



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:57 am BST

PDB ID : 5XJ0
Title : T. thermophilus RNA polymerase holoenzyme bound with gp39 and gp76
Authors : Ooi, W.Y.; Murayama, Y.; Mekler, V.; Minakhin, L.; Severinov, K.;
Yokoyama, S.; Sekine, S.
Deposited on : 2017-04-28
Resolution : 4.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

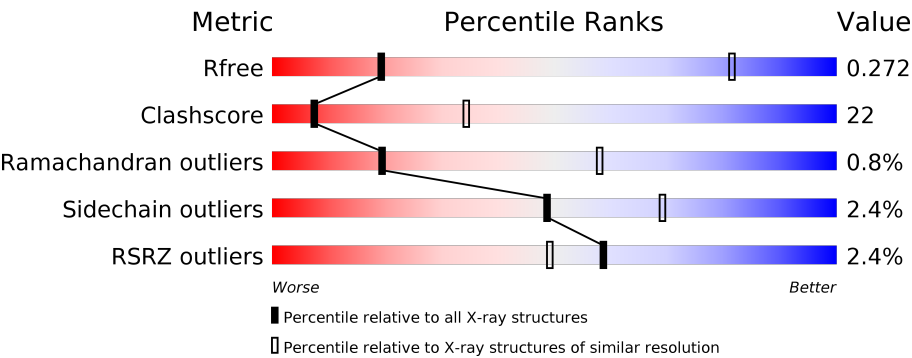
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	A	315	<div><div></div><div><div>43%</div><div>25%</div><div>..</div><div>29%</div></div></div>
1	B	315	<div><div></div><div><div>47%</div><div>26%</div><div>.</div><div>26%</div></div></div>
2	C	1119	<div><div>2%</div><div><div>54%</div><div>42%</div><div>..</div></div></div>
3	D	1524	<div><div>3%</div><div><div>54%</div><div>40%</div><div>...</div></div></div>
4	E	99	<div><div>3%</div><div><div>59%</div><div>29%</div><div>7%</div><div>..</div></div></div>
5	F	423	<div><div>3%</div><div><div>44%</div><div>28%</div><div>..</div><div>26%</div></div></div>

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Mol	Chain	Length	Quality of chain
6	G	144	<p>3% 65% 22% •• 12%</p>
6	H	144	<p>9% 40% 22% • 37%</p>
7	Y	54	<p>59% • 37%</p>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29177 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1772	1132	308	330	2			
1	B	232	Total	C	N	O	S	0	0	0
			1814	1158	316	338	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1114	Total	C	N	O	S	0	0	0
			8789	5557	1568	1640	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1462	Total	C	N	O	S	0	0	0
			11543	7322	2030	2159	32			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	313	Total	C	N	O	S	0	0	0
			2530	1600	456	471	3			

- Molecule 6 is a protein called gp39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	127	Total	C	N	O	S	0	0	0
			1035	673	175	184	3			
6	H	91	Total	C	N	O	S	0	0	0
			752	495	125	131	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP A7XX65
G	-1	SER	-	expression tag	UNP A7XX65
G	0	HIS	-	expression tag	UNP A7XX65
H	-2	GLY	-	expression tag	UNP A7XX65
H	-1	SER	-	expression tag	UNP A7XX65
H	0	HIS	-	expression tag	UNP A7XX65

- Molecule 7 is a protein called gp76.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	Y	34	Total	C	N	O	0	0	0
			171	103	34	34			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	GLY	-	expression tag	UNP A7XXA7
Y	-1	SER	-	expression tag	UNP A7XXA7
Y	0	HIS	-	expression tag	UNP A7XXA7

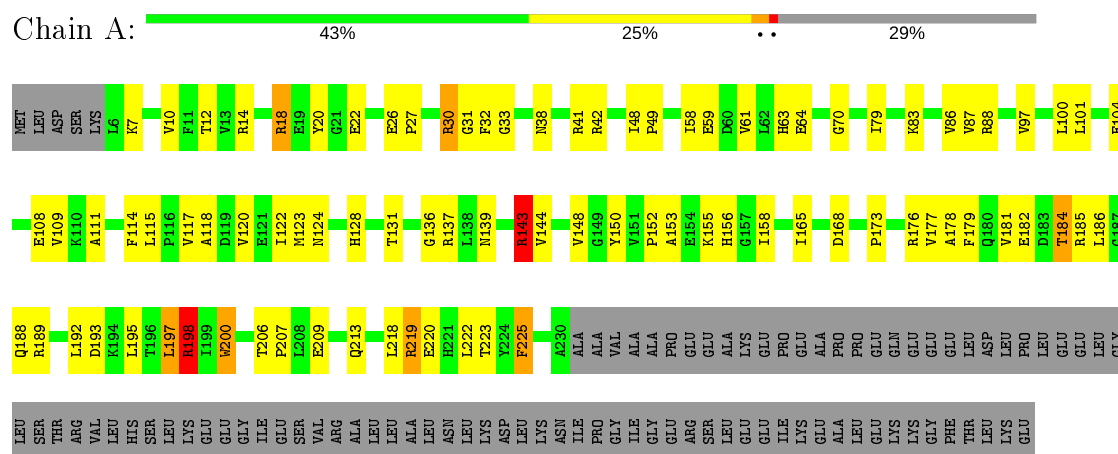
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Zn	0	0
			1	1		

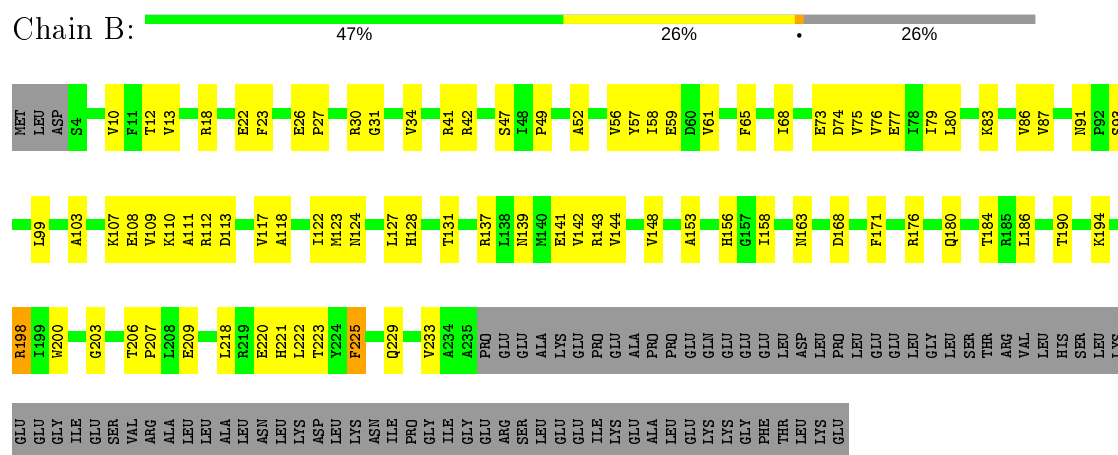
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

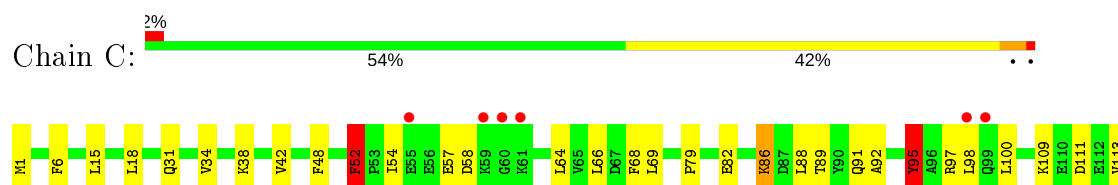
- Molecule 1: DNA-directed RNA polymerase subunit alpha

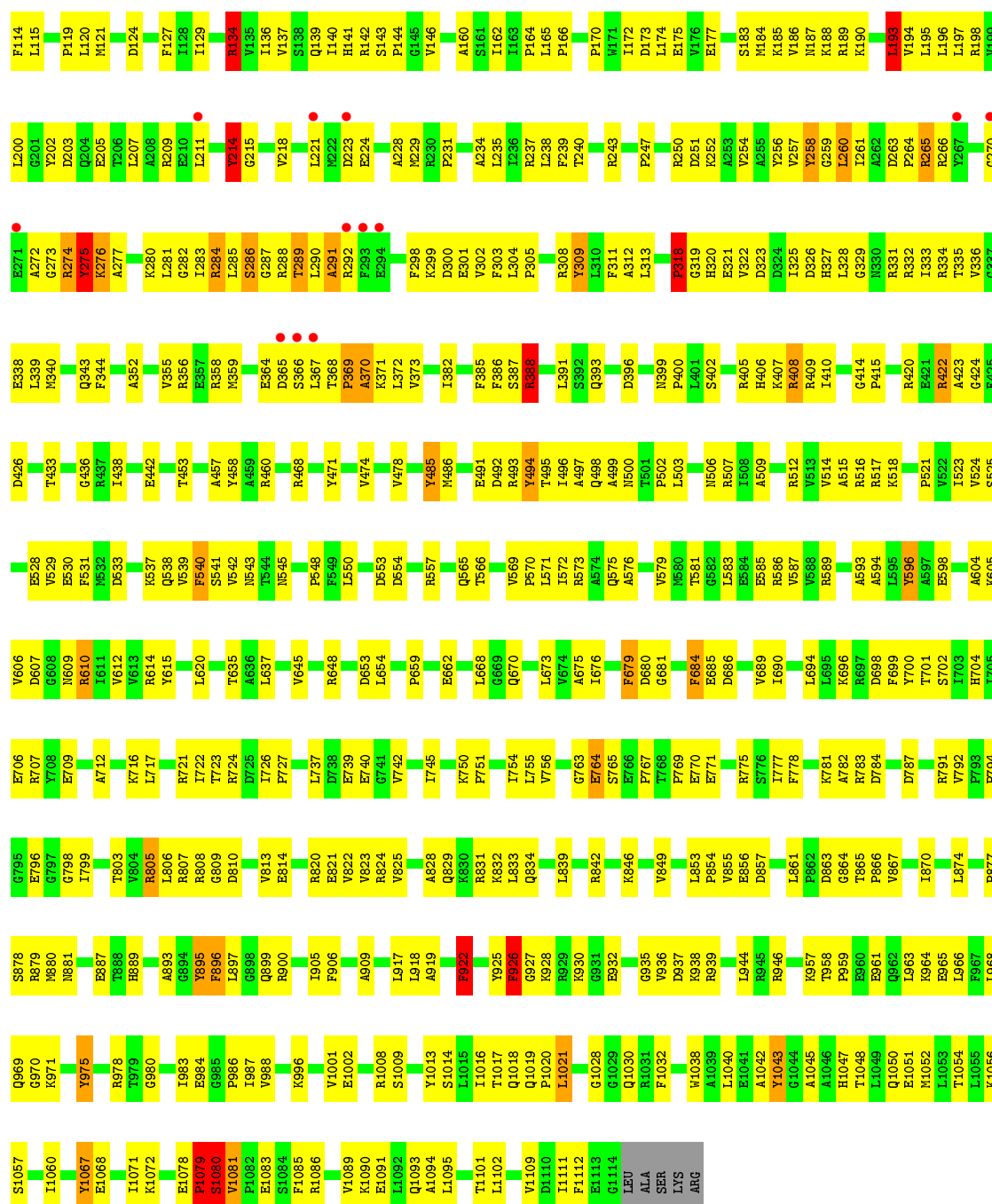


- Molecule 1: DNA-directed RNA polymerase subunit alpha

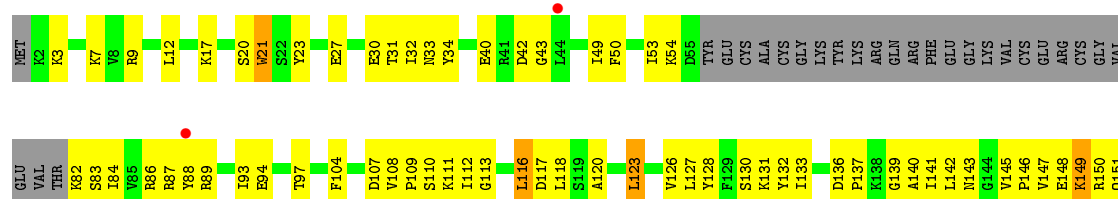


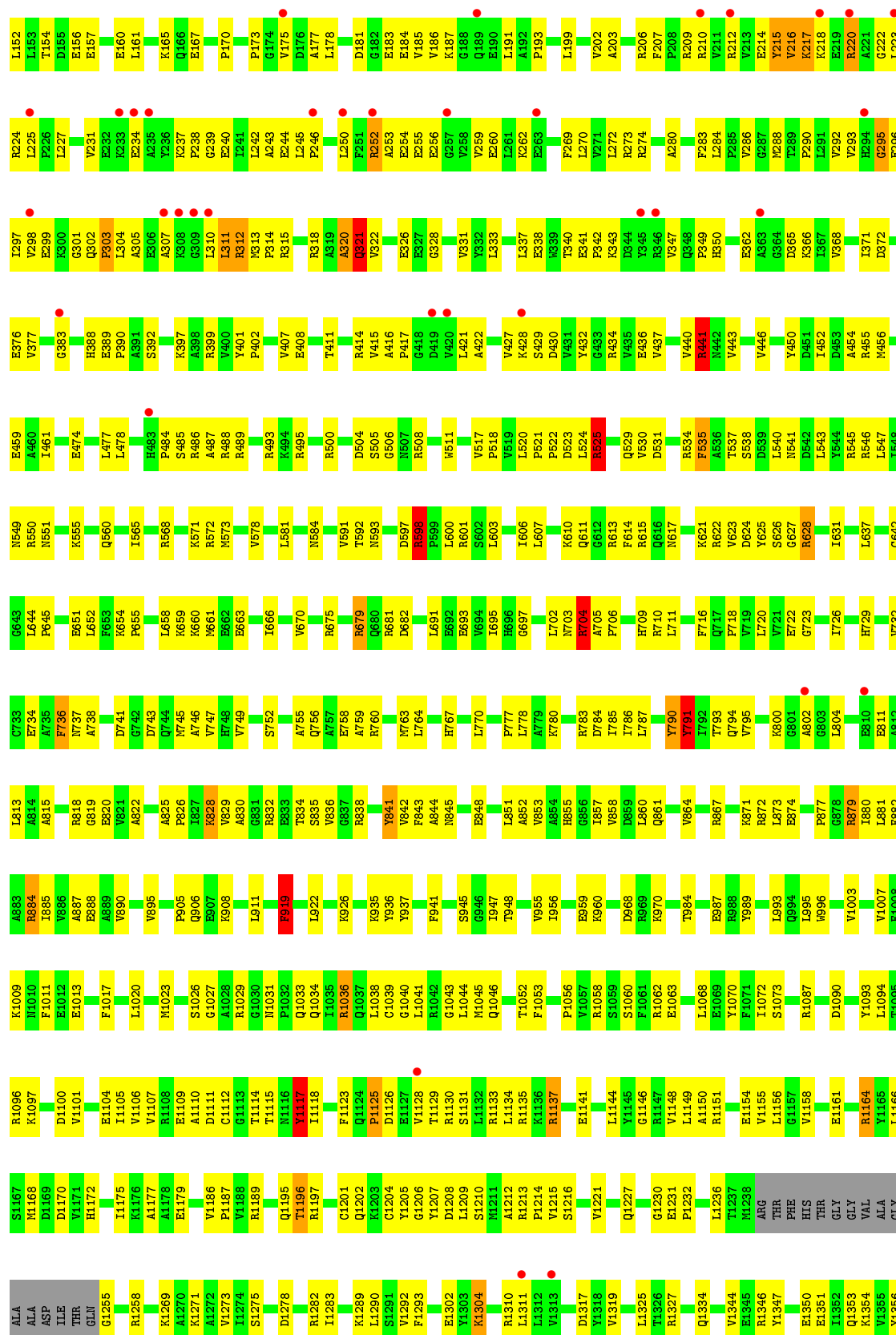
- Molecule 2: DNA-directed RNA polymerase subunit beta

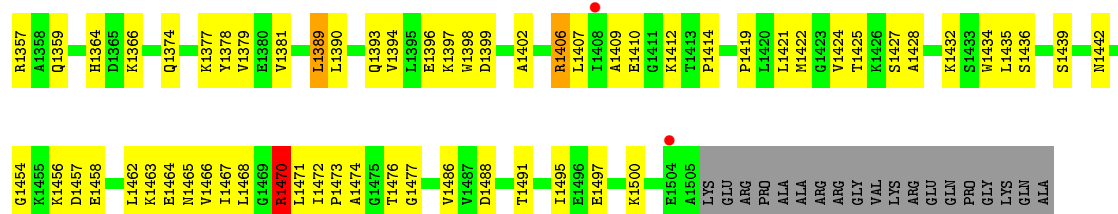




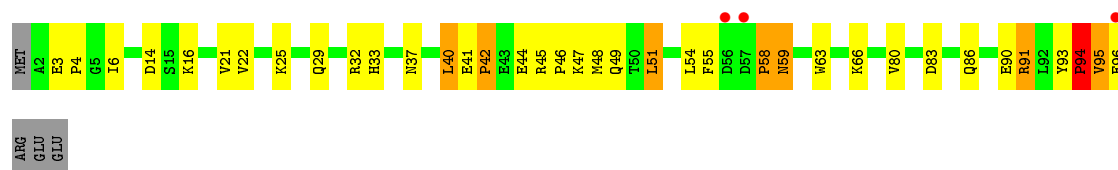
• Molecule 3: DNA-directed RNA polymerase subunit beta'



