:72:MET:HG3	5:H:6155:VAL:O	2.19	0.42
2:I:8:DT:C1'	4:A:109:GLY:HA2	2.50	0.42
5:G:5010:LEU:CD1	5:G:5190:GLN:CD	2.93	0.42
5:G:5055:TYR:HB2	5:G:5095:ALA:CB	2.49	0.42
5:H:6175:GLU:C	5:H:6176:ASN:HD22	2.27	0.42
5:H:6198:LEU:CD2	5:H:6207:ALA:HB1	2.49	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
1:E:201:PHE:O	1:E:201:PHE:CD1	2.72	0.42
4:A:159:LYS:HD3	4:A:187:TRP:NE1	2.34	0.42
5:G:5126:LEU:HD13	5:G:5165:TYR:HE2	1.83	0.42
1:B:297:ILE:HG22	1:C:295:HIS:O	2.20	0.41
1:D:48:HIS:NE2	1:D:156:THR:HB	2.35	0.41
1:D:141:ILE:C	1:D:143:GLY:N	2.78	0.41
1:D:145:ILE:HG13	1:D:147:PRO:HD2	2.02	0.41
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
4:A:178:LYS:HB3	4:A:178:LYS:HE3	1.83	0.41
5:G:5097:PRO:C	5:G:5099:THR:N	2.77	0.41
5:F:7021:ILE:HG12	5:F:7022:MSE:N	2.35	0.41
5:F:7068:ASN:O	5:F:7069:ASP:C	2.62	0.41
5:F:7113:SER:HB3	5:F:7228:PHE:CZ	2.55	0.41
1:C:146:LYS:HB3	1:C:146:LYS:HE3	1.85	0.41
1:D:111:ARG:CZ	1:E:116:GLU:HG3	2.50	0.41
2:I:27:DC:H2''	2:I:28:DT:C5	2.55	0.41
4:A:86:GLY:O	4:A:87:SER:C	2.61	0.41
4:A:147:LYS:O	4:A:147:LYS:CG	2.68	0.41
4:A:164:ASP:CB	4:A:167:LEU:HD12	2.50	0.41
5:H:6032:ARG:HH11	5:H:6036:GLY:HA2	1.84	0.41
5:F:7123:LEU:HG	5:F:7127:LEU:HD11	2.01	0.41
1:B:250:LEU:HD13	1:B:309:PHE:HB3	2.01	0.41
1:C:139:ASN:HD22	1:D:147:PRO:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ILE:HG22	1:C:149:GLN:NE2	2.36	0.41
1:E:85:ARG:O	1:E:89:THR:HB	2.20	0.41
1:E:141:ILE:C	1:E:143:GLY:N	2.77	0.41
1:E:250:LEU:HD13	1:E:309:PHE:HB3	2.02	0.41
4:A:105:GLY:O	4:A:106:LYS:HB2	2.20	0.41
1:B:108:GLU:HG3	1:C:122:ARG:HG3	2.01	0.41
4:A:157:GLU:HA	5:H:6096:ASP:HB2	2.03	0.41
4:A:163:THR:HG23	5:H:6055:TYR:HD2	1.85	0.41
5:G:5040:ALA:HB2	5:G:5216:TYR:HD1	1.80	0.41
5:G:5189:MSE:O	5:G:5189:MSE:HG2	2.19	0.41
5:H:6018:ASN:HB3	5:H:6020:GLY:O	2.20	0.41
5:H:6023:LEU:CB	5:H:6029:ILE:HG22	2.49	0.41
5:H:6153:ASN:HD22	5:H:6164:LYS:NZ	2.18	0.41
5:F:7136:ASP:C	5:F:7136:ASP:OD1	2.64	0.41
1:B:67:VAL:O	1:B:67:VAL:CG1	2.69	0.41
1:C:48:HIS:CG	1:C:141:ILE:HD11	2.51	0.41
1:C:241:SER:OG	1:C:249:GLN:HG2	2.20	0.41
1:D:131:ASN:ND2	5:G:5096:ASP:OD2	2.31	0.41
1:E:57:THR:CG2	1:E:107:ASP:OD1	2.68	0.41
1:E:141:ILE:HD13	1:E:141:ILE:HG23	1.70	0.41
1:E:235:ILE:O	1:E:235:ILE:CG2	2.69	0.41
1:E:251:ARG:HA	1:E:251:ARG:HD2	1.82	0.41
1:E:283:ARG:CZ	1:E:315:GLU:OE1	2.68	0.41
5:F:7027:GLN:O	5:F:7043:ASN:HA	2.20	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:173:ASN:C	4:A:176:GLU:HG2	2.32	0.41
5:F:7121:GLU:CD	5:F:7121:GLU:H	2.28	0.41
1:B:279:GLN:O	1:B:282:ILE:HG22	2.20	0.41
1:D:141:ILE:HG23	1:D:141:ILE:HD13	1.77	0.41
1:D:272:ILE:O	1:D:273:TYR:C	2.64	0.41
4:A:53:CYS:O	4:A:54:SER:CB	2.68	0.41
5:G:5130:SER:HA	5:G:5135:ILE:HB	2.02	0.41
5:G:5138:ILE:CD1	5:G:5187:MSE:HE2	2.50	0.41
5:G:5163:VAL:CG1	5:G:5165:TYR:O	2.69	0.41
5:H:6105:LYS:HB3	5:H:6107:ILE:CG1	2.50	0.41
5:H:6155:VAL:HG13	5:H:6156:GLU:H	1.86	0.41
5:H:6190:GLN:O	5:H:6191:PRO:O	2.39	0.41
5:F:7024:LYS:HG2	5:F:7051:ASP:OD2	2.19	0.41
5:F:7123:LEU:HD23	5:F:7191:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.71	0.41
1:C:67:VAL:O	1:C:67:VAL:CG1	2.69	0.41
1:C:67:VAL:O	1:C:67:VAL:HG12	2.20	0.41
1:D:34:LYS:HD2	1:D:34:LYS:HA	1.86	0.41
1:D:67:VAL:O	1:D:67:VAL:CG1	2.68	0.41
5:H:6027:GLN:HE21	5:H:6047:VAL:HB	1.83	0.41
5:F:7052:VAL:HG21	5:F:7081:ILE:HD11	2.02	0.41
5:F:7167:LEU:HD12	5:F:7168:THR:N	2.36	0.41
1:B:67:VAL:O	1:B:67:VAL:HG12	2.21	0.41
1:B:254:ALA:HB3	1:B:255:PRO:CD	2.51	0.41
1:D:29:ASP:O	1:D:32:THR:HG23	2.20	0.41
1:E:205:ARG:NH2	8:E:700:ADP:O2A	2.54	0.41
4:A:75:CYS:C	4:A:77:PRO:HD2	2.45	0.41
4:A:157:GLU:CD	5:H:6096:ASP:OD2	2.63	0.41
5:G:5024:LYS:HG2	5:G:5051:ASP:CG	2.46	0.41
5:G:5125:GLN:O	5:G:5125:GLN:HG2	2.20	0.41
5:H:6150:ASN:HA	5:H:6165:TYR:O	2.21	0.41
1:B:118:GLN:OE1	1:B:145:ILE:HG23	2.21	0.41
1:B:246:ASP:OD1	1:B:246:ASP:C	2.64	0.41
1:C:71:MET:CE	1:C:73:PHE:HB2	2.44	0.41
1:D:263:TRP:CZ2	1:D:267:LYS:HG3	2.56	0.41
1:D:297:ILE:HG21	1:E:297:ILE:CG1	2.49	0.41
1:E:4:VAL:HG12	1:E:15:TYR:CE1	2.56	0.41
1:E:279:GLN:O	1:E:282:ILE:HG22	2.22	0.41
5:H:6071:ALA:O	5:H:6073:ILE:N	2.54	0.41
5:H:6195:LYS:HB3	5:H:6210:GLU:CB	2.51	0.41
1:E:96:SER:N	1:E:102:LYS:HE2	2.36	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:C:48:HIS:CE1	1:C:141:ILE:HG13	2.56	0.40
1:C:93:SER:HB3	1:C:128:TYR:HE2	1.86	0.40
1:D:13:GLN:HG3	1:D:16:ARG:NH1	2.37	0.40
5:H:6208:LYS:CA	5:H:6217:VAL:HG22	2.48	0.40
5:F:7188:LYS:HD3	5:F:7188:LYS:HA	1.95	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:72:MET:HE1	5:G:5035:ASN:CB	2.52	0.40
1:C:85:ARG:O	1:C:89:THR:HB	2.22	0.40
1:C:141:ILE:C	1:C:143:GLY:H	2.28	0.40
1:D:201:PHE:O	1:D:202:PRO:C	2.64	0.40
1:D:297:ILE:HG23	1:E:297:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:15:DT:H2''	3:J:16:DA:C5'	2.51	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:B:165:LYS:HE3	1:B:169:MET:HE2	2.03	0.40
1:C:96:SER:N	1:C:102:LYS:HE2	2.37	0.40
1:C:97:PHE:C	5:G:5204:GLN:HA	2.46	0.40
1:C:169:MET:HG2	1:C:197:VAL:CG1	2.52	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
1:E:145:ILE:HG13	1:E:147:PRO:HD2	2.03	0.40
4:A:163:THR:HG23	5:H:6055:TYR:CD2	2.57	0.40
1:B:232:ARG:HD2	1:B:232:ARG:HA	1.93	0.40
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.89	0.40
1:C:169:MET:HG2	1:C:197:VAL:HG12	2.03	0.40
1:D:238:VAL:O	1:D:242:LEU:HG	2.22	0.40
1:E:107:ASP:HA	1:E:137:THR:HB	2.03	0.40
1:E:307:TYR:HD2	4:A:80:TYR:CE1	2.36	0.40
5:G:5008:THR:O	5:G:5009:ALA:C	2.64	0.40
5:H:6198:LEU:CD2	5:H:6207:ALA:HB2	2.50	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%)	36	65
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%)	7	32
5	F	226/228 (99%)	179 (79%)	44 (20%)	3 (1%)	9	35
5	G	226/228 (99%)	183 (81%)	40 (18%)	3 (1%)	9	35
5	H	226/228 (99%)	184 (81%)	35 (16%)	7 (3%)	3	20
All	All	2115/2175 (97%)	1913 (90%)	185 (9%)	17 (1%)	16	46

