



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:14 PM BST

PDB ID : 6OVR
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter variant -1G
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2019-05-08
Resolution : 2.84 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

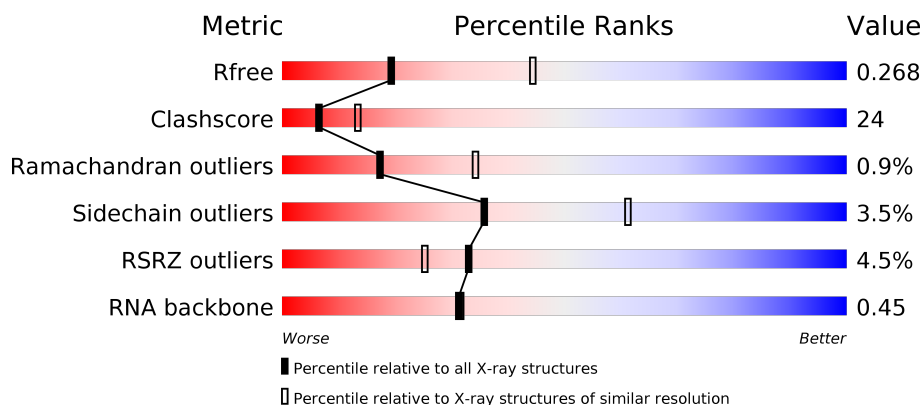
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)
RNA backbone	3102	1077 (3.10-2.58)

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>46%</div> <div>24%</div> <div>28%</div> </div>
1	B	315	<div> <div>35%</div> <div>36%</div> <div>29%</div> </div>
2	C	1119	<div> <div>4%</div> <div>61%</div> <div>35%</div> </div>
3	D	1524	<div> <div>3%</div> <div>59%</div> <div>36%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>59%32%5%</div></div>
5	F	423	<div><div></div><div>12%45%34%18%</div></div>
6	G	22	<div><div></div><div>14%50%32%5%14%</div></div>
7	H	27	<div><div></div><div>11%44%22%30%</div></div>
8	I	8	<div><div></div><div>25%38%25%38%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28535 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1107	Total	C	N	O	S	0	0	0
			8726	5523	1551	1628	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	0	0
			11722	7431	2065	2191	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2790	1760	508	518	4			

- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	19	Total	C	N	O	P	0	0	0
			387	183	75	110	19			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	19	Total	C	N	O	P	0	0	0
			394	188	76	112	18			

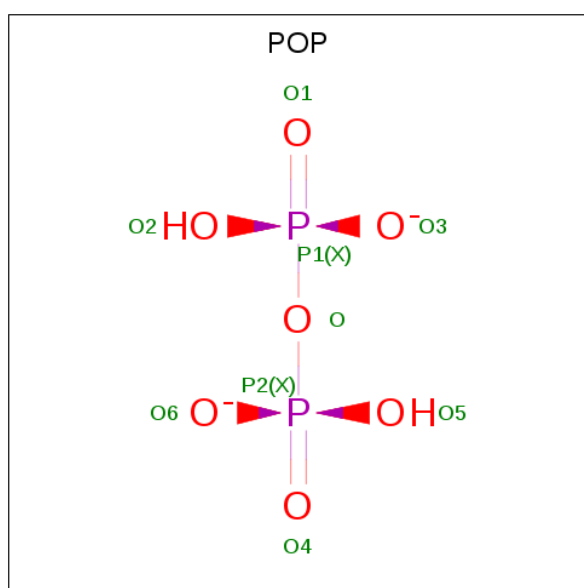
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	8	Total	C	N	O	P	0	0	0
			193	80	40	63	10			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

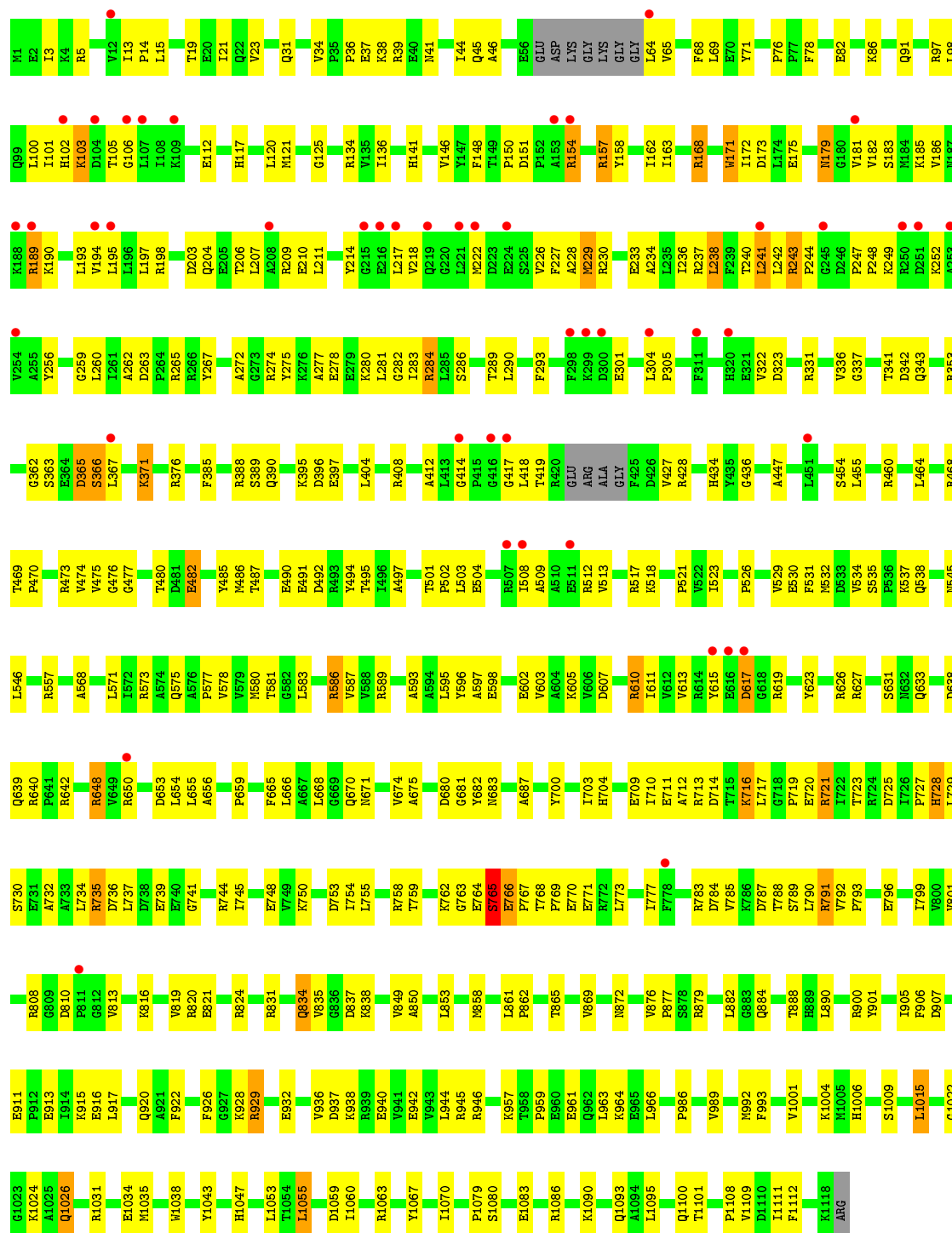
- Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

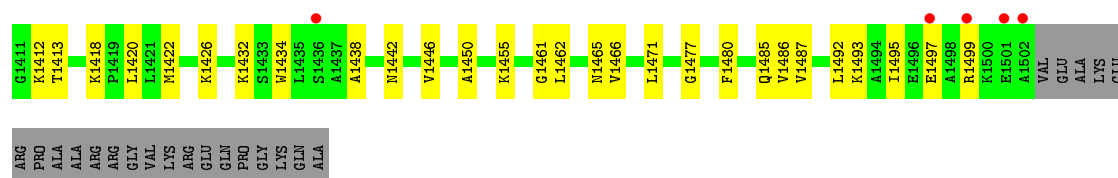
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		



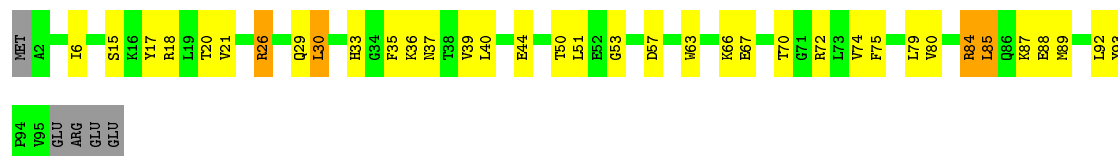
• Molecule 3: DNA-directed RNA polymerase subunit beta'



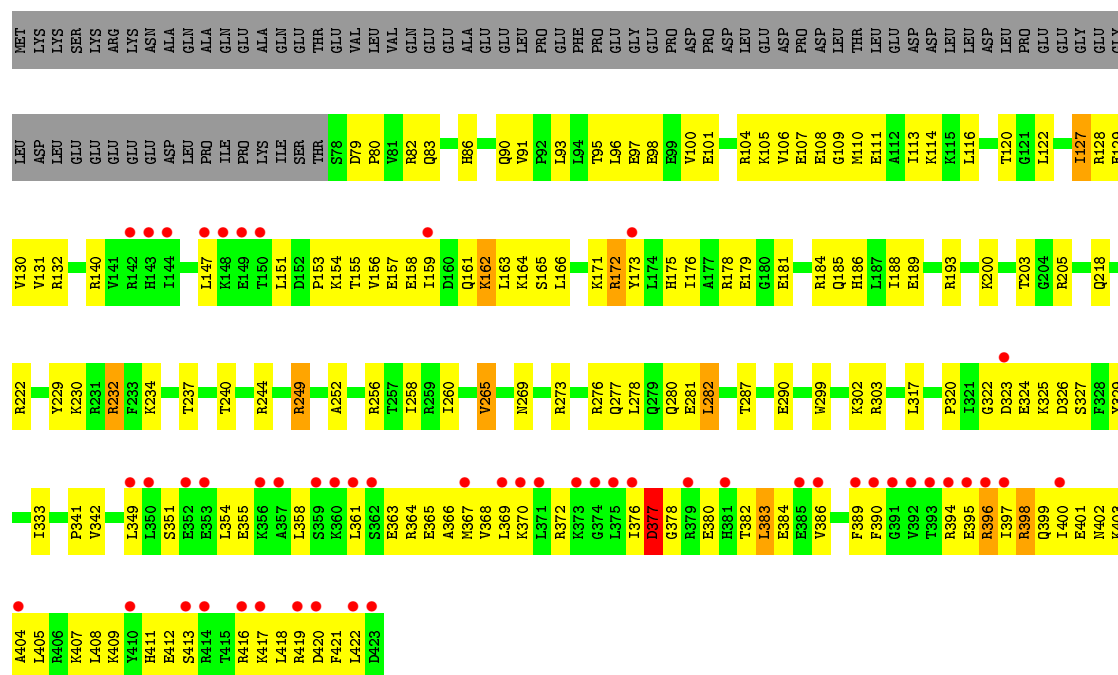
K1301	T1234	R1108	D682	Q575	R486	A398	L333	E247	P172	T97
E1302	Q1235	E1109	I603	D579	A467	Y401	L335	P243	P173	P98
K1303	L1236	A1110	K684	D579	R488	Y401	T334	Y249	G174	A99
K1304	T1237	D1111	D685	L581	R489	D405	L335	R252	L178	A100
P1306	ARG	G1112	E686	L582	A490	D405	E338	R253	L179	H101
K1307	THR	H1113	V687	L582	K491	V407	K339	R254	K180	H103
E1308	PHE	T1114	K688	R587	K494	E408	E339	D181	F104	F105
A1309	HIS	D1126	D689	R587	K495	V408	K343	V258	V105	K106
R1310	THR	E1127	L691	S602	L496	S410	D344	V259	E182	K106
R1311	GLY	H1128	L691	L603	R496	T411	E184	E183	E183	
L1312	GLY	T1129	L695	R613	R500	G412	V347	V185	V185	
V1313	VAL	R1130	V689	R613	L503	D413	Q348	K187	K111	
K1314	ALA	R1137	V700	R622	L503	V420	Q348	E266	S110	
D1315	GLY	L899	V701	R622	L503	V420	Q348	E267	I112	
G1316	ALA	L899	V701	R622	L503	V420	Q348	E268	I112	
D1317	ALA	L899	V701	R622	L503	V420	Q348	E269	L116	
Y1318	ASP	L899	V701	R622	L503	V420	Q348	E270	L117	
I1318	ILE	L899	V701	R622	L503	V420	Q348	E271	L118	
THR	THR	L899	V701	R622	L503	V420	Q348	E272	E122	
Q1254	THR	L899	V701	R622	L503	V420	Q348	E273	L123	
R1258	THR	L899	V701	R622	L503	V420	Q348	E274	E124	
P1262	THR	L899	V701	R622	L503	V420	Q348	E275	Q125	
A1265	THR	L899	V701	R622	L503	V420	Q348	E276	V126	
R1266	THR	L899	V701	R622	L503	V420	Q348	E277	L127	
R1267	THR	L899	V701	R622	L503	V420	Q348	E278	Y128	
P1268	THR	L899	V701	R622	L503	V420	Q348	E279	K131	
K1271	THR	L899	V701	R622	L503	V420	Q348	E280	Y132	
A1272	THR	L899	V701	R622	L503	V420	Q348	E281	Y133	
I1274	THR	L899	V701	R622	L503	V420	Q348	E282	Y205	
S1275	THR	L899	V701	R622	L503	V420	Q348	E283	Y206	
E1276	THR	L899	V701	R622	L503	V420	Q348	E284	Y207	
I1277	THR	L899	V701	R622	L503	V420	Q348	E285	Y208	
D1278	THR	L899	V701	R622	L503	V420	Q348	E286	Y209	
G1279	THR	L899	V701	R622	L503	V420	Q348	E287	Y210	
V1280	THR	L899	V701	R622	L503	V420	Q348	E288	Y211	
V1281	THR	L899	V701	R622	L503	V420	Q348	E289	Y212	
R1282	THR	L899	V701	R622	L503	V420	Q348	E290	Y213	
T1286	THR	L899	V701	R622	L503	V420	Q348	E291	Y214	
E1287	THR	L899	V701	R622	L503	V420	Q348	E292	Y215	
E1288	THR	L899	V701	R622	L503	V420	Q348	E293	Y216	
K1289	THR	L899	V701	R622	L503	V420	Q348	E294	Y217	
L1290	THR	L899	V701	R622	L503	V420	Q348	E295	Y218	
S1291	THR	L899	V701	R622	L503	V420	Q348	E296	Y219	
V1292	THR	L899	V701	R622	L503	V420	Q348	E297	Y220	
F1293	THR	L899	V701	R622	L503	V420	Q348	E298	Y221	
V1294	THR	L899	V701	R622	L503	V420	Q348	E299	Y222	
E1295	THR	L899	V701	R622	L503	V420	Q348	E300	Y223	
I1296	THR	L899	V701	R622	L503	V420	Q348	E301	Y224	
E1297	THR	L899	V701	R622	L503	V420	Q348	E302	Y225	
G1298	THR	L899	V701	R622	L503	V420	Q348	E303	Y226	
F1299	THR	L899	V701	R622	L503	V420	Q348	E304	Y227	
S1300	THR	L899	V701	R622	L503	V420	Q348	E305	Y228	
E1405	THR	L899	V701	R622	L503	V420	Q348	E306	Y229	
A1409	THR	L899	V701	R622	L503	V420	Q348	E307	Y230	
E1410	THR	L899	V701	R622	L503	V420	Q348	E308	Y231	
		L899	V701	R622	L503	V420	Q348	E309	Y232	
		L899	V701	R622	L503	V420	Q348	E310	Y233	
		L899	V701	R622	L503	V420	Q348	E311	Y234	
		L899	V701	R622	L503	V420	Q348	E312	Y235	
		L899	V701	R622	L503	V420	Q348	E313	Y236	
		L899	V701	R622	L503	V420	Q348	E314	Y237	
		L899	V701	R622	L503	V420	Q348	E315	Y238	
		L899	V701	R622	L503	V420	Q348	E316	Y239	
		L899	V701	R622	L503	V420	Q348	E317	Y240	
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		L899	V701	R622	L503	V420	Q348	E331	Y254	
		L899	V701	R622	L503	V420	Q348	E332	Y255	
		L899	V701	R622	L503	V420	Q348	E333	Y256	
		L899	V701	R622	L503	V420	Q348	E334	Y257	
		L899	V701	R622	L503	V420	Q348	E335	Y258	
		L899	V701	R622	L503	V420	Q348	E336	Y259	
		L899	V701	R622	L503	V420	Q348	E337	Y260	
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		L899	V701	R622	L503	V420	Q348	E389	Y312	
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		L899	V701	R622	L503	V420	Q348	E391	Y314	
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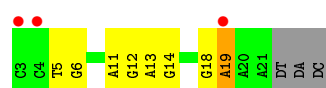
- Molecule 4: DNA-directed RNA polymerase subunit omega



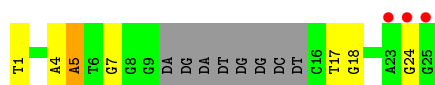
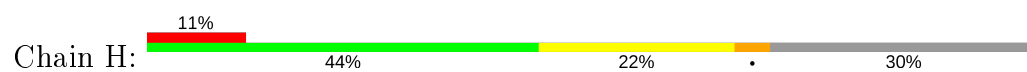
- Molecule 5: RNA polymerase sigma factor SigA