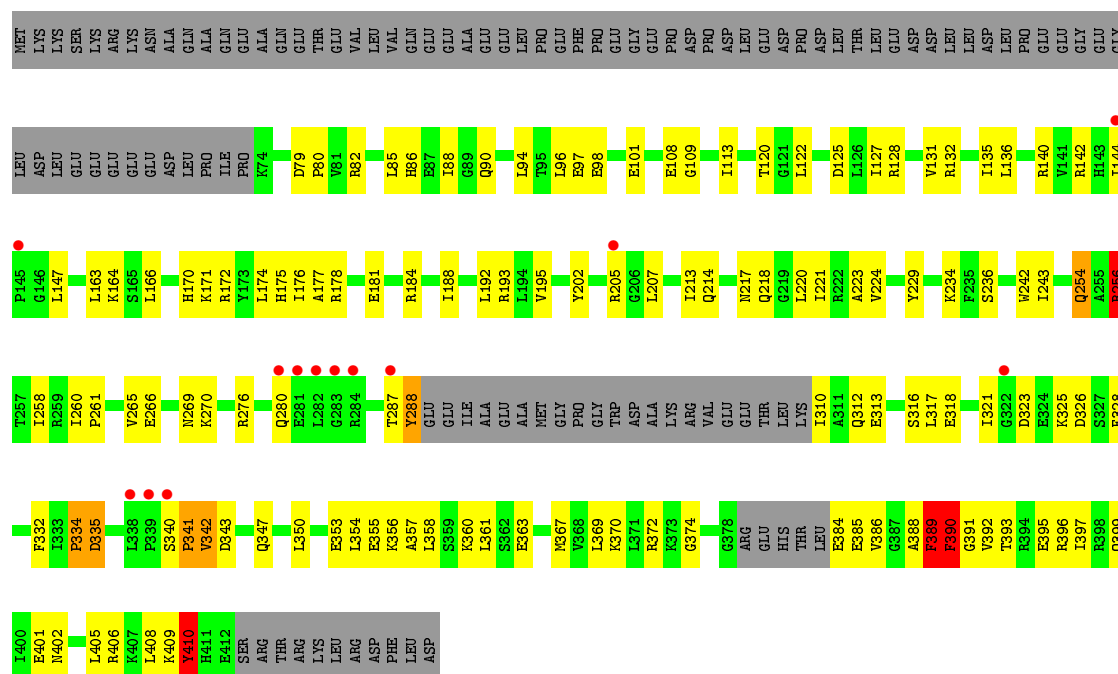
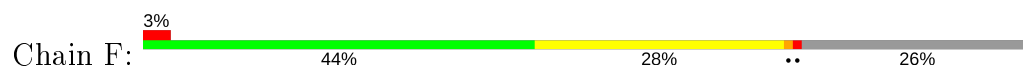




• Molecule 4: DNA-directed RNA polymerase subunit omega

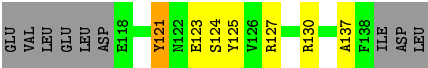


• Molecule 5: RNA polymerase sigma factor SigA

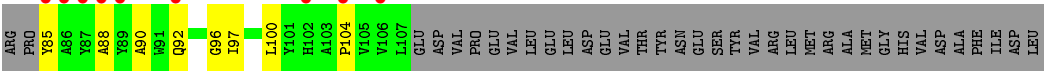


• Molecule 6: gp39

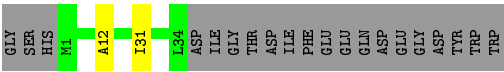




● Molecule 6: gp39



● Molecule 7: gp76



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	294.43Å 294.43Å 222.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.78 – 4.00 49.78 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.78-4.00) 96.1 (49.78-4.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.237 , 0.272 0.237 , 0.272	Depositor DCC
R_{free} test set	4644 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 127.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.105 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29177	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: ZN

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	A	0.49	3/1804 (0.2%)	0.89	10/2454 (0.4%)
1	B	0.33	0/1846	0.62	0/2511
2	C	0.43	5/8957 (0.1%)	0.81	28/12113 (0.2%)
3	D	0.44	7/11745 (0.1%)	0.80	40/15882 (0.3%)
4	E	0.52	2/784 (0.3%)	0.81	3/1057 (0.3%)
5	F	0.38	1/2568 (0.0%)	0.71	5/3453 (0.1%)
6	G	0.40	1/1065 (0.1%)	0.66	1/1449 (0.1%)
6	H	0.34	0/775	0.64	1/1057 (0.1%)
7	Y	0.29	0/171	0.48	0/238
All	All	0.43	19/29715 (0.1%)	0.78	88/40214 (0.2%)

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	A	0	2
2	C	0	13
3	D	0	11
4	E	0	1
5	F	0	2
6	G	0	1
6	H	0	1
All	All	0	31

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	254	GLN	CD-NE2	7.98	1.52	1.32
2	C	276	LYS	CG-CD	-7.36	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	879	ARG	CZ-NH2	7.36	1.42	1.33
2	C	134	ARG	CZ-NH2	7.30	1.42	1.33
3	D	1164	ARG	CG-CD	7.04	1.69	1.51
3	D	879	ARG	CG-CD	6.93	1.69	1.51
2	C	1081	VAL	C-N	6.83	1.47	1.34
3	D	220	ARG	CG-CD	6.59	1.68	1.51
1	A	143	ARG	CG-CD	6.48	1.68	1.51
3	D	628	ARG	CB-CG	-6.24	1.35	1.52
4	E	91	ARG	CG-CD	6.23	1.67	1.51
1	A	198	ARG	CG-CD	6.06	1.67	1.51
2	C	408	ARG	CB-CG	5.77	1.68	1.52
6	G	82	ALA	C-N	5.72	1.47	1.34
2	C	276	LYS	CD-CE	-5.65	1.37	1.51
1	A	200	TRP	CE3-CZ3	-5.35	1.29	1.38
3	D	1164	ARG	CZ-NH2	5.24	1.39	1.33
3	D	628	ARG	CZ-NH1	5.17	1.39	1.33
4	E	91	ARG	CZ-NH2	5.06	1.39	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	388	ARG	NE-CZ-NH2	-17.16	111.72	120.30
3	D	598	ARG	NE-CZ-NH2	-14.88	112.86	120.30
3	D	1164	ARG	NE-CZ-NH2	14.09	127.35	120.30
1	A	185	ARG	NE-CZ-NH2	12.72	126.66	120.30
1	A	185	ARG	NE-CZ-NH1	-11.93	114.34	120.30
2	C	408	ARG	NE-CZ-NH1	-11.70	114.45	120.30
2	C	408	ARG	NE-CZ-NH2	11.44	126.02	120.30
2	C	388	ARG	NE-CZ-NH1	11.39	126.00	120.30
3	D	441	ARG	NE-CZ-NH1	11.35	125.97	120.30
3	D	1164	ARG	NE-CZ-NH1	-11.19	114.70	120.30
3	D	659	LYS	CD-CE-NZ	-10.13	88.39	111.70
3	D	879	ARG	CB-CG-CD	-10.06	85.44	111.60
3	D	598	ARG	NE-CZ-NH1	9.96	125.28	120.30
3	D	879	ARG	NE-CZ-NH1	-9.95	115.32	120.30
2	C	1080	SER	N-CA-C	-9.79	84.57	111.00
1	A	18	ARG	CB-CG-CD	9.55	136.42	111.60
2	C	134	ARG	NE-CZ-NH2	-9.31	115.65	120.30
3	D	525	ARG	NE-CZ-NH2	-8.79	115.91	120.30
6	G	5	PHE	CB-CG-CD2	-8.46	114.88	120.80
1	A	143	ARG	CA-CB-CG	8.36	131.80	113.40
2	C	408	ARG	CG-CD-NE	8.36	129.35	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	NE-CZ-NH1	8.26	124.43	120.30
3	D	1164	ARG	CG-CD-NE	8.17	128.95	111.80
1	A	143	ARG	NE-CZ-NH2	-7.51	116.55	120.30
5	F	410	TYR	CB-CG-CD2	-7.29	116.63	121.00
3	D	879	ARG	NE-CZ-NH2	7.28	123.94	120.30
3	D	441	ARG	NE-CZ-NH2	-7.27	116.67	120.30
2	C	1080	SER	N-CA-CB	7.21	121.32	110.50
5	F	389	PHE	CB-CG-CD2	-7.08	115.84	120.80
3	D	321	GLN	CA-CB-CG	7.05	128.92	113.40
3	D	791	TYR	CB-CG-CD2	-6.95	116.83	121.00
3	D	1470	ARG	NE-CZ-NH1	6.93	123.77	120.30
5	F	390	PHE	CB-CG-CD2	-6.80	116.04	120.80
3	D	628	ARG	CG-CD-NE	6.78	126.03	111.80
2	C	679	PHE	CB-CA-C	6.64	123.67	110.40
2	C	134	ARG	CG-CD-NE	6.48	125.42	111.80
3	D	252	ARG	NE-CZ-NH2	-6.40	117.10	120.30
3	D	508	ARG	NE-CZ-NH2	6.39	123.50	120.30
3	D	628	ARG	CA-CB-CG	6.37	127.41	113.40
2	C	134	ARG	CD-NE-CZ	6.33	132.46	123.60
2	C	388	ARG	CD-NE-CZ	6.32	132.44	123.60
3	D	220	ARG	NE-CZ-NH1	6.23	123.42	120.30
3	D	525	ARG	CA-CB-CG	6.18	127.00	113.40
3	D	628	ARG	CD-NE-CZ	6.15	132.21	123.60
2	C	922	PHE	CB-CG-CD1	6.10	125.07	120.80
2	C	922	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	A	185	ARG	CG-CD-NE	6.04	124.48	111.80
3	D	525	ARG	NE-CZ-NH1	6.04	123.32	120.30
4	E	91	ARG	CG-CD-NE	6.03	124.46	111.80
2	C	388	ARG	CG-CD-NE	5.97	124.35	111.80
2	C	275	TYR	CB-CG-CD2	-5.95	117.43	121.00
3	D	1087	ARG	NE-CZ-NH2	-5.91	117.35	120.30
3	D	598	ARG	CD-NE-CZ	5.88	131.82	123.60
3	D	123	LEU	CB-CG-CD2	-5.87	101.03	111.00
3	D	598	ARG	CB-CG-CD	-5.87	96.35	111.60
2	C	926	PHE	CB-CG-CD2	-5.86	116.70	120.80
3	D	1470	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	30	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	C	265	ARG	NE-CZ-NH1	-5.70	117.45	120.30
3	D	628	ARG	CB-CG-CD	5.70	126.41	111.60
1	A	198	ARG	CG-CD-NE	5.68	123.73	111.80
2	C	276	LYS	CG-CD-CE	5.56	128.59	111.90
3	D	220	ARG	CA-CB-CG	5.55	125.62	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	586	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	D	295	GLY	N-CA-C	5.54	126.95	113.10
2	C	276	LYS	CB-CA-C	5.54	121.47	110.40
3	D	1470	ARG	CD-NE-CZ	5.50	131.31	123.60
4	E	40	LEU	CA-CB-CG	5.50	127.96	115.30
3	D	1117	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	C	134	ARG	CB-CG-CD	-5.45	97.44	111.60
2	C	95	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	C	319	GLY	N-CA-C	-5.37	99.69	113.10
2	C	284	ARG	C-N-CA	-5.28	108.51	121.70
5	F	254	GLN	CB-CA-C	5.27	120.94	110.40
3	D	704	ARG	NE-CZ-NH2	5.26	122.93	120.30
4	E	51	LEU	N-CA-C	-5.25	96.82	111.00
2	C	214	TYR	CB-CG-CD2	-5.24	117.85	121.00
3	D	919	PHE	CB-CG-CD2	-5.23	117.14	120.80
3	D	441	ARG	CD-NE-CZ	5.20	130.88	123.60
3	D	508	ARG	CG-CD-NE	5.18	122.69	111.80
6	H	59	ARG	NE-CZ-NH1	-5.14	117.73	120.30
2	C	52	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	A	18	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	C	193	LEU	CA-CB-CG	5.08	126.99	115.30
5	F	256	ARG	CG-CD-NE	5.04	122.39	111.80
3	D	508	ARG	NE-CZ-NH1	-5.04	117.78	120.30
3	D	1470	ARG	CG-CD-NE	-5.02	101.25	111.80
3	D	136	ASP	C-N-CD	-5.01	109.58	120.60

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	THR	Peptide
1	A	197	LEU	Peptide
2	C	1079	PRO	Peptide
2	C	214	TYR	Sidechain
2	C	260	LEU	Peptide
2	C	275	TYR	Sidechain
2	C	283	ILE	Peptide
2	C	286	SER	Peptide
2	C	291	ALA	Peptide
2	C	318	PRO	Peptide
2	C	424	GLY	Peptide
2	C	517	ARG	Peptide

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Mol	Chain	Res	Type	Group
2	C	684	PHE	Peptide
2	C	764	GLU	Peptide
2	C	794	PRO	Peptide
3	D	1117	TYR	Sidechain
3	D	116	LEU	Peptide
3	D	1196	THR	Peptide
3	D	1208	ASP	Peptide
3	D	215	TYR	Peptide
3	D	312	ARG	Peptide
3	D	320	ALA	Peptide
3	D	321	GLN	Mainchain
3	D	529	GLN	Peptide
3	D	628	ARG	Peptide
3	D	791	TYR	Sidechain
4	E	94	PRO	Peptide
5	F	390	PHE	Sidechain
5	F	410	TYR	Sidechain
6	G	5	PHE	Sidechain
6	H	58	LYS	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	A	1772	0	1821	77	0
1	B	1814	0	1868	69	0
2	C	8789	0	8886	490	0
3	D	11543	0	11785	579	0
4	E	770	0	784	40	0
5	F	2530	0	2611	131	0
6	G	1035	0	1013	30	0
6	H	752	0	748	27	0
7	Y	171	0	91	3	0
8	D	1	0	0	0	0
All	All	29177	0	29607	1305	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

