



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 03:45 PM BST

PDB ID : 6N60  
Title : Escherichia coli RNA polymerase sigma70-holoenzyme bound to upstream fork promoter DNA and Microcin J25 (MccJ25)  
Authors : Braffman, N.; Hauver, J.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2018-11-23  
Resolution : 3.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

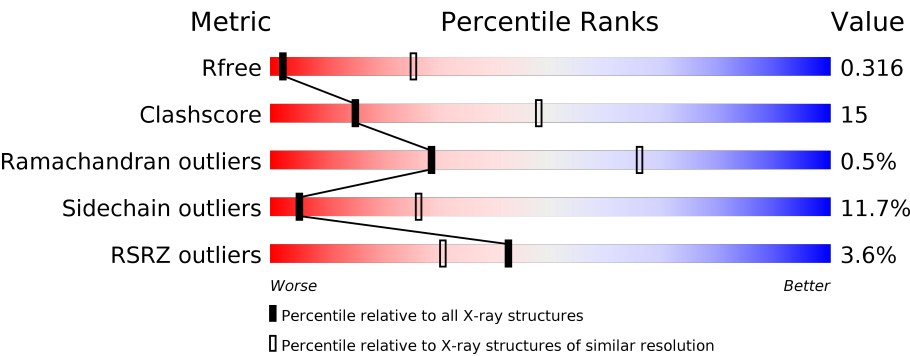
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.68 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	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RSRZ outliers	127900	1471 (3.86-3.50)

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  $\geq 3$ , 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	239	<div><div>10%</div><div><div></div><div>67%</div><div>28%</div><div>• •</div></div></div>
1	B	239	<div><div>2%</div><div><div></div><div>51%</div><div>35%</div><div>5%</div><div>9%</div></div></div>
2	C	1342	<div><div>2%</div><div><div></div><div>61%</div><div>33%</div><div>5%</div><div>•</div></div></div>
3	D	1409	<div><div>3%</div><div><div></div><div>54%</div><div>29%</div><div>5%</div><div>12%</div></div></div>
4	E	91	<div><div>8%</div><div><div></div><div>53%</div><div>29%</div><div>5%</div><div>13%</div></div></div>
5	F	612	<div><div>2%</div><div><div></div><div>35%</div><div>14%</div><div>•</div><div>48%</div></div></div>

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Mol	Chain	Length	Quality of chain
6	M	21	<div><div></div><div>10%</div><div>29%</div><div>57%</div><div>10%</div><div>5%</div></div>
7	N	29	<div><div></div><div>52%</div><div>48%</div></div>
8	T	24	<div><div></div><div>54%</div><div>42%</div><div></div></div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 27705 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	231	Total	C	N	O	S	0	0	0
			1759	1094	312	347	6			
1	B	218	Total	C	N	O	S	0	0	0
			1638	1023	284	325	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z4
A	236	VAL	-	expression tag	UNP P0A7Z4
A	237	LEU	-	expression tag	UNP P0A7Z4
A	238	PHE	-	expression tag	UNP P0A7Z4
A	239	GLN	-	expression tag	UNP P0A7Z4
B	235	GLU	-	expression tag	UNP P0A7Z4
B	236	VAL	-	expression tag	UNP P0A7Z4
B	237	LEU	-	expression tag	UNP P0A7Z4
B	238	PHE	-	expression tag	UNP P0A7Z4
B	239	GLN	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10470	6569	1822	2036	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1236	Total	C	N	O	S	0	0	0
			9578	6015	1711	1806	46			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP P0A8T7
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	318	Total	C	N	O	S	0	0	0
			2399	1499	442	446	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	conflict	UNP Q0P6L9
F	?	-	LEU	deletion	UNP Q0P6L9

- Molecule 6 is a protein called Microcin J25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	21	Total	C	N	O	0	0	0
			144	95	23	26			

- Molecule 7 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	29	Total	C	N	O	P	0	0	0
			595	284	106	176	29			

- Molecule 8 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	T	24	Total	C	N	O	P	0	0	0
			492	233	94	141	24			

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

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

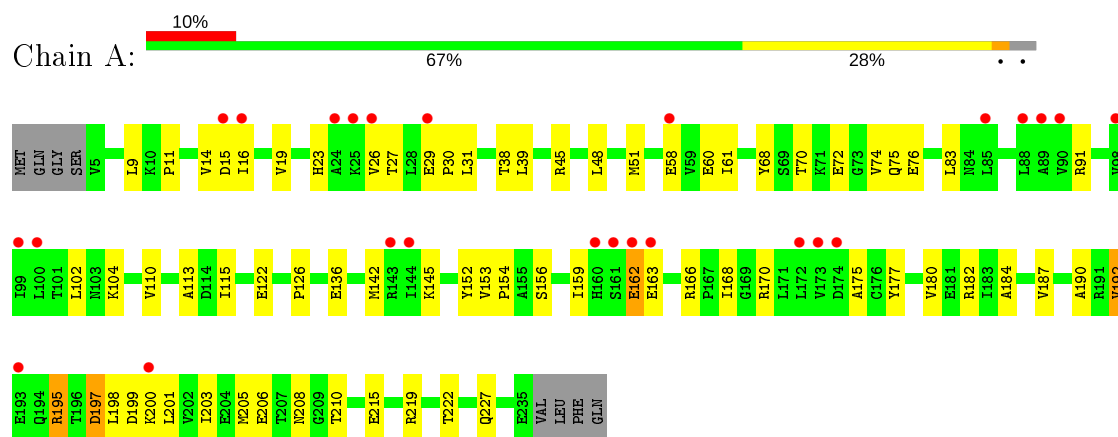
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

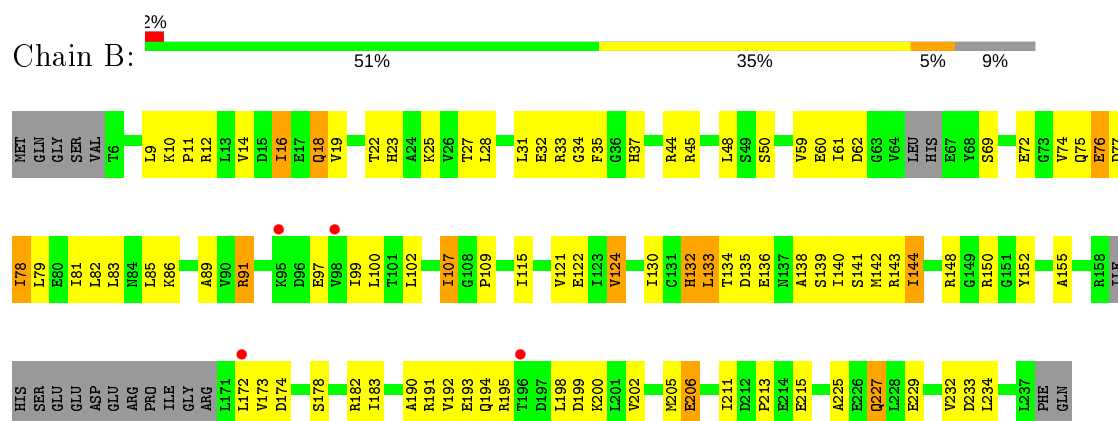
### 3 Residue-property plots [i](#)

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

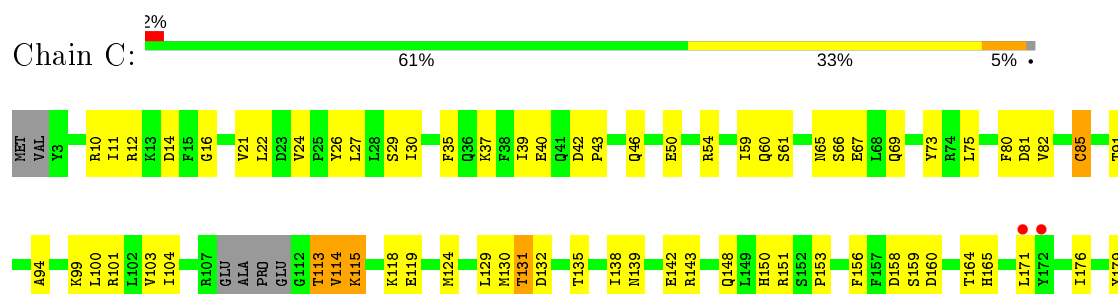
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

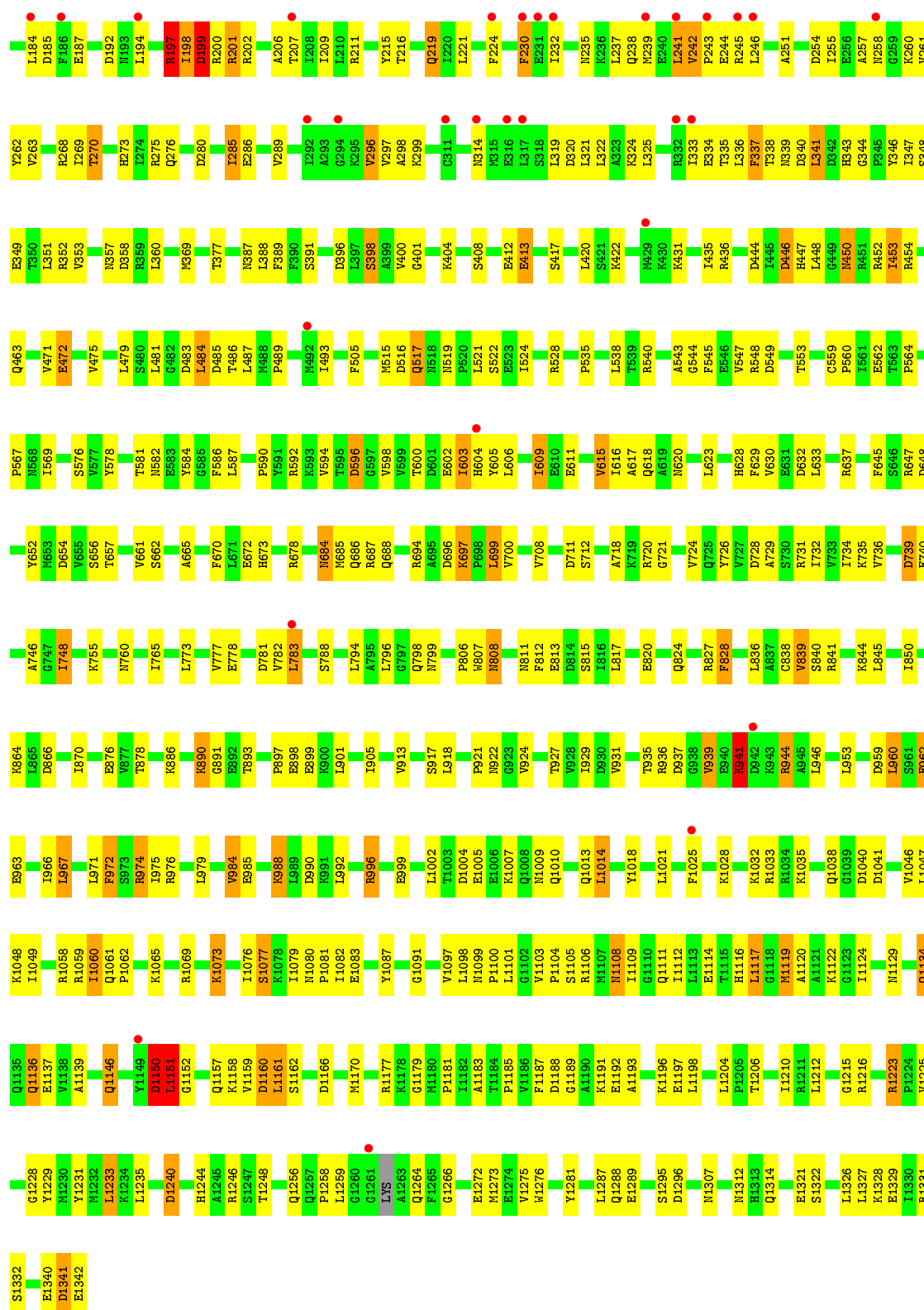


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



#### • Molecule 2: DNA-directed RNA polymerase subunit beta





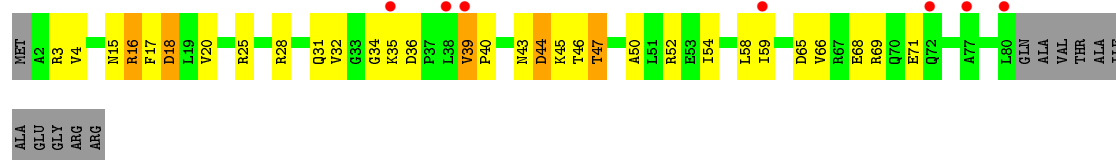
● Molecule 3: DNA-directed RNA polymerase subunit beta'