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%)	257 (93%)	20 (7%)	13	40
1	C	278/279 (100%)	254 (91%)	24 (9%)	10	34
1	D	276/279 (99%)	254 (92%)	22 (8%)	11	37
1	E	266/279 (95%)	241 (91%)	25 (9%)	8	31
4	A	161/170 (95%)	134 (83%)	27 (17%)	2	10
5	F	189/183 (103%)	184 (97%)	5 (3%)	40	63
5	G	189/183 (103%)	178 (94%)	11 (6%)	18	47
5	H	189/183 (103%)	178 (94%)	11 (6%)	18	47
All	All	1825/1835 (100%)	1680 (92%)	145 (8%)	11	37

All (145) 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	88	LEU
1	B	98	ASP
1	B	124	PHE
1	B	137	THR
1	B	141	ILE
1	B	200	ASN
1	B	235	ILE
1	B	260	ASP
1	B	265	VAL
1	B	271	GLU
1	B	272	ILE
1	B	277	THR
1	B	284	MET
1	B	303	LEU
1	B	310	ILE
1	C	4	VAL
1	C	12	GLU
1	C	20	ILE
1	C	38	SER
1	C	57	THR
1	C	58	THR
1	C	80	LYS

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Mol	Chain	Res	Type
1	C	88	LEU
1	C	97	PHE
1	C	98	ASP
1	C	112	SER
1	C	116	GLU
1	C	124	PHE
1	C	129	SER
1	C	132	CYS
1	C	137	THR
1	C	141	ILE
1	C	200	ASN
1	C	265	VAL
1	C	272	ILE
1	C	284	MET
1	C	305	LEU
1	C	310	ILE
1	C	317	GLN
1	D	4	VAL
1	D	12	GLU
1	D	20	ILE
1	D	32	THR
1	D	38	SER
1	D	57	THR
1	D	58	THR
1	D	88	LEU
1	D	97	PHE
1	D	98	ASP
1	D	112	SER
1	D	132	CYS
1	D	137	THR
1	D	141	ILE
1	D	200	ASN
1	D	213	SER
1	D	265	VAL
1	D	271	GLU
1	D	272	ILE
1	D	284	MET
1	D	305	LEU
1	D	310	ILE
1	E	8	GLU
1	E	10	ILE
1	E	20	ILE