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)
1:A:198:ARG:HD3	1:A:200:TRP:CH2	1.70	1.24
1:A:143:ARG:NH2	6:H:22:GLU:OE2	1.87	1.07
2:C:277:ALA:HB3	2:C:285:LEU:HD11	1.40	1.02
2:C:274:ARG:HA	2:C:285:LEU:HD12	1.42	1.00
1:A:198:ARG:HD3	1:A:200:TRP:HH2	1.08	0.97
2:C:260:LEU:O	2:C:265:ARG:NH1	1.96	0.96
5:F:256:ARG:HD2	5:F:260:ILE:HB	1.48	0.95
3:D:312:ARG:HA	3:D:313:MET:HB3	1.50	0.94
3:D:520:LEU:O	3:D:525:ARG:NH1	2.01	0.94
1:B:80:LEU:HD23	3:D:867:ARG:HD2	1.51	0.90
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.34	0.89
3:D:598:ARG:HH22	5:F:316:SER:CB	1.84	0.89
3:D:206:ARG:HD3	3:D:392:SER:HB2	1.54	0.89
2:C:391:LEU:HD13	2:C:415:PRO:HD3	1.56	0.88
3:D:1112:CYS:HB3	3:D:1196:THR:HG23	1.56	0.87
2:C:807:ARG:HH12	6:G:21:THR:HG22	1.40	0.87
2:C:422:ARG:HE	2:C:423:ALA:HB2	1.39	0.86
1:B:73:GLU:OE2	1:B:131:THR:OG1	1.93	0.86
6:G:56:GLU:HG3	6:G:64:ARG:HD2	1.57	0.85
3:D:224:ARG:HH11	3:D:253:ALA:HA	1.40	0.85
2:C:95:TYR:HB3	2:C:114:PHE:HA	1.57	0.85
5:F:369:LEU:HD11	5:F:401:GLU:HG3	1.57	0.85
3:D:422:ALA:HB3	3:D:427:VAL:HB	1.61	0.83
3:D:560:GLN:OE1	5:F:218:GLN:NE2	2.11	0.83
1:A:143:ARG:HE	1:A:158:ILE:HG21	1.42	0.83
2:C:846:LYS:HB3	3:D:741:ASP:HB2	1.60	0.82
1:A:198:ARG:CD	1:A:200:TRP:CH2	2.61	0.82
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.61	0.82
2:C:516:ARG:NH1	2:C:518:LYS:O	2.13	0.81
3:D:679:ARG:NE	3:D:682:ASP:OD2	2.12	0.81
3:D:601:ARG:HH22	3:D:611:GLN:HE22	1.29	0.81
2:C:257:VAL:HB	2:C:263:ASP:OD2	1.81	0.81
5:F:323:ASP:HB3	5:F:325:LYS:HE2	1.60	0.81
3:D:256:GLU:HB3	3:D:299:GLU:HG2	1.63	0.81
3:D:704:ARG:NH1	3:D:737:ASN:O	2.14	0.81
3:D:1497:GLU:HB2	3:D:1500:LYS:HE3	1.61	0.80
2:C:957:LYS:NZ	2:C:965:GLU:OE2	2.14	0.80
2:C:214:TYR:HD1	2:C:215:GLY:H	1.30	0.80
3:D:302:GLN:O	3:D:304:LEU:N	2.14	0.80
3:D:292:VAL:HG12	3:D:293:VAL:HG13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1056:LYS:HE2	3:D:623:VAL:HG13	1.64	0.80
3:D:795:VAL:HG23	3:D:879:ARG:HH12	1.47	0.80
2:C:474:VAL:HG11	2:C:529:VAL:HG12	1.63	0.79
3:D:97:THR:HG21	3:D:571:LYS:HE3	1.63	0.79
3:D:253:ALA:HB3	3:D:303:PRO:HG3	1.64	0.79
1:B:77:GLU:HB2	3:D:872:ARG:HH21	1.49	0.78
6:H:49:PRO:HD2	6:H:72:ARG:NH2	1.98	0.78
2:C:332:ARG:NH2	2:C:338:GLU:OE2	2.15	0.78
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.18	0.78
3:D:1206:GLY:HA3	3:D:1366:LYS:HE2	1.65	0.78
6:G:30:ASP:OD1	6:G:31:LEU:N	2.16	0.78
6:G:72:ARG:HD2	6:G:83:ARG:HD3	1.66	0.77
1:B:59:GLU:HG2	1:B:137:ARG:NH1	1.99	0.77
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.64	0.77
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.17	0.77
3:D:288:MET:HB3	3:D:305:ALA:HB1	1.64	0.77
2:C:164:PRO:HA	2:C:266:ARG:HH22	1.49	0.77
2:C:750:LYS:HE3	3:D:681:ARG:HE	1.46	0.76
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.67	0.76
2:C:1018:GLN:HG3	2:C:1060:ILE:HD11	1.68	0.76
2:C:1020:PRO:HD2	3:D:622:ARG:HB2	1.66	0.76
3:D:832:ARG:NE	3:D:832:ARG:O	2.18	0.76
3:D:1205:TYR:HD2	3:D:1215:VAL:HG21	1.51	0.75
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.22	0.74
3:D:455:ARG:HH12	5:F:140:ARG:HH12	1.34	0.74
2:C:537:LYS:HB3	2:C:545:ASN:HD21	1.52	0.74
3:D:1209:LEU:HD13	3:D:1215:VAL:HA	1.68	0.74
1:A:176:ARG:HH12	2:C:865:THR:HB	1.52	0.74
5:F:260:ILE:HD12	5:F:261:PRO:HD2	1.69	0.74
2:C:34:VAL:HB	2:C:38:LYS:HG3	1.68	0.74
3:D:1109:GLU:HG3	3:D:1196:THR:HG21	1.68	0.74
3:D:474:GLU:OE2	3:D:500:ARG:NH2	2.19	0.74
1:B:156:HIS:HD2	1:B:158:ILE:HG12	1.52	0.74
3:D:224:ARG:NH1	3:D:253:ALA:HA	2.02	0.74
5:F:207:LEU:HD21	5:F:254:GLN:HG3	1.70	0.74
2:C:1078:GLU:HB3	2:C:1079:PRO:HD2	1.70	0.74
2:C:273:GLY:HA2	2:C:276:LYS:NZ	2.03	0.74
2:C:833:LEU:HD21	2:C:849:VAL:HG21	1.69	0.74
2:C:573:ARG:O	2:C:670:GLN:NE2	2.18	0.73
3:D:601:ARG:HH11	5:F:318:GLU:HG2	1.52	0.73
2:C:223:ASP:OD1	2:C:224:GLU:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:890:VAL:HG12	3:D:926:LYS:HB3	1.70	0.73
2:C:498:GLN:HG3	2:C:500:ASN:OD1	1.88	0.73
3:D:259:VAL:HG21	3:D:293:VAL:HA	1.70	0.73
3:D:1378:TYR:HE1	3:D:1394:VAL:HG22	1.54	0.73
1:B:103:ALA:HB1	1:B:107:LYS:HD3	1.71	0.73
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.71	0.73
3:D:237:LYS:HB3	3:D:238:PRO:HD2	1.71	0.73
2:C:491:GLU:OE2	2:C:516:ARG:NH2	2.23	0.72
2:C:698:ASP:OD1	2:C:701:THR:OG1	2.06	0.72
4:E:42:PRO:HD2	4:E:45:ARG:HE	1.52	0.72
3:D:795:VAL:HG23	3:D:879:ARG:NH1	2.04	0.72
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.69	0.72
3:D:21:TRP:H	3:D:21:TRP:HD1	1.36	0.72
3:D:82:LYS:HG2	3:D:83:SER:H	1.52	0.72
1:B:59:GLU:HG2	1:B:137:ARG:HH12	1.54	0.72
3:D:790:TYR:HB2	3:D:906:GLN:O	1.90	0.72
2:C:607:ASP:HB3	2:C:609:ASN:H	1.53	0.72
2:C:86:LYS:HG2	2:C:813:VAL:HG12	1.72	0.72
2:C:468:ARG:HG2	2:C:485:TYR:HB3	1.71	0.71
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.04	0.71
3:D:660:LYS:HD3	3:D:663:GLU:HG3	1.73	0.71
4:E:48:MET:HG2	4:E:49:GLN:H	1.56	0.71
3:D:33:ASN:HA	5:F:258:ILE:HG23	1.73	0.71
1:A:176:ARG:HG3	1:A:200:TRP:CE3	2.26	0.70
3:D:710:ARG:NH2	3:D:1210:SER:OG	2.24	0.70
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.25	0.70
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.25	0.70
5:F:341:PRO:O	5:F:343:ASP:N	2.23	0.70
3:D:253:ALA:CB	3:D:303:PRO:HG3	2.22	0.70
3:D:225:LEU:HD13	3:D:231:VAL:HG23	1.74	0.70
2:C:141:HIS:CD2	2:C:334:ARG:HD2	2.27	0.70
3:D:34:TYR:HB3	5:F:258:ILE:HD13	1.74	0.70
3:D:416:ALA:HB2	3:D:432:TYR:HA	1.74	0.70
2:C:700:TYR:HE2	2:C:839:LEU:HD21	1.57	0.69
6:H:37:ARG:HH11	6:H:45:LEU:HD11	1.57	0.69
2:C:1056:LYS:NZ	3:D:625:TYR:HB2	2.07	0.69
3:D:1117:TYR:HE2	3:D:1151:ARG:HE	1.39	0.69
1:B:26:GLU:OE1	1:B:194:LYS:NZ	2.20	0.69
3:D:402:PRO:HA	3:D:443:VAL:HG12	1.74	0.69
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.75	0.69
2:C:493:ARG:NH1	2:C:494:TYR:OH	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:GLN:NE2	2:C:42:VAL:O	2.25	0.69
2:C:290:LEU:HD22	2:C:301:GLU:H	1.58	0.69
3:D:459:GLU:OE2	5:F:140:ARG:NH1	2.26	0.69
5:F:358:LEU:HD11	5:F:370:LYS:HD2	1.75	0.69
1:A:31:GLY:O	1:B:42:ARG:NH2	2.25	0.68
2:C:716:LYS:NZ	5:F:310:ILE:HG12	2.08	0.68
1:A:181:VAL:HG12	2:C:938:LYS:HD3	1.75	0.68
3:D:791:TYR:O	3:D:791:TYR:HD1	1.77	0.68
5:F:164:LYS:HA	5:F:171:LYS:HE2	1.76	0.68
3:D:834:THR:HA	3:D:838:ARG:HD2	1.75	0.68
5:F:347:GLN:HA	5:F:350:LEU:HB3	1.73	0.68
3:D:736:PHE:HD1	3:D:736:PHE:H	1.41	0.68
2:C:214:TYR:HD1	2:C:215:GLY:N	1.89	0.68
2:C:803:THR:HG22	2:C:825:VAL:HG12	1.76	0.68
3:D:366:LYS:NZ	3:D:376:GLU:OE1	2.22	0.68
1:A:79:ILE:HD11	1:A:165:ILE:HD12	1.75	0.68
2:C:573:ARG:HH11	2:C:699:PHE:HE1	1.42	0.68
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.74	0.68
3:D:1488:ASP:OD1	3:D:1491:THR:OG1	2.09	0.68
3:D:216:VAL:HG12	3:D:338:GLU:HB2	1.76	0.68
2:C:755:LEU:HD11	2:C:792:VAL:HG23	1.73	0.68
5:F:220:LEU:HD12	5:F:243:ILE:HD11	1.75	0.68
3:D:1101:VAL:HG21	3:D:1424:VAL:HG13	1.76	0.67
4:E:41:GLU:HG3	4:E:41:GLU:O	1.94	0.67
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.76	0.67
3:D:117:ASP:OD1	3:D:495:ARG:NH1	2.27	0.67
6:H:56:GLU:HG3	6:H:64:ARG:HD2	1.76	0.67
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.76	0.67
3:D:312:ARG:HA	3:D:313:MET:CB	2.23	0.67
3:D:1283:ILE:HG12	3:D:1292:VAL:HG22	1.76	0.67
3:D:711:LEU:HD12	3:D:778:LEU:HD23	1.74	0.67
1:A:153:ALA:HA	1:A:156:HIS:CE1	2.29	0.67
3:D:17:LYS:O	3:D:20:SER:N	2.26	0.67
2:C:140:ILE:HD13	2:C:331:ARG:HH21	1.60	0.67
2:C:606:VAL:HG22	2:C:645:VAL:HG23	1.76	0.67
3:D:1197:ARG:HD3	3:D:1396:GLU:OE1	1.94	0.67
3:D:143:ASN:OD1	3:D:145:VAL:N	2.28	0.67
3:D:401:TYR:OH	3:D:430:ASP:OD1	2.12	0.67
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.77	0.66
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.78	0.66
5:F:393:THR:HG22	5:F:395:GLU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:90:ALA:HB2	6:H:100:LEU:HD23	1.77	0.66
2:C:878:SER:HB2	3:D:1029:ARG:HD2	1.78	0.66
3:D:1155:VAL:HG12	3:D:1156:LEU:HG	1.77	0.66
6:H:71:TYR:C	6:H:72:ARG:HD2	2.16	0.66
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.31	0.66
2:C:806:LEU:HB2	2:C:822:VAL:HG12	1.78	0.66
3:D:598:ARG:NH2	5:F:316:SER:CB	2.59	0.66
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.76	0.66
5:F:234:LYS:HE3	5:F:236:SER:HB2	1.78	0.66
1:B:58:ILE:HB	1:B:61:VAL:HB	1.78	0.66
2:C:653:ASP:OD1	2:C:654:LEU:N	2.29	0.66
2:C:679:PHE:O	2:C:681:GLY:N	2.28	0.66
2:C:247:PRO:HG2	2:C:250:ARG:HD3	1.78	0.65
2:C:272:ALA:O	2:C:276:LYS:NZ	2.29	0.65
2:C:254:VAL:HG22	2:C:258:TYR:HE1	1.61	0.65
5:F:356:LYS:O	5:F:360:LYS:HG2	1.96	0.65
3:D:1406:ARG:HD3	3:D:1407:LEU:HD12	1.79	0.65
1:B:80:LEU:HB3	3:D:867:ARG:HH11	1.60	0.65
1:B:110:LYS:HD3	1:B:112:ARG:HH11	1.62	0.65
6:G:130:ARG:HE	6:G:137:ALA:HA	1.62	0.65
6:G:26:PHE:CD2	6:G:64:ARG:HD3	2.32	0.65
2:C:721:ARG:HH22	6:G:94:ASP:HB2	1.62	0.64
2:C:926:PHE:HE2	2:C:963:LEU:HD12	1.62	0.64
2:C:1051:GLU:O	2:C:1056:LYS:HG2	1.97	0.64
2:C:273:GLY:HA2	2:C:276:LYS:HZ2	1.61	0.64
2:C:197:LEU:HA	2:C:200:LEU:HD12	1.80	0.64
3:D:1053:PHE:CE2	3:D:1072:ILE:HD12	2.33	0.64
3:D:800:LYS:HD3	3:D:830:ALA:O	1.96	0.64
4:E:41:GLU:OE1	4:E:63:TRP:HH2	1.81	0.64
1:A:220:GLU:O	1:A:223:THR:HG22	1.98	0.64
2:C:175:GLU:O	2:C:183:SER:OG	2.15	0.64
2:C:763:GLY:O	2:C:764:GLU:HG2	1.97	0.64
3:D:860:LEU:HA	3:D:877:PRO:HG2	1.79	0.64
5:F:125:ASP:HA	5:F:128:ARG:HG2	1.80	0.64
1:A:58:ILE:HB	1:A:61:VAL:HB	1.80	0.64
2:C:260:LEU:C	2:C:265:ARG:HH12	2.00	0.64
3:D:679:ARG:HD3	3:D:679:ARG:H	1.62	0.64
1:A:59:GLU:HB3	1:A:139:ASN:HB3	1.78	0.63
2:C:327:HIS:HD2	2:C:329:GLY:H	1.44	0.63
3:D:1436:SER:HB2	3:D:1464:GLU:HG2	1.78	0.63
3:D:421:LEU:HD22	3:D:429:SER:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:525:ARG:HG3	3:D:540:LEU:HB2	1.80	0.63
1:A:49:PRO:HB3	1:A:148:VAL:HG22	1.79	0.63
2:C:172:ILE:HG22	2:C:186:VAL:HG12	1.80	0.63
2:C:187:ASN:O	2:C:188:LYS:HG2	1.98	0.63
2:C:309:TYR:OH	2:C:321:GLU:HG3	1.99	0.63
2:C:926:PHE:O	2:C:926:PHE:HD1	1.81	0.63
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.79	0.63
2:C:1009:SER:HB2	3:D:651:GLU:O	1.97	0.63
2:C:266:ARG:O	2:C:288:ARG:HD2	1.98	0.63
2:C:405:ARG:HD2	2:C:409:ARG:HD3	1.80	0.63
3:D:1033:GLN:OE1	3:D:1036:ARG:NH1	2.31	0.63
4:E:47:LYS:HE3	4:E:55:PHE:HZ	1.64	0.63
3:D:34:TYR:HD1	5:F:258:ILE:HG21	1.63	0.63
5:F:256:ARG:NH1	5:F:260:ILE:HD13	2.13	0.63
1:B:59:GLU:HB2	1:B:139:ASN:HB3	1.80	0.63
2:C:405:ARG:HG3	2:C:543:ASN:ND2	2.13	0.63
3:D:118:LEU:HD23	3:D:123:LEU:HB3	1.81	0.63
2:C:1094:ALA:HB2	3:D:520:LEU:HD13	1.80	0.63
3:D:209:ARG:HB2	3:D:389:GLU:HB2	1.81	0.63
3:D:215:TYR:O	3:D:217:LYS:N	2.32	0.63
2:C:275:TYR:HD1	2:C:275:TYR:O	1.81	0.63
3:D:1045:MET:HG3	3:D:1073:SER:HA	1.81	0.63
3:D:1470:ARG:HG3	3:D:1471:LEU:N	2.07	0.63
3:D:178:LEU:HD23	3:D:181:ASP:OD2	1.97	0.63
3:D:441:ARG:HD3	3:D:441:ARG:O	1.99	0.62
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.80	0.62
2:C:576:ALA:N	2:C:662:GLU:OE1	2.25	0.62
2:C:958:THR:HG23	2:C:961:GLU:H	1.65	0.62
3:D:845:ASN:HB2	3:D:848:GLU:H	1.65	0.62
6:G:90:ALA:HB2	6:G:100:LEU:HD23	1.81	0.62
2:C:491:GLU:CD	2:C:516:ARG:HH22	2.03	0.62
2:C:57:GLU:HG2	2:C:58:ASP:H	1.63	0.62
2:C:927:GLY:HA2	2:C:930:LYS:NZ	2.14	0.62
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.35	0.62
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.81	0.62
2:C:834:GLN:NE2	2:C:1002:GLU:OE2	2.32	0.62
3:D:175:VAL:HG11	3:D:193:PRO:HD2	1.82	0.62
3:D:21:TRP:CD1	3:D:21:TRP:N	2.65	0.62
2:C:57:GLU:HG2	2:C:58:ASP:N	2.15	0.62
3:D:1144:LEU:HD21	3:D:1186:VAL:HG21	1.80	0.62
2:C:290:LEU:HD11	2:C:302:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:723:THR:OG1	6:G:94:ASP:OD1	2.16	0.61
2:C:939:ARG:NH1	2:C:980:GLY:O	2.32	0.61
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.83	0.61
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.82	0.61
3:D:1412:LYS:O	3:D:1414:PRO:HD3	2.00	0.61
3:D:493:ARG:NH1	3:D:1390:LEU:HD12	2.16	0.61
3:D:546:ARG:NH1	3:D:550:ARG:NH2	2.48	0.61
2:C:1056:LYS:HE2	3:D:623:VAL:CG1	2.28	0.61
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.83	0.61
3:D:141:ILE:HG13	3:D:142:LEU:H	1.66	0.61
2:C:1038:TRP:HH2	3:D:1096:ARG:HG3	1.65	0.61
2:C:91:GLN:HA	2:C:119:PRO:HA	1.81	0.61
3:D:397:LYS:HE3	3:D:399:ARG:HH12	1.66	0.61
2:C:493:ARG:HB2	2:C:494:TYR:CE1	2.36	0.61
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.34	0.61
3:D:1236:LEU:HD11	3:D:1356:TYR:CE1	2.36	0.61
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.65	0.61
1:B:128:HIS:NE2	1:B:131:THR:HG23	2.16	0.61
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.34	0.61
3:D:615:ARG:NH1	3:D:1439:SER:O	2.33	0.61
3:D:223:LEU:HD11	3:D:333:LEU:HD12	1.81	0.61
6:G:102:HIS:CD2	6:H:11:ARG:HH21	2.19	0.61
5:F:389:PHE:O	5:F:389:PHE:HD1	1.84	0.61
2:C:495:THR:CG2	2:C:529:VAL:HA	2.30	0.60
3:D:1137:ARG:H	3:D:1137:ARG:HD3	1.65	0.60
3:D:693:GLU:HA	4:E:48:MET:HE1	1.82	0.60
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.83	0.60
4:E:32:ARG:HE	4:E:33:HIS:CE1	2.19	0.60
2:C:1111:ILE:HG13	2:C:1112:PHE:CD1	2.36	0.60
3:D:1486:VAL:HG23	4:E:29:GLN:NE2	2.17	0.60
2:C:193:LEU:HD21	2:C:303:PHE:HD2	1.67	0.60
2:C:690:ILE:HG23	2:C:694:LEU:HD12	1.82	0.60
5:F:266:GLU:HA	5:F:269:ASN:HB2	1.82	0.60
5:F:390:PHE:C	5:F:390:PHE:HD1	2.05	0.60
1:B:30:ARG:HH21	2:C:854:PRO:HB3	1.66	0.60
1:B:74:ASP:OD1	1:B:75:VAL:N	2.35	0.60
2:C:52:PHE:CE2	2:C:68:PHE:HB2	2.36	0.60
3:D:1465:ASN:OD1	3:D:1470:ARG:HG2	2.00	0.60
2:C:327:HIS:CD2	2:C:329:GLY:H	2.19	0.60
2:C:767:PRO:HG2	2:C:771:GLU:HB2	1.83	0.60
3:D:530:VAL:N	3:D:534:ARG:O	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:389:PHE:HB3	5:F:397:ILE:HD13	1.82	0.60
5:F:389:PHE:HB3	5:F:397:ILE:HG21	1.83	0.60
1:A:108:GLU:HG2	1:A:131:THR:HG22	1.83	0.60
2:C:69:LEU:HD12	2:C:97:ARG:HG2	1.85	0.59
5:F:372:ARG:HE	5:F:384:GLU:N	2.00	0.59
2:C:140:ILE:HD13	2:C:331:ARG:NH2	2.18	0.59
2:C:550:LEU:HD23	2:C:905:ILE:HD11	1.84	0.59
3:D:215:TYR:HE2	3:D:343:LYS:HD2	1.67	0.59
6:G:92:GLN:HE21	6:G:96:GLY:HA2	1.66	0.59
3:D:601:ARG:HH21	3:D:606:ILE:HA	1.67	0.59
2:C:573:ARG:HG2	2:C:699:PHE:CD1	2.38	0.59
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.84	0.59
3:D:262:LYS:HG2	3:D:269:PHE:HB2	1.84	0.59
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.85	0.59
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.36	0.59
1:B:176:ARG:NH2	3:D:888:GLU:OE2	2.36	0.59
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.18	0.59
2:C:260:LEU:O	2:C:289:THR:HG21	2.03	0.59
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.82	0.59
2:C:742:VAL:HG22	2:C:756:VAL:HG12	1.83	0.59
3:D:110:SER:HB2	3:D:120:ALA:HB1	1.84	0.59
3:D:368:VAL:HB	3:D:377:VAL:HB	1.83	0.59
1:B:153:ALA:HA	1:B:156:HIS:HE1	1.68	0.59
2:C:1089:VAL:O	2:C:1093:GLN:HG3	2.02	0.59
2:C:144:PRO:O	2:C:276:LYS:HE2	2.03	0.59
2:C:312:ALA:HB1	2:C:318:PRO:HG3	1.84	0.59
2:C:857:ASP:HB2	2:C:978:ARG:HB3	1.83	0.59
2:C:1052:MET:HA	2:C:1056:LYS:HG3	1.84	0.58
3:D:123:LEU:HD21	3:D:152:LEU:HD22	1.84	0.58
3:D:704:ARG:HH12	3:D:738:ALA:HA	1.68	0.58
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.85	0.58
6:H:21:THR:HG22	6:H:22:GLU:H	1.68	0.58
2:C:716:LYS:HZ2	5:F:310:ILE:HG12	1.68	0.58
2:C:1090:LYS:HA	2:C:1093:GLN:HB2	1.84	0.58