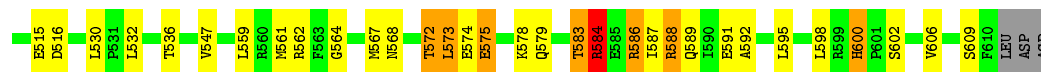
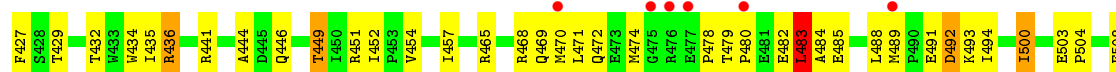
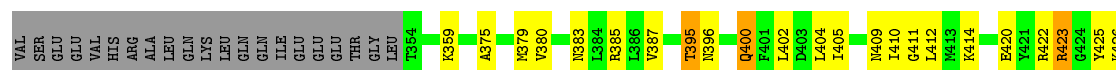
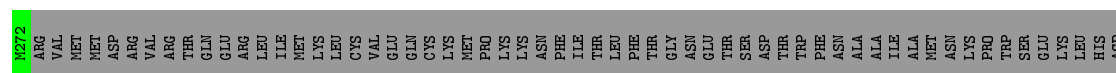
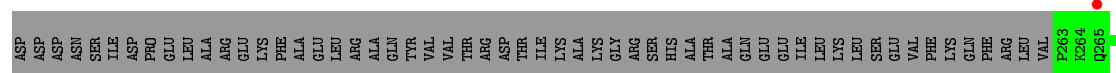
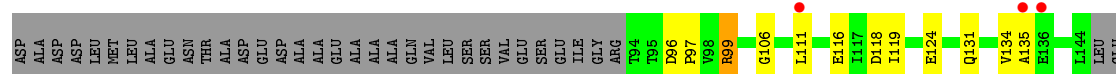
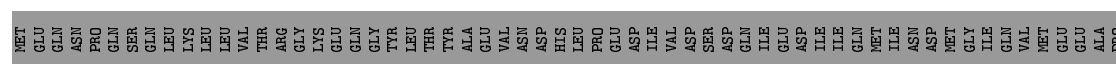
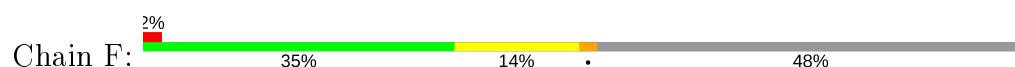


L1261	K1192	SER	SER	I975	C888	F773	V682	A577	A482	Y360	L265	E183	R98	VAL
L1262	W1193	GLY	SER	R978	D889	I774	W685	M881	W487	L361	N266	D193	R99	LYS
K1263	R1194	ASP	LEU	R979	G893	R780	W686	M882	M488	R362	D267	L194	E100	ASP
L1264	L1195	THR	VAL	R980	G894	R781	W687	K585	M489	L363	L268	E197	R101	LEU
T1265	L1196	LEU	VAL	E981	C895	L783	M690	K586	L490	R364	Y269	E198	E106	LEU
M1266	N1197	ALA	LEU	L982	A896	T786	M697	N893	L491	C367	R270	C198	P110	ARG
A1269	F1198	ILE	ASP	K983	Y899	T787	M698	Q894	M495	G367	N274	E199	P111	PHE
G1270	E1200	PRO	ALA	L984	G900	S793	M699	A895	W496	L368	R278	Q200	H113	LEU
S1271	E1201	GLN	GLU	E987	R901	S794	N700	G597	E497	A373	R279	L201	H114	GLN
R1203	E1202	GLU	ARG	E988	D902	T797	L701	K598	P498	E373	L282	R202	W115	THR
V1204	R1203	THR	THR	E993	L903	R798	Q702	K599	L499	P379	L283	E203	F116	THR
E1205	E1204	ALA	ALA	E994	L904	R799	T703	A600	L500	P379	D284	E204	L117	LYS
E1275	F1274	GLY	GLY	R905	A904	E704	E704	A601	Y382	Y382	D285	L205	K118	THR
G1277	E1276	GLY	GLY	R906	G906	D802	S602	S602	D504	T208	D289	L206	S119	GLU
E1278	E1277	LYS	LYS	H907	H907	D803	K603	K603	D505	N209	L290	S210	F117	LEU
Q1279	Q1279	ASP	ASP	I908	H908	Q805	N708	N708	W506	L120	L291	R211	D18	ASP
V1280	V1280	ARG	ARG	I909	D906	R806	R709	C608	V507	U401	V292	E211	S122	ARG
E1281	D1211	PRO	PRO	N910	N910	L807	Q712	G609	Y507	L412	E295	T212	R123	LYS
Y1282	D1212	ALA	ALA	G911	G911	R808	Q713	R609	L510	L413	E296	K213	I124	LYS
S1283	R1140	LEU	LEU	E912	E912	W809	Q716	L611	W514	D413	K296	R214	P121	LEU
R1284	A1216	LYS	LYS	E913	E913	T810	Q717	G613	T514	E414	L297	K215	S123	LEU
V1285	P1217	ILE	ILE	A914	A914	E811	F719	L614	C517	V415	L298	L216	R133	THR
K1286	H1248	VAL	VAL	W019	W019	D812	N720	K615	V518	R417	E301	L217	E136	ASP
D1249	D1249	ASP	ASP	V917	V917	D813	S721	P616	L527	E418	E302	T218	K40	LEU
E1250	F1145	ASP	ASP	Q921	Q921	C814	I722	T617	L422	R417	E303	T219	P41	LEU
E1251	E1147	GLN	GLN	E925	E925	G815	I723	T617	L423	E418	E304	R220	E42	LEU
E1252	R1148	ASN	ASN	P926	P926	T816	R731	F620	P630	L424	R312	K221	Y140	LEU
E1253	I1155	ASP	ASP	T931	T931	H817	G732	G632	K531	R425	R313	L223	F141	LEU
E1254	E1158	VAL	VAL	R931	R931	E818	S733	A633	E532	A426	T316	L224	E142	LEU
E1255	I1159	ILE	ILE	F935	F935	R842	A734	I641	E533	P427	T317	L225	S143	LEU
E1256	G1161	GLY	GLY	H936	H936	A845	Q736	I642	E534	H430	N320	V228	V144	LEU
E1257	I1162	THR	THR	I937	I937	E846	I737	V645	E535	R431	R321	Q229	V145	LEU
E1258	V1163	ASP	ASP	GLY	GLY	D847	R738	P647	L536	L432	R322	Q230	V146	LEU
E1259	S1164	MET	MET	ALA	ALA	V848	Q739	E648	S539	L433	P323	K232	I147	LEU
E1260	F1165	PRO	PRO	ALA	ALA	L849	L740	E649	H545	E439	R324	K233	L154	LEU
E1261	K1166	ARG	ARG	ALA	ALA	K850	A741	K650	H546	L442	K325	E235	E155	LEU
E1262	K1167	ALA	ALA	ALA	ALA	R854	G742	H651	V550	Q448	R330	W236	Q158	LEU
E1263	E1168	GLN	GLN	SER	SER	A854	N743	H652	V551	Q449	R331	W237	I159	LEU
E1264	K1169	THR	THR	ARG	ARG	R744	R744	A657	R551	Q449	R332	W238	I160	LEU
E1265	T1170	THR	THR	ALA	ALA	G745	L746	E658	T553	A459	R333	W239	T161	LEU
E1266	K1170	LEU	LEU	ALA	ALA	L746	M747	E659	T554	D462	R334	W240	E162	LEU
E1267	G1171	ASP	ASP	ALA	ALA	M747	I754	V661	T555	D463	R335	W241	E163	LEU
E1268	K1172	PRO	PRO	GLY	GLY	R754	I754	A662	V556	Q464	R336	W242	Q164	LEU
E1269	R1173	GLY	GLY	S948	S948	H865	P758	E663	A559	D465	R337	W243	Y165	LEU
E1270	E1174	LYS	LYS	T950	T950	E866	I759	I664	N560	Q466	R338	W244	L166	LEU
E1271	K1175	ALA	ALA	Q951	Q951	Q867	I760	E666	L563	V468	R339	W245	D167	LEU
E1272	T1176	ILE	ILE	R958	R958	N875	T760	E667	L564	V469	R340	W246	L168	LEU
E1273	P1178	VAL	VAL	K959	K959	A761	A761	A675	T567	T473	R341	W247	D174	LEU
E1274	D1181	GLN	GLN	L960	L960	N762	N762	G676	S568	L474	R342	W248	I84	LEU
E1275	D1182	LEU	LEU	L961	L961	R763	R763	E677	L569	P475	R343	W249	F176	LEU
E1276	D1183	ASP	ASP	V963	V963	R764	R764	R678	K570	A476	R344	W250	D177	LEU
E1277	F1185	GLY	GLY	K972	K972	V885	L770	E679	L571	A477	R345	W251	A178	LEU
E1278	Y1186	VAL	VAL	E972	E972	V886	Q771	N680	L478	L478	R346	W252	K180	LEU
E1279	P1191	ILE	ILE	SER	SER	S887	Y772	K681	H576	H576	R347	W253	E179	LEU

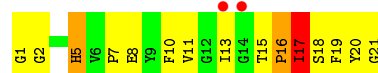
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 6: Microcin J25

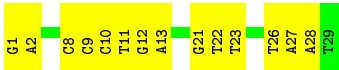


- Molecule 7: non-template strand DNA

Chain N: 

52%

48%



● Molecule 8: template strand DNA

Chain T: 

54%

42%

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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.91Å 172.91Å 387.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.68 49.55 – 3.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.55-3.68) 98.3 (49.55-3.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.263 , 0.306 0.274 , 0.316	Depositor DCC
$R_{free}$ test set	1945 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	175.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 119.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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, MG

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	0.25	0/1780	0.47	0/2415
1	B	0.25	0/1655	0.50	0/2247
2	C	0.26	0/10634	0.47	1/14353 (0.0%)
3	D	0.25	0/9724	0.47	1/13134 (0.0%)
4	E	0.23	0/629	0.40	0/847
5	F	0.25	0/2428	0.50	2/3280 (0.1%)
6	M	0.36	0/149	0.76	0/202
7	N	0.65	1/666 (0.2%)	0.96	1/1026 (0.1%)
8	T	0.64	1/552 (0.2%)	0.86	0/849
All	All	0.28	2/28217 (0.0%)	0.51	5/38353 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	5
3	D	0	3
5	F	0	1
6	M	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	12	DG	C1'-N9	-6.56	1.38	1.47
8	T	13	DC	C1'-N1	5.59	1.56	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	483	LEU	CA-CB-CG	6.04	129.20	115.30
5	F	583	THR	C-N-CA	5.44	135.30	121.70
3	D	224	LEU	CA-CB-CG	5.40	127.72	115.30
2	C	517	GLN	N-CA-C	5.20	125.04	111.00
7	N	11	DT	N3-C4-O4	5.11	122.96	119.90

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	VAL	Peptide
2	C	1150	ASP	Peptide
2	C	197	ARG	Peptide
2	C	198	ILE	Peptide
2	C	939	VAL	Peptide
2	C	941	LYS	Peptide
3	D	1166	GLY	Peptide
3	D	1168	GLU	Peptide
3	D	935	PHE	Peptide
5	F	584	ARG	Mainchain
6	M	16	PRO	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	1759	0	1759	46	0
1	B	1638	0	1629	71	0
2	C	10470	0	10445	333	0
3	D	9578	0	9710	335	0
4	E	627	0	634	21	0
5	F	2399	0	2324	69	0
6	M	144	0	131	15	0
7	N	595	0	329	14	0
8	T	492	0	269	9	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	27705	0	27230	822	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 15.