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Mol	Chain	Res	Type
1	E	38	SER
1	E	57	THR
1	E	58	THR
1	E	71	MET
1	E	80	LYS
1	E	88	LEU
1	E	97	PHE
1	E	98	ASP
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	220	LEU
1	E	235	ILE
1	E	265	VAL
1	E	271	GLU
1	E	272	ILE
1	E	277	THR
1	E	284	MET
1	E	310	ILE
4	A	3	LEU
4	A	8	ILE
4	A	12	GLU
4	A	25	VAL
4	A	26	GLN
4	A	32	PHE
4	A	52	LYS
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	126	LEU
4	A	134	ASN
4	A	139	ILE
4	A	144	ILE
4	A	145	LEU
4	A	147	LYS

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Mol	Chain	Res	Type
4	A	150	LYS
4	A	151	LEU
4	A	153	LEU
4	A	158	LEU
4	A	161	LEU
4	A	163	THR
4	A	186	GLU
5	G	5021	ILE
5	G	5044	ILE
5	G	5051	ASP
5	G	5052	VAL
5	G	5054	ILE
5	G	5063	ILE
5	G	5067	VAL
5	G	5118	ILE
5	G	5149	ILE
5	G	5182	ILE
5	G	5187	MSE
5	H	6029	ILE
5	H	6107	ILE
5	H	6111	VAL
5	H	6113	SER
5	H	6116	THR
5	H	6137	THR
5	H	6163	VAL
5	H	6187	MSE
5	H	6189	MSE
5	H	6218	VAL
5	H	6225	THR
5	F	7007	THR
5	F	7038	THR
5	F	7052	VAL
5	F	7063	ILE
5	F	7149	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	GLN
1	B	292	ASN
1	B	311	GLN
1	C	13	GLN

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Mol	Chain	Res	Type
1	C	139	ASN
1	C	230	ASN
1	C	293	GLN
1	C	311	GLN
1	D	13	GLN
1	D	295	HIS
1	D	311	GLN
1	E	140	ASN
1	E	159	GLN
1	E	295	HIS
1	E	311	GLN
4	A	13	HIS
4	A	26	GLN
4	A	96	ASN
4	A	179	GLN
5	G	5186	ASN
5	G	5215	ASN
5	H	6018	ASN
5	H	6027	GLN
5	H	6043	ASN
5	H	6068	ASN
5	H	6153	ASN
5	H	6176	ASN
5	H	6204	GLN
5	H	6215	ASN
5	F	7068	ASN
5	F	7104	ASN
5	F	7134	GLN
5	F	7153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
8	ADP	E	700	7	28,29,29	1.42	4 (14%)	43,45,45	1.87	9 (20%)
6	08T	B	700	7	31,33,33	1.84	9 (29%)	41,52,52	2.10	10 (24%)
6	08T	D	700	7	31,33,33	2.05	9 (29%)	41,52,52	2.11	11 (26%)
6	08T	C	700	7	31,33,33	1.95	9 (29%)	41,52,52	2.06	12 (29%)

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
8	ADP	E	700	7	-	3/16/32/32	0/3/3/3
6	08T	B	700	7	-	5/16/38/38	0/3/3/3
6	08T	D	700	7	-	0/16/38/38	0/3/3/3
6	08T	C	700	7	-	6/16/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	700	08T	PB-O3A	-4.91	1.54	1.59
8	E	700	ADP	C5-C4	4.85	1.47	1.39
6	D	700	08T	C2'-C3'	-4.32	1.41	1.53
6	C	700	08T	C2'-C3'	-4.20	1.42	1.53
6	B	700	08T	C2'-C3'	-4.05	1.42	1.53
6	C	700	08T	C6-N6	4.03	1.44	1.34
6	D	700	08T	C6-N6	3.93	1.44	1.34
6	D	700	08T	F2-BE	-3.75	1.45	1.54
6	B	700	08T	F2-BE	-3.71	1.45	1.54
6	C	700	08T	F2-BE	-3.67	1.45	1.54
6	C	700	08T	PB-O3A	-3.41	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	700	08T	PB-O3A	-3.37	1.55	1.59
6	B	700	08T	C6-N6	3.25	1.42	1.34
6	B	700	08T	C5-N7	-3.11	1.33	1.39
8	E	700	ADP	C5-C6	3.03	1.49	1.41
6	C	700	08T	C5-N7	-3.01	1.33	1.39
6	C	700	08T	C8-N9	-2.89	1.32	1.37
6	D	700	08T	O4'-C4'	-2.80	1.38	1.45
6	D	700	08T	C8-N9	-2.75	1.32	1.37
6	D	700	08T	C5-N7	-2.73	1.34	1.39
6	B	700	08T	C8-N9	-2.73	1.32	1.37
6	C	700	08T	O4'-C4'	-2.67	1.39	1.45
6	B	700	08T	O4'-C4'	-2.64	1.39	1.45
6	C	700	08T	C2'-C1'	-2.40	1.45	1.53
6	D	700	08T	C3'-C4'	-2.35	1.47	1.53
6	C	700	08T	C3'-C4'	-2.35	1.47	1.53
6	D	700	08T	C2'-C1'	-2.23	1.46	1.53
8	E	700	ADP	C8-N7	2.14	1.35	1.31
8	E	700	ADP	C4-N9	-2.09	1.33	1.37
6	B	700	08T	C3'-C4'	-2.08	1.47	1.53
6	B	700	08T	C2'-C1'	-2.07	1.47	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	700	08T	C5-C4-N3	-6.32	118.02	126.72
8	E	700	ADP	C5-C4-N3	-6.24	118.13	126.72
6	B	700	08T	C5-C4-N3	-5.77	118.77	126.72
6	B	700	08T	N3-C2-N1	-5.60	120.10	128.58
6	D	700	08T	N3-C2-N1	-4.89	121.18	128.58
6	C	700	08T	N3-C4-N9	4.84	135.41	127.17
8	E	700	ADP	N3-C4-N9	4.63	135.05	127.17
6	D	700	08T	C5-C4-N3	-4.48	120.55	126.72
6	D	700	08T	C2'-C1'-N9	-4.36	102.46	113.30
6	D	700	08T	N9-C8-N7	-4.32	107.81	113.94
6	C	700	08T	N3-C2-N1	-4.26	122.13	128.58
6	D	700	08T	C4-N9-C8	4.11	110.05	105.74
6	B	700	08T	N3-C4-N9	4.06	134.07	127.17
6	B	700	08T	C2-N3-C4	4.03	121.68	111.83
6	D	700	08T	N3-C4-N9	3.91	133.82	127.17
8	E	700	ADP	C2-N3-C4	3.73	120.95	111.83
6	B	700	08T	N9-C8-N7	-3.64	108.77	113.94
6	C	700	08T	C2-N3-C4	3.60	120.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	700	08T	C5-N7-C8	3.57	109.06	103.45
6	D	700	08T	C5-N7-C8	3.53	108.99	103.45
8	E	700	ADP	C4-C5-N7	-3.32	106.79	110.58
6	B	700	08T	C4-C5-N7	-3.22	106.90	110.58
6	C	700	08T	C5-N7-C8	3.19	108.46	103.45
8	E	700	ADP	C3'-C2'-C1'	3.08	107.29	101.46
6	D	700	08T	C2-N3-C4	2.99	119.14	111.83
6	C	700	08T	C4-C5-N7	-2.95	107.21	110.58
6	C	700	08T	N9-C8-N7	-2.88	109.86	113.94
6	D	700	08T	C4-C5-N7	-2.68	107.52	110.58
6	B	700	08T	C2'-C1'-N9	-2.54	107.00	113.30
8	E	700	ADP	O3'-C3'-C4'	-2.51	103.87	111.08
6	C	700	08T	C3'-C2'-C1'	2.36	105.94	101.46
8	E	700	ADP	O3B-PB-O2B	2.36	116.66	107.80
6	D	700	08T	O5'-C5'-C4'	2.31	116.86	108.99
6	C	700	08T	C1'-N9-C8	-2.28	122.03	127.09
6	C	700	08T	C6-C5-C4	2.27	120.28	117.18
6	B	700	08T	C4-N9-C8	2.24	108.09	105.74
8	E	700	ADP	N3-C2-N1	-2.15	125.33	128.58
6	B	700	08T	O5'-C5'-C4'	2.13	116.26	108.99
8	E	700	ADP	O2A-PA-O1A	2.12	122.29	112.44
6	D	700	08T	N6-C6-N1	2.09	123.03	118.38
6	C	700	08T	C4-N9-C8	2.06	107.90	105.74
6	C	700	08T	C2'-C3'-C4'	2.03	106.53	102.61