3:D:984:THR:HG23	3:D:987:GLU:H	1.68	0.58
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.85	0.58
2:C:1067:TYR:HD1	2:C:1067:TYR:C	2.07	0.58
2:C:679:PHE:HD1	2:C:680:ASP:H	1.51	0.58
3:D:408:GLU:O	5:F:171:LYS:NZ	2.19	0.58
3:D:593:ASN:ND2	5:F:313:GLU:OE2	2.36	0.58
5:F:144:ILE:HB	5:F:147:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.84	0.58
2:C:48:PHE:O	2:C:52:PHE:HB2	2.04	0.58
4:E:95:VAL:O	4:E:96:GLU:HB3	2.04	0.58
1:B:59:GLU:CG	1:B:137:ARG:HH12	2.17	0.58
2:C:922:PHE:HD1	2:C:922:PHE:C	2.07	0.58
3:D:1097:LYS:HE3	3:D:1425:THR:OG1	2.04	0.58
3:D:485:SER:H	3:D:488:ARG:HH21	1.52	0.58
5:F:390:PHE:C	5:F:390:PHE:CD1	2.77	0.58
5:F:392:VAL:HG11	5:F:396:ARG:HD2	1.86	0.58
2:C:700:TYR:HB3	2:C:833:LEU:HB2	1.86	0.57
3:D:820:GLU:HG3	3:D:836:VAL:HG21	1.86	0.57
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.85	0.57
2:C:98:LEU:O	2:C:109:LYS:HG3	2.03	0.57
3:D:531:ASP:HB2	3:D:534:ARG:HD3	1.86	0.57
2:C:1056:LYS:HZ2	3:D:625:TYR:HB2	1.70	0.57
5:F:163:LEU:HB3	5:F:174:LEU:HD12	1.86	0.57
1:A:128:HIS:NE2	1:A:131:THR:HG23	2.20	0.57
5:F:256:ARG:HE	5:F:258:ILE:HB	1.69	0.57
3:D:349:PRO:HB3	5:F:96:LEU:HB3	1.86	0.57
4:E:3:GLU:HG3	4:E:4:PRO:HD2	1.86	0.57
5:F:369:LEU:HD12	5:F:405:LEU:HD11	1.87	0.57
3:D:1397:LYS:HD2	3:D:1432:LYS:HE2	1.85	0.57
3:D:237:LYS:H	3:D:240:GLU:HG3	1.68	0.57
1:A:12:THR:HA	1:B:229:GLN:HB2	1.85	0.57
3:D:1125:PRO:HA	3:D:1131:SER:O	2.04	0.57
1:A:97:VAL:HG11	1:A:120:VAL:HG21	1.84	0.57
1:A:42:ARG:NH2	1:B:31:GLY:O	2.37	0.57
2:C:750:LYS:HG2	2:C:751:PRO:HD2	1.86	0.57
3:D:253:ALA:H	3:D:303:PRO:HG3	1.68	0.57
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.86	0.57
2:C:707:ARG:HD3	2:C:824:ARG:HD3	1.87	0.57
2:C:829:GLN:OE1	2:C:831:ARG:HD2	2.05	0.57
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.20	0.57
3:D:388:HIS:O	3:D:390:PRO:HD3	2.05	0.57
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.87	0.57
2:C:1111:ILE:HG13	2:C:1112:PHE:HD1	1.68	0.57
3:D:160:GLU:OE2	3:D:165:LYS:NZ	2.37	0.57
5:F:172:ARG:HA	5:F:175:HIS:HD2	1.70	0.56
5:F:341:PRO:C	5:F:343:ASP:H	2.08	0.56
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.87	0.56
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:LYS:CG	2:C:813:VAL:HG12	2.35	0.56
3:D:1146:GLY:HA3	3:D:1207:TYR:HB3	1.87	0.56
5:F:256:ARG:HH21	5:F:258:ILE:HD12	1.70	0.56
2:C:946:ARG:HD2	2:C:984:GLU:O	2.06	0.56
6:H:72:ARG:HD3	6:H:85:TYR:HB2	1.88	0.56
3:D:716:PHE:HZ	3:D:732:VAL:HG21	1.71	0.56
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.05	0.56
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.86	0.56
2:C:364:GLU:HG3	2:C:365:ASP:H	1.71	0.56
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.87	0.56
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.40	0.56
2:C:355:VAL:HG23	2:C:372:LEU:HD12	1.86	0.56
3:D:675:ARG:O	3:D:679:ARG:NH2	2.39	0.56
6:H:70:ILE:HG22	6:H:72:ARG:NH1	2.21	0.56
3:D:1275:SER:HB3	3:D:1325:LEU:HD21	1.88	0.56
2:C:1020:PRO:HD2	3:D:622:ARG:CB	2.34	0.56
1:A:86:VAL:HG13	1:A:123:MET:HB2	1.87	0.56
2:C:471:TYR:OH	2:C:491:GLU:OE2	2.17	0.56
2:C:537:LYS:CB	2:C:545:ASN:HD21	2.18	0.56
3:D:320:ALA:O	3:D:321:GLN:O	2.23	0.56
3:D:598:ARG:HH22	5:F:316:SER:HB3	1.69	0.56
3:D:736:PHE:CD1	3:D:736:PHE:N	2.74	0.56
2:C:1079:PRO:HA	2:C:1080:SER:HB3	1.88	0.56
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.88	0.56
2:C:717:LEU:O	2:C:783:ARG:NH1	2.37	0.56
2:C:897:LEU:HD23	2:C:899:GLN:HE21	1.69	0.56
1:B:22:GLU:HG2	1:B:198:ARG:HG3	1.88	0.56
2:C:922:PHE:HD1	2:C:922:PHE:O	1.89	0.56
3:D:1141:GLU:HG3	3:D:1168:MET:HE1	1.87	0.56
2:C:565:GLN:HE21	2:C:842:ARG:HG2	1.71	0.55
1:A:178:ALA:HB2	2:C:864:GLY:N	2.21	0.55
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.41	0.55
3:D:234:GLU:OE2	3:D:322:VAL:HG11	2.06	0.55
6:G:94:ASP:OD1	6:G:94:ASP:N	2.39	0.55
2:C:679:PHE:CD1	2:C:680:ASP:N	2.74	0.55
2:C:971:LYS:HA	2:C:988:VAL:HA	1.88	0.55
3:D:1115:THR:HG22	3:D:1151:ARG:HH22	1.71	0.55
3:D:1353:GLN:HG3	3:D:1357:ARG:NE	2.21	0.55
3:D:227:LEU:HD12	3:D:331:VAL:HG23	1.88	0.55
2:C:165:LEU:HA	2:C:166:PRO:C	2.27	0.55
2:C:335:THR:O	2:C:339:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:HB3	3:D:872:ARG:HH22	1.72	0.55
2:C:1043:TYR:CE1	3:D:710:ARG:HB2	2.41	0.55
2:C:235:LEU:HD21	2:C:251:ASP:O	2.06	0.55
2:C:541:SER:O	2:C:545:ASN:HB2	2.06	0.55
2:C:700:TYR:CD2	2:C:833:LEU:HD22	2.41	0.55
2:C:783:ARG:HG2	2:C:784:ASP:H	1.71	0.55
3:D:87:ARG:HB3	3:D:523:ASP:HB2	1.87	0.55
5:F:113:ILE:HG23	5:F:127:ILE:HB	1.89	0.55
1:B:156:HIS:CD2	1:B:158:ILE:HG12	2.38	0.55
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.72	0.55
3:D:1269:LYS:HA	3:D:1269:LYS:HE2	1.87	0.55
3:D:1422:MET:HG3	3:D:1427:SER:HB2	1.88	0.55
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.87	0.55
3:D:791:TYR:CE2	3:D:945:SER:HB2	2.42	0.55
5:F:385:GLU:HA	5:F:388:ALA:HB2	1.89	0.55
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.41	0.55
2:C:1020:PRO:HD3	2:C:1057:SER:CB	2.36	0.55
2:C:922:PHE:CD1	2:C:922:PHE:C	2.80	0.55
3:D:17:LYS:O	3:D:21:TRP:CD1	2.59	0.55
5:F:410:TYR:CD1	5:F:410:TYR:O	2.59	0.55
6:G:18:ASP:OD1	6:G:18:ASP:N	2.39	0.55
6:G:52:VAL:HG12	6:G:70:ILE:HA	1.88	0.55
3:D:240:GLU:N	3:D:313:MET:HA	2.21	0.55
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.87	0.55
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.21	0.55
3:D:644:LEU:HD21	3:D:718:PRO:HB3	1.89	0.55
2:C:807:ARG:NH1	6:G:21:THR:HG22	2.17	0.55
2:C:143:SER:HB2	2:C:332:ARG:HB2	1.88	0.55
3:D:231:VAL:HB	3:D:243:ALA:HA	1.88	0.55
3:D:407:VAL:HG22	3:D:408:GLU:H	1.72	0.55
1:A:10:VAL:N	1:A:26:GLU:O	2.35	0.54
2:C:540:PHE:CD1	2:C:540:PHE:N	2.75	0.54
3:D:908:LYS:HB3	3:D:1027:GLY:HA3	1.89	0.54
3:D:1135:ARG:NH2	3:D:1357:ARG:HH22	2.04	0.54
1:A:152:PRO:HD2	1:A:155:LYS:HD2	1.89	0.54
2:C:240:THR:OG1	2:C:243:ARG:NH2	2.39	0.54
2:C:358:ARG:NH2	2:C:372:LEU:O	2.34	0.54
2:C:724:ARG:O	2:C:726:ILE:HD12	2.06	0.54
3:D:1389:LEU:HD23	3:D:1389:LEU:H	1.71	0.54
3:D:7:LYS:HD3	3:D:1456:LYS:HE3	1.89	0.54
5:F:256:ARG:HD3	5:F:258:ILE:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1393:GLN:HB3	3:D:1398:TRP:CZ2	2.43	0.54
3:D:504:ASP:O	3:D:506:GLY:N	2.36	0.54
3:D:843:PHE:HE2	3:D:864:VAL:HG21	1.72	0.54
3:D:110:SER:CB	3:D:120:ALA:HB1	2.37	0.54
3:D:31:THR:HG23	3:D:545:ARG:HD3	1.89	0.54
2:C:1008:ARG:HD2	2:C:1028:GLY:C	2.27	0.54
3:D:1130:ARG:NH2	3:D:1317:ASP:OD2	2.40	0.54
3:D:173:PRO:HA	3:D:209:ARG:NH1	2.22	0.54
3:D:546:ARG:HH11	3:D:550:ARG:NH2	2.06	0.54
3:D:601:ARG:NE	3:D:606:ILE:HG22	2.22	0.54
3:D:955:VAL:HG22	3:D:1011:PHE:HE1	1.72	0.54
3:D:1434:TRP:CZ3	3:D:1457:ASP:HB2	2.42	0.54
3:D:546:ARG:NH1	3:D:550:ARG:HH22	2.04	0.54
4:E:46:PRO:O	4:E:54:LEU:HB3	2.07	0.54
3:D:534:ARG:NH2	7:Y:31:ILE:O	2.41	0.54
2:C:1067:TYR:CD1	2:C:1067:TYR:C	2.81	0.54
2:C:198:ARG:NH2	2:C:228:ALA:O	2.41	0.54
1:A:63:HIS:HB2	2:C:799:ILE:HD12	1.90	0.54
2:C:928:LYS:O	2:C:932:GLU:HG3	2.08	0.54
1:B:34:VAL:HG11	2:C:978:ARG:HB2	1.88	0.54
1:A:18:ARG:HH22	1:A:88:ARG:NH1	2.05	0.54
2:C:808:ARG:HG2	2:C:809:GLY:H	1.72	0.54
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.90	0.54
3:D:1213:ARG:HB2	3:D:1214:PRO:HD2	1.89	0.54
1:A:14:ARG:HE	1:B:233:VAL:HG13	1.72	0.54
2:C:436:GLY:HA2	2:C:538:GLN:O	2.08	0.54
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.42	0.54
3:D:1094:LEU:HD23	3:D:1230:GLY:HA2	1.90	0.54
3:D:441:ARG:HD3	3:D:443:VAL:HG13	1.90	0.54
2:C:124:ASP:O	2:C:407:LYS:HE3	2.07	0.54
2:C:739:GLU:HG2	6:G:18:ASP:HA	1.90	0.54
2:C:700:TYR:HD2	2:C:833:LEU:HD22	1.73	0.54
2:C:966:LEU:HD21	2:C:986:PRO:HB3	1.90	0.54
3:D:212:ARG:NH1	3:D:342:PRO:HB2	2.23	0.54
3:D:790:TYR:O	3:D:790:TYR:HD1	1.90	0.54
2:C:679:PHE:HD2	2:C:870:ILE:HD13	1.72	0.53
1:A:181:VAL:N	2:C:937:ASP:OD1	2.37	0.53
3:D:1289:LYS:HZ1	3:D:1304:LYS:HB2	1.71	0.53
3:D:206:ARG:HH21	5:F:98:GLU:HG3	1.72	0.53
3:D:301:GLY:C	3:D:303:PRO:HD2	2.27	0.53
5:F:163:LEU:HB3	5:F:174:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:206:ARG:HH22	5:F:94:LEU:HD23	1.73	0.53
3:D:601:ARG:NH2	3:D:611:GLN:HE22	2.02	0.53
3:D:1031:ASN:HB3	3:D:1034:GLN:HG3	1.89	0.53
2:C:512:ARG:HD2	2:C:523:ILE:HD11	1.91	0.53
3:D:1090:ASP:CG	3:D:1093:TYR:HB2	2.28	0.53
3:D:1189:ARG:HD2	3:D:1204:CYS:SG	2.48	0.53
3:D:371:ILE:HG13	3:D:372:ASP:H	1.72	0.53
3:D:601:ARG:HH22	3:D:611:GLN:NE2	2.01	0.53
5:F:392:VAL:HG12	5:F:393:THR:H	1.72	0.53
3:D:1168:MET:HG3	3:D:1172:HIS:HE1	1.73	0.53
3:D:215:TYR:CE2	3:D:343:LYS:HD2	2.43	0.53
3:D:598:ARG:NH2	5:F:316:SER:HB3	2.22	0.53
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.91	0.53
3:D:791:TYR:CZ	3:D:945:SER:HB2	2.44	0.53
3:D:139:GLY:HA3	3:D:452:ILE:HD12	1.90	0.53
3:D:23:TYR:O	3:D:49:ILE:HG23	2.08	0.53
3:D:785:ILE:HG12	3:D:935:LYS:HA	1.91	0.53
6:H:27:TYR:OH	6:H:34:LEU:O	2.25	0.53
1:A:41:ARG:NH1	1:A:177:VAL:O	2.42	0.53
2:C:54:ILE:HD11	2:C:356:ARG:HE	1.73	0.53
3:D:1293:PHE:CE1	3:D:1302:GLU:HG3	2.44	0.53
3:D:224:ARG:NH1	3:D:252:ARG:O	2.41	0.53
3:D:53:ILE:HD13	3:D:86:ARG:NH1	2.24	0.53
3:D:1350:GLU:O	3:D:1354:LYS:HG2	2.09	0.53
3:D:804:LEU:HD21	3:D:829:VAL:HG21	1.90	0.53
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.90	0.53
2:C:895:TYR:O	2:C:895:TYR:HD1	1.91	0.53
3:D:1141:GLU:HG3	3:D:1168:MET:CE	2.38	0.53
3:D:1168:MET:HG3	3:D:1172:HIS:CE1	2.44	0.53
6:H:16:ILE:HG21	6:H:63:VAL:HG21	1.89	0.53
1:A:209:GLU:O	1:A:213:GLN:HG3	2.08	0.52
2:C:185:LYS:HA	2:C:189:ARG:O	2.09	0.52
3:D:484:PRO:O	3:D:489:ARG:NH2	2.42	0.52
3:D:543:LEU:HB3	3:D:581:LEU:HB3	1.91	0.52
3:D:610:LYS:HG3	3:D:611:GLN:H	1.74	0.52
3:D:841:TYR:CD1	3:D:841:TYR:N	2.77	0.52
3:D:9:ARG:HD3	3:D:1456:LYS:HG3	1.90	0.52
5:F:357:ALA:HB2	6:G:124:SER:CB	2.39	0.52
1:A:198:ARG:NH2	2:C:932:GLU:OE1	2.43	0.52
3:D:254:GLU:O	3:D:255:GLU:HG2	2.09	0.52
2:C:767:PRO:HD2	2:C:771:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:214:TYR:HE1	2:C:311:PHE:HD2	1.55	0.52
2:C:751:PRO:HG3	2:C:796:GLU:HA	1.92	0.52
3:D:1290:LEU:HD23	3:D:1290:LEU:H	1.75	0.52
3:D:31:THR:O	3:D:32:ILE:HG23	2.09	0.52
1:A:156:HIS:HD2	1:A:158:ILE:H	1.56	0.52
2:C:290:LEU:HD21	2:C:302:VAL:HG23	1.90	0.52
3:D:128:TYR:CE1	3:D:461:ILE:HG13	2.45	0.52
3:D:598:ARG:NH2	5:F:316:SER:OG	2.42	0.52
2:C:569:VAL:O	2:C:571:LEU:HD12	2.10	0.52
2:C:712:ALA:HB2	2:C:722:ILE:HG12	1.91	0.52
2:C:877:PRO:HG2	3:D:1029:ARG:HG3	1.92	0.52
3:D:1105:ILE:HG22	3:D:1221:VAL:HG13	1.90	0.52
3:D:130:SER:HA	3:D:572:ARG:HH21	1.74	0.52
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.90	0.52
2:C:548:PRO:HA	2:C:581:THR:HG22	1.91	0.52
3:D:1009:LYS:O	3:D:1013:GLU:HG3	2.09	0.52
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.92	0.52
3:D:652:LEU:HD12	3:D:749:VAL:HG23	1.92	0.52
2:C:1013:TYR:HA	2:C:1020:PRO:HA	1.91	0.52
2:C:400:PRO:HD3	2:C:659:PRO:HG2	1.92	0.52
3:D:826:PRO:HD2	3:D:829:VAL:HG11	1.92	0.52
1:A:117:VAL:HG12	1:A:118:ALA:H	1.75	0.52
2:C:142:ARG:HD3	2:C:325:ILE:HG23	1.92	0.52
2:C:280:LYS:HE3	2:C:323:ASP:OD2	2.09	0.52
2:C:328:LEU:HB2	2:C:433:THR:HB	1.91	0.52
2:C:139:GLN:NE2	2:C:414:GLY:HA3	2.24	0.52
3:D:1146:GLY:CA	3:D:1207:TYR:HB3	2.40	0.52
3:D:216:VAL:HG22	3:D:340:THR:HG22	1.92	0.52
5:F:392:VAL:HG12	5:F:393:THR:N	2.24	0.52
2:C:305:PRO:HA	2:C:308:ARG:HB3	1.93	0.51
2:C:927:GLY:HA2	2:C:930:LYS:HZ3	1.73	0.51
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.92	0.51
5:F:213:ILE:O	5:F:217:ASN:N	2.41	0.51
3:D:1101:VAL:HG22	3:D:1428:ALA:HB2	1.91	0.51
3:D:302:GLN:N	3:D:303:PRO:HD2	2.26	0.51
3:D:30:GLU:HB3	3:D:40:GLU:HG2	1.92	0.51
3:D:598:ARG:C	3:D:598:ARG:HD2	2.31	0.51
5:F:184:ARG:HG3	5:F:224:VAL:HG11	1.92	0.51
2:C:410:ILE:HB	2:C:453:THR:O	2.11	0.51
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.43	0.51
3:D:1377:LYS:HE2	3:D:1378:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:TYR:HE1	3:D:154:THR:HG23	1.75	0.51
3:D:227:LEU:HD22	3:D:328:GLY:O	2.10	0.51
3:D:128:TYR:OH	3:D:461:ILE:HG21	2.11	0.51
6:H:70:ILE:HG22	6:H:72:ARG:HH12	1.76	0.51
2:C:1091:GLU:HG2	3:D:607:LEU:HD21	1.92	0.51
2:C:495:THR:HG21	2:C:529:VAL:HA	1.91	0.51
2:C:402:SER:OG	2:C:566:THR:O	2.29	0.51
4:E:44:GLU:C	4:E:45:ARG:HD2	2.31	0.51
5:F:312:GLN:HG3	5:F:313:GLU:H	1.75	0.51
5:F:405:LEU:O	5:F:409:LYS:N	2.43	0.51
1:B:122:ILE:HG22	1:B:124:ASN:H	1.76	0.51
2:C:193:LEU:HD22	2:C:193:LEU:O	2.11	0.51
2:C:426:ASP:OD1	2:C:426:ASP:N	2.37	0.51
3:D:601:ARG:NH2	3:D:611:GLN:NE2	2.59	0.51
2:C:1032:PHE:HB2	3:D:623:VAL:HG21	1.92	0.51
3:D:82:LYS:HG2	3:D:83:SER:N	2.21	0.51
5:F:353:GLU:HA	5:F:356:LYS:HD3	1.91	0.51
6:H:49:PRO:HD2	6:H:72:ARG:HH22	1.76	0.51
1:A:225:PHE:CD1	1:A:225:PHE:N	2.79	0.51
3:D:791:TYR:HE2	3:D:947:ILE:HG23	1.76	0.51
5:F:108:GLU:HB3	5:F:176:ILE:HG23	1.91	0.51
2:C:495:THR:HG22	2:C:530:GLU:H	1.76	0.51
2:C:512:ARG:HD2	2:C:523:ILE:CD1	2.41	0.51
3:D:1118:ILE:HD11	3:D:1346:ARG:HD3	1.92	0.51
3:D:21:TRP:N	3:D:21:TRP:HD1	2.01	0.51
3:D:411:THR:O	5:F:178:ARG:NH1	2.42	0.51
2:C:264:PRO:O	2:C:266:ARG:NH1	2.44	0.51
2:C:368:THR:HB	2:C:369:PRO:HD3	1.92	0.51
3:D:1109:GLU:HG3	3:D:1196:THR:CG2	2.37	0.51
3:D:1137:ARG:N	3:D:1137:ARG:HD3	2.25	0.51
3:D:1205:TYR:CE1	3:D:1221:VAL:HG21	2.46	0.51
3:D:302:GLN:O	3:D:304:LEU:HG	2.10	0.51
6:H:21:THR:HG22	6:H:22:GLU:N	2.26	0.51
3:D:286:VAL:HB	3:D:312:ARG:HG3	1.93	0.51
5:F:410:TYR:CD1	5:F:410:TYR:C	2.84	0.51
2:C:1047:HIS:ND1	2:C:1078:GLU:OE2	2.44	0.51
5:F:166:LEU:HB3	5:F:170:HIS:HB2	1.93	0.51
3:D:1112:CYS:HB2	3:D:1195:GLN:HB3	1.92	0.50
5:F:288:TYR:CD1	5:F:288:TYR:N	2.78	0.50
2:C:290:LEU:HD22	2:C:301:GLU:N	2.25	0.50
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:288:MET:CB	3:D:305:ALA:HB1	2.37	0.50
2:C:702:SER:OG	2:C:704:HIS:HE1	1.95	0.50
3:D:1117:TYR:C	3:D:1117:TYR:HD1	2.15	0.50
3:D:157:GLU:O	3:D:161:LEU:HD13	2.11	0.50
3:D:222:GLY:HA2	3:D:333:LEU:O	2.11	0.50
3:D:242:LEU:HD12	3:D:311:LEU:HD12	1.92	0.50
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.77	0.50
1:A:184:THR:O	1:A:192:LEU:HB2	2.11	0.50
3:D:525:ARG:HB2	3:D:538:SER:OG	2.10	0.50
3:D:591:VAL:CG1	3:D:597:ASP:HA	2.41	0.50
5:F:132:ARG:O	5:F:136:LEU:HG	2.12	0.50
2:C:194:VAL:HG21	2:C:221:LEU:O	2.12	0.50
2:C:265:ARG:HG2	2:C:288:ARG:HB2	1.94	0.50
1:A:42:ARG:NH1	2:C:857:ASP:HB3	2.15	0.50
3:D:535:PHE:HD1	3:D:535:PHE:N	2.10	0.50
3:D:867:ARG:O	3:D:867:ARG:HG3	2.12	0.50
3:D:919:PHE:HD1	3:D:919:PHE:O	1.94	0.50
2:C:275:TYR:CD1	2:C:275:TYR:O	2.63	0.50
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.94	0.50
3:D:477:LEU:HD11	3:D:495:ARG:HG2	1.94	0.50
5:F:405:LEU:O	5:F:409:LYS:HG3	2.12	0.50
5:F:402:ASN:O	5:F:406:ARG:HG3	2.12	0.50
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.94	0.50
1:B:220:GLU:O	1:B:223:THR:OG1	2.25	0.50
3:D:143:ASN:OD1	3:D:145:VAL:HG12	2.11	0.50
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.94	0.50
1:B:143:ARG:HD3	1:B:158:ILE:HG21	1.93	0.50
2:C:198:ARG:CZ	2:C:203:ASP:HA	2.41	0.50
3:D:601:ARG:HE	3:D:606:ILE:HG22	1.77	0.50
2:C:66:LEU:HD13	2:C:100:LEU:HB3	1.94	0.50
2:C:195:LEU:HG	2:C:238:LEU:HD12	1.93	0.50
2:C:273:GLY:HA2	2:C:276:LYS:HZ3	1.77	0.50
3:D:1344:VAL:HG11	3:D:1421:LEU:HD22	1.93	0.50
3:D:1399:ASP:HA	3:D:1402:ALA:HB3	1.93	0.50