All (822) 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)
3:D:1006:GLY:N	3:D:1009:GLU:OE2	1.92	1.01
5:F:414:LYS:HB2	5:F:434:TRP:HE1	1.30	0.94
3:D:208:THR:O	3:D:214:ARG:NH1	2.01	0.92
5:F:600:HIS:HE2	5:F:602:SER:HG	1.04	0.92
1:B:76:GLU:OE2	1:B:132:HIS:ND1	2.05	0.88
2:C:99:LYS:NZ	2:C:119:GLU:OE2	2.09	0.84
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.59	0.84
2:C:1192:GLU:OE1	3:D:764:ARG:NH1	2.11	0.83
2:C:1105:SER:HA	3:D:736:GLN:HE22	1.43	0.83
3:D:816:THR:HB	3:D:889:ASP:HB2	1.59	0.83
4:E:15:ASN:ND2	4:E:18:ASP:OD1	2.10	0.83
3:D:1263:LYS:HE3	3:D:1315:ALA:HB1	1.63	0.80
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.80
3:D:1158:GLU:OE2	3:D:1222:ARG:NH1	2.15	0.80
3:D:960:LEU:HB3	3:D:963:VAL:HG11	1.65	0.78
3:D:842:ARG:HH22	3:D:1250:ASP:HB2	1.49	0.77
5:F:474:MET:HG3	5:F:478:PRO:HB3	1.67	0.77
2:C:516:ASP:OD1	2:C:522:SER:OG	2.03	0.77
2:C:337:PHE:HD1	2:C:338:THR:H	1.32	0.77
7:N:13:DA:H61	8:T:12:DT:H3	1.29	0.77
3:D:1275:LEU:HB3	3:D:1278:GLU:HB2	1.65	0.77
2:C:941:LYS:HG3	2:C:946:LEU:HG	1.67	0.76
3:D:42:GLU:OE2	5:F:451:ARG:NE	2.18	0.75
5:F:584:ARG:H	5:F:587:ILE:HD13	1.50	0.75
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.19	0.74
2:C:700:VAL:O	2:C:1069:ARG:NH2	2.20	0.74
5:F:572:THR:HG23	5:F:575:GLU:HB2	1.68	0.73
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.34	0.73
2:C:1005:GLU:HG2	2:C:1007:LYS:H	1.54	0.72
2:C:452:ARG:NH1	2:C:584:TYR:O	2.21	0.72
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.70	0.72
1:A:197:ASP:N	1:A:197:ASP:OD1	2.23	0.72
2:C:1146:GLN:NE2	2:C:1150:ASP:OD1	2.23	0.72
2:C:199:ASP:O	2:C:201:ARG:N	2.22	0.71
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.73	0.71
1:B:9:LEU:HA	1:B:10:LYS:HB3	1.72	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.24	0.71
1:A:159:ILE:HG13	1:A:162:GLU:HB2	1.73	0.70
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.24	0.70
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.73	0.70
2:C:242:VAL:HG13	2:C:244:GLU:H	1.54	0.70
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.72	0.70
2:C:905:ILE:HG12	5:F:595:LEU:HD22	1.74	0.69
2:C:528:ARG:NH2	2:C:576:SER:O	2.25	0.69
2:C:1246:ARG:HD2	2:C:1266:GLY:H	1.58	0.69
2:C:924:VAL:HG12	2:C:1058:ARG:HH22	1.57	0.68
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.75	0.68
2:C:976:ARG:NH1	2:C:990:ASP:OD1	2.26	0.68
3:D:478:LEU:HG	4:E:47:THR:HG22	1.75	0.68
2:C:26:TYR:O	2:C:29:SER:OG	2.11	0.68
1:B:75:GLN:HG2	1:B:132:HIS:HE1	1.57	0.68
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.74	0.68
3:D:746:LEU:HD13	3:D:754:ILE:HD11	1.74	0.67
2:C:100:LEU:HD12	2:C:489:PRO:HB3	1.74	0.67
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.27	0.67
1:B:182:ARG:NH1	3:D:581:MET:SD	2.67	0.67
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.77	0.67
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.75	0.67
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.75	0.67
3:D:576:ARG:NH1	3:D:593:ASN:O	2.27	0.67
2:C:962:GLU:O	2:C:966:ILE:HG12	1.95	0.67
4:E:40:PRO:O	4:E:52:ARG:NH2	2.28	0.67
1:B:109:PRO:HA	1:B:132:HIS:HA	1.76	0.67
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.75	0.67
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.59	0.67
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.28	0.67
2:C:1073:LYS:HG2	3:D:462:ASP:HB2	1.75	0.66
3:D:205:LEU:O	3:D:214:ARG:NH2	2.28	0.66
5:F:414:LYS:HB2	5:F:434:TRP:NE1	2.09	0.66
2:C:42:ASP:OD2	2:C:46:GLN:HB3	1.95	0.66
3:D:1161:GLY:HA3	3:D:1178:THR:O	1.96	0.66
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	1.77	0.66
3:D:223:LEU:O	3:D:227:PHE:HB2	1.96	0.66
5:F:441:ARG:NH2	7:N:21:DG:OP2	2.29	0.66
2:C:239:MET:HB3	2:C:285:ILE:HD12	1.77	0.66
2:C:808:ASN:H	3:D:633:ALA:HB2	1.61	0.66
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1144:LEU:HD11	3:D:1236:GLU:HB3	1.77	0.65
3:D:850:LYS:HD3	3:D:854:ALA:HB3	1.78	0.65
1:A:45:ARG:NH1	1:B:34:GLY:O	2.30	0.65
2:C:812:PHE:O	3:D:504:GLN:NE2	2.29	0.65
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.78	0.65
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.61	0.65
3:D:736:GLN:HG3	6:M:1:GLY:HA3	1.77	0.65
6:M:8:GLU:N	6:M:18:SER:O	2.21	0.65
2:C:864:LYS:NZ	2:C:876:GLU:O	2.26	0.65
3:D:613:GLY:O	3:D:617:THR:OG1	2.13	0.64
3:D:362:ARG:H	3:D:365:GLN:HE21	1.43	0.64
3:D:612:LEU:HB3	3:D:616:PRO:HG3	1.79	0.64
5:F:561:MET:HA	5:F:567:MET:HE1	1.79	0.64
2:C:739:ASP:OD1	2:C:739:ASP:N	2.26	0.64
3:D:818:GLU:HB3	3:D:887:SER:HB2	1.80	0.64
3:D:1284:ARG:NH1	3:D:1317:GLU:OE2	2.31	0.64
3:D:1357:ILE:HG22	3:D:1359:ALA:H	1.63	0.64
3:D:220:ARG:O	3:D:224:LEU:HG	1.98	0.64
3:D:664:ILE:HD12	3:D:682:VAL:HG22	1.80	0.64
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.79	0.64
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.31	0.63
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.80	0.63
3:D:1230:THR:HB	3:D:1257:VAL:HG11	1.80	0.63
3:D:200:GLN:O	3:D:204:GLU:HG2	1.98	0.63
2:C:268:ARG:HH22	2:C:270:THR:HG23	1.64	0.63
3:D:1286:LYS:O	3:D:1290:ARG:HB2	1.98	0.63
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.26	0.63
3:D:210:SER:O	3:D:213:LYS:N	2.31	0.62
1:B:195:ARG:HB3	1:B:198:LEU:CD2	2.30	0.62
2:C:959:ASP:O	2:C:963:GLU:HG2	1.98	0.62
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.63	0.62
3:D:54:ASP:N	3:D:54:ASP:OD1	2.32	0.62
2:C:27:LEU:O	2:C:528:ARG:NH1	2.32	0.62
2:C:598:VAL:HG22	2:C:628:HIS:HE1	1.64	0.62
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.80	0.62
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.79	0.62
3:D:846:GLU:HG2	3:D:881:LYS:HB3	1.80	0.62
3:D:1232:TYR:HD1	3:D:1233:ILE:HD12	1.62	0.62
5:F:483:LEU:H	5:F:483:LEU:HD13	1.64	0.62
2:C:517:GLN:HG2	2:C:517:GLN:O	2.00	0.62
3:D:418:GLU:HG3	4:E:45:LYS:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:50:ALA:O	4:E:54:ILE:HG12	1.99	0.61
2:C:516:ASP:O	2:C:522:SER:OG	2.19	0.61
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.83	0.61
3:D:19:ALA:HB2	3:D:1343:GLU:HG3	1.81	0.61
5:F:449:THR:OG1	5:F:503:GLU:OE2	2.16	0.61
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.81	0.61
5:F:426:LYS:HD3	7:N:27:DA:H3'	1.82	0.61
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.82	0.61
1:A:75:GLN:HG3	1:A:76:GLU:OE2	2.01	0.61
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.34	0.61
3:D:678:ARG:O	3:D:682:VAL:HG23	2.01	0.61
2:C:113:THR:O	2:C:115:LYS:N	2.34	0.60
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.83	0.60
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.82	0.60
2:C:936:ARG:HH21	2:C:939:VAL:HG21	1.66	0.60
3:D:1155:ILE:HD11	3:D:1211:SER:HB3	1.83	0.60
3:D:893:GLY:O	3:D:1258:ARG:NH1	2.31	0.60
4:E:25:ARG:NH1	4:E:65:ASP:OD1	2.34	0.60
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.33	0.60
2:C:104:ILE:O	2:C:115:LYS:HA	2.01	0.60
3:D:741:ALA:O	3:D:762:ASN:ND2	2.34	0.60
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.83	0.60
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.84	0.60
3:D:1323:ALA:HB1	3:D:1328:THR:HG23	1.82	0.60
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.81	0.60
3:D:739:GLN:HG3	6:M:10:PHE:HE2	1.67	0.60
8:T:13:DC:H2"	8:T:14:DA:C8	2.36	0.60
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.83	0.60
3:D:1005:LYS:HD2	3:D:1009:GLU:HG3	1.82	0.60
2:C:199:ASP:C	2:C:201:ARG:H	2.05	0.59
2:C:941:LYS:HD3	2:C:941:LYS:H	1.67	0.59
3:D:264:ASP:N	3:D:264:ASP:OD1	2.34	0.59
2:C:1009:ASN:O	2:C:1013:GLN:HG2	2.02	0.59
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.84	0.59
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.84	0.59
2:C:67:GLU:HB3	2:C:103:VAL:HG22	1.83	0.59
3:D:1162:ILE:O	3:D:1178:THR:OG1	2.18	0.59
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.82	0.59
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.84	0.59
2:C:971:LEU:HD22	2:C:1018:TYR:HD2	1.67	0.58
3:D:1363:TYR:O	3:D:1367:GLN:N	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:337:PHE:HD1	2:C:338:THR:N	2.01	0.58
2:C:578:TYR:HE2	2:C:656:SER:HB3	1.68	0.58
3:D:317:THR:OG1	3:D:320:ASN:O	2.22	0.58
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.84	0.58
1:B:195:ARG:HB3	1:B:198:LEU:HD21	1.85	0.58
3:D:809:VAL:HB	3:D:912:GLY:H	1.69	0.58
2:C:138:ILE:HG22	2:C:139:ASN:HD22	1.67	0.58
2:C:211:ARG:NH1	2:C:357:ASN:O	2.37	0.58
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.85	0.58
2:C:185:ASP:HB2	2:C:197:ARG:HG3	1.86	0.58
1:B:191:ARG:NH2	3:D:413:ASP:OD2	2.37	0.58
2:C:431:LYS:O	2:C:435:ILE:HG12	2.03	0.58
3:D:709:ARG:O	3:D:709:ARG:NE	2.37	0.58
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.87	0.57
5:F:106:GLY:HA2	5:F:385:ARG:HH12	1.69	0.57
8:T:20:DA:H1'	8:T:21:DG:H5'	1.86	0.57
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.85	0.57
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.39	0.57
2:C:840:SER:HB3	2:C:1048:LYS:HG2	1.85	0.57
2:C:1119:MET:HG3	2:C:1204:LEU:HD13	1.86	0.57
3:D:278:ARG:HD2	3:D:295:GLU:OE2	2.04	0.57
3:D:490:ILE:HG22	3:D:500:ILE:HG13	1.85	0.57
2:C:685:MET:HA	2:C:688:GLN:HE21	1.70	0.57
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.87	0.57
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.87	0.57
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.85	0.57
3:D:813:ASP:OD1	3:D:814:CYS:N	2.38	0.57
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.87	0.57
3:D:657:ALA:O	3:D:661:VAL:HG13	2.04	0.57
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.86	0.56
3:D:432:LEU:HD21	3:D:489:ASN:HB3	1.86	0.56
6:M:5:HIS:O	6:M:5:HIS:ND1	2.37	0.56
1:B:77:ASP:O	1:B:81:ILE:HG12	2.05	0.56
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.86	0.56
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.41	0.56
3:D:317:THR:OG1	3:D:322:ARG:O	2.18	0.56
3:D:57:PHE:HD2	3:D:98:ARG:HH22	1.52	0.56
2:C:299:LYS:HE3	2:C:334:GLU:HG3	1.88	0.56
3:D:161:THR:HG22	3:D:164:GLN:HG3	1.85	0.56
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.53	0.56