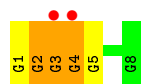
- Molecule 6: DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*G P*AP*AP*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP *AP*GP*G)-3')



● Molecule 8: RNA (5'-D*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.90Å 101.42Å 295.19Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	41.69 – 2.84 41.69 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.5 (41.69-2.84) 96.5 (41.69-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.222 , 0.268 0.222 , 0.268	Depositor DCC
R_{free} test set	1994 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28535	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: GTP, ZN, MG, POP

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	0.50	1/1814 (0.1%)	0.70	1/2466 (0.0%)
1	B	0.53	0/1799	0.72	0/2447
2	C	0.52	3/8892 (0.0%)	0.72	5/12028 (0.0%)
3	D	0.57	3/11928 (0.0%)	0.75	12/16127 (0.1%)
4	E	0.52	0/775	0.80	3/1045 (0.3%)
5	F	0.58	5/2835 (0.2%)	0.74	6/3816 (0.2%)
6	G	1.14	1/434 (0.2%)	1.06	1/666 (0.2%)
7	H	0.87	0/442	1.00	2/680 (0.3%)
8	I	0.79	0/181	1.36	1/283 (0.4%)
All	All	0.57	13/29100 (0.0%)	0.75	31/39558 (0.1%)

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	1
3	D	0	2
5	F	0	1
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	249	ARG	CB-CG	10.78	1.81	1.52
2	C	37	GLU	CB-CG	-10.32	1.32	1.52
2	C	37	GLU	CD-OE1	-8.63	1.16	1.25
5	F	249	ARG	CZ-NH2	-8.59	1.21	1.33
5	F	249	ARG	NE-CZ	8.53	1.44	1.33
2	C	37	GLU	CD-OE2	7.38	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	19	DA	P-O5'	6.97	1.66	1.59
3	D	1148	VAL	CB-CG2	-6.40	1.39	1.52
3	D	749	VAL	CB-CG2	-5.64	1.41	1.52
3	D	299	GLU	CB-CG	5.47	1.62	1.52
5	F	249	ARG	CD-NE	5.30	1.55	1.46
1	A	75	VAL	CB-CG1	-5.05	1.42	1.52
5	F	265	VAL	CB-CG1	-5.04	1.42	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	249	ARG	NE-CZ-NH2	13.02	126.81	120.30
6	G	19	DA	O4'-C4'-C3'	-8.25	101.05	106.00
5	F	249	ARG	NH1-CZ-NH2	-7.98	110.62	119.40
3	D	513	ILE	CG1-CB-CG2	-7.95	93.91	111.40
3	D	35	ARG	NE-CZ-NH2	-7.32	116.64	120.30
3	D	1151	ARG	CA-CB-CG	7.21	129.26	113.40
5	F	249	ARG	CD-NE-CZ	7.10	133.54	123.60
3	D	152	LEU	CA-CB-CG	6.97	131.34	115.30
3	D	1151	ARG	NE-CZ-NH1	-6.76	116.92	120.30
3	D	170	PRO	C-N-CA	-6.73	104.88	121.70
4	E	85	LEU	CB-CG-CD1	-6.34	100.22	111.00
3	D	204	LEU	CB-CG-CD1	-6.32	100.26	111.00
5	F	127	ILE	CG1-CB-CG2	-6.13	97.91	111.40
4	E	30	LEU	CB-CG-CD1	-5.99	100.83	111.00
2	C	203	ASP	CB-CG-OD1	5.87	123.58	118.30
3	D	191	LEU	CB-CG-CD2	-5.82	101.10	111.00
2	C	260	LEU	CA-CB-CG	5.78	128.60	115.30
4	E	26	ARG	CG-CD-NE	5.72	123.80	111.80
7	H	1	DT	O4'-C1'-N1	5.70	111.99	108.00
1	A	99	LEU	CB-CG-CD2	-5.46	101.72	111.00
7	H	5	DA	O4'-C1'-N9	5.43	111.80	108.00
5	F	282	LEU	CA-CB-CG	5.43	127.79	115.30
2	C	241	LEU	CA-CB-CG	5.43	127.78	115.30
5	F	383	LEU	CA-CB-CG	5.29	127.47	115.30
2	C	1055	LEU	CA-CB-CG	5.23	127.33	115.30
8	I	2	G	O4'-C1'-N9	-5.22	104.03	108.20
3	D	1422	MET	CA-CB-CG	5.18	122.11	113.30
3	D	739	ASP	CB-CG-OD2	5.05	122.85	118.30
3	D	713	ILE	CG1-CB-CG2	-5.02	100.35	111.40
2	C	37	GLU	CB-CA-C	-5.02	100.36	110.40
3	D	191	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Peptide
3	D	1129	THR	Peptide
3	D	65	ARG	Peptide
5	F	389	PHE	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	1782	0	1834	86	0
1	B	1767	0	1816	118	0
2	C	8726	0	8814	428	0
3	D	11722	0	11950	601	13
4	E	761	0	778	43	0
5	F	2790	0	2853	183	11
6	G	387	0	212	9	0
7	H	394	0	217	9	0
8	I	193	0	88	3	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28535	0	28562	1358	13

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 24.