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	700	08T	C5'-O5'-PA-O2A
6	B	700	08T	C5'-O5'-PA-O3A
6	C	700	08T	C5'-O5'-PA-O1A
6	C	700	08T	C5'-O5'-PA-O2A
6	C	700	08T	C5'-O5'-PA-O3A
8	E	700	ADP	C5'-O5'-PA-O2A
6	C	700	08T	O4'-C4'-C5'-O5'
6	C	700	08T	C3'-C4'-C5'-O5'
6	C	700	08T	PA-O3A-PB-O1B
8	E	700	ADP	C3'-C4'-C5'-O5'
6	B	700	08T	C5'-O5'-PA-O1A
6	B	700	08T	PA-O3A-PB-O1B
8	E	700	ADP	O4'-C4'-C5'-O5'

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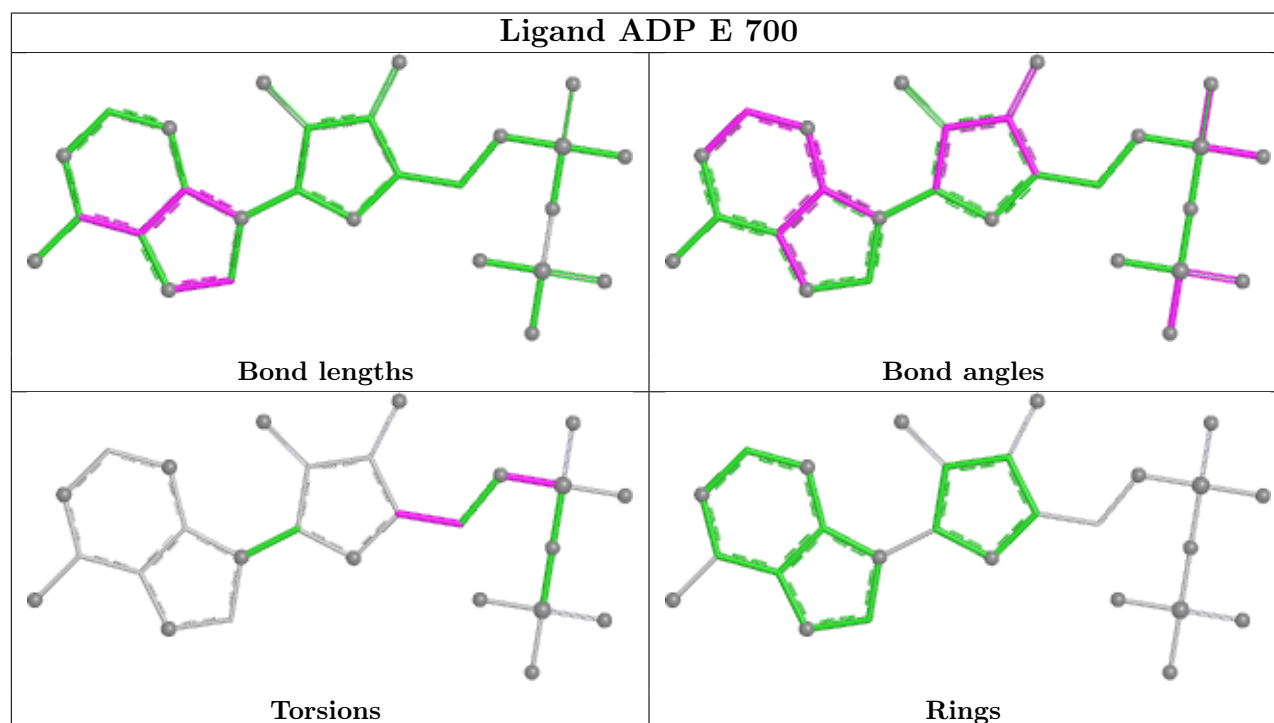
Mol	Chain	Res	Type	Atoms
6	B	700	08T	PA-O3A-PB-O2B

There are no ring outliers.