1:B:190:ALA:N	1:B:198:LEU:O	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	1.87	0.56
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.71	0.56
3:D:917:VAL:HG12	3:D:921:GLN:HE21	1.70	0.56
7:N:22:DT:H2"	7:N:23:DT:H5"	1.87	0.56
1:A:72:GLU:OE2	2:C:726:TYR:OH	2.23	0.56
1:B:18:GLN:HE21	1:B:18:GLN:HA	1.70	0.56
2:C:238:GLN:HG2	2:C:286:GLU:HG2	1.88	0.56
2:C:224:PHE:CD2	2:C:347:ILE:HG13	2.41	0.56
3:D:127:LEU:HD11	3:D:194:LEU:HD21	1.87	0.56
8:T:9:DC:H1'	8:T:10:DC:H5'	1.87	0.56
1:B:155:ALA:HB1	1:B:172:LEU:HB3	1.88	0.56
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.32	0.56
5:F:588:ARG:O	5:F:588:ARG:NE	2.37	0.56
6:M:7:PRO:HA	6:M:19:PHE:H	1.69	0.56
3:D:1173:ARG:HB2	3:D:1192:LYS:HB3	1.88	0.56
3:D:905:ARG:H	3:D:905:ARG:HD2	1.71	0.56
5:F:588:ARG:HH21	5:F:592:ALA:HB2	1.71	0.56
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.88	0.55
5:F:482:GLU:O	5:F:485:GLU:HG3	2.06	0.55
2:C:1272:GLU:OE2	3:D:798:ARG:NH2	2.38	0.55
2:C:142:GLU:OE2	2:C:515:MET:SD	2.64	0.55
3:D:1265:THR:N	3:D:1305:ASP:OD2	2.38	0.55
3:D:232:ASN:N	3:D:232:ASN:HD22	2.05	0.55
3:D:491:LEU:HD11	3:D:610:ARG:HH12	1.70	0.55
3:D:972:LYS:HD3	3:D:1004:ALA:HA	1.88	0.55
8:T:19:DA:H2"	8:T:20:DA:H5'	1.88	0.55
3:D:394:ILE:HG23	5:F:536:THR:HG22	1.89	0.55
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.07	0.55
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.89	0.55
3:D:810:THR:O	3:D:1363:TYR:OH	2.24	0.55
2:C:1069:ARG:HG2	2:C:1233:LEU:HD21	1.87	0.55
5:F:379:MET:O	5:F:383:ASN:ND2	2.39	0.55
3:D:786:THR:HG23	6:M:7:PRO:HD3	1.88	0.55
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.07	0.55
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.87	0.55
2:C:960:LEU:HB3	2:C:1025:PHE:HE2	1.72	0.55
2:C:1160:ASP:OD1	2:C:1162:SER:N	2.40	0.55
2:C:1062:PRO:HA	2:C:1076:ILE:HG22	1.89	0.54
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.89	0.54
3:D:268:LEU:HD21	3:D:324:LEU:HD13	1.89	0.54
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:562:GLU:OE2	2:C:662:SER:OG	2.15	0.54
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.88	0.54
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.88	0.54
5:F:606:VAL:O	5:F:609:SER:OG	2.20	0.54
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.06	0.54
2:C:890:LYS:NZ	2:C:891:GLY:O	2.41	0.54
2:C:898:GLU:OE1	2:C:898:GLU:N	2.40	0.54
2:C:731:ARG:NH2	2:C:962:GLU:OE2	2.40	0.54
3:D:147:ILE:HG13	3:D:177:ASP:HB3	1.89	0.54
2:C:1258:PRO:HD2	3:D:346:ARG:HB2	1.89	0.54
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.89	0.54
6:M:7:PRO:HA	6:M:19:PHE:N	2.22	0.54
1:B:192:VAL:HB	1:B:195:ARG:HG2	1.90	0.54
2:C:158:ASP:OD1	2:C:159:SER:N	2.40	0.54
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.90	0.54
3:D:214:ARG:O	3:D:218:THR:HG22	2.08	0.54
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.90	0.54
1:B:60:GLU:O	1:B:142:MET:HB2	2.08	0.54
2:C:1060:ILE:HD11	2:C:1076:ILE:HG12	1.90	0.54
2:C:1105:SER:HA	3:D:736:GLN:NE2	2.19	0.54
2:C:748:ILE:HD11	2:C:966:ILE:HG22	1.89	0.54
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.43	0.54
3:D:739:GLN:HG3	6:M:10:PHE:CE2	2.42	0.54
2:C:40:GLU:O	2:C:73:TYR:OH	2.25	0.53
2:C:721:GLY:N	2:C:740:GLU:OE1	2.41	0.53
3:D:1328:THR:HG22	3:D:1332:LEU:HD23	1.89	0.53
3:D:141:PHE:HD1	3:D:180:MET:HE3	1.73	0.53
1:B:99:ILE:HA	1:B:144:ILE:O	2.09	0.53
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.74	0.53
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.91	0.53
2:C:268:ARG:NH2	2:C:270:THR:HG23	2.24	0.53
2:C:412:GLU:HB3	2:C:413:GLU:OE2	2.09	0.53
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.90	0.53
2:C:349:GLU:O	2:C:353:VAL:HG23	2.09	0.53
3:D:473:THR:HG23	3:D:476:ALA:H	1.72	0.53
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.90	0.53
3:D:555:TYR:HB3	3:D:563:LEU:HD21	1.90	0.53
3:D:648:GLU:OE1	3:D:648:GLU:N	2.42	0.53
2:C:489:PRO:O	2:C:493:ILE:HG22	2.08	0.53
3:D:50:LYS:HB3	3:D:71:LEU:HD11	1.91	0.53
5:F:530:LEU:H	5:F:530:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:1:DG:H2"	7:N:2:DA:C8	2.43	0.53
1:A:74:VAL:HG22	1:A:76:GLU:H	1.74	0.53
3:D:658:GLU:O	3:D:661:VAL:HG22	2.09	0.53
5:F:492:ASP:N	5:F:492:ASP:OD1	2.42	0.53
1:B:9:LEU:HA	1:B:10:LYS:CB	2.37	0.52
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.90	0.52
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.09	0.52
1:B:193:GLU:HG3	1:B:194:GLN:HG3	1.91	0.52
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.90	0.52
2:C:408:SER:O	2:C:431:LYS:NZ	2.42	0.52
3:D:559:ALA:O	3:D:560:ASN:ND2	2.42	0.52
3:D:700:ASN:O	3:D:704:GLU:HB2	2.09	0.52
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.90	0.52
6:M:8:GLU:HB2	6:M:18:SER:HB2	1.91	0.52
3:D:478:LEU:HB3	4:E:20:VAL:HG13	1.92	0.52
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.92	0.52
2:C:118:LYS:NZ	2:C:485:ASP:OD1	2.40	0.52
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.45	0.52
2:C:521:LEU:HB2	2:C:794:LEU:HD21	1.92	0.52
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.74	0.52
3:D:845:ALA:HB3	3:D:881:LYS:HG2	1.91	0.52
5:F:411:GLY:O	5:F:434:TRP:HD1	1.92	0.52
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.92	0.52
1:A:227:GLN:NE2	1:B:9:LEU:O	2.43	0.52
2:C:148:GLN:NE2	2:C:535:PRO:O	2.42	0.52
3:D:747:MET:N	3:D:747:MET:SD	2.83	0.52
3:D:793:SER:O	3:D:797:THR:HG23	2.10	0.52
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.91	0.52
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.91	0.52
3:D:744:ARG:HG3	3:D:759:ILE:HB	1.91	0.52
3:D:847:ASP:N	3:D:847:ASP:OD1	2.42	0.52
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.09	0.52
3:D:334:LYS:HA	3:D:339:ARG:HD2	1.92	0.52
1:B:16:ILE:HG23	1:B:25:LYS:O	2.09	0.52
5:F:583:THR:HG22	5:F:584:ARG:HB2	1.92	0.52
1:B:28:LEU:HG	1:B:31:LEU:HD21	1.92	0.51
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.92	0.51
3:D:495:ASN:HD22	3:D:497:GLU:HB2	1.74	0.51
3:D:812:ASP:O	3:D:896:ALA:N	2.42	0.51
3:D:93:THR:HG22	3:D:94:GLN:H	1.75	0.51
5:F:586:ARG:NH1	5:F:589:GLN:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.25	0.51
8:T:12:DT:H2"	8:T:13:DC:C6	2.45	0.51
1:B:152:TYR:HB2	3:D:535:ARG:HH21	1.75	0.51
1:B:81:ILE:O	1:B:85:LEU:HG	2.09	0.51
2:C:230:PHE:HD2	2:C:335:THR:HG21	1.76	0.51
3:D:1019:ASN:OD1	3:D:1020:TRP:N	2.44	0.51
5:F:562:ARG:HG2	5:F:591:GLU:OE2	2.10	0.51
2:C:27:LEU:HD12	2:C:711:ASP:HB2	1.92	0.51
2:C:728:ASP:OD1	2:C:729:ALA:N	2.44	0.51
1:A:58:GLU:HB2	1:A:145:LYS:HD2	1.91	0.51
2:C:263:VAL:HG22	2:C:273:HIS:CD2	2.45	0.51
3:D:356:THR:OG1	3:D:357:VAL:N	2.44	0.51
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.93	0.51
2:C:1105:SER:HB2	3:D:731:ARG:HG3	1.92	0.51
2:C:321:LEU:HD23	2:C:324:LYS:HD2	1.92	0.51
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.45	0.51
3:D:733:SER:O	3:D:737:ILE:HG12	2.11	0.51
1:B:102:LEU:O	1:B:141:SER:HA	2.11	0.51
2:C:322:LEU:HD23	2:C:325:LEU:HD21	1.91	0.51
1:A:14:VAL:HG22	1:A:15:ASP:H	1.75	0.51
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.93	0.51
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.44	0.51
3:D:123:ARG:HD2	3:D:1337:VAL:HG21	1.93	0.51
3:D:1325:PHE:CD2	3:D:1326:GLN:HG3	2.46	0.51
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.91	0.51
3:D:813:ASP:OD1	3:D:815:GLY:N	2.43	0.51
1:B:11:PRO:HG3	1:B:31:LEU:HD13	1.92	0.51
3:D:322:ARG:HG2	3:D:323:PRO:HD2	1.93	0.51
3:D:848:VAL:HG11	3:D:858:VAL:HG23	1.93	0.51
2:C:548:ARG:NH2	2:C:567:PRO:O	2.44	0.50
3:D:1173:ARG:CB	3:D:1192:LYS:HB3	2.41	0.50
3:D:42:GLU:OE1	3:D:42:GLU:N	2.44	0.50
5:F:584:ARG:N	5:F:587:ILE:HD13	2.24	0.50
2:C:12:ARG:O	2:C:1157:GLN:NE2	2.45	0.50
2:C:890:LYS:HG3	2:C:891:GLY:N	2.26	0.50
2:C:941:LYS:N	2:C:941:LYS:HD3	2.25	0.50
3:D:62:PHE:O	3:D:101:ARG:HD2	2.10	0.50
1:A:23:HIS:HB2	1:A:205:MET:O	2.12	0.50
1:B:44:ARG:HA	1:B:183:ILE:HD13	1.92	0.50
2:C:198:ILE:O	2:C:199:ASP:O	2.29	0.50
2:C:798:GLN:HE22	2:C:827:ARG:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:507:VAL:HG11	3:D:598:LYS:HB2	1.92	0.50
3:D:110:PRO:HD2	3:D:183:GLU:HG2	1.94	0.50
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.10	0.50
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.93	0.50
1:A:11:PRO:HD2	1:B:227:GLN:NE2	2.26	0.50
2:C:450:ASN:N	2:C:450:ASN:OD1	2.45	0.50
2:C:487:LEU:H	2:C:487:LEU:HD23	1.75	0.50
7:N:8:DC:H2"	7:N:9:DC:C6	2.47	0.50
2:C:543:ALA:O	2:C:548:ARG:NH1	2.44	0.50
5:F:489:MET:HB3	5:F:493:LYS:HG3	1.94	0.49
2:C:206:ALA:O	2:C:209:ILE:HG22	2.12	0.49
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.93	0.49
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.93	0.49
1:A:31:LEU:HD21	1:A:39:LEU:HD12	1.94	0.49
2:C:1101:LEU:HB3	3:D:731:ARG:HD3	1.95	0.49
2:C:255:ILE:HD12	2:C:263:VAL:HG23	1.94	0.49
2:C:257:ALA:HB3	2:C:262:TYR:HE1	1.77	0.49
3:D:45:ASN:HB3	3:D:48:THR:O	2.12	0.49
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.45	0.49
1:B:182:ARG:HD3	1:B:206:GLU:OE2	2.11	0.49
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.93	0.49
2:C:1340:GLU:HB2	3:D:19:ALA:O	2.13	0.49
3:D:909:ILE:HD11	3:D:913:GLU:HB3	1.94	0.49
3:D:291:ILE:HD13	5:F:409:ASN:HB3	1.94	0.49
2:C:996:ARG:HD2	2:C:999:GLU:OE2	2.13	0.49
5:F:452:ILE:HG13	5:F:457:ILE:HD11	1.95	0.49
1:B:225:ALA:O	1:B:229:GLU:N	2.46	0.49
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.93	0.49
2:C:684:ASN:OD1	2:C:687:ARG:NH1	2.46	0.49
3:D:362:ARG:N	3:D:365:GLN:HE21	2.11	0.49
2:C:603:ILE:HD13	2:C:603:ILE:H	1.77	0.49
3:D:1284:ARG:HH12	3:D:1317:GLU:HG3	1.77	0.49
3:D:1295:ASN:OD1	3:D:1296:GLY:N	2.46	0.49
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.94	0.49
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.27	0.49
2:C:251:ALA:H	2:C:268:ARG:HA	1.77	0.49
2:C:678:ARG:NH2	6:M:21:GLY:O	2.46	0.49
2:C:901:LEU:O	2:C:905:ILE:HG13	2.13	0.49
3:D:352:ARG:HE	3:D:465:GLN:NE2	2.10	0.49
3:D:978:ARG:CZ	3:D:999:TYR:HB3	2.42	0.49
6:M:11:VAL:HG11	6:M:17:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:632:ASP:N	2:C:632:ASP:OD1	2.39	0.48