All (1358) 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:249:ARG:CG	5:F:249:ARG:CB	1.81	1.58
3:D:371:ILE:CD1	3:D:372:ASP:H	1.36	1.38
2:C:605:LYS:HB3	2:C:610:ARG:NH2	1.35	1.36
3:D:411:THR:O	5:F:178:ARG:NH2	1.58	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:411:THR:C	5:F:178:ARG:NH2	1.90	1.23
2:C:605:LYS:CB	2:C:610:ARG:NH2	2.06	1.19
5:F:258:ILE:O	5:F:258:ILE:HD12	1.39	1.17
3:D:371:ILE:HD12	3:D:372:ASP:N	1.58	1.16
2:C:367:LEU:HA	2:C:371:LYS:HE3	1.29	1.13
3:D:411:THR:O	5:F:178:ARG:CZ	1.97	1.11
2:C:13:ILE:HD12	2:C:14:PRO:HD2	1.33	1.11
2:C:68:PHE:HA	2:C:98:LEU:HD12	1.28	1.10
3:D:135:LEU:O	3:D:149:LYS:HE2	1.52	1.09
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.34	1.07
3:D:411:THR:O	5:F:178:ARG:NE	1.88	1.06
2:C:366:SER:O	2:C:371:LYS:NZ	1.90	1.04
2:C:1101:THR:OG1	2:C:1111:ILE:HD11	1.55	1.04
3:D:572:ARG:HH12	5:F:83:GLN:HG2	1.22	1.03
3:D:218:LYS:NZ	3:D:338:GLU:CA	2.23	1.01
3:D:992:ILE:HD11	3:D:1054:GLU:HB3	1.42	1.01
1:A:57:TYR:CD1	1:A:161:ARG:NH1	2.28	1.01
3:D:371:ILE:CD1	3:D:372:ASP:N	2.17	1.01
3:D:890:VAL:CG1	3:D:922:LEU:HD13	1.90	1.00
3:D:1047:LYS:CE	3:D:1048:PRO:HG2	1.93	0.99
5:F:230:LYS:O	5:F:232:ARG:HD2	1.63	0.98
3:D:218:LYS:HE3	3:D:338:GLU:HG2	1.45	0.97
5:F:258:ILE:O	5:F:258:ILE:CD1	2.12	0.97
1:B:71:VAL:HG12	1:B:132:LEU:HG	1.45	0.97
3:D:218:LYS:NZ	3:D:338:GLU:HA	1.78	0.96
2:C:605:LYS:CB	2:C:610:ARG:HH22	1.70	0.96
3:D:371:ILE:HD13	3:D:372:ASP:CG	1.84	0.96
1:A:57:TYR:CE2	1:A:161:ARG:NH2	2.34	0.96
2:C:1067:TYR:OH	3:D:674:ARG:NH1	1.99	0.96
3:D:36:THR:HG23	3:D:38:LYS:H	1.29	0.96
2:C:723:THR:HG22	2:C:725:ASP:H	1.29	0.95
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.47	0.94
3:D:218:LYS:NZ	3:D:339:TRP:N	2.17	0.92
2:C:486:MET:HG3	2:C:490:GLU:HG3	1.48	0.92
3:D:168:THR:HG22	3:D:394:LEU:HD13	1.52	0.92
3:D:361:VAL:HG23	3:D:365:ASP:HB2	1.49	0.92
3:D:371:ILE:HD12	3:D:372:ASP:H	0.75	0.91
3:D:371:ILE:HD13	3:D:372:ASP:OD1	1.69	0.91
3:D:218:LYS:CE	3:D:338:GLU:CB	2.49	0.90
1:B:102:LYS:HG3	1:B:139:ASN:HB2	1.51	0.90
1:B:56:VAL:HG23	1:B:142:VAL:HG12	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:237:THR:HG1	7:H:4:DA:H8	1.13	0.90
3:D:205:TYR:HD1	3:D:390:PRO:HB3	1.36	0.90
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.52	0.89
3:D:218:LYS:HZ2	3:D:338:GLU:HA	1.33	0.89
1:B:124:ASN:HD22	1:B:127:LEU:CD1	1.85	0.89
3:D:828:LYS:HD2	3:D:833:GLU:HB3	1.55	0.88
1:B:124:ASN:ND2	1:B:127:LEU:HD12	1.89	0.88
3:D:174:GLY:H	3:D:209:ARG:HH12	1.20	0.88
2:C:367:LEU:HA	2:C:371:LYS:CE	2.04	0.87
1:A:99:LEU:HD11	1:A:114:PHE:HB3	1.54	0.87
2:C:575:GLN:OE1	2:C:671:ASN:N	2.07	0.86
3:D:116:LEU:HD11	3:D:465:LEU:HD21	1.55	0.86
2:C:210:GLU:HB3	2:C:211:LEU:HD22	1.55	0.86
3:D:142:LEU:HD12	3:D:161:LEU:HD11	1.56	0.86
3:D:181:ASP:HB2	3:D:205:TYR:HD2	1.40	0.86
3:D:209:ARG:HA	3:D:347:VAL:HG12	1.55	0.86
5:F:372:ARG:HH12	5:F:380:GLU:HA	1.40	0.85
3:D:208:PRO:O	3:D:347:VAL:HG11	1.75	0.85
5:F:372:ARG:NH1	5:F:372:ARG:O	2.08	0.85
2:C:605:LYS:HB3	2:C:610:ARG:HH22	0.77	0.84
3:D:241:ILE:HD11	3:D:310:LEU:HD11	1.59	0.84
3:D:631:ILE:HD11	3:D:745:MET:SD	2.17	0.84
3:D:1047:LYS:HE2	3:D:1048:PRO:CG	2.08	0.84
3:D:173:PRO:HA	3:D:209:ARG:HH22	1.43	0.84
3:D:1047:LYS:NZ	3:D:1048:PRO:HG2	1.93	0.84
3:D:218:LYS:HZ1	3:D:338:GLU:CA	1.91	0.84
3:D:896:ALA:O	3:D:900:ILE:HD12	1.78	0.83
1:A:76:VAL:O	1:A:79:ILE:HG22	1.79	0.83
2:C:428:ARG:NH2	2:C:447:ALA:O	2.12	0.83
1:B:112:ARG:HG2	1:B:125:PRO:HB2	1.59	0.83
3:D:496:LEU:HD23	3:D:1390:LEU:HD21	1.60	0.82
1:A:57:TYR:CZ	1:A:161:ARG:NH2	2.44	0.82
1:A:85:LEU:HD21	1:A:87:VAL:HG13	1.61	0.82
2:C:23:VAL:HA	2:C:121:MET:HE1	1.61	0.82
2:C:607:ASP:HB3	2:C:610:ARG:HG3	1.62	0.82
5:F:116:LEU:HD22	5:F:127:ILE:HG21	1.61	0.82
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.61	0.81
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.60	0.81
2:C:367:LEU:HD12	2:C:371:LYS:NZ	1.93	0.81
3:D:890:VAL:HG11	3:D:922:LEU:CD1	2.09	0.81
3:D:218:LYS:HZ1	3:D:338:GLU:C	1.84	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.45	0.81
6:G:18:DG:H2'	6:G:19:DA:H5'	1.62	0.81
2:C:716:LYS:HE2	2:C:716:LYS:H	1.45	0.80
3:D:1047:LYS:CE	3:D:1048:PRO:CG	2.58	0.80
3:D:218:LYS:HE3	3:D:338:GLU:CG	2.11	0.80
2:C:503:LEU:HD12	2:C:508:ILE:HA	1.63	0.80
3:D:218:LYS:CE	3:D:338:GLU:HB3	2.11	0.80
3:D:413:ASP:H	5:F:178:ARG:HH22	1.28	0.80
3:D:628:ARG:HH21	3:D:746:ALA:HB2	1.43	0.80
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.47	0.80
1:A:57:TYR:CD2	1:A:161:ARG:NH2	2.50	0.79
2:C:229:MET:HG3	2:C:233:GLU:HB2	1.64	0.79
3:D:203:ALA:HB1	3:D:393:ILE:HD11	1.64	0.79
3:D:218:LYS:HZ2	3:D:339:TRP:H	1.31	0.79
3:D:800:LYS:NZ	3:D:819:GLY:O	2.16	0.79
2:C:728:HIS:ND1	5:F:422:LEU:O	2.15	0.79
2:C:890:LEU:HD23	2:C:890:LEU:O	1.82	0.79
3:D:65:ARG:HH21	5:F:377:ASP:H	1.28	0.79
2:C:367:LEU:HD12	2:C:371:LYS:HZ2	1.45	0.78
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.18	0.78
2:C:589:ARG:HE	2:C:596:TYR:HE2	1.32	0.78
3:D:218:LYS:HE2	3:D:338:GLU:HB3	1.66	0.78
3:D:218:LYS:NZ	3:D:339:TRP:H	1.80	0.78
3:D:218:LYS:CE	3:D:338:GLU:CG	2.62	0.78
3:D:259:VAL:HG12	3:D:296:GLU:O	1.85	0.77
5:F:116:LEU:HD21	5:F:163:LEU:HD21	1.65	0.77
1:A:108:GLU:HG2	1:A:131:THR:HG23	1.67	0.77
2:C:474:VAL:HG11	2:C:529:VAL:HG22	1.65	0.77
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.66	0.77
3:D:371:ILE:HD13	3:D:372:ASP:CB	2.14	0.77
3:D:209:ARG:HA	3:D:347:VAL:CG1	2.14	0.77
3:D:224:ARG:NH1	3:D:254:GLU:OE1	2.16	0.77
4:E:26:ARG:HD3	4:E:30:LEU:HD11	1.64	0.77
5:F:131:VAL:HG13	5:F:178:ARG:HG2	1.66	0.77
3:D:1047:LYS:HE2	3:D:1048:PRO:HD2	1.65	0.77
4:E:80:VAL:CG2	4:E:85:LEU:HD11	2.14	0.77
1:A:111:ALA:HA	1:A:114:PHE:HE2	1.50	0.76
3:D:1047:LYS:HE2	3:D:1048:PRO:CD	2.15	0.76
3:D:218:LYS:NZ	3:D:338:GLU:C	2.39	0.76
3:D:631:ILE:HD11	3:D:745:MET:HB2	1.66	0.76
3:D:33:ASN:HB3	3:D:36:THR:HG22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:HA	1:A:201:THR:HG22	1.67	0.76
2:C:162:ILE:HD11	2:C:172:ILE:HD12	1.66	0.76
2:C:711:GLU:OE1	2:C:713:ARG:NH2	2.20	0.75
1:B:18:ARG:NH1	1:B:204:SER:O	2.20	0.75
5:F:265:VAL:O	5:F:269:ASN:ND2	2.19	0.75
4:E:50:THR:HG22	4:E:53:GLY:O	1.86	0.75
2:C:226:VAL:O	2:C:229:MET:HE2	1.87	0.75
2:C:150:PRO:HA	2:C:158:TYR:HD1	1.50	0.75
2:C:78:PHE:HB3	2:C:82:GLU:HG2	1.68	0.75
3:D:1126:ASP:O	3:D:1130:ARG:HA	1.87	0.75
3:D:675:ARG:HH22	5:F:420:ASP:HA	1.50	0.74
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.68	0.74
3:D:171:LEU:HD21	3:D:390:PRO:HG2	1.69	0.74
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.69	0.74
3:D:224:ARG:HH11	3:D:254:GLU:CD	1.90	0.74
3:D:808:THR:HG23	3:D:811:GLU:HB2	1.70	0.74
1:A:111:ALA:HA	1:A:114:PHE:CE2	2.22	0.73
2:C:23:VAL:HA	2:C:121:MET:CE	2.18	0.73
3:D:691:LEU:HD22	3:D:720:LEU:HD21	1.69	0.73
5:F:120:THR:HB	5:F:122:LEU:HD13	1.67	0.73
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.71	0.73
1:A:79:ILE:HD11	1:A:167:VAL:CG2	2.19	0.73
1:B:128:HIS:HE1	1:B:131:THR:HG22	1.54	0.73
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.03	0.73
2:C:605:LYS:HB2	2:C:610:ARG:NH2	2.04	0.73
2:C:267:TYR:CZ	2:C:290:LEU:HD11	2.24	0.73
3:D:1286:THR:O	3:D:1307:LYS:NZ	2.18	0.72
4:E:39:VAL:HG11	4:E:72:ARG:HB2	1.69	0.72
2:C:280:LYS:HE3	2:C:323:ASP:OD2	1.89	0.72
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.21	0.72
3:D:686:GLU:N	3:D:686:GLU:OE1	2.22	0.72
2:C:495:THR:HG23	2:C:530:GLU:OE1	1.90	0.72
3:D:572:ARG:NH1	5:F:83:GLN:HG2	2.01	0.72
3:D:798:GLU:OE2	3:D:824:ASN:ND2	2.20	0.72
3:D:828:LYS:CD	3:D:833:GLU:HB3	2.20	0.72
3:D:100:ALA:HB3	3:D:575:GLN:HE22	1.54	0.72
3:D:625:TYR:HB3	3:D:749:VAL:HG22	1.71	0.72
3:D:1155:VAL:HG11	3:D:1177:ALA:HB2	1.71	0.72
3:D:975:GLU:OE2	3:D:988:ARG:NH1	2.21	0.72
3:D:767:HIS:CE1	4:E:6:ILE:HD13	2.24	0.72
3:D:218:LYS:HZ2	3:D:339:TRP:N	1.85	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:875:THR:HG21	3:D:902:LEU:HD21	1.72	0.72
1:A:94:LEU:O	1:A:146:ARG:NH1	2.23	0.71
5:F:122:LEU:HB3	5:F:127:ILE:HD11	1.72	0.71
1:B:124:ASN:HB2	1:B:127:LEU:HG	1.70	0.71
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.70	0.71
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.71	0.71
1:A:104:GLU:HG2	1:A:137:ARG:HD3	1.72	0.71
3:D:169:TYR:HE1	3:D:395:VAL:HG12	1.56	0.71
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.71	0.71
1:A:39:PRO:O	1:A:43:ILE:HG13	1.91	0.71
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.24	0.71
3:D:1305:LEU:HD21	3:D:1309:ALA:HB3	1.72	0.71
3:D:218:LYS:CE	3:D:338:GLU:HA	2.21	0.71
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.23	0.70
3:D:231:VAL:O	3:D:236:TYR:OH	2.08	0.70
3:D:408:GLU:HA	5:F:164:LYS:NZ	2.07	0.70
3:D:297:ILE:O	3:D:297:ILE:HD12	1.92	0.70
3:D:1267:ARG:NH1	3:D:1331:ASP:OD2	2.23	0.70
3:D:581:LEU:HD23	3:D:582:LEU:HD23	1.73	0.70
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.74	0.70
3:D:513:ILE:HD12	3:D:513:ILE:O	1.92	0.70
3:D:36:THR:HG23	3:D:38:LYS:N	2.02	0.70
3:D:116:LEU:HD21	3:D:465:LEU:CD2	2.22	0.70
3:D:809:PRO:HG3	3:D:829:VAL:HG11	1.74	0.70
1:B:101:LEU:HD21	1:B:113:ASP:O	1.92	0.69
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	1.91	0.69
1:A:222:LEU:HD22	1:B:215:VAL:HG23	1.75	0.69
2:C:753:ASP:OD2	3:D:681:ARG:NH2	2.25	0.69
3:D:368:VAL:HG22	3:D:377:VAL:HG22	1.73	0.69
3:D:984:THR:HB	3:D:987:GLU:H	1.55	0.69
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.73	0.69
2:C:150:PRO:HA	2:C:158:TYR:CD1	2.26	0.69
2:C:242:LEU:HD22	2:C:242:LEU:N	2.08	0.69
1:A:101:LEU:HD12	1:A:114:PHE:CE1	2.28	0.69
3:D:64:LYS:O	3:D:65:ARG:HG3	1.93	0.69
2:C:495:THR:HG22	2:C:517:ARG:HD3	1.73	0.69
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.28	0.69
2:C:719:PRO:HB3	2:C:820:ARG:HH12	1.58	0.68
3:D:1294:VAL:O	3:D:1300:SER:HB3	1.93	0.68
2:C:13:ILE:HD12	2:C:14:PRO:CD	2.19	0.68
1:B:58:ILE:HG13	1:B:61:VAL:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HD21	1:B:122:ILE:HG23	1.76	0.68
2:C:395:LYS:HD3	2:C:397:GLU:HB3	1.74	0.68
2:C:754:ILE:HG13	2:C:791:ARG:HE	1.58	0.68
2:C:890:LEU:HD21	2:C:901:TYR:CD2	2.28	0.68
3:D:218:LYS:HZ1	3:D:338:GLU:HB3	1.58	0.68
1:B:58:ILE:HD11	1:B:61:VAL:HB	1.75	0.68
3:D:413:ASP:N	5:F:178:ARG:HH22	1.92	0.68
5:F:363:GLU:O	5:F:367:MET:N	2.27	0.68
3:D:179:VAL:HG21	3:D:191:LEU:HD12	1.74	0.67
2:C:163:ILE:HG13	2:C:171:TRP:HD1	1.59	0.67
3:D:218:LYS:NZ	3:D:338:GLU:CB	2.56	0.67
3:D:411:THR:HA	3:D:435:VAL:HG13	1.76	0.67
3:D:371:ILE:HD13	3:D:372:ASP:N	2.09	0.67
3:D:245:LEU:HD12	3:D:309:GLY:O	1.94	0.67
5:F:365:GLU:HG2	5:F:403:LYS:HE3	1.76	0.67
2:C:535:SER:OG	2:C:537:LYS:HG3	1.95	0.67
3:D:992:ILE:CD1	3:D:1054:GLU:HB3	2.22	0.67
1:B:124:ASN:HD22	1:B:127:LEU:HD11	1.57	0.67
3:D:1271:LYS:HD2	3:D:1331:ASP:HB2	1.77	0.67
3:D:133:ILE:HD12	3:D:152:LEU:HB3	1.76	0.67
3:D:218:LYS:CE	3:D:338:GLU:HG2	2.22	0.67
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.75	0.67
2:C:244:PRO:O	5:F:82:ARG:NH1	2.27	0.67
3:D:218:LYS:HZ1	3:D:338:GLU:CB	2.08	0.67
3:D:485:SER:O	3:D:487:ALA:N	2.24	0.67
3:D:1019:PRO:O	3:D:1023:MET:HG3	1.95	0.67
3:D:1273:VAL:H	3:D:1326:THR:HG22	1.59	0.67
1:A:4:SER:O	1:A:189:ARG:NH1	2.27	0.66
2:C:189:ARG:NH1	2:C:242:LEU:O	2.27	0.66
2:C:390:GLN:NE2	2:C:414:GLY:HA2	2.09	0.66
2:C:835:VAL:HA	2:C:849:VAL:HG23	1.76	0.66
5:F:110:MET:HG2	5:F:128:ARG:HH22	1.60	0.66
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.11	0.66
3:D:1235:GLN:O	3:D:1236:LEU:HD12	1.96	0.66
1:A:211:LEU:O	1:A:215:VAL:HG12	1.95	0.66
2:C:241:LEU:CB	2:C:242:LEU:HD22	2.26	0.66
2:C:728:HIS:C	2:C:729:LEU:HD22	2.16	0.66
3:D:640:HIS:CD2	3:D:641:GLN:HG3	2.30	0.66
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.77	0.66
3:D:191:LEU:HD21	3:D:197:SER:CB	2.26	0.66
4:E:39:VAL:HG12	4:E:72:ARG:HH11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:193:ARG:HB3	7:H:7:DG:H5'	1.78	0.66
2:C:154:ARG:NH2	2:C:175:GLU:OE2	2.29	0.66
2:C:615:TYR:HD2	2:C:619:ARG:HE	1.42	0.66
5:F:104:ARG:O	5:F:108:GLU:HG3	1.96	0.66
3:D:407:VAL:O	5:F:164:LYS:NZ	2.29	0.66
1:B:110:LYS:HZ2	1:B:112:ARG:HG3	1.59	0.66
3:D:1046:GLN:HE21	3:D:1076:GLY:HA3	1.60	0.66
2:C:168:ARG:NH2	2:C:265:ARG:O	2.29	0.65
2:C:503:LEU:CD1	2:C:508:ILE:HA	2.25	0.65
2:C:229:MET:CE	2:C:237:ARG:HE	2.08	0.65
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.65
2:C:913:GLU:O	2:C:917:LEU:HD12	1.95	0.65
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.10	0.65
1:B:153:ALA:O	1:B:155:LYS:N	2.29	0.65
2:C:233:GLU:N	2:C:233:GLU:OE1	2.20	0.65
3:D:93:ILE:HB	3:D:517:VAL:HG12	1.79	0.65
2:C:1047:HIS:CE1	3:D:1471:LEU:HD11	2.31	0.65
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.77	0.65
2:C:495:THR:HG22	2:C:517:ARG:CD	2.26	0.65
3:D:1151:ARG:HB3	3:D:1151:ARG:CZ	2.22	0.65
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.77	0.65
5:F:154:LYS:NZ	5:F:155:THR:HG22	2.12	0.65
3:D:218:LYS:CE	3:D:338:GLU:CA	2.75	0.65
3:D:762:GLN:OE1	4:E:20:THR:HG21	1.96	0.65
2:C:105:THR:HG23	2:C:106:GLY:H	1.60	0.65
2:C:884:GLN:O	2:C:888:THR:HG23	1.97	0.65
5:F:322:GLY:O	5:F:324:GLU:N	2.30	0.65
5:F:372:ARG:NH1	5:F:380:GLU:HA	2.10	0.64
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.79	0.64
3:D:1144:LEU:O	3:D:1147:ARG:HG3	1.96	0.64
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.77	0.64
5:F:363:GLU:HA	5:F:363:GLU:OE1	1.95	0.64
1:B:95:GLN:HE21	1:B:146:ARG:HD2	1.62	0.64
3:D:1033:GLN:N	3:D:1033:GLN:OE1	2.30	0.64
3:D:408:GLU:HA	5:F:164:LYS:HZ1	1.61	0.64
1:A:215:VAL:HG23	1:B:222:LEU:HD22	1.78	0.64
1:B:124:ASN:HD22	1:B:127:LEU:HD12	1.47	0.64
1:A:57:TYR:CE1	1:A:161:ARG:NH1	2.62	0.64
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.79	0.64
2:C:68:PHE:HA	2:C:98:LEU:CD1	2.16	0.64
3:D:1047:LYS:CD	3:D:1048:PRO:HG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:674:VAL:HG23	2:C:869:VAL:HG13	1.79	0.64
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.78	0.64
5:F:326:ASP:O	6:G:19:DA:N6	2.31	0.64
2:C:853:LEU:HB2	2:C:858:MET:CE	2.28	0.64
3:D:361:VAL:CG2	3:D:365:ASP:HB2	2.24	0.64
1:B:95:GLN:NE2	1:B:146:ARG:HD2	2.12	0.64
3:D:205:TYR:CD1	3:D:390:PRO:HB3	2.27	0.64
5:F:365:GLU:HG3	5:F:404:ALA:HB2	1.80	0.64
3:D:280:ALA:HB1	3:D:282:TYR:CE2	2.33	0.64
5:F:265:VAL:HG22	5:F:269:ASN:HD21	1.63	0.64
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.13	0.63
3:D:218:LYS:NZ	3:D:338:GLU:HB3	2.14	0.63
3:D:116:LEU:HD21	3:D:465:LEU:HD22	1.80	0.63
1:B:61:VAL:CG2	1:B:66:SER:HB2	2.29	0.63
5:F:122:LEU:CB	5:F:127:ILE:HD11	2.27	0.63
1:B:110:LYS:HZ1	1:B:112:ARG:HD2	1.63	0.63
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.81	0.63
4:E:80:VAL:HG21	4:E:85:LEU:HD11	1.80	0.63
5:F:101:GLU:O	5:F:105:LYS:HG3	1.97	0.63
1:B:124:ASN:ND2	1:B:127:LEU:CD1	2.53	0.63
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.80	0.63
3:D:218:LYS:HE2	3:D:338:GLU:CB	2.24	0.63
5:F:116:LEU:O	5:F:120:THR:OG1	2.08	0.63
5:F:132:ARG:HH21	5:F:184:ARG:CZ	2.11	0.63
2:C:238:LEU:O	2:C:242:LEU:CD2	2.47	0.63
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.81	0.63
3:D:1273:VAL:HG12	3:D:1326:THR:HG22	1.81	0.62
2:C:716:LYS:NZ	3:D:529:GLN:HE22	1.96	0.62
4:E:88:GLU:O	4:E:92:LEU:HD13	1.99	0.62
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.33	0.62
2:C:473:ARG:O	2:C:480:THR:HG22	1.99	0.62
3:D:631:ILE:CD1	3:D:745:MET:HB2	2.29	0.62
3:D:367:ILE:HB	3:D:377:VAL:HG23	1.82	0.62
5:F:269:ASN:O	5:F:273:ARG:HG3	2.00	0.62
1:B:72:LYS:HE2	1:B:133:GLU:HG3	1.82	0.61
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.30	0.61
2:C:163:ILE:HG13	2:C:171:TRP:CD1	2.34	0.61
2:C:495:THR:CG2	2:C:517:ARG:HE	2.13	0.61
2:C:946:ARG:HH12	3:D:861:GLN:HE22	1.46	0.61
3:D:808:THR:CG2	3:D:811:GLU:HB2	2.29	0.61
1:A:35:THR:OG1	1:B:42:ARG:HD3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.82	0.61
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.83	0.61
8:I:3:G:N3	8:I:4:G:N2	2.48	0.61
2:C:238:LEU:O	2:C:242:LEU:HD23	2.00	0.61
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.81	0.61
3:D:116:LEU:HB3	3:D:118:LEU:HD13	1.81	0.61
3:D:412:GLY:N	5:F:178:ARG:NH2	2.47	0.61
2:C:390:GLN:HE21	2:C:414:GLY:HA2	1.65	0.61
3:D:1151:ARG:CB	3:D:1151:ARG:CZ	2.78	0.61
2:C:1101:THR:OG1	2:C:1111:ILE:CD1	2.43	0.61
3:D:530:VAL:HG22	3:D:531:ASP:H	1.64	0.61
1:A:57:TYR:CD1	1:A:161:ARG:CZ	2.84	0.61
2:C:390:GLN:HG2	2:C:390:GLN:O	2.01	0.61
2:C:545:ASN:O	2:C:581:THR:HG21	2.01	0.61
2:C:97:ARG:NH1	2:C:112:GLU:OE2	2.34	0.61
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.81	0.61
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.83	0.61
1:A:85:LEU:HD21	1:A:87:VAL:CG1	2.31	0.61
2:C:468:ARG:NH2	2:C:490:GLU:OE2	2.34	0.61
3:D:258:VAL:HG12	3:D:297:ILE:HG22	1.83	0.61
3:D:500:ARG:NH1	3:D:1390:LEU:HD11	2.15	0.61
3:D:761:ILE:HD12	4:E:20:THR:HB	1.83	0.61
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.83	0.60
2:C:241:LEU:HB2	2:C:242:LEU:HD22	1.83	0.60
2:C:640:ARG:HD3	2:C:642:ARG:HH22	1.64	0.60
3:D:956:ILE:HD13	3:D:1039:CYS:O	2.01	0.60
3:D:286:VAL:O	3:D:311:LEU:HD12	2.01	0.60
3:D:671:LYS:HE3	5:F:421:PHE:HA	1.83	0.60
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.01	0.60
5:F:185:GLN:O	5:F:189:GLU:HG3	2.01	0.60
3:D:199:LEU:HD11	3:D:397:LYS:HD2	1.83	0.60
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.34	0.60
3:D:500:ARG:HH11	3:D:1390:LEU:HD11	1.66	0.60
2:C:64:LEU:N	2:C:103:LYS:HB3	2.17	0.60
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.84	0.60
1:B:110:LYS:NZ	1:B:112:ARG:HG3	2.16	0.60
1:B:206:THR:HG22	1:B:209:GLU:CB	2.31	0.60
2:C:277:ALA:O	2:C:281:LEU:HD12	2.02	0.60
3:D:199:LEU:HD21	3:D:397:LYS:HG3	1.84	0.60
8:I:2:G:H2'	8:I:2:G:N3	2.16	0.60
2:C:711:GLU:O	2:C:758:ARG:NH1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:572:ARG:HH12	5:F:83:GLN:CG	2.07	0.60
1:B:206:THR:HG22	1:B:209:GLU:CG	2.32	0.60
3:D:631:ILE:HG22	3:D:740:PHE:CE2	2.37	0.60
3:D:631:ILE:HD11	3:D:745:MET:CB	2.31	0.60
2:C:727:PRO:O	2:C:729:LEU:HD23	2.01	0.59
2:C:607:ASP:CB	2:C:610:ARG:HG3	2.31	0.59
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.00	0.59
1:B:64:GLU:HG2	1:B:76:VAL:HG12	1.84	0.59
3:D:208:PRO:HG3	3:D:387:LEU:HD12	1.84	0.59
3:D:988:ARG:HG3	3:D:989:TYR:N	2.17	0.59
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.01	0.59
3:D:410:SER:O	3:D:435:VAL:HG11	2.03	0.59
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.34	0.59
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.85	0.59
2:C:154:ARG:CZ	2:C:175:GLU:OE2	2.51	0.59
2:C:501:THR:O	2:C:503:LEU:HD22	2.01	0.59
5:F:109:GLY:O	5:F:113:ILE:HG13	2.02	0.59
2:C:723:THR:O	2:C:741:GLY:HA3	2.03	0.59
4:E:30:LEU:N	4:E:30:LEU:HD12	2.18	0.59
5:F:164:LYS:HZ2	5:F:171:LYS:HE3	1.67	0.59
5:F:372:ARG:HH22	5:F:380:GLU:HB3	1.68	0.59
2:C:586:ARG:O	2:C:586:ARG:HG3	2.00	0.59
3:D:1405:GLU:OE2	3:D:1409:ALA:N	2.35	0.59
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.38	0.59
3:D:241:ILE:HD11	3:D:310:LEU:CD1	2.31	0.59
3:D:65:ARG:NH2	5:F:376:ILE:HA	2.17	0.59
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.84	0.59
1:A:18:ARG:O	1:A:201:THR:HG21	2.02	0.58
3:D:288:MET:HB2	3:D:311:LEU:HD11	1.85	0.58
3:D:65:ARG:HH21	5:F:376:ILE:HA	1.68	0.58
5:F:376:ILE:O	5:F:377:ASP:HB3	2.03	0.58
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.84	0.58
2:C:436:GLY:HA2	2:C:538:GLN:O	2.02	0.58
2:C:238:LEU:O	2:C:241:LEU:HB2	2.03	0.58
2:C:768:THR:HG23	2:C:771:GLU:H	1.66	0.58
3:D:184:GLU:OE1	3:D:184:GLU:N	2.36	0.58
3:D:209:ARG:CA	3:D:347:VAL:HG12	2.29	0.58
4:E:26:ARG:HD3	4:E:30:LEU:CD1	2.31	0.58
3:D:82:LYS:HB2	3:D:84:ILE:HG22	1.86	0.58
2:C:711:GLU:HB2	2:C:713:ARG:HH21	1.68	0.58
2:C:890:LEU:HD21	2:C:901:TYR:CG	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:985:ASP:HA	3:D:988:ARG:HG2	1.86	0.58
5:F:361:LEU:HD13	5:F:407:LYS:HB3	1.84	0.58
1:A:85:LEU:CD2	1:A:87:VAL:HG13	2.32	0.58
1:B:85:LEU:HD22	1:B:87:VAL:HG13	1.86	0.58
2:C:162:ILE:HD13	2:C:290:LEU:HD21	1.85	0.58
2:C:290:LEU:N	2:C:290:LEU:HD12	2.18	0.58
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.03	0.58
3:D:174:GLY:N	3:D:209:ARG:HH12	1.97	0.58
3:D:899:LEU:HD21	3:D:921:ARG:HD3	1.86	0.58
2:C:745:ILE:H	2:C:745:ILE:HD12	1.68	0.58
1:A:44:LEU:O	1:A:174:VAL:HG11	2.04	0.58
3:D:465:LEU:N	3:D:465:LEU:HD23	2.18	0.58
2:C:719:PRO:CB	2:C:820:ARG:HH12	2.15	0.58
3:D:1495:ILE:O	3:D:1499:ARG:HG3	2.04	0.58
3:D:218:LYS:HZ1	3:D:339:TRP:N	1.99	0.58
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.68	0.57
1:B:110:LYS:NZ	1:B:112:ARG:HD2	2.18	0.57
2:C:15:LEU:O	2:C:586:ARG:NH2	2.31	0.57
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.68	0.57
3:D:1272:ALA:HA	3:D:1326:THR:HG23	1.85	0.57
5:F:398:ARG:O	5:F:398:ARG:NH1	2.37	0.57
6:G:5:DT:H2"	6:G:6:DG:C8	2.39	0.57
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.86	0.57
5:F:162:LYS:HE2	5:F:165:SER:HB2	1.86	0.57
5:F:230:LYS:O	5:F:232:ARG:CD	2.47	0.57
3:D:352:ASN:HB3	5:F:104:ARG:CZ	2.34	0.57
2:C:173:ASP:HB2	2:C:185:LYS:HE3	1.86	0.57
3:D:165:LYS:HD2	3:D:166:GLN:H	1.69	0.57
3:D:312:ARG:NH1	3:D:315:ARG:HH22	2.03	0.57
2:C:209:ARG:HG3	2:C:210:GLU:N	2.19	0.57
3:D:218:LYS:HZ2	3:D:338:GLU:CA	1.99	0.57
3:D:218:LYS:HE2	3:D:338:GLU:CG	2.32	0.57