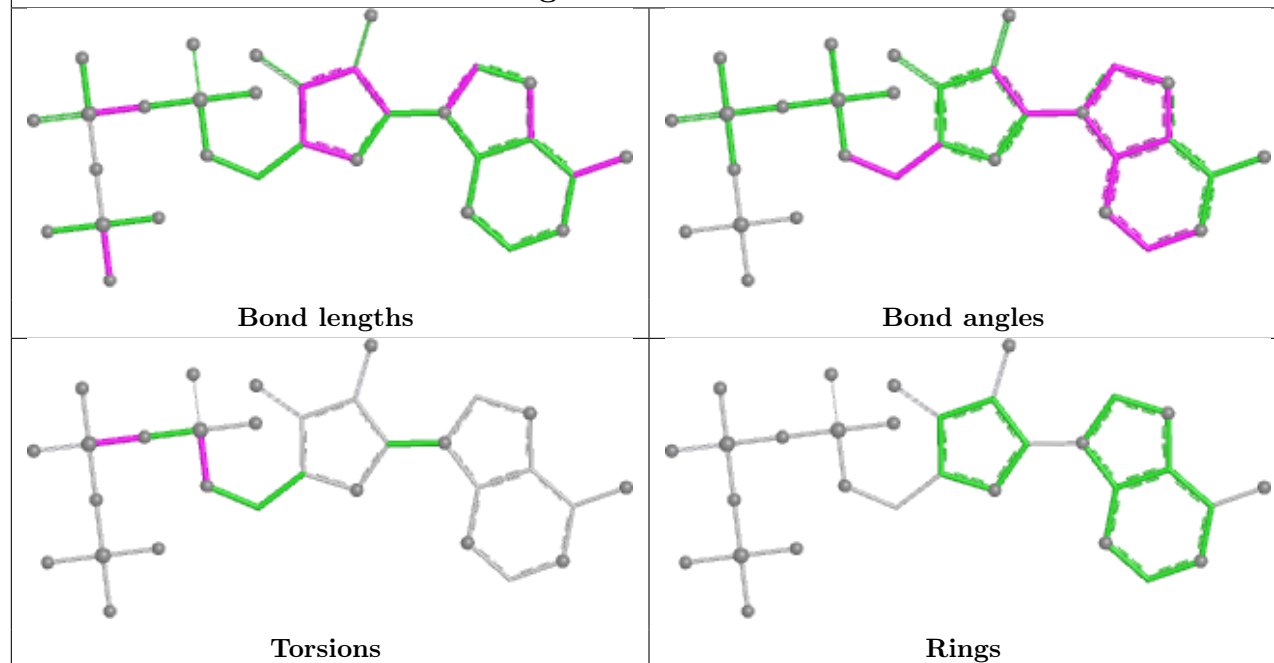
4 monomers are involved in 17 short contacts:

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

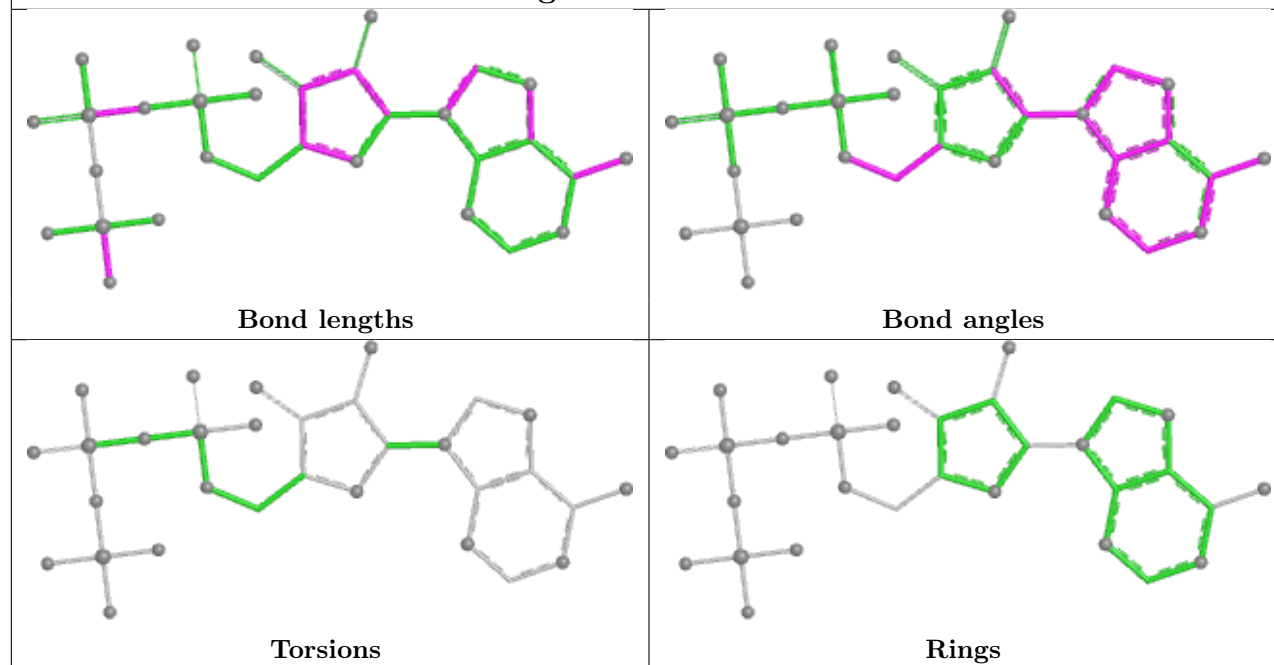
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