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.13	0.48
1:B:60:GLU:N	1:B:143:ARG:O	2.46	0.48
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.46	0.48
3:D:805:GLN:HE22	3:D:1348:LYS:HD2	1.78	0.48
1:B:191:ARG:NH1	3:D:413:ASP:OD1	2.41	0.48
3:D:744:ARG:HG2	3:D:761:ALA:O	2.13	0.48
4:E:32:VAL:O	4:E:34:GLY:N	2.42	0.48
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.48	0.48
2:C:446:ASP:OD2	2:C:547:VAL:HA	2.14	0.48
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.49	0.48
3:D:364:HIS:ND1	3:D:364:HIS:O	2.47	0.48
1:B:19:VAL:HB	1:B:23:HIS:HB3	1.95	0.48
2:C:813:GLU:HA	3:D:504:GLN:NE2	2.28	0.48
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.78	0.48
2:C:1120:ALA:O	2:C:1124:ILE:HG12	2.14	0.48
2:C:16:GLY:HA3	2:C:1188:ASP:OD2	2.14	0.48
2:C:617:ALA:N	2:C:652:TYR:O	2.40	0.48
3:D:1191:PRO:HB2	3:D:1194:ARG:HD2	1.96	0.48
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.95	0.48
3:D:745:GLY:O	3:D:758:PRO:HB3	2.13	0.48
2:C:216:THR:OG1	2:C:219:GLN:OE1	2.29	0.48
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.48
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.48	0.48
2:C:1342:GLU:OXT	3:D:18:ASP:OD2	2.32	0.48
2:C:1259:LEU:HB2	3:D:346:ARG:HD2	1.95	0.48
5:F:600:HIS:CE1	5:F:602:SER:HG	2.26	0.48
2:C:1069:ARG:HD3	2:C:1231:TYR:HD2	1.79	0.48
2:C:341:LEU:H	2:C:341:LEU:HG	1.36	0.48
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.96	0.48
6:M:2:GLY:O	6:M:20:TYR:HA	2.14	0.47
2:C:606:LEU:HD23	2:C:611:GLU:HA	1.96	0.47
3:D:850:LYS:HE2	3:D:875:ASN:ND2	2.29	0.47
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.95	0.47
2:C:138:ILE:HD13	2:C:143:ARG:HD3	1.94	0.47
3:D:487:THR:HG21	4:E:4:VAL:HG23	1.96	0.47
7:N:27:DA:H2''	7:N:28:DA:H5'	1.96	0.47
1:A:27:THR:HA	1:A:201:LEU:O	2.15	0.47
1:B:152:TYR:HB2	3:D:535:ARG:NH2	2.29	0.47
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.15	0.47
2:C:1273:MET:HA	2:C:1276:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:802:ASP:OD2	3:D:1325:PHE:CD2	2.67	0.47
3:D:217:LEU:O	3:D:221:ILE:HG22	2.14	0.47
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.97	0.47
7:N:9:DC:H2"	7:N:10:DC:C6	2.48	0.47
1:B:182:ARG:HB3	1:B:206:GLU:HG3	1.96	0.47
2:C:12:ARG:HG2	2:C:1183:ALA:HB2	1.97	0.47
2:C:198:ILE:HD13	2:C:388:LEU:HD13	1.96	0.47
2:C:207:THR:HG21	2:C:351:LEU:HG	1.96	0.47
2:C:398:SER:O	2:C:401:GLY:N	2.48	0.47
2:C:746:ALA:HB2	2:C:974:ARG:NE	2.29	0.47
3:D:118:LYS:NZ	3:D:136:GLU:OE2	2.47	0.47
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.97	0.47
3:D:807:LEU:HD12	3:D:808:VAL:N	2.29	0.47
5:F:124:GLU:OE2	5:F:422:ARG:NH2	2.46	0.47
1:A:192:VAL:HB	1:A:198:LEU:HD12	1.95	0.47
1:B:136:GLU:C	1:B:138:ALA:H	2.17	0.47
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.96	0.47
2:C:199:ASP:C	2:C:201:ARG:N	2.68	0.47
3:D:1216:ALA:HB1	3:D:1218:HIS:CD2	2.50	0.47
1:A:222:THR:HA	1:B:232:VAL:HB	1.95	0.47
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.80	0.47
3:D:1215:GLU:HB2	3:D:1220:ILE:HD11	1.96	0.47
3:D:1216:ALA:O	3:D:1220:ILE:HG12	2.15	0.47
2:C:1032:LYS:HA	2:C:1035:LYS:HD3	1.97	0.47
2:C:521:LEU:HD23	2:C:708:VAL:HG11	1.96	0.47
3:D:1261:LEU:HD13	3:D:1304:ARG:CZ	2.45	0.47
3:D:551:ARG:HA	3:D:568:SER:O	2.14	0.47
5:F:429:THR:OG1	7:N:27:DA:H2'	2.14	0.47
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.96	0.47
2:C:357:ASN:ND2	2:C:358:ASP:OD1	2.48	0.47
2:C:817:LEU:HD21	2:C:1080:ASN:HD22	1.79	0.47
3:D:708:ASN:N	3:D:708:ASN:OD1	2.48	0.47
3:D:641:ILE:HD12	3:D:764:ARG:HH11	1.80	0.47
4:E:44:ASP:OD2	4:E:52:ARG:NH1	2.48	0.47
5:F:465:ARG:HG2	5:F:468:ARG:HH22	1.80	0.47
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.15	0.47
2:C:807:TRP:HB2	2:C:1097:VAL:HG11	1.97	0.47
2:C:841:ARG:CZ	3:D:256:ASP:HB3	2.44	0.47
3:D:198:CYS:O	3:D:202:ARG:HG3	2.15	0.47
3:D:360:TYR:OH	3:D:442:ILE:HD11	2.14	0.47
3:D:647:PRO:O	3:D:650:LYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:31:GLN:HB2	4:E:46:THR:HG21	1.96	0.47
5:F:96:ASP:OD2	5:F:99:ARG:HB2	2.15	0.47
3:D:144:TYR:CD2	3:D:180:MET:HB2	2.50	0.47
3:D:349:TYR:HE1	3:D:379:PRO:HG2	1.80	0.47
2:C:1065:LYS:HE3	3:D:463:GLY:HA3	1.95	0.47
3:D:53:ARG:HA	3:D:54:ASP:HA	1.50	0.47
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.48	0.46
2:C:582:ASN:HB3	2:C:586:PHE:H	1.80	0.46
3:D:127:LEU:HD21	3:D:234:PRO:HB3	1.97	0.46
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.96	0.46
2:C:936:ARG:HG2	2:C:937:ASP:H	1.79	0.46
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	1.97	0.46
3:D:857:LEU:HD22	3:D:875:ASN:ND2	2.30	0.46
5:F:573:LEU:HD23	5:F:574:GLU:H	1.80	0.46
6:M:18:SER:HA	6:M:19:PHE:CB	2.46	0.46
1:A:91:ARG:HB2	1:A:210:THR:HG23	1.97	0.46
1:B:34:GLY:N	1:B:199:ASP:OD2	2.48	0.46
3:D:1218:HIS:H	3:D:1218:HIS:CD2	2.32	0.46
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.97	0.46
3:D:246:PRO:HD2	3:D:249:LEU:HD12	1.98	0.46
3:D:301:GLU:OE2	5:F:97:PRO:HG3	2.15	0.46
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.97	0.46
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.97	0.46
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.98	0.46
1:B:192:VAL:HG12	1:B:193:GLU:H	1.81	0.46
3:D:1252:HIS:O	3:D:1255:VAL:HG12	2.15	0.46
3:D:735:ALA:O	3:D:739:GLN:HG2	2.15	0.46
2:C:1119:MET:HE3	2:C:1204:LEU:HD22	1.98	0.46
2:C:1256:GLN:HG2	2:C:1321:GLU:HG2	1.98	0.46
3:D:1179:PRO:HD3	3:D:1184:ASP:OD1	2.16	0.46
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.98	0.46
2:C:836:LEU:HD23	2:C:918:LEU:HD11	1.97	0.46
3:D:113:HIS:HB3	3:D:116:PHE:HD1	1.81	0.46
3:D:1271:SER:HB3	3:D:1298:VAL:O	2.15	0.46
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.48	0.46
2:C:59:ILE:HD12	2:C:472:GLU:HG2	1.98	0.46
2:C:609:ILE:H	2:C:609:ILE:HG13	1.31	0.46
3:D:1226:VAL:O	3:D:1230:THR:HG22	2.16	0.46
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.97	0.46
1:A:156:SER:H	2:C:1059:ARG:NH2	2.13	0.46
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:VAL:HG22	2:C:319:LEU:HG	1.97	0.46
2:C:348:SER:O	2:C:352:ARG:HG3	2.16	0.46
2:C:984:VAL:HG23	2:C:985:GLU:HG3	1.98	0.46
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	1.99	0.45
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.51	0.45
2:C:396:ASP:OD2	2:C:398:SER:HB3	2.16	0.45
2:C:517:GLN:OE1	2:C:760:ASN:N	2.44	0.45
2:C:781:ASP:OD1	2:C:782:VAL:N	2.49	0.45
2:C:815:SER:HB2	2:C:1077:SER:OG	2.15	0.45
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.75	0.45
3:D:662:ALA:O	3:D:666:GLU:HG3	2.16	0.45
1:B:50:SER:HA	1:B:150:ARG:O	2.16	0.45
2:C:629:PHE:HB2	2:C:647:ARG:HG3	1.98	0.45
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.98	0.45
4:E:44:ASP:OD1	4:E:44:ASP:N	2.50	0.45
2:C:796:LEU:H	2:C:796:LEU:HD12	1.80	0.45
2:C:941:LYS:HG3	2:C:946:LEU:CG	2.41	0.45
1:B:76:GLU:HB2	1:B:81:ILE:HD11	1.98	0.45
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.81	0.45
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.98	0.45
3:D:514:THR:HG21	3:D:596:LEU:HD23	1.98	0.45
5:F:359:LYS:HA	5:F:359:LYS:HD2	1.79	0.45
2:C:1272:GLU:HG2	2:C:1276:TRP:NE1	2.32	0.45
2:C:600:THR:HG22	2:C:602:GLU:H	1.82	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.45
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.35	0.45
7:N:21:DG:H2'	7:N:22:DT:H71	1.98	0.45
1:A:208:ASN:ND2	1:A:210:THR:OG1	2.50	0.45
2:C:1060:ILE:HG12	2:C:1061:GLN:N	2.31	0.45
2:C:596:ASP:N	2:C:596:ASP:OD1	2.50	0.45
3:D:530:PRO:HB3	3:D:577:ALA:O	2.17	0.45
2:C:1150:ASP:O	2:C:1151:LEU:HB2	2.16	0.45
2:C:890:LYS:NZ	2:C:891:GLY:H	2.15	0.45
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.99	0.45
3:D:1325:PHE:HD2	3:D:1326:GLN:HG3	1.81	0.45
3:D:709:ARG:H	3:D:709:ARG:HE	1.65	0.45
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.50	0.45
2:C:251:ALA:HB2	2:C:269:ILE:HD12	1.99	0.45
2:C:984:VAL:HA	2:C:985:GLU:HA	1.66	0.45
3:D:1220:ILE:HD12	3:D:1224:ARG:NH2	2.31	0.45
3:D:600:ALA:O	3:D:603:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:914:ALA:HB2	3:D:1359:ALA:HB1	1.98	0.45
1:B:211:ILE:HD11	1:B:215:GLU:HB3	1.99	0.44
2:C:1329:GLU:O	2:C:1332:SER:OG	2.29	0.44
2:C:135:THR:HG21	2:C:515:MET:SD	2.57	0.44
3:D:963:VAL:HB	3:D:980:THR:HG23	1.99	0.44
2:C:298:ALA:HB2	2:C:336:LEU:HD21	1.99	0.44
2:C:35:PHE:O	2:C:39:ILE:HG22	2.18	0.44
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.53	0.44
3:D:1271:SER:OG	3:D:1271:SER:O	2.36	0.44
3:D:197:GLU:O	3:D:201:LEU:HG	2.17	0.44
3:D:232:ASN:HD22	3:D:232:ASN:H	1.64	0.44
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.52	0.44
3:D:1167:LYS:HZ3	3:D:1170:LYS:HD2	1.83	0.44
3:D:1332:LEU:HD13	3:D:1332:LEU:HA	1.78	0.44
3:D:661:VAL:O	3:D:664:ILE:HG12	2.16	0.44
3:D:289:ASP:HA	3:D:292:VAL:HG22	2.00	0.44
3:D:664:ILE:CD1	3:D:682:VAL:HG22	2.47	0.44
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.83	0.44
2:C:1240:ASP:OD1	2:C:1240:ASP:N	2.39	0.44
2:C:962:GLU:HG2	2:C:963:GLU:N	2.33	0.44
3:D:1268:ASN:HD22	3:D:1269:ALA:N	2.16	0.44
5:F:432:THR:HG21	7:N:28:DA:C5	2.53	0.44
2:C:1134:GLN:HG3	2:C:1134:GLN:H	1.64	0.44
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.35	0.44
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.75	0.44
3:D:907:HIS:CD2	3:D:908:ILE:H	2.35	0.44
5:F:402:LEU:HA	5:F:405:ILE:HG12	2.00	0.44
7:N:26:DT:C2	7:N:27:DA:C8	3.05	0.44
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.53	0.44
3:D:412:LEU:O	3:D:416:ILE:HB	2.18	0.44
1:B:69:SER:H	1:B:78:ILE:HD11	1.83	0.44
2:C:1134:GLN:O	2:C:1136:GLN:HG2	2.18	0.44
2:C:544:GLY:O	2:C:548:ARG:HD2	2.18	0.44
2:C:545:PHE:CE2	2:C:549:ASP:HB2	2.53	0.44
3:D:1146:GLU:OE2	3:D:1310:THR:HG22	2.18	0.44
3:D:16:GLU:HG3	3:D:17:PHE:HD1	1.82	0.44
3:D:786:THR:CG2	6:M:7:PRO:HD3	2.48	0.44
8:T:17:DG:H2"	8:T:18:DG:C8	2.53	0.44
1:B:115:ILE:HD11	1:B:130:ILE:HD11	2.00	0.44
1:B:31:LEU:HB2	1:B:199:ASP:O	2.18	0.44
2:C:1244:HIS:CD2	2:C:1264:GLN:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:453:ILE:HD12	2:C:587:LEU:HD21	2.00	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.58	0.43