2:C:475:VAL:O	2:C:477:GLY:N	2.37	0.57
5:F:111:GLU:HA	5:F:114:LYS:HG2	1.87	0.57
5:F:91:VAL:O	5:F:193:ARG:NH2	2.33	0.57
1:A:64:GLU:O	1:A:75:VAL:HG13	2.05	0.57
1:B:94:LEU:HD11	1:B:96:THR:O	2.05	0.57
2:C:272:ALA:HA	2:C:464:LEU:HD13	1.86	0.57
3:D:1048:PRO:HD3	3:D:1075:HIS:ND1	2.19	0.57
3:D:1342:GLU:H	3:D:1342:GLU:CD	2.07	0.57
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:179:ASN:ND2	2:C:181:VAL:HG12	2.19	0.56
2:C:34:VAL:HG23	2:C:39:ARG:HG2	1.86	0.56
3:D:218:LYS:HE3	3:D:338:GLU:HA	1.87	0.56
1:A:201:THR:HG23	1:A:203:GLY:H	1.70	0.56
2:C:367:LEU:CD1	2:C:371:LYS:HZ2	2.16	0.56
2:C:650:ARG:HB2	2:C:650:ARG:HH11	1.70	0.56
3:D:956:ILE:CD1	3:D:1039:CYS:O	2.53	0.56
2:C:1060:ILE:HD11	2:C:1083:GLU:HG2	1.87	0.56
3:D:170:PRO:HA	3:D:392:SER:OG	2.04	0.56
3:D:347:VAL:CG2	3:D:351:MET:HG3	2.36	0.56
3:D:44:LEU:HB3	3:D:525:ARG:HH22	1.69	0.56
5:F:398:ARG:HH12	5:F:402:ASN:ND2	2.03	0.56
1:B:38:ASN:O	1:B:42:ARG:HG3	2.06	0.56
2:C:249:LYS:HB2	2:C:252:LYS:HG2	1.86	0.56
3:D:122:GLU:HG2	3:D:152:LEU:HD21	1.88	0.56
3:D:628:ARG:NH2	3:D:746:ALA:HB2	2.17	0.56
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.86	0.56
1:B:41:ARG:HG3	1:B:177:VAL:CG2	2.35	0.56
2:C:916:GLU:O	2:C:920:GLN:HG3	2.06	0.56
2:C:366:SER:O	2:C:367:LEU:HD12	2.06	0.56
1:B:132:LEU:HD21	1:B:136:GLY:HA3	1.88	0.56
3:D:565:ILE:H	3:D:565:ILE:HD12	1.70	0.56
1:B:110:LYS:NZ	1:B:112:ARG:CG	2.69	0.56
1:B:132:LEU:HD21	1:B:136:GLY:CA	2.35	0.56
2:C:198:ARG:HH22	2:C:230:ARG:HA	1.70	0.56
3:D:1047:LYS:HD3	3:D:1048:PRO:HG2	1.88	0.56
3:D:699:VAL:N	3:D:756:GLN:OE1	2.36	0.56
5:F:154:LYS:HD3	5:F:155:THR:HG22	1.87	0.56
5:F:91:VAL:HG11	5:F:189:GLU:O	2.05	0.56
1:B:153:ALA:C	1:B:155:LYS:H	2.09	0.55
1:B:58:ILE:HD13	1:B:68:ILE:HD11	1.88	0.55
2:C:146:VAL:HG13	2:C:162:ILE:HG22	1.88	0.55
2:C:238:LEU:HG	2:C:242:LEU:HD21	1.88	0.55
4:E:57:ASP:O	4:E:63:TRP:NE1	2.38	0.55
2:C:668:LEU:HD12	2:C:668:LEU:H	1.70	0.55
3:D:258:VAL:HG22	3:D:273:ARG:O	2.06	0.55
3:D:272:LEU:HD21	3:D:298:VAL:CG1	2.36	0.55
1:B:101:LEU:HG	1:B:114:PHE:HA	1.88	0.55
1:B:170:VAL:HG11	3:D:848:GLU:HG3	1.87	0.55
2:C:14:PRO:HB2	2:C:586:ARG:NH2	2.21	0.55
3:D:405:ASP:CG	3:D:406:ASP:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.89	0.55
1:B:99:LEU:HB2	1:B:142:VAL:HG22	1.88	0.55
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.89	0.55
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.87	0.55
3:D:173:PRO:HA	3:D:209:ARG:NH2	2.17	0.55
3:D:508:ARG:NH1	3:D:509:PRO:HD2	2.22	0.55
2:C:750:LYS:HE3	3:D:680:GLN:OE1	2.07	0.55
2:C:376:ARG:HE	5:F:276:ARG:HG2	1.71	0.55
2:C:602:GLU:CG	2:C:648:ARG:HE	2.19	0.55
3:D:1372:VAL:HA	3:D:1375:MET:SD	2.47	0.55
3:D:203:ALA:O	3:D:204:LEU:HD23	2.07	0.55
1:A:57:TYR:CG	1:A:161:ARG:CZ	2.89	0.55
1:B:58:ILE:HG22	1:B:140:MET:HB3	1.88	0.55
1:B:208:LEU:HD23	1:B:208:LEU:H	1.72	0.55
3:D:185:VAL:HG13	3:D:189:GLN:HB3	1.89	0.55
3:D:326:GLU:OE2	3:D:326:GLU:N	2.40	0.55
3:D:348:GLN:HB2	3:D:351:MET:CE	2.37	0.55
3:D:704:ARG:HB2	3:D:745:MET:CE	2.37	0.55
3:D:95:LEU:HD22	3:D:574:LEU:HD21	1.89	0.55
5:F:232:ARG:HG2	5:F:232:ARG:HH11	1.72	0.55
1:B:85:LEU:HD22	1:B:87:VAL:CG1	2.36	0.54
3:D:481:MET:O	3:D:489:ARG:HD3	2.08	0.54
1:B:108:GLU:HA	1:B:131:THR:HA	1.90	0.54
3:D:1145:TYR:CD1	3:D:1168:MET:HE2	2.43	0.54
3:D:669:ASN:HB3	5:F:417:LYS:HE2	1.88	0.54
3:D:808:THR:HG23	3:D:811:GLU:H	1.72	0.54
3:D:881:LEU:O	3:D:885:ILE:HG12	2.07	0.54
3:D:886:VAL:O	3:D:890:VAL:HG23	2.08	0.54
3:D:875:THR:HG21	3:D:902:LEU:CD2	2.36	0.54
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.87	0.54
1:A:87:VAL:CG2	1:A:144:VAL:HG11	2.37	0.54
1:A:201:THR:HG23	1:A:203:GLY:N	2.22	0.54
3:D:317:VAL:HG12	3:D:339:TRP:CB	2.36	0.54
3:D:666:ILE:HD11	3:D:684:LYS:HZ2	1.72	0.54
5:F:401:GLU:O	5:F:405:LEU:HD13	2.07	0.54
3:D:1047:LYS:CE	3:D:1048:PRO:HD2	2.35	0.54
3:D:100:ALA:HA	3:D:513:ILE:HG22	1.88	0.54
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.89	0.54
1:A:99:LEU:CD1	1:A:114:PHE:HB3	2.34	0.54
3:D:1046:GLN:NE2	3:D:1076:GLY:HA3	2.23	0.54
3:D:181:ASP:CB	3:D:205:TYR:HD2	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:LEU:HD11	3:D:390:PRO:O	2.07	0.54
3:D:554:LEU:HB2	3:D:570:GLU:HG2	1.88	0.54
5:F:299:TRP:HA	5:F:303:ARG:HD3	1.89	0.54
1:B:206:THR:HG22	1:B:209:GLU:CD	2.28	0.54
2:C:1111:ILE:HD12	2:C:1111:ILE:H	1.73	0.54
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.90	0.54
2:C:480:THR:HG21	2:C:482:GLU:HG2	1.89	0.54
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.90	0.54
3:D:661:MET:CE	3:D:677:LEU:HD11	2.38	0.54
5:F:129:GLU:HG3	5:F:147:LEU:HD21	1.90	0.54
1:A:57:TYR:CE1	1:A:161:ARG:NH2	2.72	0.54
3:D:890:VAL:HG13	3:D:922:LEU:HD13	1.87	0.54
3:D:361:VAL:O	3:D:382:GLU:HA	2.08	0.54
3:D:544:TYR:O	3:D:548:ILE:HG13	2.08	0.54
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.88	0.54
1:B:72:LYS:HG3	1:B:131:THR:OG1	2.07	0.54
3:D:1295:GLU:OE2	3:D:1300:SER:HB2	2.08	0.54
3:D:200:ASP:O	3:D:397:LYS:HG2	2.08	0.54
3:D:661:MET:HE2	3:D:677:LEU:HD11	1.90	0.54
5:F:164:LYS:NZ	5:F:171:LYS:HE3	2.23	0.54
5:F:277:GLN:O	5:F:281:GLU:HG2	2.07	0.54
3:D:275:GLU:OE1	3:D:275:GLU:N	2.40	0.54
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.89	0.54
5:F:132:ARG:HH21	5:F:184:ARG:NH2	2.06	0.54
1:B:110:LYS:HZ1	1:B:112:ARG:CD	2.20	0.53
2:C:64:LEU:HA	2:C:103:LYS:H	1.72	0.53
2:C:816:LYS:O	2:C:819:VAL:HG12	2.08	0.53
3:D:1273:VAL:H	3:D:1326:THR:CG2	2.20	0.53
3:D:135:LEU:O	3:D:149:LYS:CE	2.42	0.53
3:D:695:ILE:HD12	3:D:718:PRO:HG2	1.90	0.53
2:C:179:ASN:HD21	2:C:181:VAL:HG12	1.71	0.53
2:C:227:PHE:O	2:C:229:MET:N	2.41	0.53
2:C:666:LEU:HG	2:C:668:LEU:HD11	1.91	0.53
3:D:828:LYS:CD	3:D:833:GLU:CB	2.86	0.53
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.42	0.53
2:C:280:LYS:HE3	2:C:323:ASP:CG	2.28	0.53
2:C:3:ILE:HA	2:C:900:ARG:O	2.08	0.53
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.90	0.53
3:D:669:ASN:ND2	5:F:417:LYS:HG2	2.24	0.53
2:C:262:ALA:HA	2:C:289:THR:OG1	2.07	0.53
3:D:1286:THR:HG22	3:D:1287:GLU:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:936:TYR:O	3:D:940:THR:HG23	2.08	0.53
2:C:890:LEU:CD2	2:C:901:TYR:CD2	2.92	0.53
2:C:97:ARG:O	2:C:98:LEU:HD13	2.09	0.53
1:B:132:LEU:HD23	1:B:133:GLU:N	2.24	0.53
2:C:1109:VAL:O	2:C:1111:ILE:HD12	2.08	0.53
2:C:367:LEU:CA	2:C:371:LYS:HE3	2.21	0.53
2:C:495:THR:HG22	2:C:517:ARG:NE	2.23	0.53
2:C:683:ASN:CB	2:C:872:ASN:HD22	2.22	0.53
3:D:15:PRO:O	3:D:19:ARG:HG3	2.08	0.53
3:D:666:ILE:CD1	3:D:684:LYS:HZ2	2.21	0.53
3:D:865:THR:HG22	3:D:874:GLU:HG2	1.91	0.53
3:D:675:ARG:HH22	5:F:420:ASP:CA	2.20	0.53
1:B:68:ILE:HB	1:B:71:VAL:HG22	1.90	0.53
7:H:17:DT:H2'	7:H:18:DG:C8	2.44	0.53
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.91	0.53
1:B:110:LYS:HZ1	1:B:112:ARG:CG	2.22	0.53
1:A:70:GLY:N	2:C:607:ASP:OD1	2.42	0.53
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.41	0.53
3:D:142:LEU:HD12	3:D:161:LEU:CD1	2.33	0.53
3:D:657:LEU:HG	3:D:661:MET:CE	2.39	0.53
5:F:278:LEU:C	5:F:282:LEU:HD12	2.29	0.53
2:C:1100:GLN:OE1	2:C:1108:PRO:HB3	2.08	0.53
2:C:595:LEU:C	2:C:596:TYR:HD1	2.13	0.53
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.90	0.53
2:C:102:HIS:HE1	2:C:365:ASP:HA	1.73	0.53
2:C:473:ARG:NE	2:C:482:GLU:OE2	2.33	0.53
3:D:1155:VAL:HG11	3:D:1177:ALA:CB	2.38	0.53
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.23	0.53
5:F:154:LYS:HD3	5:F:155:THR:CG2	2.38	0.53
5:F:398:ARG:NH2	5:F:399:GLN:HG3	2.24	0.53
1:B:216:GLU:OE1	1:B:219:ARG:NE	2.43	0.52
2:C:229:MET:HE1	2:C:237:ARG:HE	1.73	0.52
2:C:97:ARG:HG2	2:C:112:GLU:HB2	1.90	0.52
3:D:1286:THR:HG22	3:D:1287:GLU:N	2.24	0.52
3:D:361:VAL:HG23	3:D:365:ASP:CB	2.30	0.52
3:D:491:LYS:HD2	3:D:494:LYS:HE3	1.90	0.52
3:D:1487:VAL:HG23	4:E:74:VAL:HG13	1.91	0.52
5:F:106:VAL:O	5:F:110:MET:HG3	2.10	0.52
1:A:209:GLU:O	1:A:213:GLN:HG2	2.09	0.52
2:C:492:ASP:HB3	2:C:518:LYS:HG2	1.92	0.52
3:D:581:LEU:O	3:D:603:LEU:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:473:ARG:HB3	2:C:480:THR:HG21	1.91	0.52
2:C:495:THR:HG22	2:C:517:ARG:HE	1.74	0.52
2:C:654:LEU:HD11	2:C:656:ALA:O	2.09	0.52
3:D:1033:GLN:H	3:D:1033:GLN:CD	2.13	0.52
3:D:809:PRO:O	3:D:813:LEU:HD12	2.09	0.52
1:A:110:LYS:HD3	1:A:128:HIS:HA	1.91	0.52
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.92	0.52
2:C:911:GLU:O	2:C:915:LYS:HG2	2.10	0.52
3:D:1290:LEU:HD12	3:D:1307:LYS:HD3	1.90	0.52
2:C:154:ARG:CB	2:C:157:ARG:HG2	2.40	0.52
2:C:470:PRO:HD3	2:C:485:TYR:CE1	2.44	0.52
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.91	0.52
3:D:1492:LEU:CD1	3:D:1493:LYS:HE2	2.39	0.52
4:E:26:ARG:CD	4:E:30:LEU:HD11	2.36	0.52
4:E:39:VAL:HG12	4:E:72:ARG:NH1	2.25	0.52
1:B:14:ARG:HG2	1:B:14:ARG:HH11	1.74	0.52
1:B:31:GLY:N	1:B:193:ASP:OD1	2.43	0.52
3:D:1287:GLU:C	3:D:1307:LYS:HZ2	2.12	0.52
3:D:191:LEU:HD21	3:D:197:SER:HB3	1.91	0.52
5:F:256:ARG:HH21	5:F:258:ILE:HD11	1.74	0.52
2:C:214:TYR:O	2:C:218:VAL:HG23	2.09	0.52
2:C:611:ILE:HG13	2:C:611:ILE:O	2.09	0.52
2:C:793:PRO:HG2	2:C:796:GLU:OE1	2.10	0.52
3:D:804:LEU:O	3:D:827:ILE:HG23	2.10	0.52
1:A:65:PHE:CE2	2:C:703:ILE:HD13	2.45	0.52
2:C:154:ARG:HB3	2:C:157:ARG:HG2	1.91	0.52
2:C:727:PRO:HB2	2:C:728:HIS:CD2	2.45	0.52
3:D:1047:LYS:HZ2	3:D:1048:PRO:HG2	1.73	0.52
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.90	0.52
3:D:750:PRO:O	3:D:756:GLN:NE2	2.43	0.52
3:D:828:LYS:NZ	3:D:833:GLU:HB2	2.25	0.52
5:F:96:LEU:O	5:F:100:VAL:HG12	2.10	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.91	0.52
1:A:57:TYR:CG	1:A:161:ARG:NH2	2.77	0.51
2:C:179:ASN:CG	2:C:181:VAL:H	2.12	0.51
2:C:603:VAL:HA	2:C:613:VAL:HG23	1.91	0.51
2:C:758:ARG:HH21	2:C:788:THR:HG22	1.74	0.51
3:D:1486:VAL:HG13	4:E:29:GLN:NE2	2.24	0.51
3:D:470:LEU:HB2	3:D:503:LEU:HD21	1.91	0.51
3:D:65:ARG:HH21	5:F:377:ASP:N	2.01	0.51
5:F:403:LYS:O	5:F:407:LYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD11	1:A:109:VAL:HG11	1.92	0.51
1:B:107:LYS:HE2	1:B:108:GLU:O	2.11	0.51
1:B:58:ILE:HG22	1:B:140:MET:CB	2.39	0.51
2:C:1055:LEU:HD13	2:C:1079:PRO:HB3	1.91	0.51
2:C:764:GLU:HA	2:C:766:GLU:OE1	2.10	0.51
2:C:770:GLU:N	2:C:770:GLU:OE2	2.37	0.51
2:C:788:THR:HG22	2:C:788:THR:O	2.10	0.51
5:F:166:LEU:HB2	5:F:171:LYS:CG	2.41	0.51
1:A:9:PRO:HD2	1:B:224:TYR:CD1	2.46	0.51
3:D:178:LEU:HD23	3:D:190:GLU:OE1	2.10	0.51
3:D:371:ILE:CD1	3:D:372:ASP:CB	2.87	0.51
3:D:116:LEU:CD1	3:D:465:LEU:HD21	2.34	0.51
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.40	0.51
2:C:263:ASP:O	2:C:265:ARG:N	2.40	0.51
2:C:36:PRO:HA	2:C:39:ARG:HG3	1.93	0.51
3:D:413:ASP:H	5:F:178:ARG:NH2	2.04	0.51
3:D:93:ILE:HB	3:D:517:VAL:CG1	2.40	0.51
2:C:412:ALA:O	2:C:417:GLY:HA3	2.11	0.51
5:F:349:LEU:HD22	5:F:421:PHE:HZ	1.76	0.51
2:C:236:ILE:O	2:C:240:THR:HG23	2.11	0.51
3:D:208:PRO:O	3:D:347:VAL:CG1	2.54	0.51
3:D:285:PRO:HG2	3:D:311:LEU:HG	1.92	0.51
3:D:702:LEU:O	3:D:713:ILE:HA	2.11	0.51
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.46	0.51
3:D:374:GLU:OE2	3:D:374:GLU:N	2.31	0.51
3:D:522:PRO:HA	3:D:525:ARG:HG3	1.92	0.51
6:G:12:DG:H8	6:G:12:DG:H5"	1.76	0.51
3:D:527:MET:HE2	3:D:537:THR:HB	1.92	0.51
2:C:1031:ARG:HB2	3:D:622:ARG:NH1	2.26	0.51
2:C:502:PRO:O	2:C:503:LEU:HD13	2.11	0.51
3:D:258:VAL:O	3:D:272:LEU:HA	2.11	0.51
4:E:33:HIS:O	4:E:36:LYS:HG3	2.11	0.51
2:C:267:TYR:CE1	2:C:290:LEU:HD11	2.46	0.50
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.93	0.50
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.27	0.50
2:C:768:THR:OG1	2:C:770:GLU:OE2	2.30	0.50
3:D:1485:GLN:O	4:E:75:PHE:HA	2.11	0.50
3:D:657:LEU:HG	3:D:661:MET:HE2	1.93	0.50
5:F:162:LYS:HA	5:F:162:LYS:HE2	1.92	0.50
5:F:394:ARG:NH1	5:F:395:GLU:OE2	2.44	0.50
1:A:79:ILE:HD11	1:A:167:VAL:HG22	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.46	0.50
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.11	0.50
3:D:988:ARG:O	3:D:992:ILE:HG23	2.10	0.50
5:F:129:GLU:HA	5:F:132:ARG:HB2	1.92	0.50
3:D:65:ARG:NH2	5:F:377:ASP:H	2.05	0.50
1:A:19:GLU:HA	1:A:201:THR:CG2	2.41	0.50
1:A:9:PRO:HB3	1:A:27:PRO:O	2.12	0.50
2:C:589:ARG:NE	2:C:596:TYR:HE2	2.05	0.50
3:D:1280:VAL:HG12	3:D:1318:TYR:HA	1.93	0.50
3:D:288:MET:HA	3:D:306:GLU:O	2.11	0.50
3:D:631:ILE:HD11	3:D:745:MET:CG	2.41	0.50
2:C:64:LEU:HD13	2:C:102:HIS:CD2	2.47	0.50
2:C:575:GLN:HG3	2:C:670:GLN:HA	1.92	0.50
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.93	0.50
1:A:65:PHE:HE2	2:C:703:ILE:HD13	1.76	0.50
2:C:286:SER:OG	2:C:301:GLU:OE1	2.28	0.50
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.46	0.50
3:D:124:GLU:OE2	3:D:128:TYR:CD1	2.64	0.50
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.93	0.50
1:A:170:VAL:O	1:A:170:VAL:HG23	2.12	0.50
1:B:112:ARG:CG	1:B:125:PRO:HB2	2.35	0.50
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.94	0.50
3:D:412:GLY:CA	5:F:178:ARG:NH2	2.74	0.50
2:C:1067:TYR:CZ	5:F:342:VAL:HG12	2.46	0.50
2:C:650:ARG:HB2	2:C:650:ARG:NH1	2.26	0.50
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.46	0.50
3:D:1159:ARG:HG3	3:D:1159:ARG:O	2.11	0.50
2:C:283:ILE:HD13	2:C:305:PRO:HB3	1.94	0.50
6:G:12:DG:N2	7:H:17:DT:O2	2.45	0.50
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.47	0.49
2:C:31:GLN:HB3	2:C:34:VAL:HG22	1.94	0.49
3:D:695:ILE:CD1	3:D:720:LEU:HD11	2.42	0.49
1:A:19:GLU:CA	1:A:201:THR:HG22	2.39	0.49
2:C:1111:ILE:HD12	2:C:1111:ILE:N	2.27	0.49
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.94	0.49
2:C:719:PRO:HB3	2:C:820:ARG:HH22	1.77	0.49
3:D:1289:LYS:C	3:D:1307:LYS:HE2	2.33	0.49
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.94	0.49
5:F:154:LYS:O	5:F:158:GLU:HG2	2.12	0.49
1:A:74:ASP:HB3	2:C:627:ARG:NH2	2.28	0.49
3:D:1305:LEU:HD23	3:D:1306:PRO:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1364:HIS:CE1	3:D:1366:LYS:HB2	2.47	0.49
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.95	0.49
2:C:835:VAL:HA	2:C:849:VAL:CG2	2.42	0.49
2:C:69:LEU:HB2	2:C:97:ARG:O	2.13	0.49
2:C:877:PRO:HG3	3:D:1023:MET:CE	2.42	0.49
3:D:218:LYS:HE3	3:D:338:GLU:CB	2.35	0.49
3:D:362:GLU:HG3	3:D:363:ALA:N	2.27	0.49
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.48	0.49
3:D:513:ILE:HD12	3:D:513:ILE:C	2.31	0.49
4:E:30:LEU:HD12	4:E:30:LEU:H	1.78	0.49
5:F:128:ARG:NH1	5:F:181:GLU:OE1	2.45	0.49
5:F:265:VAL:HG22	5:F:269:ASN:ND2	2.28	0.49
2:C:209:ARG:NE	2:C:210:GLU:OE1	2.45	0.49
2:C:597:ALA:HB2	2:C:655:LEU:HD11	1.94	0.49
2:C:719:PRO:HB3	2:C:820:ARG:NH1	2.26	0.49
3:D:102:ILE:HB	3:D:579:ASP:OD2	2.12	0.49
3:D:581:LEU:O	3:D:602:SER:HB2	2.12	0.49
3:D:810:GLU:OE2	3:D:810:GLU:N	2.30	0.49
3:D:82:LYS:O	3:D:85:VAL:HG22	2.13	0.49
3:D:907:GLU:OE2	3:D:910:SER:N	2.33	0.49
4:E:39:VAL:CG1	4:E:72:ARG:HH11	2.25	0.49
5:F:365:GLU:OE2	5:F:365:GLU:HA	2.13	0.49
2:C:148:PHE:HD1	2:C:280:LYS:NZ	2.11	0.49
2:C:640:ARG:HB2	2:C:642:ARG:NH2	2.28	0.49
2:C:838:LYS:HE3	3:D:741:ASP:O	2.12	0.49
2:C:97:ARG:HG2	2:C:112:GLU:CB	2.43	0.49
2:C:633:GLN:OE1	2:C:633:GLN:N	2.46	0.49
5:F:349:LEU:HD22	5:F:421:PHE:CZ	2.48	0.49
2:C:682:TYR:CE1	3:D:635:PRO:HD2	2.48	0.49
5:F:166:LEU:HB2	5:F:171:LYS:HG3	1.94	0.49
1:B:220:GLU:O	1:B:223:THR:OG1	2.24	0.48
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.93	0.48
2:C:890:LEU:HD21	2:C:901:TYR:CE2	2.47	0.48
2:C:97:ARG:HG3	2:C:97:ARG:HH11	1.78	0.48
3:D:1165:TYR:CE1	3:D:1214:PRO:HB3	2.48	0.48
3:D:270:LEU:HB2	3:D:284:LEU:HD11	1.95	0.48
3:D:34:TYR:CB	5:F:260:ILE:HG22	2.43	0.48
3:D:553:ARG:HG3	3:D:557:LEU:HD13	1.95	0.48
3:D:66:GLN:HB3	5:F:376:ILE:CG2	2.43	0.48
3:D:695:ILE:HD11	3:D:720:LEU:HD11	1.95	0.48
5:F:162:LYS:CE	5:F:165:SER:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:229:TYR:CE1	5:F:230:LYS:HD3	2.47	0.48
2:C:1009:SER:O	3:D:624:ASP:HB3	2.13	0.48
2:C:157:ARG:N	2:C:157:ARG:HD2	2.27	0.48
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.94	0.48
5:F:365:GLU:CD	5:F:400:ILE:HB	2.33	0.48
3:D:207:PHE:CE2	5:F:97:GLU:HB2	2.48	0.48
1:A:66:SER:O	1:A:75:VAL:HG12	2.13	0.48
1:A:85:LEU:C	1:A:85:LEU:HD23	2.34	0.48
3:D:191:LEU:HD21	3:D:197:SER:HB2	1.96	0.48
3:D:33:ASN:HB2	3:D:40:GLU:OE2	2.12	0.48
3:D:556:LYS:NZ	5:F:222:ARG:HH21	2.11	0.48
5:F:398:ARG:O	5:F:401:GLU:HB3	2.13	0.48
1:A:103:ALA:O	1:A:104:GLU:HG3	2.12	0.48
1:A:111:ALA:O	1:A:114:PHE:HD2	1.95	0.48
1:B:206:THR:HG23	1:B:209:GLU:H	1.79	0.48
2:C:234:ALA:O	2:C:237:ARG:HB2	2.14	0.48
2:C:243:ARG:HD3	2:C:256:TYR:CE2	2.48	0.48
3:D:137:PRO:HA	3:D:452:ILE:CD1	2.42	0.48
3:D:437:VAL:HG21	5:F:175:HIS:CE1	2.48	0.48
5:F:386:VAL:HG13	5:F:390:PHE:CE1	2.48	0.48
3:D:179:VAL:HG12	3:D:180:LYS:N	2.29	0.48
3:D:828:LYS:HZ2	3:D:833:GLU:HB2	1.79	0.48
5:F:234:LYS:HD2	7:H:5:DA:OP2	2.12	0.48
1:A:97:VAL:HG13	1:A:98:THR:N	2.29	0.48
2:C:64:LEU:HD12	2:C:101:ILE:O	2.13	0.48
2:C:194:VAL:HG23	2:C:197:LEU:HD12	1.95	0.48
2:C:586:ARG:HA	2:C:589:ARG:HB3	1.96	0.48
2:C:734:LEU:HD23	2:C:737:LEU:HD12	1.96	0.48
2:C:765:SER:O	2:C:765:SER:OG	2.31	0.48
3:D:186:VAL:HG12	3:D:189:GLN:HB2	1.94	0.48
3:D:834:THR:HB	3:D:838:ARG:HD2	1.95	0.48
2:C:728:HIS:CE1	5:F:422:LEU:O	2.67	0.48
3:D:347:VAL:HG23	3:D:351:MET:HG3	1.96	0.48
3:D:204:LEU:HD11	3:D:445:ARG:HH11	1.78	0.48
7:H:17:DT:H2''	7:H:18:DG:H5'	1.96	0.48
1:B:132:LEU:HD21	1:B:136:GLY:C	2.34	0.48
3:D:1047:LYS:CG	3:D:1048:PRO:HD2	2.44	0.48
3:D:1084:THR:O	3:D:1088:THR:HG23	2.14	0.48
3:D:1379:VAL:HA	3:D:1420:LEU:HB2	1.95	0.48
3:D:556:LYS:NZ	5:F:222:ARG:NH2	2.61	0.48
5:F:287:THR:HG22	5:F:290:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:LEU:CD2	2:C:242:LEU:N	2.77	0.48
2:C:148:PHE:HD1	2:C:280:LYS:HZ2	1.62	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.14	0.48
3:D:1167:SER:O	3:D:1171:VAL:HG23	2.13	0.48
3:D:701:LEU:HB2	3:D:748:HIS:HB2	1.96	0.48
4:E:80:VAL:HG23	4:E:85:LEU:HD11	1.95	0.48
5:F:372:ARG:HH12	5:F:380:GLU:CA	2.19	0.48
1:A:53:VAL:HG21	1:A:82:LEU:O	2.14	0.48
1:B:159:LYS:HE2	1:B:164:ALA:O	2.13	0.48
2:C:31:GLN:O	2:C:34:VAL:HG22	2.13	0.48
2:C:627:ARG:NH1	2:C:640:ARG:HA	2.29	0.48
3:D:1047:LYS:CD	3:D:1048:PRO:HD2	2.44	0.48
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.49	0.48
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.96	0.48
3:D:1499:ARG:NH1	4:E:84:ARG:HG2	2.28	0.48
1:A:99:LEU:HD12	1:A:100:LEU:H	1.79	0.47
2:C:290:LEU:O	2:C:301:GLU:HB2	2.14	0.47
3:D:348:GLN:HB2	3:D:351:MET:HE2	1.95	0.47
3:D:401:TYR:C	3:D:443:VAL:HG23	2.34	0.47
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.96	0.47
3:D:896:ALA:O	3:D:900:ILE:CD1	2.57	0.47
4:E:44:GLU:O	4:E:66:LYS:HE2	2.14	0.47
2:C:777:ILE:HD13	5:F:408:LEU:HD13	1.95	0.47
3:D:1266:ARG:CZ	7:H:18:DG:H4'	2.45	0.47
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.94	0.47
1:B:64:GLU:HG3	1:B:79:ILE:HD12	1.94	0.47
3:D:1047:LYS:NZ	3:D:1048:PRO:CG	2.71	0.47
3:D:1282:ARG:HD2	3:D:1293:PHE:HB2	1.95	0.47
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.96	0.47
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.29	0.47
1:B:112:ARG:HG2	1:B:125:PRO:CB	2.37	0.47
2:C:14:PRO:HB2	2:C:586:ARG:HH21	1.79	0.47
2:C:568:ALA:CB	2:C:668:LEU:HB3	2.45	0.47
2:C:367:LEU:HD12	2:C:371:LYS:HZ1	1.75	0.47
2:C:627:ARG:HA	2:C:638:ASP:OD1	2.14	0.47
3:D:1293:PHE:CD1	3:D:1302:GLU:HB3	2.50	0.47
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.50	0.47
3:D:897:TRP:CH2	3:D:902:LEU:HD13	2.49	0.47
5:F:130:VAL:HG11	5:F:159:ILE:HG22	1.95	0.47
3:D:411:THR:HG22	5:F:178:ARG:HB2	1.97	0.47
1:B:9:PRO:HB2	1:B:25:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:468:ARG:HG3	2:C:485:TYR:HB3	1.97	0.47
3:D:126:VAL:O	3:D:457:GLY:N	2.42	0.47
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.49	0.47
3:D:212:ARG:HG3	3:D:344:ASP:OD1	2.14	0.47
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.45	0.47
2:C:1111:ILE:O	2:C:1111:ILE:HG22	2.15	0.47
2:C:247:PRO:O	2:C:252:LYS:HD3	2.14	0.47
2:C:730:SER:O	2:C:734:LEU:HD12	2.15	0.47
3:D:1275:SER:OG	3:D:1277:ILE:O	2.33	0.47
3:D:1305:LEU:HD11	3:D:1326:THR:HB	1.97	0.47
3:D:266:GLU:OE2	3:D:315:ARG:NH2	2.43	0.47
3:D:420:VAL:HG23	3:D:425:GLY:HA2	1.96	0.47
3:D:885:ILE:HD12	3:D:937:TYR:CG	2.50	0.47
2:C:190:LYS:HB3	2:C:190:LYS:HE3	1.50	0.47
2:C:283:ILE:HG22	2:C:284:ARG:N	2.30	0.47
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.49	0.47
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.97	0.47
3:D:316:GLN:HG3	3:D:316:GLN:O	2.15	0.47
3:D:357:GLU:HB2	3:D:387:LEU:HD23	1.97	0.47
3:D:530:VAL:HG22	3:D:531:ASP:N	2.28	0.47
3:D:613:ARG:HA	3:D:613:ARG:HD3	1.76	0.47
5:F:147:LEU:HD23	5:F:151:LEU:HD11	1.95	0.47
2:C:185:LYS:HB2	2:C:190:LYS:HD2	1.96	0.47
3:D:207:PHE:HB2	3:D:391:ALA:HB2	1.96	0.47
3:D:398:ALA:HB2	3:D:447:VAL:HG12	1.96	0.47
4:E:30:LEU:HB3	4:E:35:PHE:CD1	2.49	0.47
3:D:156:GLU:CD	3:D:156:GLU:H	2.14	0.46
3:D:252:ARG:HB3	3:D:301:GLY:HA2	1.97	0.46
5:F:403:LYS:HG3	5:F:404:ALA:N	2.30	0.46
1:A:4:SER:HB3	1:A:189:ARG:HH22	1.80	0.46
1:A:76:VAL:O	1:A:80:LEU:HD13	2.14	0.46
1:B:117:VAL:HB	1:B:120:VAL:HG22	1.98	0.46
1:A:11:PHE:O	1:B:228:PRO:HA	2.14	0.46
2:C:243:ARG:HD3	2:C:256:TYR:CZ	2.50	0.46
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.48	0.46