3:D:186:VAL:HG12	3:D:187:LYS:H	1.77	0.50
3:D:421:LEU:HD22	3:D:429:SER:H	1.75	0.50
5:F:355:GLU:OE1	5:F:358:LEU:HD22	2.12	0.50
6:H:72:ARG:HD2	6:H:72:ARG:N	2.26	0.50
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.94	0.49
2:C:387:SER:C	2:C:388:ARG:HG3	2.31	0.49
2:C:585:GLU:O	2:C:589:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:775:ARG:HH22	2:C:781:LYS:HA	1.76	0.49
3:D:145:VAL:CG2	3:D:146:PRO:HD2	2.42	0.49
3:D:752:SER:HB3	3:D:755:ALA:H	1.76	0.49
3:D:835:SER:H	3:D:838:ARG:HH11	1.60	0.49
6:G:124:SER:HA	6:G:127:ARG:HB2	1.94	0.49
3:D:852:ALA:HB1	3:D:857:ILE:HD11	1.92	0.49
3:D:1476:THR:HG23	4:E:21:VAL:HG22	1.94	0.49
5:F:276:ARG:O	5:F:280:GLN:HG2	2.12	0.49
1:A:179:PHE:HA	1:A:197:LEU:HA	1.93	0.49
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.94	0.49
2:C:119:PRO:HG2	2:C:386:PHE:CE2	2.47	0.49
2:C:896:PHE:CD2	2:C:925:TYR:HB2	2.48	0.49
3:D:1110:ALA:O	3:D:1202:GLN:HB3	2.12	0.49
2:C:229:MET:O	2:C:229:MET:HG3	2.13	0.49
2:C:328:LEU:HD21	2:C:438:ILE:HD12	1.93	0.49
2:C:679:PHE:HD1	2:C:680:ASP:N	2.09	0.49
3:D:209:ARG:HA	3:D:347:VAL:HG22	1.94	0.49
3:D:50:PHE:CD1	3:D:522:PRO:HD3	2.48	0.49
2:C:18:LEU:HA	2:C:408:ARG:HH21	1.77	0.49
2:C:211:LEU:HD12	2:C:304:LEU:HG	1.93	0.49
2:C:458:TYR:HB2	2:C:538:GLN:HB2	1.94	0.49
2:C:557:ARG:HG3	2:C:879:ARG:HB3	1.94	0.49
5:F:85:LEU:HD22	5:F:193:ARG:NE	2.27	0.49
6:H:88:ALA:HB2	6:H:104:PRO:HA	1.95	0.49
2:C:808:ARG:NH2	2:C:820:ARG:HG3	2.28	0.49
3:D:955:VAL:HG22	3:D:1011:PHE:CE1	2.47	0.49
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.13	0.49
3:D:93:ILE:HB	3:D:517:VAL:HB	1.93	0.49
2:C:144:PRO:HD2	2:C:276:LYS:HE3	1.95	0.49
2:C:495:THR:HG22	2:C:529:VAL:HA	1.94	0.49
3:D:1156:LEU:O	3:D:1158:VAL:HG23	2.12	0.49
3:D:126:VAL:HG13	3:D:132:TYR:CD2	2.47	0.49
3:D:1409:ALA:O	3:D:1410:GLU:HG2	2.12	0.49
3:D:209:ARG:N	3:D:389:GLU:O	2.46	0.49
1:B:180:GLN:NE2	3:D:936:TYR:HE2	2.11	0.49
2:C:614:ARG:HD3	2:C:620:LEU:HD12	1.93	0.49
2:C:814:GLU:HG3	2:C:814:GLU:O	2.13	0.49
3:D:906:GLN:HB3	3:D:911:LEU:HD11	1.94	0.49
1:A:33:GLY:HA2	1:A:195:LEU:HB2	1.94	0.49
1:B:225:PHE:N	1:B:225:PHE:CD1	2.81	0.49
2:C:1085:PHE:CD1	3:D:1468:LEU:HG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:498:GLN:HB3	2:C:514:VAL:HG23	1.95	0.49
2:C:553:ASP:HA	2:C:881:ASN:HA	1.94	0.49
3:D:238:PRO:HD3	3:D:318:ARG:CG	2.42	0.49
3:D:214:GLU:O	3:D:383:GLY:HA2	2.12	0.49
1:B:111:ALA:HB2	1:B:127:LEU:HB3	1.94	0.49
3:D:313:MET:O	3:D:313:MET:HG2	2.12	0.49
3:D:661:MET:HA	3:D:666:ILE:HD12	1.94	0.49
1:B:80:LEU:HB3	3:D:867:ARG:NH1	2.27	0.49
2:C:896:PHE:N	2:C:896:PHE:CD1	2.81	0.48
3:D:1126:ASP:HA	3:D:1129:THR:O	2.13	0.48
5:F:82:ARG:O	5:F:86:HIS:HB2	2.13	0.48
2:C:1019:GLN:HA	2:C:1057:SER:HB3	1.94	0.48
2:C:280:LYS:HZ1	2:C:321:GLU:HB3	1.78	0.48
2:C:405:ARG:HG3	2:C:543:ASN:HD21	1.76	0.48
3:D:1036:ARG:HH21	3:D:1043:GLY:H	1.61	0.48
3:D:1439:SER:OG	3:D:1467:ILE:HD11	2.12	0.48
2:C:1056:LYS:HZ1	3:D:625:TYR:HB2	1.76	0.48
2:C:352:ALA:O	2:C:356:ARG:HG2	2.13	0.48
2:C:893:ALA:HB2	2:C:918:LEU:HD12	1.95	0.48
3:D:218:LYS:HA	3:D:337:LEU:O	2.14	0.48
3:D:591:VAL:HG11	3:D:597:ASP:HA	1.95	0.48
4:E:3:GLU:CG	4:E:4:PRO:HD2	2.43	0.48
5:F:363:GLU:O	5:F:367:MET:HG2	2.12	0.48
5:F:384:GLU:HG3	5:F:386:VAL:HG22	1.95	0.48
1:B:65:PHE:CE2	3:D:813:LEU:HD22	2.49	0.48
2:C:259:GLY:HA2	2:C:290:LEU:O	2.13	0.48
2:C:537:LYS:HB3	2:C:545:ASN:ND2	2.26	0.48
3:D:127:LEU:HD11	3:D:461:ILE:HD11	1.94	0.48
3:D:430:ASP:N	3:D:430:ASP:OD1	2.41	0.48
3:D:786:ILE:HD13	3:D:908:LYS:HB3	1.95	0.48
3:D:790:TYR:CD2	3:D:1026:SER:HB3	2.47	0.48
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.14	0.48
3:D:756:GLN:O	3:D:760:ARG:HG2	2.13	0.48
2:C:539:VAL:HB	2:C:540:PHE:CE1	2.49	0.48
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.96	0.48
3:D:1161:GLU:HG2	3:D:1164:ARG:HG2	1.95	0.48
3:D:691:LEU:HD23	3:D:720:LEU:HD21	1.95	0.48
2:C:137:VAL:HG13	2:C:409:ARG:HB2	1.95	0.48
2:C:589:ARG:HD3	2:C:596:TYR:CE2	2.49	0.48
3:D:1175:ILE:O	3:D:1179:GLU:HB2	2.14	0.48
3:D:1209:LEU:HD23	4:E:16:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:260:GLU:OE2	3:D:273:ARG:NH2	2.40	0.48
3:D:456:MET:SD	3:D:568:ARG:NE	2.87	0.48
3:D:94:GLU:O	3:D:551:ASN:ND2	2.44	0.48
4:E:54:LEU:HD23	4:E:58:PRO:HD2	1.96	0.48
5:F:410:TYR:HD1	5:F:410:TYR:C	2.16	0.48
6:H:92:GLN:HE21	6:H:96:GLY:HA2	1.79	0.48
1:A:20:TYR:HE1	1:A:198:ARG:CG	2.26	0.48
2:C:1008:ARG:NH2	2:C:1020:PRO:HB2	2.29	0.48
2:C:200:LEU:HD13	2:C:300:ASP:CG	2.34	0.48
2:C:572:ILE:HG13	2:C:573:ARG:N	2.28	0.48
2:C:604:ALA:HB3	2:C:612:VAL:HG12	1.95	0.48
3:D:1146:GLY:O	3:D:1207:TYR:N	2.47	0.48
3:D:288:MET:O	3:D:290:PRO:HD3	2.13	0.48
3:D:505:SER:O	3:D:1454:GLY:HA3	2.13	0.48
3:D:535:PHE:CD1	3:D:535:PHE:N	2.80	0.48
3:D:790:TYR:C	3:D:790:TYR:HD1	2.16	0.48
3:D:800:LYS:HE2	3:D:830:ALA:HB3	1.96	0.48
1:B:18:ARG:NH1	1:B:203:GLY:O	2.46	0.48
2:C:15:LEU:HD11	2:C:457:ALA:HB1	1.94	0.48
3:D:1107:VAL:HG21	3:D:1215:VAL:HG11	1.96	0.48
3:D:1378:TYR:CE1	3:D:1394:VAL:HG22	2.43	0.48
3:D:884:ARG:O	3:D:888:GLU:N	2.44	0.48
5:F:389:PHE:CD2	5:F:392:VAL:O	2.67	0.48
2:C:1042:ALA:HB1	3:D:710:ARG:HD3	1.95	0.47
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.96	0.47
2:C:256:TYR:CE1	2:C:261:ILE:HD11	2.48	0.47
2:C:493:ARG:HB2	2:C:494:TYR:CD1	2.48	0.47
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.14	0.47
3:D:310:LEU:O	3:D:311:LEU:HD22	2.14	0.47
2:C:755:LEU:HD23	2:C:825:VAL:HG21	1.96	0.47
2:C:861:LEU:HB2	2:C:865:THR:HG23	1.96	0.47
3:D:835:SER:N	3:D:838:ARG:HH11	2.12	0.47
1:A:20:TYR:HE1	1:A:198:ARG:HG3	1.79	0.47
2:C:770:GLU:HG2	5:F:354:LEU:CD1	2.45	0.47
3:D:1034:GLN:O	3:D:1038:LEU:HD12	2.14	0.47
3:D:1117:TYR:C	3:D:1117:TYR:CD1	2.88	0.47
3:D:154:THR:CG2	3:D:156:GLU:HG2	2.44	0.47
3:D:270:LEU:HD23	3:D:284:LEU:HD11	1.96	0.47
2:C:1071:ILE:CG2	3:D:670:VAL:HG21	2.44	0.47
3:D:884:ARG:HA	3:D:887:ALA:HB3	1.96	0.47
3:D:207:PHE:HZ	5:F:101:GLU:OE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG12	1:A:118:ALA:N	2.29	0.47
1:B:156:HIS:HD2	1:B:158:ILE:CG1	2.26	0.47
2:C:257:VAL:HG23	2:C:258:TYR:CD1	2.49	0.47
3:D:1364:HIS:CD2	3:D:1366:LYS:HE3	2.49	0.47
3:D:546:ARG:O	3:D:550:ARG:HG2	2.14	0.47
3:D:819:GLY:HA2	3:D:822:ALA:HB3	1.96	0.47
4:E:14:ASP:N	4:E:14:ASP:OD1	2.47	0.47
5:F:288:TYR:N	5:F:288:TYR:HD1	2.11	0.47
2:C:214:TYR:CD1	2:C:215:GLY:N	2.77	0.47
2:C:570:PRO:HD2	2:C:635:THR:HB	1.97	0.47
2:C:839:LEU:HD13	2:C:849:VAL:HG23	1.96	0.47
2:C:975:TYR:N	2:C:975:TYR:CD1	2.83	0.47
3:D:1020:LEU:HA	3:D:1023:MET:HE2	1.96	0.47
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.54	0.47
3:D:1166:LEU:H	3:D:1166:LEU:HD23	1.79	0.47
3:D:1278:ASP:N	3:D:1278:ASP:OD1	2.42	0.47
3:D:697:GLY:O	3:D:760:ARG:NH1	2.45	0.47
2:C:170:PRO:HG3	2:C:258:TYR:HD2	1.79	0.47
2:C:569:VAL:HG12	2:C:996:LYS:O	2.15	0.47
2:C:737:LEU:HD21	2:C:754:ILE:HB	1.97	0.47
2:C:97:ARG:HA	2:C:111:ASP:O	2.14	0.47
5:F:195:VAL:HG22	5:F:243:ILE:HD13	1.96	0.47
2:C:494:TYR:CD2	2:C:531:PHE:HE2	2.33	0.47
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.95	0.47
2:C:810:ASP:HB3	2:C:813:VAL:HG22	1.96	0.47
3:D:547:LEU:HD11	3:D:578:VAL:HG23	1.97	0.47
3:D:729:HIS:NE2	3:D:935:LYS:HE2	2.29	0.47
2:C:1089:VAL:HG21	2:C:1111:ILE:HD11	1.96	0.47
2:C:165:LEU:HA	2:C:166:PRO:O	2.14	0.47
2:C:745:ILE:HD11	2:C:803:THR:HG23	1.96	0.47
2:C:922:PHE:CD2	2:C:964:LYS:HA	2.50	0.47
3:D:1123:PHE:HD1	3:D:1133:ARG:C	2.18	0.47
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.50	0.47
2:C:113:VAL:O	2:C:115:LEU:HD23	2.15	0.47
2:C:364:GLU:HG3	2:C:365:ASP:N	2.29	0.47
2:C:596:TYR:N	2:C:596:TYR:CD1	2.83	0.47
3:D:210:ARG:HE	3:D:388:HIS:CB	2.27	0.47
4:E:25:LYS:O	4:E:29:GLN:HG2	2.13	0.47
2:C:344:PHE:HD1	2:C:382:ILE:HD11	1.79	0.47
2:C:807:ARG:HG2	2:C:821:GLU:OE1	2.15	0.47
2:C:854:PRO:HB2	2:C:856:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1128:VAL:HG13	3:D:1129:THR:HG22	1.97	0.47
3:D:1154:GLU:HA	3:D:1158:VAL:O	2.14	0.47
3:D:1381:VAL:HB	3:D:1389:LEU:O	2.14	0.47
3:D:297:ILE:HG23	3:D:298:VAL:H	1.80	0.47
6:H:52:VAL:HG12	6:H:70:ILE:HG23	1.97	0.47
2:C:69:LEU:HB2	2:C:97:ARG:HB3	1.96	0.47
2:C:778:PHE:HE1	6:G:125:TYR:CE1	2.33	0.47
3:D:170:PRO:HA	3:D:392:SER:OG	2.15	0.47
3:D:525:ARG:O	3:D:541:ASN:ND2	2.44	0.47
1:A:86:VAL:HG12	1:A:124:ASN:HB2	1.97	0.46
1:A:32:PHE:HE2	1:B:221:HIS:CE1	2.32	0.46
2:C:6:PHE:HZ	2:C:917:LEU:HD11	1.79	0.46
2:C:252:LYS:HG3	2:C:298:PHE:CZ	2.50	0.46
2:C:889:HIS:ND1	2:C:970:GLY:HA3	2.30	0.46
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.15	0.46
4:E:40:LEU:HB2	4:E:45:ARG:CZ	2.45	0.46
2:C:164:PRO:CA	2:C:266:ARG:HH22	2.22	0.46
2:C:905:ILE:HG23	2:C:906:PHE:H	1.80	0.46
6:H:23:LEU:HD23	6:H:61:ARG:HG3	1.97	0.46
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.33	0.46
2:C:257:VAL:HG23	2:C:258:TYR:CE1	2.51	0.46
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.16	0.46
3:D:139:GLY:O	3:D:147:VAL:HG22	2.16	0.46
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.98	0.46
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.31	0.46
5:F:181:GLU:O	5:F:184:ARG:HB3	2.15	0.46
3:D:1112:CYS:CB	3:D:1196:THR:HG23	2.37	0.46
3:D:474:GLU:O	3:D:478:LEU:HG	2.14	0.46
3:D:486:ARG:HG2	3:D:487:ALA:H	1.81	0.46
3:D:815:ALA:O	3:D:818:ARG:HB3	2.16	0.46
5:F:321:ILE:HD11	5:F:332:PHE:CE2	2.51	0.46
2:C:1016:ILE:HG21	5:F:317:LEU:HD21	1.98	0.46
2:C:252:LYS:HG3	2:C:298:PHE:HZ	1.81	0.46
3:D:1488:ASP:N	3:D:1488:ASP:OD1	2.48	0.46
1:B:206:THR:HG23	1:B:209:GLU:H	1.78	0.46
2:C:1078:GLU:HB3	2:C:1079:PRO:CD	2.42	0.46
2:C:554:ASP:N	2:C:880:MET:O	2.41	0.46
1:A:182:GLU:OE2	2:C:935:GLY:N	2.48	0.46
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.31	0.46
3:D:1397:LYS:NZ	3:D:1432:LYS:HE2	2.31	0.46
3:D:132:TYR:CE1	3:D:154:THR:HG23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:216:VAL:O	3:D:216:VAL:HG12	2.15	0.46
3:D:434:ARG:NH1	3:D:436:GLU:OE2	2.48	0.46
3:D:50:PHE:O	3:D:89:ARG:HD2	2.15	0.46
1:B:190:THR:HB	3:D:722:GLU:HG2	1.98	0.46
3:D:790:TYR:CD1	3:D:790:TYR:C	2.89	0.46
1:A:20:TYR:OH	1:A:22:GLU:OE2	2.18	0.46
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.28	0.46
2:C:1067:TYR:HD1	2:C:1067:TYR:O	1.99	0.46
2:C:420:ARG:HG3	2:C:422:ARG:HG3	1.98	0.46
2:C:525:SER:OG	2:C:528:GLU:HG3	2.15	0.46
2:C:605:LYS:HD3	2:C:610:ARG:NH2	2.31	0.46
3:D:250:LEU:HA	3:D:250:LEU:HD12	1.75	0.46
1:B:110:LYS:HD3	1:B:112:ARG:NH1	2.30	0.46
3:D:645:PRO:HB3	3:D:723:GLY:O	2.15	0.46
3:D:655:PRO:HA	3:D:658:LEU:HD12	1.98	0.46
3:D:704:ARG:NH1	3:D:738:ALA:HA	2.30	0.46
2:C:777:ILE:HA	5:F:409:LYS:HE2	1.96	0.46
2:C:1032:PHE:HZ	2:C:1040:LEU:HD13	1.81	0.46
2:C:177:GLU:HG2	2:C:183:SER:OG	2.15	0.46
2:C:263:ASP:HB2	2:C:264:PRO:HD3	1.98	0.46
2:C:326:ASP:HA	2:C:331:ARG:HD3	1.97	0.46
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.36	0.46
3:D:1394:VAL:HG21	3:D:1432:LYS:NZ	2.31	0.46
3:D:767:HIS:CE1	4:E:6:ILE:HD12	2.51	0.46
5:F:321:ILE:HD11	5:F:332:PHE:HE2	1.80	0.46
1:B:109:VAL:HA	1:B:113:ASP:OD2	2.16	0.45
2:C:196:LEU:HD13	2:C:303:PHE:CE2	2.50	0.45
2:C:275:TYR:HD1	2:C:275:TYR:C	2.19	0.45
3:D:1155:VAL:HG11	3:D:1177:ALA:HB1	1.98	0.45
3:D:183:GLU:O	3:D:202:VAL:HG13	2.16	0.45
3:D:238:PRO:HB2	3:D:315:ARG:O	2.16	0.45
3:D:253:ALA:H	3:D:303:PRO:CG	2.30	0.45
3:D:485:SER:H	3:D:488:ARG:NH2	2.13	0.45
1:A:156:HIS:CD2	1:A:158:ILE:H	2.34	0.45
1:A:38:ASN:HD22	2:C:980:GLY:CA	2.29	0.45
2:C:146:VAL:HG11	2:C:281:LEU:HD21	1.98	0.45
2:C:207:LEU:HB3	2:C:221:LEU:HD21	1.98	0.45
3:D:113:GLY:HA3	3:D:120:ALA:HA	1.97	0.45
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.97	0.45
5:F:207:LEU:HD13	5:F:254:GLN:HE21	1.81	0.45
2:C:673:LEU:HD13	2:C:895:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.46	0.45
3:D:295:GLY:HA3	3:D:302:GLN:HB2	1.97	0.45
3:D:658:LEU:HB3	3:D:670:VAL:HG13	1.97	0.45
3:D:631:ILE:HG12	3:D:743:ASP:O	2.17	0.45
5:F:88:ILE:HG21	5:F:193:ARG:HB2	1.97	0.45
1:A:18:ARG:HG3	1:A:18:ARG:NH1	2.30	0.45
2:C:679:PHE:CD2	2:C:870:ILE:HD13	2.50	0.45
3:D:654:LYS:O	3:D:658:LEU:HG	2.17	0.45
4:E:83:ASP:O	4:E:86:GLN:HG2	2.17	0.45
2:C:121:MET:HB2	2:C:127:PHE:HE1	1.82	0.45
2:C:689:VAL:HB	2:C:870:ILE:HB	1.98	0.45
3:D:1282:ARG:O	3:D:1292:VAL:HA	2.17	0.45
3:D:362:GLU:HB2	3:D:365:ASP:HB2	1.99	0.45
5:F:202:TYR:HD1	5:F:205:ARG:HE	1.63	0.45
5:F:410:TYR:HD1	5:F:410:TYR:O	1.98	0.45
1:A:225:PHE:HD1	1:A:225:PHE:N	2.14	0.45
1:B:10:VAL:HG12	1:B:12:THR:HG23	1.98	0.45
2:C:184:MET:SD	2:C:193:LEU:HD23	2.57	0.45
2:C:265:ARG:HE	2:C:288:ARG:NH2	2.15	0.45
2:C:575:GLN:HB3	2:C:670:GLN:HA	1.99	0.45
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.50	0.45
2:C:896:PHE:N	2:C:896:PHE:HD1	2.15	0.45
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.98	0.45
3:D:794:GLN:HG3	3:D:1017:PHE:CZ	2.50	0.45
6:G:5:PHE:CD1	6:G:5:PHE:C	2.90	0.45
6:G:73:PHE:CD1	6:G:80:LEU:HB3	2.52	0.45
2:C:399:ASN:ND2	2:C:668:LEU:HD22	2.31	0.45
2:C:679:PHE:CE2	2:C:853:LEU:HD11	2.52	0.45
2:C:965:GLU:O	2:C:969:GLN:HG3	2.17	0.45
3:D:206:ARG:HG3	3:D:207:PHE:N	2.32	0.45
3:D:27:GLU:HB2	3:D:42:ASP:HB3	1.99	0.45
3:D:693:GLU:HA	4:E:48:MET:CE	2.46	0.45
3:D:825:ALA:HA	3:D:826:PRO:HD3	1.81	0.45
3:D:853:VAL:HG22	3:D:858:VAL:HG23	1.99	0.45
3:D:861:GLN:N	3:D:861:GLN:OE1	2.49	0.45
3:D:537:THR:O	5:F:317:LEU:N	2.50	0.45
2:C:367:LEU:HA	2:C:371:LYS:HD2	1.99	0.45
2:C:18:LEU:HD23	2:C:542:VAL:HG21	1.99	0.45
3:D:1393:GLN:HB3	3:D:1398:TRP:NE1	2.32	0.45
3:D:1458:GLU:HG2	3:D:1458:GLU:H	1.59	0.45
3:D:216:VAL:HG13	3:D:340:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:17:LYS:HB3	3:D:21:TRP:HE1	1.81	0.45
3:D:626:SER:HA	3:D:747:VAL:O	2.16	0.45
5:F:220:LEU:O	5:F:224:VAL:HG23	2.17	0.45
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.16	0.45
3:D:1442:ASN:OD1	3:D:1442:ASN:N	2.49	0.45
3:D:253:ALA:N	3:D:303:PRO:HG3	2.30	0.45
3:D:402:PRO:CA	3:D:443:VAL:HG12	2.46	0.45
3:D:729:HIS:HE2	3:D:935:LYS:HE2	1.82	0.45
4:E:40:LEU:O	4:E:45:ARG:HG2	2.16	0.45
6:G:123:GLU:O	6:G:127:ARG:HG2	2.17	0.45
1:B:99:LEU:O	1:B:141:GLU:HA	2.16	0.45
2:C:922:PHE:CD1	2:C:922:PHE:O	2.70	0.45
3:D:186:VAL:HG12	3:D:187:LYS:N	2.32	0.45
3:D:591:VAL:HG12	3:D:592:THR:N	2.32	0.45
5:F:372:ARG:HA	5:F:372:ARG:HD2	1.52	0.45
3:D:584:ASN:ND2	3:D:600:LEU:O	2.47	0.44
3:D:610:LYS:HD2	5:F:328:PHE:CZ	2.53	0.44
2:C:1043:TYR:HE1	3:D:710:ARG:HB2	1.82	0.44
2:C:1079:PRO:HA	2:C:1080:SER:CB	2.47	0.44
2:C:239:PHE:CZ	2:C:254:VAL:HG12	2.52	0.44
2:C:497:ALA:HA	2:C:515:ALA:HA	1.99	0.44
3:D:1111:ASP:HA	3:D:1201:CYS:HB2	1.99	0.44
3:D:17:LYS:C	3:D:21:TRP:HE1	2.21	0.44
2:C:1093:GLN:CB	3:D:21:TRP:HZ3	2.30	0.44
2:C:186:VAL:O	2:C:189:ARG:N	2.46	0.44
2:C:340:MET:HE3	2:C:340:MET:HB3	1.89	0.44
2:C:500:ASN:OD1	2:C:500:ASN:N	2.38	0.44
2:C:906:PHE:HZ	3:D:1070:TYR:HD2	1.64	0.44
3:D:1115:THR:HG22	3:D:1151:ARG:NH2	2.32	0.44
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.99	0.44
4:E:93:TYR:HA	4:E:94:PRO:HD2	1.84	0.44
5:F:389:PHE:C	5:F:391:GLY:H	2.20	0.44
5:F:94:LEU:HD23	5:F:97:GLU:HB2	2.00	0.44
1:A:156:HIS:CD2	1:A:158:ILE:HG12	2.53	0.44
2:C:184:MET:O	2:C:190:LYS:HA	2.17	0.44
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.00	0.44