3:D:608:CYS:HG	3:D:620:PHE:HD2	1.64	0.43
5:F:483:LEU:HD13	5:F:483:LEU:N	2.31	0.43
2:C:230:PHE:O	2:C:333:ILE:HB	2.18	0.43
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.53	0.43
1:A:182:ARG:H	1:A:206:GLU:HB3	1.82	0.43
1:A:190:ALA:H	1:A:199:ASP:HA	1.84	0.43
3:D:1226:VAL:O	3:D:1229:VAL:HG12	2.18	0.43
1:B:48:LEU:HD22	3:D:539:SER:HB3	2.00	0.43
1:B:79:LEU:HA	1:B:82:LEU:HD12	2.00	0.43
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.52	0.43
3:D:482:ALA:O	3:D:488:ASN:ND2	2.49	0.43
3:D:56:LEU:HD12	3:D:56:LEU:H	1.83	0.43
1:B:100:LEU:HD21	1:B:121:VAL:HG11	2.00	0.43
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.48	0.43
2:C:471:VAL:O	2:C:475:VAL:HG23	2.19	0.43
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.84	0.43
3:D:1166:GLY:O	3:D:1173:ARG:HG2	2.18	0.43
3:D:1262:ARG:O	3:D:1282:TYR:N	2.33	0.43
3:D:200:GLN:HE21	3:D:200:GLN:HB2	1.63	0.43
5:F:400:GLN:O	5:F:404:LEU:HG	2.19	0.43
2:C:1158:LYS:HA	2:C:1158:LYS:HD3	1.83	0.43
2:C:273:HIS:HA	2:C:276:GLN:HB3	1.99	0.43
2:C:524:ILE:HD11	2:C:712:SER:HB2	2.00	0.43
2:C:799:ASN:N	2:C:799:ASN:OD1	2.52	0.43
3:D:770:LEU:O	3:D:774:ILE:HG13	2.19	0.43
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.88	0.43
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.98	0.43
1:B:107:ILE:HG23	1:B:135:ASP:HA	2.01	0.43
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.54	0.43
2:C:594:VAL:HA	2:C:598:VAL:O	2.18	0.43
3:D:1265:THR:HG23	3:D:1305:ASP:OD2	2.19	0.43
2:C:1295:SER:OG	3:D:346:ARG:O	2.23	0.43
5:F:111:LEU:HD22	5:F:116:GLU:HG2	1.99	0.43
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.18	0.43
2:C:192:ASP:OD1	2:C:436:ARG:NH2	2.52	0.43
2:C:80:PHE:HB2	2:C:85:CYS:SG	2.58	0.43
3:D:343:LEU:HD11	3:D:1324:SER:HB2	2.01	0.43
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.54	0.43
3:D:981:GLU:OE2	3:D:983:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:9:DC:H2"	7:N:10:DC:C5	2.54	0.43
2:C:1166:ASP:O	2:C:1170:MET:HG2	2.19	0.43
2:C:216:THR:H	2:C:219:GLN:NE2	2.16	0.43
3:D:1162:ILE:O	3:D:1178:THR:CB	2.66	0.43
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.84	0.43
3:D:1211:SER:OG	3:D:1212:ASP:N	2.52	0.43
3:D:266:ASN:O	3:D:270:ARG:HB2	2.19	0.43
2:C:1101:LEU:HD12	3:D:505:ASP:OD1	2.19	0.43
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.99	0.43
3:D:554:GLU:OE1	3:D:570:LYS:NZ	2.50	0.43
3:D:555:TYR:HB2	3:D:585:LYS:O	2.18	0.43
3:D:889:ASP:OD1	3:D:1286:LYS:NZ	2.41	0.43
3:D:813:ASP:HA	3:D:895:CYS:HB2	2.01	0.43
5:F:575:GLU:O	5:F:579:GLN:HG2	2.19	0.43
2:C:967:LEU:HD23	2:C:1021:LEU:HD13	2.01	0.42
2:C:1108:ASN:O	2:C:1111:GLN:HG2	2.18	0.42
2:C:42:ASP:HA	2:C:43:PRO:HD3	1.89	0.42
2:C:484:LEU:HD12	2:C:485:ASP:H	1.84	0.42
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.01	0.42
3:D:499:ILE:HD12	3:D:499:ILE:HA	1.87	0.42
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.54	0.42
4:E:66:VAL:HG22	4:E:69:ARG:NH2	2.34	0.42
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.19	0.42
1:B:62:ASP:HB2	1:B:141:SER:O	2.19	0.42
3:D:1263:LYS:HA	3:D:1281:GLU:HA	2.00	0.42
3:D:1313:SER:O	3:D:1316:THR:OG1	2.34	0.42
3:D:422:LEU:O	3:D:468:VAL:HA	2.19	0.42
3:D:708:ASN:HB3	3:D:712:GLN:O	2.19	0.42
3:D:858:VAL:HG12	3:D:862:THR:OG1	2.20	0.42
3:D:902:ASP:OD1	3:D:903:LEU:N	2.52	0.42
2:C:699:LEU:HB2	2:C:799:ASN:HD22	1.83	0.42
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.77	0.42
3:D:641:ILE:HG23	3:D:764:ARG:NH1	2.34	0.42
5:F:532:LEU:O	5:F:536:THR:HG23	2.19	0.42
2:C:1159:VAL:HA	2:C:1160:ASP:HA	1.82	0.42
2:C:142:GLU:OE2	2:C:515:MET:CE	2.67	0.42
3:D:949:SER:OG	3:D:1019:ASN:OD1	2.30	0.42
3:D:41:PRO:HG3	3:D:274:ASN:OD1	2.20	0.42
1:B:233:ASP:OD1	1:B:234:LEU:N	2.53	0.42
2:C:1160:ASP:CG	2:C:1161:LEU:N	2.73	0.42
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:985:GLU:HB3	2:C:988:LYS:HG2	2.02	0.42
3:D:19:ALA:HB2	3:D:1343:GLU:HA	2.01	0.42
3:D:432:LEU:HD13	3:D:499:ILE:HG21	2.02	0.42
2:C:560:PRO:O	3:D:780:ARG:NH2	2.52	0.42
3:D:925:GLU:HB3	3:D:926:PRO:HD3	2.02	0.42
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.54	0.42
2:C:1281:TYR:HE1	3:D:489:ASN:HD21	1.67	0.42
2:C:81:ASP:O	2:C:85:CYS:HB2	2.19	0.42
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.85	0.42
3:D:161:THR:HG23	3:D:163:GLU:H	1.85	0.42
3:D:46:TYR:CD2	5:F:500:ILE:HG12	2.54	0.42
3:D:801:VAL:O	3:D:805:GLN:HB3	2.19	0.42
3:D:885:VAL:HG22	3:D:899:TYR:HA	2.00	0.42
1:A:11:PRO:HD2	1:B:227:GLN:HE22	1.83	0.42
1:A:166:ARG:O	1:A:168:ILE:N	2.53	0.42
3:D:1179:PRO:HD3	3:D:1184:ASP:HB3	2.00	0.42
1:B:178:SER:H	3:D:535:ARG:HH22	1.68	0.42
2:C:215:TYR:HE2	2:C:422:LYS:HD2	1.83	0.42
2:C:50:GLU:O	2:C:54:ARG:HG3	2.20	0.42
2:C:806:PRO:O	3:D:633:ALA:HA	2.19	0.42
3:D:910:ASN:HB3	4:E:15:ASN:OD1	2.20	0.42
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.42
2:C:1152:GLY:N	2:C:1197:GLU:OE2	2.51	0.42
2:C:387:ASN:HA	2:C:391:SER:HB2	2.01	0.42
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.35	0.42
2:C:972:PHE:HA	2:C:972:PHE:HD1	1.71	0.42
1:B:135:ASP:O	1:B:136:GLU:HB2	2.20	0.42
2:C:242:VAL:HG12	2:C:245:ARG:HG3	2.02	0.42
2:C:886:LYS:H	2:C:917:SER:HB3	1.85	0.42
3:D:1167:LYS:HB3	3:D:1167:LYS:HE3	1.91	0.42
2:C:1101:LEU:O	3:D:731:ARG:HG2	2.20	0.42
3:D:814:CYS:HB2	3:D:889:ASP:HB3	2.02	0.42
3:D:848:VAL:HB	3:D:858:VAL:H	1.85	0.42
5:F:478:PRO:HB2	5:F:483:LEU:HD12	2.02	0.42
8:T:13:DC:H2"	8:T:14:DA:N7	2.35	0.42
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.20	0.41
2:C:897:PRO:HB3	5:F:564:GLY:H	1.85	0.41
3:D:198:CYS:HB2	3:D:224:LEU:HD13	2.02	0.41
3:D:57:PHE:CZ	3:D:252:LEU:HB2	2.55	0.41
3:D:722:ILE:HG12	3:D:737:ILE:HD12	2.02	0.41
4:E:58:LEU:HD12	4:E:59:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:515:GLU:HA	5:F:516:ASP:HA	1.60	0.41
8:T:24:DC:H5'	8:T:24:DC:C6	2.55	0.41
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.00	0.41
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	2.02	0.41
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.21	0.41
3:D:1263:LYS:HE2	3:D:1281:GLU:HB3	2.02	0.41
3:D:362:ARG:H	3:D:365:GLN:NE2	2.15	0.41
1:B:195:ARG:HB3	1:B:198:LEU:HD23	2.02	0.41
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.56	0.41
3:D:97:VAL:HG13	3:D:100:GLU:OE2	2.20	0.41
3:D:347:VAL:HG12	3:D:348:ASP:O	2.20	0.41
3:D:612:LEU:HB3	3:D:616:PRO:CG	2.49	0.41
6:M:11:VAL:HG11	6:M:17:ILE:HD12	2.02	0.41
7:N:8:DC:H2''	7:N:9:DC:C5	2.55	0.41
1:A:222:THR:HG23	1:B:232:VAL:HG23	2.02	0.41
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.56	0.41
2:C:194:LEU:HA	2:C:194:LEU:HD12	1.88	0.41
2:C:444:ASP:OD1	2:C:444:ASP:N	2.53	0.41
2:C:866:ASP:OD2	2:C:944:ARG:HD2	2.20	0.41
3:D:45:ASN:O	3:D:46:TYR:HD1	2.03	0.41
3:D:598:LYS:O	3:D:601:ILE:HG22	2.21	0.41
2:C:1028:LYS:HB3	2:C:1028:LYS:HE2	1.84	0.41
2:C:130:MET:HG2	2:C:131:THR:O	2.20	0.41
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.56	0.41
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.85	0.41
3:D:527:LEU:HD23	3:D:532:GLU:HG2	2.02	0.41
3:D:807:LEU:HD11	3:D:894:VAL:HG23	2.02	0.41
1:A:51:MET:HB3	1:A:51:MET:HE3	1.92	0.41
2:C:935:THR:O	2:C:1040:ASP:N	2.53	0.41
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.94	0.41
3:D:278:ARG:NH2	5:F:446:GLN:OE1	2.54	0.41
3:D:365:GLN:HA	3:D:438:GLU:H	1.86	0.41
3:D:609:TYR:HB2	3:D:617:THR:HG21	2.03	0.41
3:D:677:GLU:O	3:D:681:LYS:HD3	2.20	0.41
5:F:131:GLN:O	5:F:135:ALA:HB2	2.20	0.41
5:F:436:ARG:HB3	5:F:436:ARG:HH11	1.85	0.41
1:A:156:SER:H	2:C:1059:ARG:HH22	1.69	0.41
2:C:1331:ARG:HD3	3:D:33:TRP:CE2	2.56	0.41
3:D:1282:TYR:O	3:D:1286:LYS:HB2	2.20	0.41
3:D:325:LYS:HE2	3:D:330:MET:SD	2.61	0.41
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HA	1:A:222:THR:HB	2.02	0.41
2:C:257:ALA:HB3	2:C:262:TYR:CE1	2.55	0.41
2:C:260:LYS:HG2	2:C:261:VAL:H	1.86	0.41
2:C:483:ASP:HB2	2:C:486:THR:HG22	2.03	0.41
3:D:123:ARG:HD3	3:D:123:ARG:HA	1.89	0.41
5:F:402:LEU:O	5:F:405:ILE:HG12	2.21	0.41
5:F:547:VAL:HG13	5:F:598:LEU:HD22	2.03	0.41
1:B:225:ALA:O	1:B:229:GLU:HG2	2.20	0.41
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.21	0.41
2:C:813:GLU:HA	3:D:504:GLN:HE22	1.85	0.41
3:D:553:THR:HG22	3:D:567:THR:HB	2.03	0.41
3:D:417:ARG:NH2	4:E:43:ASN:O	2.53	0.41
1:B:59:VAL:HG22	1:B:144:ILE:HG13	2.01	0.41
3:D:1326:GLN:H	3:D:1326:GLN:HG3	1.45	0.41
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.53	0.41
3:D:798:ARG:O	3:D:801:VAL:HG22	2.21	0.41
1:A:83:LEU:HD23	2:C:694:ARG:NH1	2.36	0.41
2:C:246:LEU:HB3	2:C:269:ILE:HG21	2.03	0.41
2:C:615:VAL:HG21	2:C:645:PHE:HD2	1.86	0.41
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.86	0.41
3:D:697:MET:HG3	3:D:698:MET:N	2.35	0.41
2:C:242:VAL:HG22	2:C:243:PRO:HD2	2.03	0.40
2:C:275:ARG:HH11	2:C:275:ARG:HB2	1.86	0.40
2:C:696:ASP:O	2:C:697:LYS:HB3	2.21	0.40
3:D:292:VAL:O	3:D:296:LYS:HG3	2.20	0.40
3:D:682:VAL:HG12	3:D:686:TRP:HD1	1.85	0.40
4:E:15:ASN:O	4:E:17:PHE:N	2.54	0.40
5:F:395:THR:OG1	5:F:396:ASN:N	2.54	0.40
2:C:1328:LYS:HA	2:C:1328:LYS:HD3	1.85	0.40
2:C:153:PRO:HB2	2:C:401:GLY:HA3	2.02	0.40
3:D:1330:ARG:HA	3:D:1333:THR:OG1	2.22	0.40
1:B:89:ALA:HB3	1:B:124:VAL:HG12	2.04	0.40
2:C:820:GLU:N	2:C:1080:ASN:O	2.55	0.40
2:C:1296:ASP:OD2	2:C:1322:SER:OG	2.28	0.40
3:D:1333:THR:O	3:D:1337:VAL:HG13	2.22	0.40
3:D:367:GLY:HA3	3:D:448:GLN:HB2	2.02	0.40
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.51	0.40
3:D:984:LEU:CB	3:D:993:GLU:HB2	2.52	0.40
2:C:1159:VAL:HG23	2:C:1160:ASP:HB2	2.03	0.40
2:C:296:VAL:HG12	2:C:297:VAL:H	1.86	0.40
1:A:68:TYR:HE2	2:C:927:THR:HG1	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:325:LYS:HE3	3:D:330:MET:HA	2.04	0.40
3:D:338:PHE:HD1	3:D:338:PHE:HA	1.70	0.40
3:D:124:ILE:H	3:D:124:ILE:HG13	1.61	0.40
3:D:615:LYS:HG3	3:D:615:LYS:H	1.61	0.40
3:D:84:ILE:H	3:D:84:ILE:HD13	1.85	0.40
3:D:857:LEU:HG	3:D:858:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