1:A:176:ARG:NH2	2:C:865:THR:HG22	2.30	0.46
3:D:1261:GLU:OE1	3:D:1268:PRO:HA	2.16	0.46
3:D:237:LYS:O	3:D:240:GLU:HB2	2.15	0.46
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.44	0.46
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.81	0.46
3:D:999:THR:O	3:D:1003:VAL:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1004:LYS:HD3	3:D:744:GLN:HE22	1.80	0.46
2:C:13:ILE:HG13	2:C:14:PRO:O	2.16	0.46
2:C:928:LYS:HG3	2:C:932:GLU:OE1	2.15	0.46
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.97	0.46
2:C:1101:THR:CG2	2:C:1111:ILE:HD11	2.46	0.46
2:C:727:PRO:O	2:C:729:LEU:CD2	2.63	0.46
2:C:82:GLU:HG3	2:C:86:LYS:NZ	2.31	0.46
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.50	0.46
1:A:191:ASP:OD1	2:C:938:LYS:NZ	2.37	0.46
6:G:12:DG:C6	6:G:13:DA:C6	3.04	0.46
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.50	0.46
3:D:1399:ASP:OD2	3:D:1432:LYS:NZ	2.49	0.46
3:D:1492:LEU:HD11	3:D:1493:LYS:HE2	1.98	0.46
5:F:105:LYS:HE2	5:F:179:GLU:OE2	2.15	0.46
2:C:238:LEU:HG	2:C:242:LEU:CD2	2.45	0.46
2:C:97:ARG:HG3	2:C:97:ARG:NH1	2.30	0.46
3:D:347:VAL:HG22	3:D:351:MET:HG3	1.97	0.46
3:D:409:VAL:HG23	3:D:435:VAL:HG21	1.96	0.46
3:D:666:ILE:HD11	3:D:684:LYS:NZ	2.30	0.46
1:A:99:LEU:HD21	1:A:114:PHE:CG	2.50	0.46
1:B:124:ASN:HB2	1:B:127:LEU:CG	2.42	0.46
1:B:97:VAL:HG13	1:B:144:VAL:HG22	1.96	0.46
1:B:153:ALA:HB2	1:B:168:ASP:N	2.31	0.46
2:C:31:GLN:HB3	2:C:34:VAL:CG2	2.46	0.46
2:C:337:GLY:O	2:C:341:THR:HG23	2.15	0.46
2:C:497:ALA:HB3	2:C:532:MET:HG3	1.98	0.46
2:C:668:LEU:N	2:C:668:LEU:HD12	2.30	0.46
2:C:762:LYS:HE2	2:C:783:ARG:O	2.14	0.46
3:D:704:ARG:HD3	3:D:736:PHE:O	2.15	0.46
1:A:185:ARG:CZ	1:A:187:GLY:HA2	2.46	0.46
1:B:64:GLU:HB2	1:B:165:ILE:HG21	1.98	0.46
2:C:501:THR:CG2	2:C:513:VAL:HG23	2.35	0.46
2:C:602:GLU:HG3	2:C:648:ARG:HE	1.81	0.46
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.37	0.46
2:C:716:LYS:HZ2	3:D:529:GLN:HE22	1.64	0.46
5:F:107:GLU:O	5:F:111:GLU:HG3	2.16	0.46
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.97	0.46
3:D:556:LYS:HZ1	5:F:222:ARG:HH21	1.64	0.46
2:C:204:GLN:HA	2:C:207:LEU:HD23	1.98	0.46
2:C:627:ARG:HD2	2:C:639:GLN:O	2.16	0.46
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.81	0.46
3:D:155:ASP:OD1	3:D:159:ARG:NH2	2.49	0.46
3:D:683:ILE:CG2	3:D:687:VAL:HG11	2.45	0.46
2:C:946:ARG:NH1	3:D:861:GLN:HE22	2.14	0.46
5:F:382:THR:HB	5:F:383:LEU:HD12	1.96	0.46
2:C:627:ARG:NH1	2:C:639:GLN:O	2.49	0.45
2:C:810:ASP:HB2	2:C:813:VAL:CG1	2.46	0.45
2:C:68:PHE:HD2	2:C:98:LEU:HD11	1.81	0.45
3:D:1277:ILE:HG13	3:D:1278:ASP:N	2.30	0.45
3:D:1410:GLU:HB3	3:D:1412:LYS:HE2	1.97	0.45
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.98	0.45
3:D:97:THR:HG22	3:D:98:PRO:O	2.15	0.45
5:F:366:ALA:O	5:F:370:LYS:HB2	2.16	0.45
2:C:206:THR:HA	2:C:209:ARG:HD3	1.98	0.45
2:C:366:SER:OG	2:C:366:SER:O	2.29	0.45
3:D:1148:VAL:HG22	3:D:1189:ARG:HB2	1.97	0.45
4:E:26:ARG:HD2	4:E:67:GLU:OE1	2.17	0.45
1:A:104:GLU:HG2	1:A:137:ARG:CD	2.43	0.45
2:C:282:GLY:C	2:C:283:ILE:HD12	2.37	0.45
2:C:739:GLU:CD	2:C:739:GLU:H	2.20	0.45
3:D:169:TYR:O	3:D:392:SER:HB3	2.16	0.45
3:D:556:LYS:HD3	5:F:218:GLN:NE2	2.32	0.45
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.99	0.45
3:D:437:VAL:HG11	5:F:175:HIS:ND1	2.32	0.45
2:C:716:LYS:HZ1	3:D:529:GLN:HE22	1.64	0.45
3:D:773:ALA:HB1	3:D:1363:LEU:HD12	1.99	0.45
4:E:84:ARG:HG3	4:E:88:GLU:OE1	2.16	0.45
3:D:1148:VAL:HA	3:D:1164:ARG:O	2.17	0.45
2:C:769:PRO:HD2	3:D:65:ARG:NH1	2.32	0.45
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.51	0.45
2:C:5:ARG:HH11	2:C:5:ARG:HB3	1.82	0.45
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.56	0.45
3:D:1438:ALA:N	3:D:1446:VAL:HG11	2.31	0.45
3:D:199:LEU:HG	3:D:200:ASP:O	2.15	0.45
3:D:131:LYS:N	3:D:456:MET:HE2	2.32	0.45
2:C:1001:VAL:HG22	3:D:724:GLN:HB2	1.98	0.45
5:F:164:LYS:HD2	5:F:171:LYS:CD	2.45	0.45
5:F:278:LEU:O	5:F:282:LEU:HD12	2.15	0.45
2:C:175:GLU:O	2:C:183:SER:OG	2.20	0.45
2:C:687:ALA:HB1	2:C:850:ALA:HB2	1.99	0.45
4:E:85:LEU:HD12	4:E:85:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:162:LYS:NZ	5:F:165:SER:HB2	2.31	0.45
1:A:133:GLU:OE2	2:C:610:ARG:NH2	2.49	0.45
3:D:1295:GLU:HA	3:D:1300:SER:CB	2.47	0.45
3:D:3:LYS:HG3	3:D:4:GLU:H	1.82	0.45
3:D:432:TYR:O	3:D:448:GLU:HA	2.17	0.45
3:D:628:ARG:HE	3:D:628:ARG:HB2	1.70	0.45
3:D:632:VAL:O	3:D:727:GLN:HA	2.16	0.45
5:F:181:GLU:O	5:F:185:GLN:HG2	2.17	0.45
5:F:232:ARG:NH1	5:F:232:ARG:HG2	2.31	0.45
5:F:369:LEU:O	5:F:372:ARG:HB3	2.17	0.45
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.81	0.45
2:C:681:GLY:HA2	3:D:939:PHE:CE1	2.52	0.45
2:C:820:ARG:H	2:C:820:ARG:HG2	1.65	0.45
3:D:1003:VAL:HG21	3:D:1041:LEU:HD22	1.98	0.45
3:D:199:LEU:HD12	3:D:199:LEU:HA	1.72	0.45
3:D:354:VAL:O	3:D:354:VAL:HG22	2.17	0.45
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.50	0.45
1:B:161:ARG:HG3	1:B:162:ILE:O	2.17	0.45
2:C:278:GLU:HG2	2:C:284:ARG:HA	1.99	0.45
2:C:882:LEU:HA	2:C:882:LEU:HD23	1.70	0.45
3:D:23:TYR:CE1	3:D:89:ARG:HD3	2.51	0.45
3:D:431:VAL:HG11	3:D:448:GLU:CD	2.38	0.45
3:D:63:TYR:CZ	3:D:71:LYS:HE2	2.51	0.45
5:F:368:VAL:O	5:F:390:PHE:HE2	1.99	0.45
2:C:195:LEU:HD22	2:C:238:LEU:HB2	1.98	0.44
2:C:263:ASP:C	2:C:265:ARG:H	2.20	0.44
3:D:1028:ALA:O	3:D:1029:ARG:HG2	2.18	0.44
3:D:1054:GLU:HG3	3:D:1054:GLU:H	1.62	0.44
5:F:97:GLU:HA	5:F:100:VAL:HG12	2.00	0.44
2:C:583:LEU:O	2:C:587:VAL:HG23	2.17	0.44
2:C:766:GLU:O	2:C:767:PRO:C	2.55	0.44
2:C:68:PHE:CA	2:C:98:LEU:HD12	2.21	0.44
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.50	0.44
3:D:916:TYR:CZ	3:D:920:LEU:HD21	2.52	0.44
3:D:669:ASN:HD22	5:F:417:LYS:HG2	1.82	0.44
1:A:36:LEU:O	1:A:39:PRO:HD2	2.18	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.53	0.44
1:B:29:GLU:HG2	1:B:30:ARG:N	2.33	0.44
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.97	0.44
2:C:259:GLY:HA2	2:C:263:ASP:CB	2.48	0.44
2:C:385:PHE:O	2:C:389:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:573:ARG:HB2	2:C:670:GLN:HE21	1.81	0.44
3:D:165:LYS:HD2	3:D:166:GLN:N	2.32	0.44
3:D:361:VAL:HG21	3:D:379:ALA:CB	2.47	0.44
3:D:792:ILE:HD13	3:D:941:PHE:CE2	2.53	0.44
1:A:16:GLN:OE1	1:A:17:GLY:N	2.51	0.44
2:C:460:ARG:HD2	2:C:485:TYR:CE1	2.52	0.44
2:C:650:ARG:NH1	2:C:653:ASP:OD1	2.49	0.44
3:D:171:LEU:HD21	3:D:390:PRO:CG	2.44	0.44
3:D:187:LYS:HG2	3:D:200:ASP:OD2	2.18	0.44
3:D:310:LEU:HA	3:D:310:LEU:HD12	1.68	0.44
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.98	0.44
3:D:534:ARG:HB3	3:D:534:ARG:HE	1.69	0.44
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.38	0.44
4:E:17:TYR:O	4:E:21:VAL:HG23	2.18	0.44
5:F:252:ALA:HB1	5:F:265:VAL:HG11	2.00	0.44
1:B:40:LEU:HD21	1:B:218:LEU:HD22	1.98	0.44
3:D:1047:LYS:CD	3:D:1048:PRO:CD	2.96	0.44
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.52	0.44
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.53	0.44
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.77	0.44
3:D:348:GLN:HB2	3:D:351:MET:HE3	2.00	0.44
3:D:56:TYR:HA	3:D:80:VAL:HG23	1.99	0.44
2:C:1053:LEU:HD11	3:D:1466:VAL:HG13	2.00	0.44
2:C:290:LEU:HD12	2:C:290:LEU:H	1.82	0.44
2:C:280:LYS:HE3	2:C:323:ASP:OD1	2.17	0.44
2:C:34:VAL:CG2	2:C:39:ARG:HG2	2.47	0.44
2:C:470:PRO:HB2	2:C:534:VAL:HG21	2.00	0.44
3:D:1314:LYS:O	3:D:1317:ASP:HB2	2.18	0.44
3:D:297:ILE:HD12	3:D:297:ILE:C	2.37	0.44
3:D:799:LYS:NZ	3:D:1014:ASN:HA	2.32	0.44
5:F:101:GLU:O	5:F:104:ARG:HB3	2.17	0.44
5:F:364:ARG:HE	5:F:364:ARG:C	2.20	0.44
1:A:18:ARG:O	1:A:201:THR:CG2	2.66	0.44
2:C:404:LEU:O	2:C:408:ARG:HG3	2.18	0.44
3:D:1045:MET:HB3	3:D:1045:MET:HE2	1.88	0.44
3:D:1053:PHE:CE2	3:D:1072:ILE:HD12	2.53	0.44
3:D:124:GLU:OE2	3:D:128:TYR:HD1	1.99	0.44
3:D:169:TYR:HE1	3:D:395:VAL:CG1	2.26	0.44
3:D:186:VAL:HG13	3:D:187:LYS:O	2.18	0.44
5:F:105:LYS:HB3	5:F:105:LYS:HE3	1.53	0.44
5:F:412:GLU:OE1	5:F:418:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HG13	1:B:61:VAL:CG1	2.44	0.44
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.36	0.44
2:C:207:LEU:C	2:C:207:LEU:HD12	2.38	0.44
2:C:719:PRO:CB	2:C:820:ARG:HH22	2.31	0.44
2:C:732:ALA:O	2:C:735:ARG:HG2	2.17	0.44
3:D:1048:PRO:HD3	3:D:1075:HIS:CG	2.53	0.44
3:D:1053:PHE:CD2	3:D:1072:ILE:HG23	2.52	0.44
3:D:1262:LEU:CD1	3:D:1351:GLU:HB3	2.47	0.44
3:D:1442:ASN:OD1	6:G:11:DA:H4'	2.18	0.44
3:D:85:VAL:C	3:D:87:ARG:H	2.20	0.44
2:C:197:LEU:HA	2:C:197:LEU:HD23	1.76	0.44
2:C:304:LEU:HA	2:C:304:LEU:HD22	1.71	0.44
2:C:759:THR:HB	2:C:785:VAL:HB	1.99	0.44
2:C:905:ILE:O	2:C:907:ASP:N	2.51	0.44
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.17	0.44
3:D:1267:ARG:HD2	3:D:1331:ASP:OD2	2.17	0.44
3:D:1386:ASP:OD2	3:D:1413:THR:HG22	2.17	0.44
3:D:808:THR:OG1	3:D:810:GLU:OE2	2.28	0.44
5:F:354:LEU:O	5:F:358:LEU:HD13	2.18	0.44
1:B:128:HIS:CE1	1:B:131:THR:CG2	2.97	0.43
1:B:173:PRO:HB2	1:B:205:VAL:HG12	1.99	0.43
3:D:231:VAL:HG22	3:D:242:LEU:O	2.18	0.43
3:D:34:TYR:HB3	5:F:260:ILE:HG22	1.99	0.43
3:D:794:GLN:HG3	3:D:795:VAL:N	2.32	0.43
3:D:876:SER:OG	3:D:879:ARG:HG3	2.18	0.43
5:F:172:ARG:HG3	5:F:173:TYR:CD1	2.53	0.43
1:B:219:ARG:HH11	1:B:219:ARG:HG2	1.83	0.43
2:C:1022:GLY:O	2:C:1026:GLN:NE2	2.51	0.43
2:C:675:ALA:HA	2:C:989:VAL:HG22	2.00	0.43
3:D:204:LEU:O	3:D:393:ILE:HD12	2.17	0.43
3:D:483:HIS:O	3:D:489:ARG:HG2	2.18	0.43
3:D:660:LYS:HA	3:D:660:LYS:HD3	1.82	0.43
3:D:711:LEU:HD13	3:D:778:LEU:CD1	2.49	0.43
1:B:219:ARG:HG2	1:B:219:ARG:NH1	2.34	0.43
2:C:230:ARG:HB2	2:C:233:GLU:OE1	2.18	0.43
2:C:755:LEU:HD11	2:C:792:VAL:HG22	2.00	0.43
3:D:209:ARG:N	3:D:389:GLU:O	2.32	0.43
3:D:684:LYS:O	3:D:687:VAL:HG12	2.18	0.43
1:A:152:PRO:O	1:A:155:LYS:HB2	2.17	0.43
1:B:170:VAL:HG23	1:B:170:VAL:O	2.17	0.43
2:C:957:LYS:HD3	2:C:961:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:LYS:HE3	3:D:200:ASP:OD2	2.17	0.43
3:D:520:LEU:O	3:D:525:ARG:HD3	2.18	0.43
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.54	0.43
3:D:900:ILE:H	3:D:900:ILE:HD12	1.83	0.43
5:F:193:ARG:NH1	7:H:7:DG:N7	2.66	0.43
2:C:229:MET:HE2	2:C:229:MET:HB3	1.82	0.43
2:C:627:ARG:HE	2:C:627:ARG:HB3	1.61	0.43
2:C:64:LEU:HD11	2:C:100:LEU:HD11	2.00	0.43
2:C:763:GLY:O	2:C:765:SER:N	2.52	0.43
2:C:890:LEU:C	2:C:890:LEU:HD23	2.37	0.43
2:C:905:ILE:C	2:C:907:ASP:H	2.21	0.43
3:D:317:VAL:HG12	3:D:339:TRP:HB3	2.00	0.43
3:D:818:ARG:HB3	3:D:820:GLU:HG3	2.00	0.43
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.19	0.43
5:F:164:LYS:HZ2	5:F:171:LYS:CE	2.32	0.43
1:B:48:ILE:C	1:B:148:VAL:HG12	2.39	0.43
1:B:85:LEU:HD23	1:B:86:VAL:N	2.34	0.43
1:A:176:ARG:CZ	2:C:865:THR:HG22	2.48	0.43
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.66	0.43
3:D:266:GLU:CD	3:D:315:ARG:HD2	2.39	0.43
4:E:79:LEU:HA	4:E:79:LEU:HD23	1.70	0.43
5:F:184:ARG:O	5:F:188:ILE:HG13	2.18	0.43
1:B:13:VAL:HG22	1:B:23:PHE:CD1	2.54	0.43
2:C:754:ILE:CG1	2:C:791:ARG:HE	2.27	0.43
3:D:1047:LYS:HD3	3:D:1048:PRO:CG	2.49	0.43
3:D:1293:PHE:CE1	3:D:1302:GLU:HG2	2.54	0.43
3:D:362:GLU:HG3	3:D:363:ALA:H	1.82	0.43
3:D:631:ILE:CG1	3:D:745:MET:HB2	2.48	0.43
3:D:526:PRO:HG2	5:F:317:LEU:HD11	2.01	0.43
1:A:97:VAL:HG12	1:A:144:VAL:HB	1.99	0.43
2:C:713:ARG:HG2	2:C:720:GLU:OE1	2.18	0.43
2:C:748:GLU:HA	2:C:799:ILE:HD13	1.99	0.43
3:D:116:LEU:CB	3:D:118:LEU:HD13	2.48	0.43
3:D:1371:VAL:O	3:D:1374:GLN:N	2.52	0.43
3:D:1487:VAL:HG23	4:E:74:VAL:CG1	2.49	0.43
3:D:41:ARG:HH21	3:D:48:ARG:NH1	2.17	0.43
3:D:408:GLU:HA	5:F:164:LYS:CE	2.49	0.43
5:F:132:ARG:NH2	5:F:184:ARG:NH2	2.66	0.43
5:F:200:LYS:O	5:F:203:THR:HG23	2.19	0.43
2:C:605:LYS:HD3	2:C:610:ARG:HH12	1.84	0.43
2:C:763:GLY:C	2:C:765:SER:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:890:LEU:CD2	2:C:901:TYR:CE2	3.02	0.43
3:D:208:PRO:CG	3:D:387:LEU:HD12	2.49	0.43
1:A:185:ARG:NH2	1:A:187:GLY:O	2.52	0.43
2:C:283:ILE:CG2	2:C:284:ARG:N	2.82	0.43
2:C:274:ARG:HH22	2:C:284:ARG:CZ	2.32	0.43
2:C:508:ILE:HG21	2:C:526:PRO:HB3	2.01	0.43
3:D:1262:LEU:HD11	3:D:1351:GLU:HB3	2.01	0.43
3:D:335:LEU:HA	3:D:335:LEU:HD23	1.82	0.43
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.01	0.42
2:C:172:ILE:HG12	2:C:186:VAL:CG2	2.45	0.42
2:C:206:THR:HA	2:C:209:ARG:HG2	2.00	0.42
3:D:361:VAL:HG22	3:D:362:GLU:O	2.18	0.42
3:D:626:SER:HA	3:D:747:VAL:O	2.19	0.42
3:D:640:HIS:H	3:D:640:HIS:CD2	2.37	0.42
5:F:396:ARG:O	5:F:400:ILE:HG12	2.19	0.42
1:B:104:GLU:HA	1:B:132:LEU:HD13	2.00	0.42
2:C:229:MET:SD	2:C:237:ARG:HG3	2.58	0.42
3:D:272:LEU:CD2	3:D:298:VAL:CG1	2.97	0.42
5:F:163:LEU:HD23	5:F:163:LEU:HA	1.52	0.42
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.39	0.42
3:D:1148:VAL:CG2	3:D:1189:ARG:HG3	2.49	0.42
3:D:128:TYR:CE1	3:D:587:ARG:HD2	2.54	0.42
3:D:213:VAL:HG13	3:D:215:TYR:CE2	2.54	0.42
1:B:94:LEU:HD12	1:B:95:GLN:N	2.33	0.42
2:C:595:LEU:C	2:C:596:TYR:CD1	2.93	0.42
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.50	0.42
2:C:736:ASP:O	2:C:744:ARG:HG2	2.19	0.42
2:C:876:VAL:H	2:C:877:PRO:HD2	1.85	0.42
3:D:1092:GLY:HA3	6:G:14:DG:O4'	2.20	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.54	0.42
3:D:33:ASN:HB3	3:D:36:THR:CG2	2.45	0.42
3:D:352:ASN:N	3:D:352:ASN:OD1	2.52	0.42
3:D:486:ARG:O	3:D:489:ARG:HB2	2.20	0.42
3:D:984:THR:HG22	3:D:986:ARG:H	1.84	0.42
5:F:240:THR:O	5:F:244:ARG:HG3	2.19	0.42
3:D:949:ILE:HD11	3:D:1023:MET:HE1	2.00	0.42
3:D:1286:THR:HB	3:D:1289:LYS:H	1.85	0.42
3:D:258:VAL:HG12	3:D:297:ILE:CG2	2.48	0.42
3:D:273:ARG:HB2	3:D:277:GLU:O	2.20	0.42
3:D:314:PRO:HB2	3:D:317:VAL:HG22	2.01	0.42
3:D:413:ASP:N	5:F:178:ARG:NH2	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	2.00	0.42
3:D:684:LYS:HG3	3:D:684:LYS:HZ3	1.76	0.42
2:C:241:LEU:HB2	2:C:242:LEU:CD2	2.50	0.42
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.53	0.42
2:C:773:LEU:O	2:C:777:ILE:HG13	2.19	0.42
2:C:783:ARG:HB3	2:C:783:ARG:CZ	2.49	0.42
3:D:1286:THR:N	3:D:1289:LYS:O	2.49	0.42
3:D:1291:SER:HB2	3:D:1304:LYS:HG2	2.01	0.42
3:D:352:ASN:HB3	5:F:104:ARG:NH2	2.35	0.42
5:F:320:PRO:HA	5:F:327:SER:O	2.20	0.42
1:A:57:TYR:CD1	1:A:161:ARG:NH2	2.87	0.42
2:C:280:LYS:CE	2:C:323:ASP:OD2	2.62	0.42
3:D:128:TYR:HD2	3:D:128:TYR:HA	1.70	0.42
3:D:317:VAL:HG12	3:D:339:TRP:HB2	2.01	0.42
3:D:210:ARG:HG2	3:D:388:HIS:HB2	2.02	0.42
3:D:394:LEU:HD11	3:D:396:VAL:HG12	2.01	0.42
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.42
5:F:166:LEU:O	5:F:171:LYS:NZ	2.30	0.42
2:C:1063:ARG:HG3	5:F:341:PRO:HG3	2.02	0.42
5:F:364:ARG:CZ	5:F:368:VAL:HG23	2.50	0.42
1:B:185:ARG:NH1	1:B:187:GLY:O	2.53	0.42
1:B:212:ASN:HA	1:B:215:VAL:HG12	2.02	0.42
2:C:762:LYS:HD2	2:C:784:ASP:C	2.40	0.42
2:C:926:PHE:O	2:C:929:ARG:HB3	2.19	0.42
1:B:73:GLU:N	1:B:73:GLU:OE1	2.40	0.42
2:C:966:LEU:HD13	2:C:986:PRO:HB3	2.01	0.42
3:D:148:GLU:H	3:D:148:GLU:HG2	1.49	0.42
3:D:112:ILE:HG23	3:D:465:LEU:HD11	2.02	0.42
3:D:553:ARG:HG3	3:D:557:LEU:CD1	2.50	0.42
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.55	0.42
5:F:260:ILE:CD1	5:F:265:VAL:HB	2.49	0.42
5:F:351:SER:HA	5:F:354:LEU:HB2	2.02	0.42
2:C:64:LEU:HD12	2:C:65:VAL:H	1.85	0.42
3:D:1047:LYS:CE	3:D:1048:PRO:CD	2.88	0.42
3:D:371:ILE:CD1	3:D:372:ASP:CA	2.95	0.42
3:D:71:LYS:O	3:D:80:VAL:HG12	2.20	0.42
1:A:97:VAL:HG22	1:A:98:THR:H	1.85	0.41
2:C:1015:LEU:HD21	5:F:333:ILE:HG22	2.02	0.41
2:C:121:MET:CE	2:C:125:GLY:HA2	2.50	0.41
2:C:283:ILE:CD1	2:C:305:PRO:HB3	2.50	0.41
2:C:331:ARG:NH1	2:C:427:VAL:HG23	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:611:ILE:HD11	2:C:655:LEU:HB3	2.02	0.41
3:D:1034:GLN:O	3:D:1038:LEU:HD12	2.20	0.41
3:D:1098:LEU:HA	3:D:1098:LEU:HD23	1.82	0.41
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.20	0.41
3:D:273:ARG:HH11	3:D:278:PRO:HD3	1.85	0.41
3:D:128:TYR:HE1	3:D:587:ARG:HD2	1.85	0.41
3:D:711:LEU:HB3	3:D:714:GLN:OE1	2.20	0.41
3:D:641:GLN:HE21	3:D:717:GLN:NE2	2.18	0.41
4:E:30:LEU:HD23	4:E:35:PHE:HD1	1.85	0.41
4:E:50:THR:CG2	4:E:53:GLY:H	2.32	0.41
5:F:95:THR:OG1	5:F:98:GLU:HG3	2.20	0.41
1:A:30:ARG:HB2	1:A:191:ASP:O	2.19	0.41
2:C:1059:ASP:OD2	2:C:1080:SER:HB3	2.20	0.41
2:C:207:LEU:O	2:C:211:LEU:HD23	2.21	0.41
2:C:768:THR:HG23	2:C:771:GLU:N	2.33	0.41
2:C:834:GLN:HG2	2:C:837:ASP:OD2	2.20	0.41
2:C:959:PRO:O	2:C:963:LEU:HG	2.19	0.41
3:D:36:THR:C	3:D:38:LYS:H	2.23	0.41
4:E:40:LEU:HA	4:E:72:ARG:HH12	1.85	0.41
5:F:154:LYS:HZ3	5:F:155:THR:HG22	1.83	0.41
1:A:213:GLN:HG2	1:A:213:GLN:H	1.57	0.41
1:B:106:PRO:HD3	1:B:134:GLU:HG2	2.03	0.41
2:C:388:ARG:HH11	2:C:388:ARG:HG2	1.83	0.41
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	2.01	0.41
3:D:14:SER:HB2	3:D:16:GLU:OE2	2.20	0.41
3:D:437:VAL:HG11	5:F:175:HIS:CE1	2.56	0.41
3:D:450:TYR:C	3:D:452:ILE:H	2.23	0.41
5:F:157:GLU:O	5:F:161:GLN:HG2	2.20	0.41
6:G:5:DT:O2	7:H:24:DG:N2	2.53	0.41
2:C:719:PRO:HG2	2:C:721:ARG:NH2	2.35	0.41
1:B:128:HIS:CE1	1:B:131:THR:HG22	2.43	0.41
2:C:365:ASP:OD2	2:C:365:ASP:N	2.54	0.41
2:C:717:LEU:HD21	2:C:763:GLY:HA2	2.02	0.41
3:D:127:LEU:HA	3:D:127:LEU:HD23	1.78	0.41
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.56	0.41
3:D:272:LEU:HD21	3:D:298:VAL:HG11	2.01	0.41
3:D:222:GLY:HA2	3:D:333:LEU:O	2.21	0.41
3:D:431:VAL:HG12	3:D:432:TYR:N	2.35	0.41
3:D:860:LEU:O	3:D:876:SER:HB2	2.21	0.41
4:E:26:ARG:O	4:E:29:GLN:HB2	2.20	0.41
1:B:23:PHE:HE1	1:B:208:LEU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:THR:O	2:C:23:VAL:HG23	2.20	0.41
2:C:495:THR:HA	2:C:517:ARG:HG2	2.01	0.41
2:C:754:ILE:CG2	2:C:789:SER:HB3	2.51	0.41
3:D:105:VAL:O	3:D:110:SER:HB2	2.21	0.41
3:D:1110:ALA:O	3:D:1203:LYS:HG2	2.20	0.41
3:D:800:LYS:HZ3	3:D:820:GLU:C	2.23	0.41
5:F:383:LEU:HB2	5:F:384:GLU:OE2	2.20	0.41
1:B:150:TYR:CE2	1:B:170:VAL:HG12	2.56	0.41
1:B:188:GLN:CD	1:B:188:GLN:H	2.23	0.41
2:C:580:MET:HE1	2:C:665:PHE:CE2	2.55	0.41
2:C:763:GLY:C	2:C:765:SER:N	2.74	0.41
2:C:808:ARG:NH1	2:C:820:ARG:HD2	2.36	0.41
3:D:116:LEU:HD11	3:D:465:LEU:CD2	2.38	0.41
3:D:137:PRO:HB3	3:D:147:VAL:CG1	2.50	0.41
3:D:313:MET:HA	3:D:314:PRO:HD3	1.94	0.41
3:D:720:LEU:H	3:D:720:LEU:HD12	1.85	0.41
1:B:53:VAL:HG22	1:B:144:VAL:HG12	2.02	0.41
1:B:32:PHE:HA	1:B:35:THR:HB	2.02	0.41
2:C:91:GLN:HG3	2:C:117:HIS:HB3	2.02	0.41
2:C:207:LEU:HD11	2:C:222:MET:CE	2.51	0.41
2:C:487:THR:OG1	2:C:490:GLU:HG2	2.21	0.41
2:C:810:ASP:HB2	2:C:813:VAL:HG11	2.02	0.41
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.90	0.41
3:D:191:LEU:N	3:D:191:LEU:HD22	2.35	0.41
3:D:218:LYS:HE2	3:D:338:GLU:CD	2.41	0.41
3:D:343:LYS:NZ	3:D:380:GLU:OE2	2.41	0.41
5:F:363:GLU:OE1	5:F:366:ALA:HB3	2.21	0.41
1:B:36:LEU:O	1:B:39:PRO:HD2	2.21	0.41
2:C:151:ASP:HB3	2:C:157:ARG:O	2.21	0.41
2:C:884:GLN:HB2	2:C:992:MET:CE	2.51	0.41
3:D:1217:ILE:HG21	3:D:1480:PHE:CG	2.55	0.41
3:D:231:VAL:O	3:D:231:VAL:HG23	2.21	0.41
5:F:276:ARG:O	5:F:280:GLN:HB2	2.21	0.41
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.91	0.41
8:I:3:G:C2	8:I:4:G:N2	2.89	0.41
2:C:714:ASP:OD2	2:C:820:ARG:HD3	2.20	0.41
3:D:181:ASP:N	3:D:205:TYR:HE2	2.19	0.41
3:D:245:LEU:CD2	3:D:249:TYR:HB3	2.50	0.41
5:F:172:ARG:O	5:F:176:ILE:HG12	2.21	0.41
2:C:546:LEU:HA	2:C:581:THR:HG21	2.03	0.41
3:D:1145:TYR:CG	3:D:1168:MET:HE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:50:THR:HG23	4:E:53:GLY:H	1.86	0.41
5:F:166:LEU:HB2	5:F:171:LYS:HG2	2.03	0.41
1:B:18:ARG:O	1:B:207:PRO:HD3	2.22	0.40
3:D:1237:THR:O	3:D:1237:THR:HG22	2.22	0.40
3:D:1471:LEU:HD21	3:D:1477:GLY:HA2	2.03	0.40
3:D:169:TYR:CE1	3:D:395:VAL:HG12	2.46	0.40
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.65	0.40
4:E:44:GLU:O	4:E:66:LYS:CE	2.69	0.40
1:A:186:LEU:HA	1:A:186:LEU:HD12	1.92	0.40
1:B:124:ASN:N	1:B:124:ASN:OD1	2.47	0.40
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.54	0.40
1:B:211:LEU:O	1:B:215:VAL:HG12	2.21	0.40
1:B:40:LEU:N	1:B:40:LEU:HD23	2.36	0.40
2:C:1086:ARG:HE	2:C:1111:ILE:HG22	1.86	0.40
2:C:195:LEU:CD2	2:C:238:LEU:HB2	2.51	0.40
3:D:355:VAL:CG1	3:D:367:ILE:HA	2.51	0.40
3:D:845:ASN:OD1	3:D:848:GLU:N	2.46	0.40
2:C:41:ASN:OD1	2:C:46:ALA:HA	2.22	0.40
2:C:494:TYR:CD2	2:C:531:PHE:CE2	3.09	0.40
2:C:573:ARG:HB2	2:C:670:GLN:NE2	2.36	0.40
2:C:758:ARG:HE	2:C:788:THR:HG22	1.86	0.40
2:C:799:ILE:O	2:C:801:VAL:HG13	2.21	0.40
2:C:876:VAL:HG22	2:C:884:GLN:NE2	2.37	0.40
2:C:877:PRO:HG3	3:D:1023:MET:HE3	2.01	0.40
3:D:359:ALA:H	3:D:385:VAL:HG22	1.85	0.40
2:C:376:ARG:NE	5:F:276:ARG:HG2	2.36	0.40
1:A:190:THR:OG1	1:A:191:ASP:N	2.55	0.40
1:B:75:VAL:O	1:B:79:ILE:HG13	2.21	0.40
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.86	0.40
2:C:598:GLU:HG3	2:C:615:TYR:OH	2.21	0.40
2:C:861:LEU:HD13	2:C:865:THR:OG1	2.21	0.40
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.22	0.40
3:D:1265:ALA:O	3:D:1333:HIS:HE1	2.04	0.40
3:D:16:GLU:N	3:D:16:GLU:OE2	2.30	0.40
3:D:703:ASN:HA	3:D:712:GLY:O	2.22	0.40
5:F:140:ARG:HE	5:F:140:ARG:HB2	1.62	0.40
5:F:358:LEU:CB	5:F:366:ALA:HB1	2.51	0.40
2:C:1093:GLN:HG2	3:D:21:TRP:CH2	2.56	0.40
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.77	0.40
2:C:486:MET:SD	2:C:491:GLU:HA	2.62	0.40
3:D:204:LEU:CD1	3:D:445:ARG:HH11	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:86:HIS:O	5:F:90:GLN:NE2	2.53	0.40