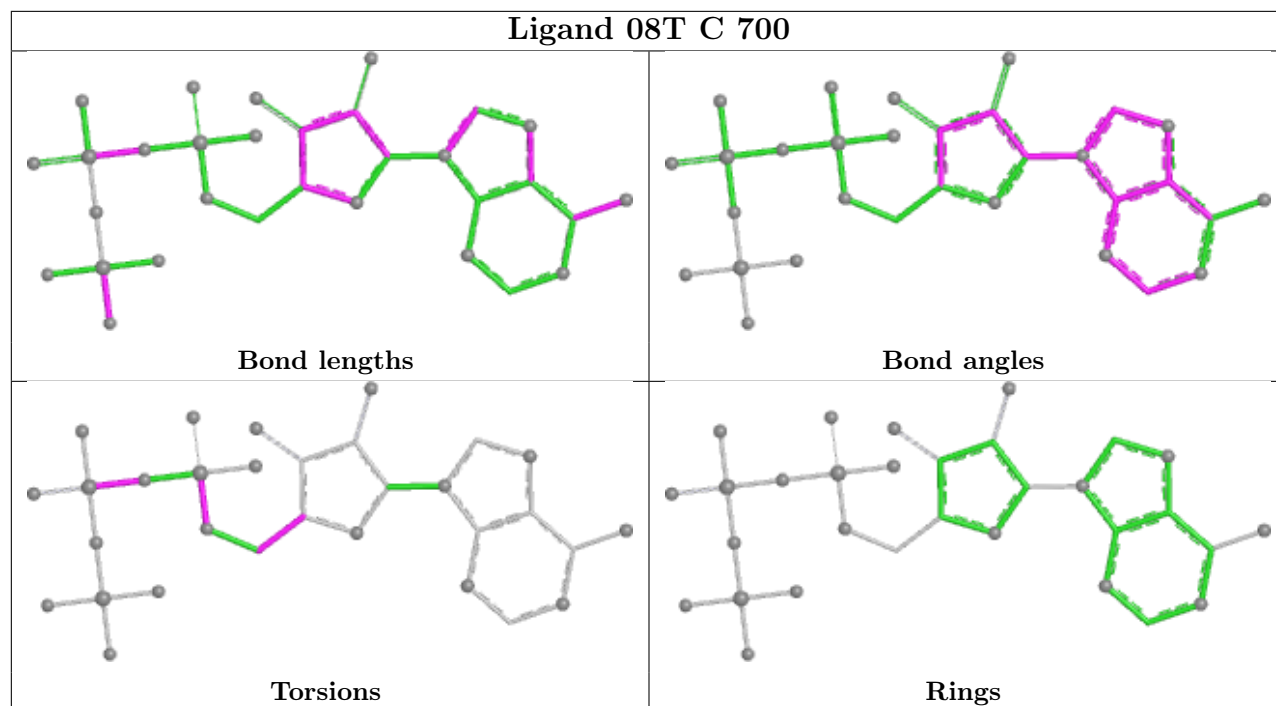


Ligand 08T B 700



Ligand 08T D 700





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	319/324 (98%)	0.40	16 (5%) 34 23	24, 54, 94, 158	0
1	C	320/324 (98%)	0.16	6 (1%) 66 48	26, 45, 82, 131	0
1	D	319/324 (98%)	0.16	12 (3%) 44 30	25, 48, 95, 170	0
1	E	305/324 (94%)	0.67	30 (9%) 13 11	31, 63, 110, 185	0
2	I	24/30 (80%)	0.18	1 (4%) 40 26	35, 66, 216, 261	0
3	J	20/20 (100%)	0.43	0 100 100	54, 92, 235, 258	0
4	A	186/195 (95%)	0.25	6 (3%) 50 34	29, 70, 122, 157	0
5	F	222/228 (97%)	0.84	13 (5%) 28 19	76, 129, 172, 202	0
5	G	222/228 (97%)	0.75	12 (5%) 31 21	54, 80, 121, 136	0
5	H	222/228 (97%)	1.04	25 (11%) 10 9	67, 99, 147, 185	0
All	All	2159/2225 (97%)	0.50	121 (5%) 30 21	24, 66, 146, 261	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	5036	GLY	6.1
1	E	112	SER	5.7
1	B	120	HIS	5.5
1	E	110	ASP	5.5
1	E	214	TYR	4.5
1	E	211	LEU	4.4
1	E	111	ARG	4.3
1	D	231	ASP	4.3
1	B	131	ASN	4.1
1	E	159	GLN	4.0
1	B	96	SER	3.9
1	E	143	GLY	3.8
1	E	158	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	131	ASN	3.8
1	B	231	ASP	3.8
1	D	131	ASN	3.7
5	G	5140	ILE	3.7
1	B	97	PHE	3.6
5	G	5058	ASN	3.6
5	H	6023	LEU	3.6
5	F	7029	ILE	3.6
1	E	192	VAL	3.4
5	F	7055	TYR	3.4
1	B	293	GLN	3.4
1	C	231	ASP	3.3
1	B	95	ALA	3.2
1	D	232	ARG	3.2
1	B	1	MET	3.2
1	E	26	PRO	3.2
1	E	28	PHE	3.1
1	B	93	SER	3.1
1	E	220	LEU	3.1
5	H	6190	GLN	3.0
1	E	234	ALA	3.0
1	E	113	GLY	3.0
5	G	5035	ASN	3.0
1	D	8	GLU	2.9
1	C	97	PHE	2.9
5	F	7123	LEU	2.8
5	H	6054	ILE	2.8
5	H	6045	SER	2.7
1	C	131	ASN	2.7
5	H	6034	VAL	2.7
1	D	153	ARG	2.6
1	E	97	PHE	2.6
1	E	300	ASN	2.6
5	H	6132	GLY	2.6
1	D	92	ALA	2.6
5	H	6155	VAL	2.6
5	H	6127	LEU	2.6
5	H	6060	PHE	2.5
1	B	18	SER	2.5
1	E	56	LYS	2.5
4	A	54	SER	2.5
4	A	179	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	2	ILE	2.5
1	C	93	SER	2.5
1	E	303	LEU	2.5
1	E	140	ASN	2.4
5	H	6058	ASN	2.4
1	B	49	SER	2.4
1	B	123	SER	2.4
1	B	215	SER	2.4
5	G	5014	PHE	2.4
5	H	6221	GLU	2.4
1	D	49	SER	2.4
1	E	156	THR	2.3
1	B	92	ALA	2.3
1	B	299	ALA	2.3
5	H	6114	ALA	2.3
1	D	93	SER	2.3
5	F	7222	ALA	2.3
1	C	1	MET	2.3
5	H	6191	PRO	2.3
5	F	7107	ILE	2.3
5	F	7182	ILE	2.3
1	E	115	ALA	2.3
4	A	53	CYS	2.3
1	E	157	PHE	2.3
4	A	2	SER	2.3
1	D	260	ASP	2.3
5	H	6218	VAL	2.3
5	G	5151	GLY	2.2
5	H	6011	LEU	2.2
5	H	6031	THR	2.2
1	E	27	ALA	2.2
4	A	186	GLU	2.2
5	G	5093	PRO	2.2
5	F	7014	PHE	2.2
5	G	5074	SER	2.2
5	F	7138	ILE	2.2
1	D	230	ASN	2.2
5	F	7068	ASN	2.2
5	H	6116	THR	2.2
5	H	6142	VAL	2.2
1	E	20	ILE	2.2
1	B	284	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	142	ASP	2.2
5	H	6171	ASP	2.2
5	G	5037	THR	2.1
1	E	196	LEU	2.1
1	E	90	ASN	2.1
5	G	5161	THR	2.1
5	F	7021	ILE	2.1
5	G	5101	VAL	2.1
5	F	7056	ASP	2.1
5	H	6063	ILE	2.1
5	H	6115	VAL	2.1
5	H	6196	LEU	2.1
5	F	7010	LEU	2.1
1	C	233	GLY	2.1
5	H	6109	PHE	2.1
4	A	185	LEU	2.0
5	F	7122	ASP	2.0
1	D	296	GLY	2.0
5	H	6101	VAL	2.0
1	E	282	ILE	2.0
1	D	259	ALA	2.0
2	I	30	DC	2.0
5	G	5142	VAL	2.0
5	H	6117	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