## 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	229/239 (96%)	204 (89%)	23 (10%)	2 (1%)	17	54
1	B	212/239 (89%)	189 (89%)	23 (11%)	0	100	100
2	C	1329/1342 (99%)	1243 (94%)	77 (6%)	9 (1%)	22	59
3	D	1230/1409 (87%)	1166 (95%)	62 (5%)	2 (0%)	47	78
4	E	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	12	47
5	F	312/612 (51%)	293 (94%)	18 (6%)	1 (0%)	41	74
6	M	19/21 (90%)	13 (68%)	4 (21%)	2 (10%)	0	7
All	All	3408/3953 (86%)	3181 (93%)	210 (6%)	17 (0%)	29	66

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	199	ASP
2	C	200	ARG
2	C	1151	LEU
1	A	177	TYR
2	C	340	ASP

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Mol	Chain	Res	Type
3	D	1326	GLN
6	M	17	ILE
4	E	16	ARG
5	F	134	VAL
6	M	16	PRO
1	A	163	GLU
2	C	114	VAL
2	C	339	ASN
2	C	398	SER
2	C	1150	ASP
2	C	1341	ASP
3	D	1167	LYS

### 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	190/206 (92%)	178 (94%)	12 (6%)	18	49
1	B	176/206 (85%)	154 (88%)	22 (12%)	4	23
2	C	1138/1157 (98%)	1001 (88%)	137 (12%)	5	25
3	D	1022/1170 (87%)	901 (88%)	121 (12%)	5	26
4	E	67/75 (89%)	59 (88%)	8 (12%)	5	25
5	F	232/539 (43%)	205 (88%)	27 (12%)	5	27
6	M	13/14 (93%)	9 (69%)	4 (31%)	0	2
All	All	2838/3367 (84%)	2507 (88%)	331 (12%)	5	26