All (13) 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)
3:D:301:GLY:N	5:F:249:ARG:NH1[4_1349]	1.44	0.76
3:D:300:LYS:O	5:F:249:ARG:NE[4_1349]	1.58	0.62
3:D:302:GLN:N	5:F:249:ARG:NH2[4_1349]	1.66	0.54
3:D:302:GLN:N	5:F:249:ARG:CZ[4_1349]	1.77	0.43
3:D:300:LYS:C	5:F:249:ARG:NE[4_1349]	1.80	0.40
3:D:302:GLN:CG	5:F:249:ARG:NH2[4_1349]	1.81	0.39
3:D:301:GLY:N	5:F:249:ARG:CZ[4_1349]	1.91	0.29
3:D:35:ARG:NH2	3:D:327:GLU:OE1[4_1359]	1.98	0.22
3:D:300:LYS:C	5:F:249:ARG:NH1[4_1349]	2.00	0.20
3:D:299:GLU:O	5:F:249:ARG:NH1[4_1349]	2.14	0.06
3:D:301:GLY:C	5:F:249:ARG:CZ[4_1349]	2.16	0.04
3:D:985:ASP:CB	3:D:1497:GLU:OE2[1_545]	2.16	0.04
3:D:300:LYS:C	5:F:249:ARG:CZ[4_1349]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	211 (94%)	13 (6%)	0	100	100
1	B	222/315 (70%)	202 (91%)	18 (8%)	2 (1%)	17	34
2	C	1101/1119 (98%)	1036 (94%)	53 (5%)	12 (1%)	14	30
3	D	1480/1524 (97%)	1398 (94%)	71 (5%)	11 (1%)	22	42
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423 (81%)	316 (92%)	23 (7%)	5 (2%)	10	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3463/3795 (91%)	3252 (94%)	181 (5%)	30 (1%)	17	34