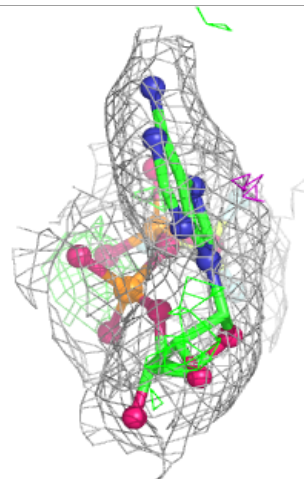
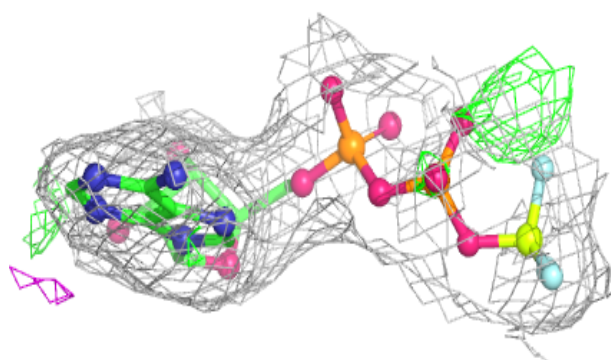
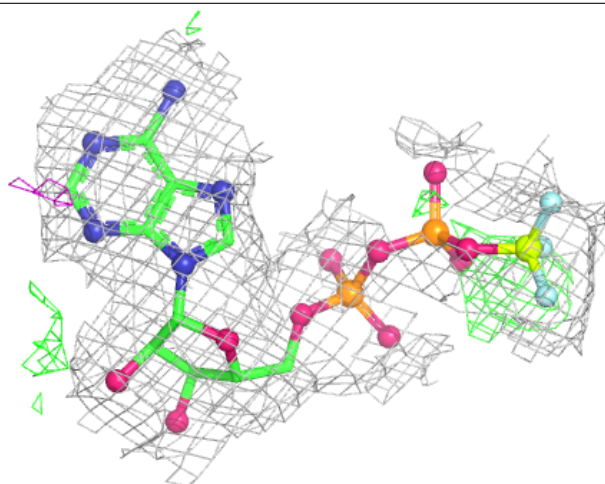
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	E	801	1/1	0.86	0.23	47,47,47,47	0
7	MG	D	800	1/1	0.87	0.24	47,47,47,47	0
7	MG	C	800	1/1	0.89	0.24	47,47,47,47	0
7	MG	B	800	1/1	0.94	0.20	47,47,47,47	0
6	08T	C	700	31/31	0.96	0.08	47,47,48,48	0
6	08T	D	700	31/31	0.96	0.08	47,47,48,48	0
6	08T	B	700	31/31	0.96	0.07	47,47,48,48	0
8	ADP	E	700	27/27	0.96	0.08	47,47,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

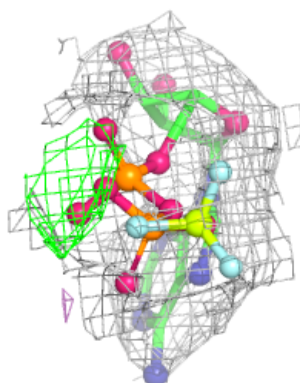
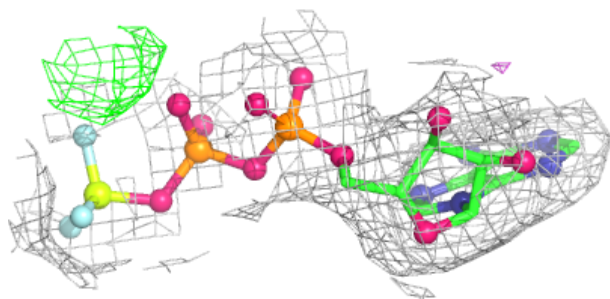
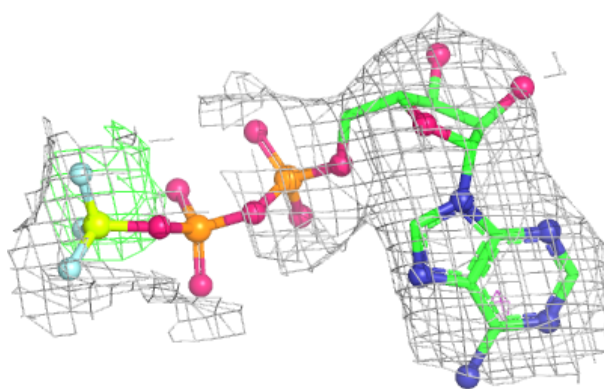
Electron density around 08T C 700:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