3:D:167:GLU:HB2	3:D:199:LEU:HD22	1.99	0.44
3:D:759:ALA:O	3:D:763:MET:HB2	2.18	0.44
5:F:108:GLU:HB3	5:F:176:ILE:CG2	2.48	0.44
5:F:389:PHE:CB	5:F:397:ILE:HG21	2.48	0.44
5:F:86:HIS:O	5:F:90:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:CG	2:C:832:LYS:HZ3	2.20	0.44
2:C:1016:ILE:HG13	2:C:1017:THR:N	2.33	0.44
2:C:771:GLU:O	2:C:775:ARG:HG2	2.17	0.44
3:D:1474:ALA:O	3:D:1477:GLY:N	2.50	0.44
3:D:440:VAL:HG23	3:D:441:ARG:H	1.81	0.44
3:D:828:LYS:HG2	3:D:828:LYS:O	2.17	0.44
3:D:959:GLU:N	3:D:959:GLU:OE1	2.45	0.44
3:D:970:LYS:HD2	3:D:995:LEU:HD13	2.00	0.44
4:E:42:PRO:CD	4:E:45:ARG:HE	2.26	0.44
3:D:697:GLY:HA3	4:E:59:ASN:OD1	2.18	0.44
6:H:57:ILE:HG22	6:H:58:LYS:HG2	1.99	0.44
1:A:219:ARG:HE	1:A:219:ARG:HB3	1.69	0.44
2:C:1043:TYR:CE2	3:D:763:MET:HA	2.53	0.44
2:C:1090:LYS:HD3	2:C:1093:GLN:OE1	2.18	0.44
2:C:162:ILE:HB	2:C:172:ILE:CG1	2.48	0.44
2:C:202:TYR:HE2	2:C:300:ASP:OD1	2.00	0.44
3:D:598:ARG:HH11	3:D:598:ARG:HG3	1.82	0.44
3:D:610:LYS:NZ	5:F:326:ASP:HA	2.32	0.44
3:D:695:ILE:HG23	3:D:718:PRO:HG2	2.00	0.44
4:E:40:LEU:HD13	4:E:45:ARG:HG3	1.98	0.44
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.99	0.44
1:B:87:VAL:HG21	1:B:144:VAL:HG11	2.00	0.44
2:C:209:ARG:HD2	2:C:209:ARG:N	2.33	0.44
2:C:369:PRO:HB2	2:C:370:ALA:H	1.54	0.44
3:D:112:ILE:O	3:D:116:LEU:N	2.48	0.44
3:D:149:LYS:HG2	3:D:150:ARG:N	2.33	0.44
3:D:350:HIS:HB2	3:D:371:ILE:HG23	2.00	0.44
3:D:703:ASN:HB3	3:D:746:ALA:HB3	2.00	0.44
3:D:82:LYS:HB3	3:D:84:ILE:HG12	1.99	0.44
1:A:104:GLU:HB3	1:A:137:ARG:HD2	1.99	0.44
3:D:256:GLU:HB2	3:D:296:GLU:HG2	2.00	0.44
3:D:411:THR:HB	3:D:437:VAL:H	1.83	0.44
3:D:133:ILE:CG2	3:D:454:ALA:HB1	2.41	0.44
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.83	0.44
2:C:1068:GLU:O	2:C:1072:LYS:HG2	2.18	0.44
2:C:327:HIS:HE1	2:C:492:ASP:OD2	2.01	0.44
2:C:579:VAL:CG1	2:C:887:GLU:HG3	2.47	0.44
3:D:214:GLU:HA	3:D:341:GLU:O	2.18	0.44
4:E:46:PRO:HG3	4:E:66:LYS:HG3	2.00	0.44
5:F:334:PRO:HG2	5:F:335:ASP:H	1.82	0.44
6:H:90:ALA:HB2	6:H:100:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1001:VAL:HG12	2:C:1001:VAL:O	2.18	0.43
2:C:234:ALA:HA	2:C:237:ARG:HB3	1.99	0.43
2:C:673:LEU:HD13	2:C:895:TYR:CE2	2.53	0.43
3:D:1123:PHE:CE1	3:D:1134:LEU:HG	2.53	0.43
3:D:1412:LYS:HA	3:D:1412:LYS:HD2	1.65	0.43
3:D:86:ARG:O	3:D:522:PRO:HD2	2.17	0.43
3:D:937:TYR:HB3	3:D:941:PHE:CE2	2.53	0.43
2:C:637:LEU:HA	2:C:659:PRO:HB3	1.99	0.43
2:C:798:GLY:HA3	2:C:828:ALA:O	2.18	0.43
3:D:989:TYR:CE2	3:D:993:LEU:HD11	2.52	0.43
3:D:1216:SER:OG	4:E:16:LYS:N	2.51	0.43
5:F:361:LEU:HA	5:F:361:LEU:HD23	1.85	0.43
1:A:27:PRO:HB3	1:A:186:LEU:HD12	2.00	0.43
2:C:289:THR:OG1	2:C:290:LEU:N	2.52	0.43
2:C:290:LEU:HD21	2:C:302:VAL:CG2	2.48	0.43
2:C:86:LYS:O	2:C:88:LEU:N	2.51	0.43
3:D:956:ILE:HG22	3:D:1039:CYS:O	2.17	0.43
3:D:244:GLU:HB3	3:D:245:LEU:HD23	2.00	0.43
3:D:411:THR:HB	3:D:437:VAL:HG12	2.00	0.43
2:C:1091:GLU:OE1	3:D:613:ARG:HD2	2.18	0.43
4:E:49:GLN:C	4:E:51:LEU:H	2.22	0.43
6:G:127:ARG:HD3	6:G:127:ARG:HA	1.61	0.43
2:C:874:LEU:HD13	3:D:783:ARG:HB3	2.00	0.43
5:F:260:ILE:CD1	5:F:261:PRO:HD2	2.44	0.43
2:C:716:LYS:HZ3	5:F:310:ILE:HG12	1.81	0.43
2:C:877:PRO:HG2	3:D:1029:ARG:CG	2.47	0.43
3:D:243:ALA:O	3:D:311:LEU:HD23	2.19	0.43
5:F:396:ARG:HA	5:F:399:GLN:HB2	2.00	0.43
1:B:56:VAL:HG13	1:B:142:VAL:HG12	2.01	0.43
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.54	0.43
2:C:140:ILE:HA	2:C:332:ARG:O	2.18	0.43
2:C:291:ALA:O	2:C:299:LYS:HE2	2.19	0.43
2:C:79:PRO:O	2:C:82:GLU:HB3	2.18	0.43
2:C:700:TYR:CB	2:C:833:LEU:HB2	2.47	0.43
3:D:1137:ARG:O	3:D:1141:GLU:HB2	2.17	0.43
3:D:485:SER:N	3:D:488:ARG:HH21	2.17	0.43
3:D:131:LYS:CE	3:D:568:ARG:HG3	2.49	0.43
3:D:811:GLU:O	3:D:815:ALA:HB3	2.19	0.43
1:A:206:THR:HB	1:A:207:PRO:HD2	2.01	0.43
2:C:1030:GLN:HE21	3:D:627:GLY:HA2	1.84	0.43
2:C:18:LEU:HG	2:C:408:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:280:LYS:HZ3	2:C:309:TYR:HE2	1.65	0.43
2:C:134:ARG:NH1	2:C:393:GLN:HA	2.34	0.43
2:C:494:TYR:CD1	2:C:494:TYR:N	2.87	0.43
2:C:975:TYR:N	2:C:975:TYR:HD1	2.17	0.43
3:D:1205:TYR:CZ	3:D:1366:LYS:HD3	2.54	0.43
3:D:1406:ARG:CD	3:D:1407:LEU:HD12	2.46	0.43
3:D:565:ILE:HD11	5:F:192:LEU:HD22	2.00	0.43
2:C:1:MET:HE2	2:C:900:ARG:HE	1.84	0.43
2:C:54:ILE:CD1	2:C:356:ARG:HE	2.30	0.43
3:D:1164:ARG:NH2	3:D:1170:ASP:OD1	2.51	0.43
3:D:704:ARG:HB2	3:D:745:MET:HG2	2.00	0.43
2:C:164:PRO:HA	2:C:266:ARG:NH2	2.26	0.43
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.18	0.43
3:D:631:ILE:HG21	3:D:745:MET:SD	2.59	0.43
3:D:793:THR:HA	3:D:879:ARG:HG3	2.00	0.43
5:F:166:LEU:O	5:F:171:LYS:HD2	2.19	0.43
6:H:65:LEU:HD12	6:H:90:ALA:O	2.19	0.43
1:A:188:GLN:HG2	1:A:189:ARG:N	2.34	0.43
2:C:170:PRO:HG3	2:C:258:TYR:CD2	2.54	0.43
2:C:927:GLY:HA2	2:C:930:LYS:HZ1	1.83	0.43
3:D:1310:ARG:HE	3:D:1327:ARG:HD2	1.83	0.43
3:D:371:ILE:HG13	3:D:372:ASP:N	2.33	0.43
2:C:1048:THR:N	3:D:758:GLU:OE2	2.42	0.43
5:F:389:PHE:O	5:F:389:PHE:CD1	2.69	0.43
1:A:88:ARG:HD2	1:A:123:MET:CE	2.49	0.42
2:C:275:TYR:CD1	2:C:275:TYR:C	2.92	0.42
2:C:571:LEU:HD23	2:C:700:TYR:HA	2.01	0.42
2:C:805:ARG:HD3	2:C:823:VAL:HG23	2.00	0.42
3:D:1104:GLU:OE1	3:D:1374:GLN:NE2	2.52	0.42
2:C:1085:PHE:HD1	3:D:1468:LEU:HG	1.84	0.42
5:F:265:VAL:O	5:F:269:ASN:ND2	2.51	0.42
6:H:39:PHE:CD2	6:H:97:ILE:HD11	2.54	0.42
1:A:100:LEU:HB2	1:A:115:LEU:HD21	2.01	0.42
1:A:188:GLN:HG2	1:A:189:ARG:HG3	2.01	0.42
2:C:1014:SER:HB3	2:C:1017:THR:O	2.18	0.42
2:C:1052:MET:HA	2:C:1056:LYS:CG	2.49	0.42
2:C:313:LEU:HD13	2:C:321:GLU:O	2.19	0.42
2:C:320:HIS:O	2:C:322:VAL:HG23	2.19	0.42
2:C:57:GLU:OE1	2:C:57:GLU:N	2.50	0.42
1:A:70:GLY:N	2:C:607:ASP:OD1	2.37	0.42
2:C:712:ALA:O	2:C:820:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.18	0.42
3:D:185:VAL:HG21	3:D:203:ALA:HB2	2.01	0.42
3:D:702:LEU:HD21	3:D:726:ILE:HG21	2.01	0.42
3:D:770:LEU:HB2	3:D:1210:SER:O	2.18	0.42
4:E:33:HIS:C	4:E:37:ASN:HD21	2.23	0.42
1:A:32:PHE:HZ	1:B:47:SER:HG	1.64	0.42
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.00	0.42
2:C:460:ARG:HD2	2:C:485:TYR:CE2	2.54	0.42
2:C:926:PHE:C	2:C:926:PHE:CD1	2.93	0.42
3:D:288:MET:HG2	3:D:305:ALA:HB1	2.01	0.42
3:D:520:LEU:HD11	3:D:524:LEU:HD12	2.00	0.42
5:F:132:ARG:HG2	5:F:181:GLU:CD	2.39	0.42
3:D:185:VAL:CG2	3:D:203:ALA:HB2	2.50	0.42
4:E:33:HIS:CD2	4:E:90:GLU:HG3	2.54	0.42
5:F:342:VAL:O	5:F:342:VAL:HG12	2.18	0.42
1:A:111:ALA:O	1:A:114:PHE:HD2	2.03	0.42
1:B:26:GLU:HG3	1:B:184:THR:HG21	2.01	0.42
1:B:27:PRO:HG3	1:B:186:LEU:HD12	2.00	0.42
2:C:1083:GLU:OE2	3:D:87:ARG:NH1	2.52	0.42
2:C:358:ARG:HE	2:C:372:LEU:HA	1.83	0.42
2:C:594:ALA:HB3	2:C:596:TYR:CE1	2.54	0.42
2:C:598:GLU:HB2	2:C:615:TYR:CE2	2.53	0.42
2:C:863:ASP:O	2:C:865:THR:N	2.52	0.42
2:C:889:HIS:CE1	2:C:988:VAL:HG21	2.55	0.42
2:C:936:VAL:HG11	2:C:959:PRO:HB2	2.02	0.42
3:D:1207:TYR:CE2	3:D:1212:ALA:O	2.73	0.42
3:D:1393:GLN:HB3	3:D:1398:TRP:CE2	2.55	0.42
3:D:30:GLU:O	3:D:43:GLY:HA3	2.19	0.42
3:D:614:PHE:HD1	3:D:1467:ILE:HG21	1.84	0.42
3:D:617:ASN:OD1	3:D:621:LYS:NZ	2.52	0.42
5:F:142:ARG:HG3	5:F:142:ARG:O	2.19	0.42
5:F:166:LEU:O	5:F:171:LYS:HG3	2.19	0.42
5:F:384:GLU:O	5:F:388:ALA:HB2	2.19	0.42
6:G:121:TYR:CD1	6:G:121:TYR:N	2.88	0.42
6:H:39:PHE:CE2	6:H:97:ILE:HD11	2.54	0.42
1:B:65:PHE:CD2	3:D:813:LEU:HD22	2.55	0.42
3:D:1101:VAL:CG2	3:D:1428:ALA:HB2	2.49	0.42
3:D:140:ALA:HA	3:D:147:VAL:HG22	2.00	0.42
3:D:239:GLY:H	3:D:314:PRO:C	2.22	0.42
3:D:573:MET:SD	5:F:214:GLN:HG3	2.59	0.42
2:C:365:ASP:OD1	2:C:366:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1271:LYS:NZ	3:D:1273:VAL:HG12	2.34	0.42
3:D:882:PHE:HA	3:D:885:ILE:HD12	2.02	0.42
4:E:41:GLU:OE1	4:E:63:TRP:CH2	2.67	0.42
4:E:47:LYS:HE3	4:E:55:PHE:CZ	2.49	0.42
5:F:172:ARG:HA	5:F:175:HIS:CD2	2.52	0.42
3:D:54:LYS:HE3	5:F:340:SER:O	2.20	0.42
3:D:206:ARG:HH21	5:F:98:GLU:CG	2.32	0.42
2:C:218:VAL:O	2:C:221:LEU:HB3	2.19	0.42
2:C:285:LEU:O	2:C:301:GLU:HG2	2.20	0.42
2:C:554:ASP:HB2	2:C:880:MET:CB	2.50	0.42
2:C:64:LEU:HD22	2:C:359:MET:HG3	2.01	0.42
2:C:54:ILE:HG22	2:C:66:LEU:O	2.19	0.42
3:D:1255:GLY:O	3:D:1258:ARG:HB3	2.19	0.42
3:D:421:LEU:HB3	3:D:428:LYS:HA	2.01	0.42
3:D:802:ALA:O	3:D:804:LEU:N	2.53	0.42
3:D:820:GLU:HG3	3:D:836:VAL:HG11	2.01	0.42
4:E:95:VAL:HG12	4:E:95:VAL:O	2.20	0.42
5:F:266:GLU:O	5:F:270:LYS:HB2	2.20	0.42
5:F:79:ASP:HB3	5:F:80:PRO:HD3	2.02	0.42
6:G:72:ARG:HB2	6:G:85:TYR:HB2	2.02	0.42
1:B:52:ALA:HB3	1:B:171:PHE:CD1	2.54	0.42
2:C:1020:PRO:HD3	2:C:1057:SER:HB3	2.01	0.42
2:C:260:LEU:HB3	2:C:261:ILE:CD1	2.49	0.42
2:C:724:ARG:NH1	6:G:16:ILE:HG23	2.34	0.42
2:C:926:PHE:HD1	2:C:926:PHE:C	2.24	0.42
2:C:676:ILE:CG2	2:C:988:VAL:HG13	2.49	0.42
3:D:734:GLU:HG2	3:D:778:LEU:O	2.19	0.42
3:D:877:PRO:HA	3:D:880:ILE:HG22	2.01	0.42
1:B:76:VAL:O	1:B:79:ILE:HG12	2.20	0.42
2:C:18:LEU:HG	2:C:408:ARG:NH2	2.34	0.42
2:C:261:ILE:O	2:C:265:ARG:NH1	2.53	0.42
2:C:309:TYR:CZ	2:C:321:GLU:HG3	2.54	0.42
2:C:442:GLU:HG3	2:C:442:GLU:O	2.20	0.42
2:C:496:ILE:O	2:C:516:ARG:N	2.42	0.42
2:C:684:PHE:O	2:C:686:ASP:N	2.53	0.42
2:C:670:GLN:OE1	2:C:699:PHE:HB3	2.20	0.42
3:D:107:ASP:OD2	3:D:111:LYS:HE3	2.20	0.42
3:D:1271:LYS:HZ3	3:D:1273:VAL:HG12	1.84	0.42
2:C:1093:GLN:CG	3:D:21:TRP:HZ3	2.32	0.42
2:C:256:TYR:CE1	2:C:261:ILE:CD1	3.03	0.41
2:C:370:ALA:HA	2:C:373:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:648:ARG:HD2	2:C:648:ARG:N	2.35	0.41
3:D:1495:ILE:HG13	4:E:80:VAL:HG11	2.01	0.41
2:C:769:PRO:HA	5:F:374:GLY:HA2	2.02	0.41
3:D:131:LYS:HE3	3:D:568:ARG:HG3	2.00	0.41
3:D:845:ASN:CB	3:D:848:GLU:H	2.32	0.41
5:F:223:ALA:HB2	5:F:242:TRP:HB2	2.01	0.41
1:B:91:ASN:O	1:B:93:SER:N	2.49	0.41
2:C:18:LEU:CB	2:C:408:ARG:HH21	2.33	0.41
3:D:246:PRO:HG2	3:D:307:ALA:HB1	2.02	0.41
4:E:42:PRO:HD2	4:E:45:ARG:HH21	1.85	0.41
1:A:193:ASP:OD1	2:C:938:LYS:HE2	2.20	0.41
2:C:302:VAL:O	2:C:305:PRO:HD2	2.20	0.41
2:C:136:ILE:HG21	2:C:336:VAL:HG23	2.02	0.41
2:C:468:ARG:HG3	2:C:486:MET:C	2.40	0.41
3:D:118:LEU:HB3	3:D:123:LEU:HB2	2.03	0.41
3:D:1278:ASP:HA	3:D:1319:VAL:O	2.20	0.41
3:D:206:ARG:NH2	5:F:98:GLU:OE2	2.54	0.41
3:D:269:PHE:HD1	3:D:283:PHE:HD1	1.69	0.41
3:D:441:ARG:HD3	3:D:443:VAL:CG1	2.51	0.41
3:D:851:LEU:O	3:D:855:HIS:HD2	2.04	0.41
3:D:935:LYS:HB3	3:D:935:LYS:HE3	1.90	0.41
6:G:31:LEU:HA	6:G:51:PRO:HB2	2.02	0.41
1:A:143:ARG:HE	1:A:158:ILE:CG2	2.23	0.41
2:C:89:THR:OG1	2:C:129:ILE:O	2.20	0.41
2:C:258:TYR:CD1	2:C:258:TYR:N	2.88	0.41
2:C:332:ARG:NH1	2:C:338:GLU:OE2	2.54	0.41
2:C:486:MET:CE	2:C:491:GLU:HA	2.51	0.41
2:C:889:HIS:CE1	2:C:970:GLY:HA3	2.55	0.41
3:D:414:ARG:NH1	3:D:450:TYR:OH	2.52	0.41
5:F:287:THR:OG1	5:F:288:TYR:N	2.51	0.41
1:A:122:ILE:HG22	1:A:124:ASN:H	1.85	0.41
2:C:1094:ALA:O	3:D:518:PRO:HG2	2.21	0.41
2:C:686:ASP:OD2	2:C:879:ARG:NH2	2.54	0.41
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.85	0.41
3:D:1346:ARG:HA	3:D:1346:ARG:HD2	1.67	0.41
3:D:184:GLU:O	3:D:185:VAL:HG23	2.21	0.41
5:F:405:LEU:HA	5:F:408:LEU:HD12	2.01	0.41
6:H:46:TYR:CZ	6:H:104:PRO:HG2	2.55	0.41
1:B:117:VAL:HG12	1:B:118:ALA:H	1.86	0.41
1:B:176:ARG:H	1:B:200:TRP:HB2	1.85	0.41
1:B:18:ARG:O	1:B:207:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:GLN:O	2:C:333:ILE:HA	2.21	0.41
2:C:6:PHE:HD2	2:C:909:ALA:HB2	1.85	0.41
2:C:919:ALA:HB2	2:C:968:LEU:HD21	2.01	0.41
3:D:17:LYS:O	3:D:21:TRP:HD1	2.02	0.41
3:D:871:LYS:HD2	3:D:873:LEU:HD21	2.03	0.41
3:D:895:VAL:HG11	3:D:922:LEU:HD21	2.03	0.41
2:C:270:GLY:O	2:C:274:ARG:HD2	2.21	0.41
2:C:557:ARG:HH12	2:C:879:ARG:HE	1.68	0.41
2:C:782:ALA:HB3	6:G:34:LEU:HD12	2.03	0.41
2:C:557:ARG:CZ	2:C:879:ARG:HD3	2.51	0.41
2:C:1093:GLN:HG2	3:D:21:TRP:HZ3	1.85	0.41
3:D:417:PRO:HA	3:D:429:SER:O	2.21	0.41
1:A:188:GLN:CD	1:A:188:GLN:H	2.24	0.41
1:B:68:ILE:HD11	1:B:75:VAL:HG22	2.03	0.41
2:C:1081:VAL:HB	2:C:1086:ARG:NE	2.35	0.41
2:C:214:TYR:N	2:C:214:TYR:CD1	2.88	0.41
2:C:396:ASP:H	2:C:406:HIS:HD1	1.68	0.41
3:D:1495:ILE:HG21	4:E:80:VAL:HG13	2.03	0.41
3:D:434:ARG:O	3:D:446:VAL:HA	2.20	0.41
2:C:706:GLU:HG3	2:C:707:ARG:H	1.85	0.41
3:D:791:TYR:C	3:D:791:TYR:HD1	2.24	0.41
1:B:80:LEU:HD11	3:D:842:VAL:HG12	2.01	0.41
2:C:1021:LEU:HD12	7:Y:12:ALA:CB	2.51	0.41
2:C:1056:LYS:HE3	3:D:625:TYR:H	1.86	0.41
2:C:478:VAL:HG13	2:C:506:ASN:HB3	2.03	0.41
2:C:524:VAL:HG22	2:C:525:SER:H	1.85	0.41
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	2.03	0.41
3:D:1161:GLU:O	3:D:1164:ARG:HG2	2.21	0.41
3:D:1434:TRP:CE3	3:D:1457:ASP:HB2	2.56	0.41
3:D:237:LYS:O	3:D:240:GLU:HB2	2.21	0.41
3:D:660:LYS:HA	3:D:663:GLU:CG	2.51	0.41
3:D:838:ARG:HD3	3:D:874:GLU:OE1	2.21	0.41
3:D:793:THR:O	3:D:905:PRO:HA	2.21	0.41
6:G:121:TYR:N	6:G:121:TYR:HD1	2.19	0.41
1:A:70:GLY:HA3	1:A:136:GLY:HA2	2.03	0.40
1:B:225:PHE:HD1	1:B:225:PHE:N	2.17	0.40
2:C:309:TYR:CE2	2:C:321:GLU:HG3	2.56	0.40
2:C:855:VAL:HG23	2:C:866:PRO:HG3	2.02	0.40
3:D:1101:VAL:CG2	3:D:1424:VAL:HG13	2.47	0.40
3:D:415:VAL:O	3:D:416:ALA:HB2	2.21	0.40
3:D:551:ASN:O	3:D:555:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:844:ALA:HA	3:D:867:ARG:HG2	2.04	0.40
1:B:110:LYS:HB2	1:B:112:ARG:HG2	2.04	0.40
2:C:265:ARG:HE	2:C:288:ARG:HH21	1.69	0.40
2:C:292:ARG:HD3	2:C:299:LYS:HD3	2.03	0.40
2:C:503:LEU:HA	2:C:507:ARG:O	2.21	0.40
2:C:971:LYS:HG2	2:C:988:VAL:HB	2.02	0.40
3:D:1206:GLY:HA3	3:D:1366:LYS:CE	2.43	0.40
3:D:1209:LEU:CD1	3:D:1215:VAL:HA	2.43	0.40
3:D:1271:LYS:NZ	3:D:1334:GLN:HE22	2.19	0.40
3:D:177:ALA:HB3	3:D:191:LEU:O	2.21	0.40
3:D:338:GLU:HG2	3:D:338:GLU:O	2.21	0.40
5:F:361:LEU:HD12	5:F:408:LEU:HG	2.02	0.40
2:C:54:ILE:O	2:C:54:ILE:HG23	2.20	0.40
2:C:583:LEU:O	2:C:587:VAL:HG23	2.21	0.40
2:C:670:GLN:OE1	2:C:700:TYR:HD1	2.04	0.40
3:D:1236:LEU:HD23	3:D:1359:GLN:HG3	2.02	0.40
3:D:326:GLU:HA	3:D:331:VAL:HG22	2.03	0.40
3:D:770:LEU:HA	3:D:777:PRO:HA	2.02	0.40
3:D:804:LEU:HD21	3:D:829:VAL:CG2	2.51	0.40
5:F:131:VAL:O	5:F:135:ILE:HG12	2.22	0.40
6:H:28:ASP:OD1	6:H:64:ARG:NH2	2.54	0.40
2:C:1021:LEU:HD12	7:Y:12:ALA:HB1	2.02	0.40
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.02	0.40
2:C:937:ASP:OD2	2:C:939:ARG:NE	2.50	0.40
5:F:109:GLY:HA2	5:F:177:ALA:HA	2.04	0.40
6:G:88:ALA:HA	6:G:102:HIS:CE1	2.56	0.40
2:C:1050:GLN:O	2:C:1054:THR:N	2.55	0.40
2:C:205:GLU:O	2:C:209:ARG:HD3	2.21	0.40
2:C:364:GLU:HG2	2:C:364:GLU:H	1.70	0.40
3:D:1129:THR:HG23	3:D:1131:SER:HB3	2.03	0.40
3:D:1148:VAL:HG12	3:D:1149:LEU:O	2.22	0.40
3:D:256:GLU:O	3:D:274:ARG:HG3	2.21	0.40
3:D:298:VAL:O	3:D:298:VAL:HG12	2.22	0.40
3:D:786:ILE:HG21	3:D:1027:GLY:H	1.87	0.40
3:D:881:LEU:HD21	3:D:941:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/315 (71%)	207 (93%)	16 (7%)	0	100	100
1	B	230/315 (73%)	216 (94%)	14 (6%)	0	100	100
2	C	1112/1119 (99%)	960 (86%)	138 (12%)	14 (1%)	12	48
3	D	1456/1524 (96%)	1271 (87%)	179 (12%)	6 (0%)	34	71
4	E	93/99 (94%)	78 (84%)	11 (12%)	4 (4%)	2	25
5	F	307/423 (73%)	271 (88%)	32 (10%)	4 (1%)	12	48
6	G	123/144 (85%)	120 (98%)	3 (2%)	0	100	100
6	H	87/144 (60%)	82 (94%)	5 (6%)	0	100	100
7	Y	32/54 (59%)	28 (88%)	4 (12%)	0	100	100
All	All	3663/4137 (88%)	3233 (88%)	402 (11%)	28 (1%)	19	58