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	GLU
2	C	363	SER
2	C	418	LEU
2	C	419	THR
3	D	486	ARG
3	D	664	LYS
3	D	1130	ARG
5	F	323	ASP
5	F	377	ASP
2	C	362	GLY
2	C	476	GLY
3	D	743	ASP
3	D	984	THR
2	C	228	ALA
3	D	320	ALA
3	D	442	ASN
2	C	229	MET
3	D	37	LEU
3	D	86	ARG
3	D	187	LYS
3	D	484	PRO
2	C	766	GLU
2	C	1015	LEU
2	C	1034	GLU
5	F	325	LYS
5	F	378	GLY
5	F	416	ARG
1	B	59	GLU
2	C	728	HIS
2	C	765	SER

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	199/273 (73%)	192 (96%)	7 (4%)	36	61
1	B	197/273 (72%)	194 (98%)	3 (2%)	65	82
2	C	931/941 (99%)	892 (96%)	39 (4%)	30	54
3	D	1250/1279 (98%)	1213 (97%)	37 (3%)	41	65
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	60
5	F	296/371 (80%)	281 (95%)	15 (5%)	24	45
All	All	2956/3225 (92%)	2852 (96%)	104 (4%)	36	61

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	126	ASP
1	A	145	ASP
1	A	161	ARG
1	A	175	ARG
1	A	188	GLN
1	A	219	ARG
1	B	74	ASP
1	B	110	LYS
1	B	126	ASP
2	C	38	LYS
2	C	103	LYS
2	C	134	ARG
2	C	141	HIS
2	C	154	ARG
2	C	157	ARG
2	C	168	ARG
2	C	171	TRP
2	C	179	ASN
2	C	189	ARG
2	C	238	LEU
2	C	243	ARG
2	C	275	TYR
2	C	284	ARG
2	C	293	PHE
2	C	342	ASP
2	C	353	ARG