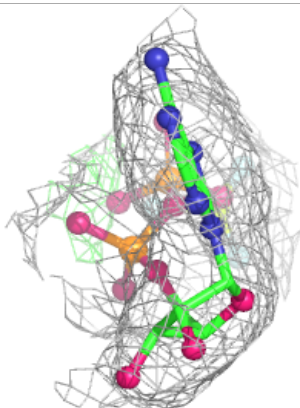
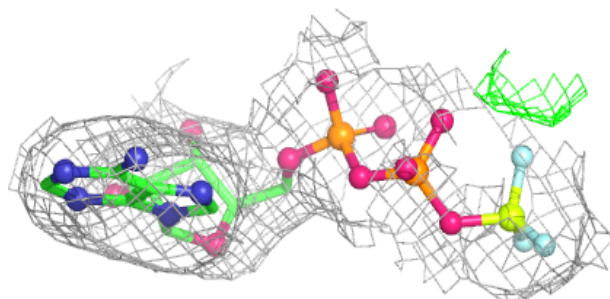
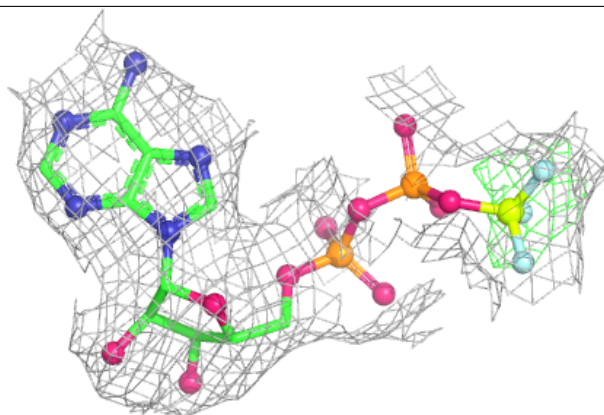


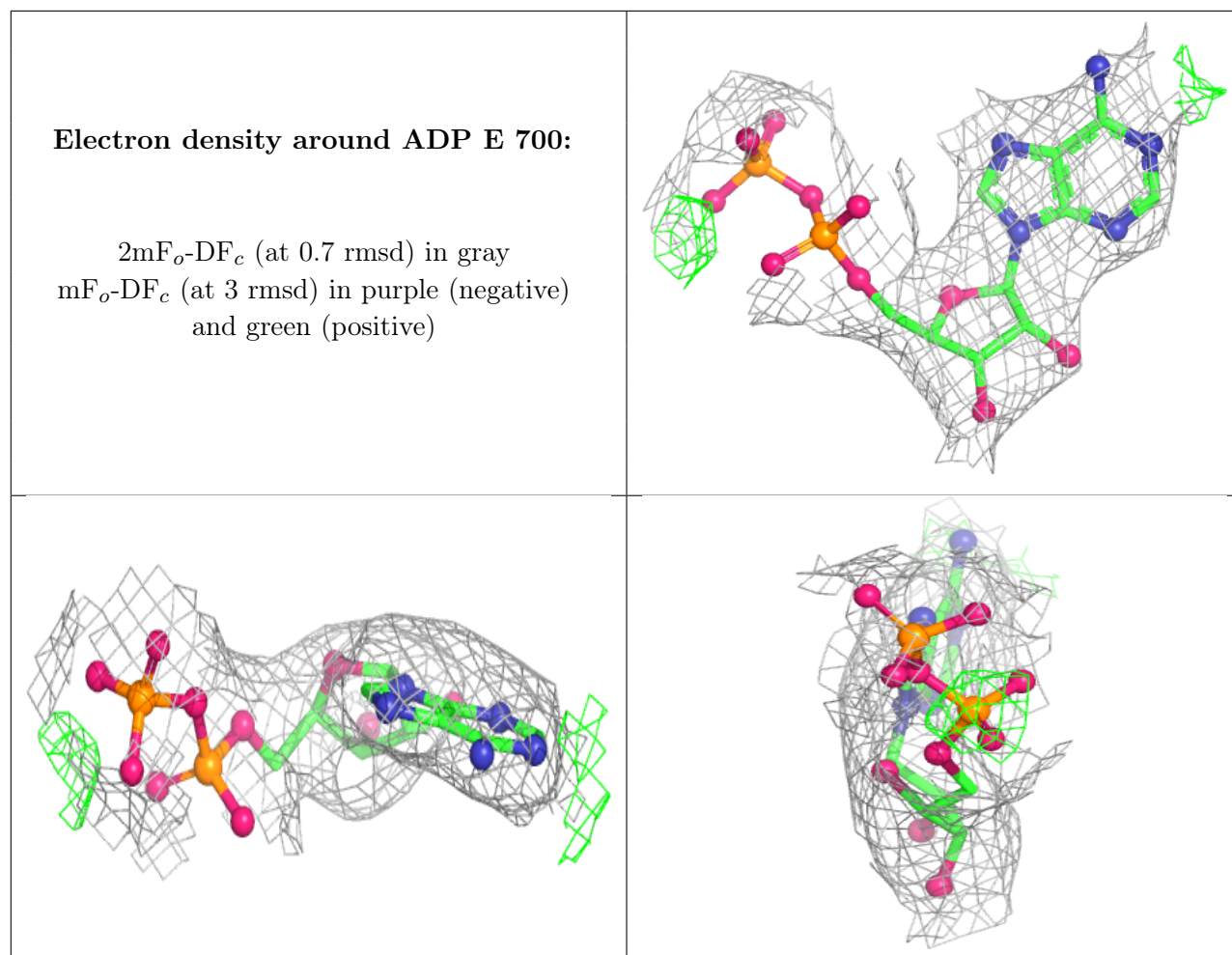
Electron density around 08T D 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 08T B 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.