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	284	ARG
2	C	286	SER
2	C	370	ALA
2	C	765	SER
2	C	1080	SER
3	D	216	VAL
3	D	321	GLN
4	E	94	PRO
4	E	95	VAL
5	F	342	VAL
3	D	217	LYS
4	E	58	PRO
5	F	335	ASP
5	F	341	PRO
2	C	231	PRO
2	C	685	GLU

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Mol	Chain	Res	Type
3	D	1125	PRO
5	F	334	PRO
2	C	287	GLY
2	C	369	PRO
2	C	1079	PRO
4	E	42	PRO
2	C	282	GLY
2	C	289	THR
2	C	318	PRO
2	C	727	PRO
3	D	303	PRO
3	D	137	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	A	197/273 (72%)	191 (97%)	6 (3%)	41	64
1	B	200/273 (73%)	197 (98%)	3 (2%)	65	80
2	C	937/941 (100%)	911 (97%)	26 (3%)	43	65
3	D	1232/1279 (96%)	1204 (98%)	28 (2%)	50	70
4	E	84/88 (96%)	82 (98%)	2 (2%)	49	69
5	F	273/371 (74%)	267 (98%)	6 (2%)	52	71
6	G	107/123 (87%)	103 (96%)	4 (4%)	34	60
6	H	79/123 (64%)	78 (99%)	1 (1%)	69	82
7	Y	1/45 (2%)	1 (100%)	0	100	100
All	All	3110/3516 (88%)	3034 (98%)	76 (2%)	49	69