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Mol	Chain	Res	Type
2	C	365	ASP
2	C	366	SER
2	C	371	LYS
2	C	434	HIS
2	C	454	SER
2	C	482	GLU
2	C	557	ARG
2	C	586	ARG
2	C	610	ARG
2	C	617	ASP
2	C	626	ARG
2	C	648	ARG
2	C	680	ASP
2	C	716	LYS
2	C	721	ARG
2	C	735	ARG
2	C	765	SER
2	C	791	ARG
2	C	834	GLN
2	C	879	ARG
2	C	929	ARG
2	C	1026	GLN
3	D	3	LYS
3	D	9	ARG
3	D	106	LYS
3	D	190	GLU
3	D	220	ARG
3	D	224	ARG
3	D	247	GLU
3	D	276	ASP
3	D	302	GLN
3	D	316	GLN
3	D	351	MET
3	D	434	ARG
3	D	500	ARG
3	D	508	ARG
3	D	525	ARG
3	D	638	LYS
3	D	640	HIS
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU

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Mol	Chain	Res	Type
3	D	784	ASP
3	D	797	LYS
3	D	832	ARG
3	D	907	GLU
3	D	982	PHE
3	D	986	ARG
3	D	988	ARG
3	D	1011	PHE
3	D	1159	ARG
3	D	1188	VAL
3	D	1234	THR
3	D	1282	ARG
3	D	1308	GLU
3	D	1317	ASP
3	D	1363	LEU
3	D	1418	LYS
3	D	1426	LYS
4	E	15	SER
4	E	84	ARG
4	E	87	LYS
5	F	93	LEU
5	F	162	LYS
5	F	172	ARG
5	F	186	HIS
5	F	205	ARG
5	F	232	ARG
5	F	302	LYS
5	F	355	GLU
5	F	377	ASP
5	F	396	ARG
5	F	398	ARG
5	F	409	LYS
5	F	411	HIS
5	F	413	SER
5	F	419	ARG

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

Mol	Chain	Res	Type
1	A	128	HIS
1	A	213	GLN
1	B	95	GLN

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Mol	Chain	Res	Type
1	B	124	ASN
1	B	163	ASN
1	B	229	GLN
2	C	102	HIS
2	C	139	GLN
2	C	204	GLN
2	C	647	GLN
2	C	1047	HIS
3	D	33	ASN
3	D	151	GLN
3	D	529	GLN
3	D	611	GLN
3	D	640	HIS
3	D	717	GLN
3	D	744	GLN
3	D	861	GLN
3	D	1046	GLN
3	D	1445	HIS
5	F	175	HIS
5	F	248	ASN
5	F	402	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	7/8 (87%)	3 (42%)	2 (28%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	3	G
8	I	4	G
8	I	5	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	1	GTP
8	I	4	G

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
10	POP	C	1201	-	6,8,8	0.51	0	13,13,13	1.31	1 (7%)

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
10	POP	C	1201	-	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	POP	P2-O-P1	-2.86	123.03	132.83

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 [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	A	226/315 (71%)	-0.11	3 (1%) 77 74	71, 95, 118, 132	0
1	B	224/315 (71%)	-0.02	1 (0%) 92 91	68, 96, 127, 146	0
2	C	1107/1119 (98%)	0.16	48 (4%) 35 27	54, 94, 165, 203	0
3	D	1484/1524 (97%)	0.13	47 (3%) 47 41	49, 87, 149, 204	0
4	E	94/99 (94%)	0.01	0 100 100	64, 102, 152, 157	0
5	F	346/423 (81%)	0.65	52 (15%) 2 1	62, 107, 206, 228	0
6	G	19/22 (86%)	0.63	3 (15%) 2 1	66, 123, 229, 241	0
7	H	19/27 (70%)	0.11	3 (15%) 2 1	92, 125, 233, 239	0
8	I	7/8 (87%)	1.04	2 (28%) 0 0	68, 83, 172, 195	0
All	All	3526/3852 (91%)	0.17	159 (4%) 33 25	49, 94, 165, 241	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	392	VAL	9.6
5	F	397	ILE	8.2
5	F	376	ILE	8.1
5	F	396	ARG	8.0
5	F	374	GLY	7.7
5	F	375	LEU	7.5
5	F	419	ARG	6.6
5	F	390	PHE	6.1
5	F	422	LEU	6.1
3	D	173	PRO	5.8
5	F	356	LYS	5.6
5	F	400	ILE	5.5
5	F	149	GLU	5.5
5	F	357	ALA	5.4
5	F	361	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
5	F	414	ARG	5.1
5	F	147	LEU	5.0
5	F	370	LYS	4.9
5	F	148	LYS	4.9
6	G	3	DC	4.8
5	F	394	ARG	4.8
2	C	107	LEU	4.7
5	F	391	GLY	4.7
2	C	188	LYS	4.6
5	F	393	THR	4.6
3	D	1129	THR	4.5
3	D	144	GLY	4.5
5	F	367	MET	4.5
2	C	245	GLY	4.5
2	C	311	PHE	4.4
5	F	371	LEU	4.3
3	D	1128	VAL	4.3
3	D	1301	LYS	4.2
3	D	1297	GLU	4.1
5	F	349	LEU	4.1
2	C	219	GLN	4.0
2	C	194	VAL	4.0
5	F	389	PHE	3.9
7	H	25	DG	3.9
7	H	24	DG	3.9
2	C	216	GLU	3.8
3	D	1502	ALA	3.8
5	F	386	VAL	3.8
8	I	4	G	3.8
5	F	352	GLU	3.7
5	F	395	GLU	3.7
5	F	369	LEU	3.7
2	C	617	ASP	3.6
5	F	413	SER	3.6
5	F	416	ARG	3.6
7	H	23	DA	3.6
5	F	417	LYS	3.6
3	D	1298	GLY	3.6
3	D	174	GLY	3.6
2	C	104	ASP	3.3
5	F	353	GLU	3.3
5	F	362	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	3.3
2	C	304	LEU	3.2
5	F	150	THR	3.2
5	F	381	HIS	3.2
5	F	410	TYR	3.1
5	F	173	TYR	3.1
3	D	188	GLY	3.1
3	D	409	VAL	3.1
3	D	310	LEU	3.1
2	C	416	GLY	3.1
5	F	142	ARG	3.0
2	C	102	HIS	3.0
5	F	385	GLU	2.9
3	D	268	ALA	2.9
2	C	254	VAL	2.9
5	F	143	HIS	2.9
3	D	1299	PHE	2.9
3	D	363	ALA	2.9
2	C	64	LEU	2.8
2	C	811	PRO	2.8
2	C	417	GLY	2.8
2	C	221	LEU	2.8
3	D	67	ARG	2.7
3	D	1278	ASP	2.7
3	D	1294	VAL	2.7
2	C	109	LYS	2.7
2	C	189	ARG	2.7
3	D	1289	LYS	2.7
3	D	384	VAL	2.7
3	D	1293	PHE	2.7
3	D	1313	VAL	2.7
3	D	142	LEU	2.6
5	F	379	ARG	2.6
3	D	170	PRO	2.6
2	C	208	ALA	2.6
2	C	217	LEU	2.5
2	C	251	ASP	2.5
8	I	3	G	2.5
3	D	978	TYR	2.5
3	D	152	LEU	2.5
2	C	181	VAL	2.5
3	D	1497	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
5	F	323	ASP	2.5
2	C	215	GLY	2.5
5	F	360	LYS	2.5
2	C	367	LEU	2.5
1	A	137	ARG	2.4
2	C	195	LEU	2.4
5	F	420	ASP	2.4
2	C	778	PHE	2.4
3	D	143	ASN	2.4
2	C	153	ALA	2.4
1	A	99	LEU	2.4
2	C	12	VAL	2.4
2	C	106	GLY	2.4
5	F	373	LYS	2.4
2	C	250	ARG	2.3
3	D	183	GLU	2.3
3	D	241	ILE	2.3
3	D	1305	LEU	2.3
3	D	1288	GLU	2.3
3	D	1327	ARG	2.3
3	D	369	ALA	2.3
5	F	350	LEU	2.3
3	D	195	VAL	2.3
5	F	359	SER	2.3
2	C	224	GLU	2.3
3	D	1387	SER	2.3
2	C	650	ARG	2.3
5	F	404	ALA	2.3
6	G	4	DC	2.2
2	C	320	HIS	2.2
3	D	63	TYR	2.2
3	D	1501	GLU	2.2
6	G	19	DA	2.2
2	C	299	LYS	2.2
2	C	241	LEU	2.2
3	D	1292	VAL	2.2
2	C	154	ARG	2.2
5	F	423	ASP	2.2
3	D	189	GLN	2.2
2	C	507	ARG	2.2
2	C	253	ALA	2.2
2	C	508	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1436	SER	2.2
2	C	222	MET	2.2
2	C	300	ASP	2.2
3	D	321	GLN	2.2
3	D	1311	LEU	2.1
2	C	414	GLY	2.1
3	D	203	ALA	2.1
1	A	100	LEU	2.1
2	C	298	PHE	2.1
2	C	451	LEU	2.1
2	C	616	GLU	2.1
5	F	144	ILE	2.1
2	C	511	GLU	2.1
3	D	339	TRP	2.1
3	D	236	TYR	2.1
2	C	615	TYR	2.0
5	F	159	ILE	2.0
3	D	1499	ARG	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 monosaccharides 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
10	POP	C	1201	9/9	0.91	0.15	78,95,107,114	0
9	MG	D	2001	1/1	0.92	0.25	48,48,48,48	0
9	MG	B	1001	1/1	0.93	0.37	78,78,78,78	0
11	ZN	D	2002	1/1	0.97	0.12	113,113,113,113	0
11	ZN	D	2003	1/1	0.99	0.28	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.