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	30	ARG

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Mol	Chain	Res	Type
1	A	143	ARG
1	A	198	ARG
1	A	219	ARG
1	A	225	PHE
1	B	41	ARG
1	B	198	ARG
1	B	225	PHE
2	C	52	PHE
2	C	86	LYS
2	C	95	TYR
2	C	134	ARG
2	C	193	LEU
2	C	214	TYR
2	C	258	TYR
2	C	274	ARG
2	C	275	TYR
2	C	309	TYR
2	C	388	ARG
2	C	422	ARG
2	C	485	TYR
2	C	494	TYR
2	C	540	PHE
2	C	596	TYR
2	C	610	ARG
2	C	805	ARG
2	C	895	TYR
2	C	896	PHE
2	C	922	PHE
2	C	926	PHE
2	C	975	TYR
2	C	1021	LEU
2	C	1043	TYR
2	C	1067	TYR
3	D	3	LYS
3	D	21	TRP
3	D	149	LYS
3	D	220	ARG
3	D	311	LEU
3	D	441	ARG
3	D	511	TRP
3	D	525	ARG
3	D	535	PHE

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Mol	Chain	Res	Type
3	D	549	ASN
3	D	598	ARG
3	D	679	ARG
3	D	704	ARG
3	D	736	PHE
3	D	790	TYR
3	D	791	TYR
3	D	828	LYS
3	D	841	TYR
3	D	884	ARG
3	D	919	PHE
3	D	1036	ARG
3	D	1062	ARG
3	D	1117	TYR
3	D	1137	ARG
3	D	1304	LYS
3	D	1389	LEU
3	D	1406	ARG
3	D	1470	ARG
4	E	59	ASN
4	E	91	ARG
5	F	229	TYR
5	F	256	ARG
5	F	288	TYR
5	F	389	PHE
5	F	390	PHE
5	F	410	TYR
6	G	5	PHE
6	G	18	ASP
6	G	61	ARG
6	G	121	TYR
6	H	61	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
2	C	139	GLN
2	C	327	HIS
2	C	545	ASN
2	C	565	GLN
2	C	704	HIS

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Mol	Chain	Res	Type
2	C	899	GLN
3	D	611	GLN
3	D	744	GLN
3	D	767	HIS
3	D	824	ASN
3	D	1334	GLN
4	E	33	HIS
4	E	37	ASN
5	F	218	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	225/315 (71%)	-0.34	0	100 100	74, 112, 158, 227	0
1	B	232/315 (73%)	-0.30	0	100 100	70, 122, 170, 236	0
2	C	1114/1119 (99%)	-0.17	18 (1%)	72 62	63, 135, 222, 329	0
3	D	1462/1524 (95%)	0.03	39 (2%)	54 44	69, 160, 249, 295	0
4	E	95/99 (95%)	0.04	3 (3%)	47 37	99, 158, 242, 266	0
5	F	313/423 (73%)	0.08	13 (4%)	36 29	144, 205, 276, 332	0
6	G	127/144 (88%)	0.16	4 (3%)	49 38	108, 172, 219, 238	0
6	H	91/144 (63%)	1.05	13 (14%)	2 3	186, 217, 248, 264	0
7	Y	34/54 (62%)	-0.81	0	100 100	204, 241, 270, 283	0
All	All	3693/4137 (89%)	-0.05	90 (2%)	59 49	63, 153, 245, 332	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	270	GLY	5.4
5	F	282	LEU	5.4
2	C	59	LYS	5.2
3	D	1408	ILE	4.7
5	F	281	GLU	4.6
4	E	56	ASP	4.6
2	C	60	GLY	4.3
5	F	339	PRO	4.2
6	H	87	TYR	4.2
4	E	57	ASP	4.1
6	H	86	ALA	4.1
3	D	298	VAL	4.0
3	D	294	HIS	3.8
6	H	89	TYR	3.7
3	D	802	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	61	LYS	3.5
5	F	287	THR	3.5
2	C	292	ARG	3.3
3	D	233	LYS	3.3
3	D	420	VAL	3.2
3	D	235	ALA	3.2
6	G	73	PHE	3.1
3	D	1311	LEU	3.0
2	C	223	ASP	3.0
5	F	145	PRO	3.0
3	D	810	GLU	3.0
3	D	1313	VAL	3.0
3	D	345	TYR	3.0
4	E	96	GLU	3.0
6	H	88	ALA	2.9
6	H	85	TYR	2.9
5	F	205	ARG	2.8
5	F	284	ARG	2.8
6	H	36	PRO	2.8
3	D	234	GLU	2.7
3	D	346	ARG	2.7
3	D	483	HIS	2.7
5	F	338	LEU	2.6
2	C	293	PHE	2.6
2	C	55	GLU	2.6
2	C	221	LEU	2.6
6	H	37	ARG	2.6
2	C	271	GLU	2.6
3	D	309	GLY	2.6
3	D	88	TYR	2.5
5	F	280	GLN	2.5
3	D	212	ARG	2.5
2	C	367	LEU	2.5
6	H	106	VAL	2.5
3	D	263	GLU	2.4
3	D	419	ASP	2.4
5	F	322	GLY	2.4
3	D	257	GLY	2.4
3	D	189	GLN	2.4
6	G	88	ALA	2.4
6	H	104	PRO	2.4
5	F	340	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	267	TYR	2.3
3	D	246	PRO	2.3
3	D	218	LYS	2.3
3	D	44	LEU	2.3
3	D	1128	VAL	2.3
3	D	383	GLY	2.3
3	D	363	ALA	2.3
3	D	220	ARG	2.3
3	D	250	LEU	2.3
5	F	283	GLY	2.3
3	D	308	LYS	2.2
2	C	98	LEU	2.2
3	D	210	ARG	2.2
6	G	82	ALA	2.2
3	D	252	ARG	2.2
6	H	92	GLN	2.2
3	D	307	ALA	2.2
6	H	54	LEU	2.1
2	C	366	SER	2.1
2	C	99	GLN	2.1
2	C	294	GLU	2.1
6	H	38	MET	2.1
6	H	102	HIS	2.1
2	C	211	LEU	2.1
3	D	310	LEU	2.1
3	D	175	VAL	2.1
2	C	365	ASP	2.1
3	D	223	LEU	2.1
6	G	89	TYR	2.1
5	F	144	ILE	2.1
3	D	1504	GLU	2.1
3	D	428	LYS	2.0
3	D	225	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
8	ZN	D	2001	1/1	0.97	0.17	225,225,225,225	0

6.5 Other polymers [i](#)

There are no such residues in this entry.