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	16	ILE
1	A	19	VAL
1	A	61	ILE
1	A	115	ILE

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Mol	Chain	Res	Type
1	A	122	GLU
1	A	136	GLU
1	A	162	GLU
1	A	187	VAL
1	A	192	VAL
1	A	195	ARG
1	A	197	ASP
1	B	12	ARG
1	B	16	ILE
1	B	18	GLN
1	B	22	THR
1	B	61	ILE
1	B	72	GLU
1	B	74	VAL
1	B	76	GLU
1	B	78	ILE
1	B	83	LEU
1	B	91	ARG
1	B	97	GLU
1	B	107	ILE
1	B	124	VAL
1	B	132	HIS
1	B	133	LEU
1	B	134	THR
1	B	139	SER
1	B	144	ILE
1	B	148	ARG
1	B	206	GLU
1	B	227	GLN
2	C	11	ILE
2	C	22	LEU
2	C	24	VAL
2	C	30	ILE
2	C	60	GLN
2	C	65	ASN
2	C	66	SER
2	C	82	VAL
2	C	85	CYS
2	C	91	THR
2	C	113	THR
2	C	114	VAL
2	C	115	LYS

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Mol	Chain	Res	Type
2	C	124	MET
2	C	131	THR
2	C	132	ASP
2	C	151	ARG
2	C	160	ASP
2	C	164	THR
2	C	165	HIS
2	C	171	LEU
2	C	179	TYR
2	C	197	ARG
2	C	199	ASP
2	C	201	ARG
2	C	219	GLN
2	C	230	PHE
2	C	232	ILE
2	C	235	ASN
2	C	237	LEU
2	C	241	LEU
2	C	242	VAL
2	C	254	ASP
2	C	258	ASN
2	C	270	THR
2	C	280	ASP
2	C	285	ILE
2	C	296	VAL
2	C	320	ASP
2	C	337	PHE
2	C	341	LEU
2	C	343	HIS
2	C	360	LEU
2	C	377	THR
2	C	413	GLU
2	C	417	SER
2	C	446	ASP
2	C	448	LEU
2	C	450	ASN
2	C	453	ILE
2	C	472	GLU
2	C	481	LEU
2	C	484	LEU
2	C	538	LEU
2	C	540	ARG

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Mol	Chain	Res	Type
2	C	569	ILE
2	C	581	THR
2	C	596	ASP
2	C	603	ILE
2	C	604	HIS
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	630	VAL
2	C	633	LEU
2	C	637	ARG
2	C	648	ASP
2	C	654	ASP
2	C	672	GLU
2	C	684	ASN
2	C	697	LYS
2	C	699	LEU
2	C	724	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	783	LEU
2	C	788	SER
2	C	808	ASN
2	C	828	PHE
2	C	839	VAL
2	C	844	LYS
2	C	845	LEU
2	C	878	THR
2	C	890	LYS
2	C	893	THR
2	C	899	GLU
2	C	913	VAL
2	C	922	ASN
2	C	929	ILE
2	C	941	LYS
2	C	944	ARG
2	C	960	LEU
2	C	962	GLU

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Mol	Chain	Res	Type
2	C	967	LEU
2	C	972	PHE
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	988	LYS
2	C	992	LEU
2	C	996	ARG
2	C	1002	LEU
2	C	1004	ASP
2	C	1014	LEU
2	C	1038	GLN
2	C	1041	ASP
2	C	1047	LEU
2	C	1060	ILE
2	C	1073	LYS
2	C	1077	SER
2	C	1082	ILE
2	C	1083	GLU
2	C	1098	LEU
2	C	1106	ARG
2	C	1108	ASN
2	C	1114	GLU
2	C	1117	LEU
2	C	1119	MET
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1150	ASP
2	C	1151	LEU
2	C	1160	ASP
2	C	1161	LEU
2	C	1210	ILE
2	C	1223	ARG
2	C	1233	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1326	LEU
2	C	1327	LEU
2	C	1341	ASP
3	D	45	ASN
3	D	46	TYR

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Mol	Chain	Res	Type
3	D	54	ASP
3	D	74	LYS
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	97	VAL
3	D	99	ARG
3	D	158	GLN
3	D	161	THR
3	D	167	ASP
3	D	174	ASP
3	D	177	ASP
3	D	193	ASP
3	D	211	GLU
3	D	216	LYS
3	D	219	LYS
3	D	223	LEU
3	D	224	LEU
3	D	229	GLN
3	D	232	ASN
3	D	244	VAL
3	D	251	PRO
3	D	252	LEU
3	D	255	LEU
3	D	264	ASP
3	D	284	ASP
3	D	299	LEU
3	D	316	ILE
3	D	317	THR
3	D	321	LYS
3	D	324	LEU
3	D	338	PHE
3	D	394	ILE
3	D	416	ILE
3	D	474	LEU
3	D	497	GLU
3	D	505	ASP
3	D	506	VAL
3	D	514	THR
3	D	518	VAL
3	D	536	LEU
3	D	545	HIS

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Mol	Chain	Res	Type
3	D	571	ASP
3	D	594	GLN
3	D	610	ARG
3	D	641	ILE
3	D	646	ILE
3	D	650	LYS
3	D	651	HIS
3	D	663	GLU
3	D	678	ARG
3	D	680	ASN
3	D	697	MET
3	D	702	GLN
3	D	707	ILE
3	D	708	ASN
3	D	709	ARG
3	D	712	GLN
3	D	720	ASN
3	D	731	ARG
3	D	740	LEU
3	D	746	LEU
3	D	747	MET
3	D	764	ARG
3	D	772	TYR
3	D	780	ARG
3	D	783	LEU
3	D	805	GLN
3	D	807	LEU
3	D	808	VAL
3	D	817	HIS
3	D	818	GLU
3	D	847	ASP
3	D	850	LYS
3	D	858	VAL
3	D	862	THR
3	D	867	GLN
3	D	882	VAL
3	D	895	CYS
3	D	901	ARG
3	D	905	ARG
3	D	907	HIS
3	D	908	ILE
3	D	931	THR

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Mol	Chain	Res	Type
3	D	951	GLN
3	D	987	GLU
3	D	1009	GLU
3	D	1010	GLN
3	D	1138	LEU
3	D	1140	ARG
3	D	1145	PHE
3	D	1148	ARG
3	D	1155	ILE
3	D	1163	VAL
3	D	1164	SER
3	D	1170	LYS
3	D	1178	THR
3	D	1181	ASP
3	D	1186	TYR
3	D	1209	VAL
3	D	1211	SER
3	D	1215	GLU
3	D	1218	HIS
3	D	1221	LEU
3	D	1223	LEU
3	D	1242	ARG
3	D	1268	ASN
3	D	1276	GLU
3	D	1289	ASN
3	D	1291	GLU
3	D	1293	GLU
3	D	1310	THR
3	D	1316	THR
3	D	1326	GLN
3	D	1329	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1349	GLU
4	E	3	ARG
4	E	16	ARG
4	E	18	ASP
4	E	28	ARG
4	E	36	ASP
4	E	39	VAL
4	E	44	ASP

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Mol	Chain	Res	Type
4	E	47	THR
5	F	99	ARG
5	F	118	ASP
5	F	395	THR
5	F	400	GLN
5	F	423	ARG
5	F	425	TYR
5	F	427	PHE
5	F	436	ARG
5	F	449	THR
5	F	469	GLN
5	F	470	MET
5	F	471	LEU
5	F	472	GLN
5	F	483	LEU
5	F	488	LEU
5	F	492	ASP
5	F	494	ILE
5	F	500	ILE
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	575	GLU
5	F	578	LYS
5	F	584	ARG
5	F	586	ARG
5	F	588	ARG
5	F	600	HIS
6	M	5	HIS
6	M	13	ILE
6	M	15	THR
6	M	17	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	GLN
1	B	75	GLN
1	B	84	ASN
1	B	147	GLN
1	B	227	GLN
2	C	69	GLN

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Mol	Chain	Res	Type
2	C	139	ASN
2	C	258	ASN
2	C	357	ASN
2	C	490	GLN
2	C	513	GLN
2	C	573	ASN
2	C	620	ASN
2	C	628	HIS
2	C	688	GLN
2	C	922	ASN
2	C	1017	GLN
2	C	1038	GLN
2	C	1080	ASN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1134	GLN
2	C	1237	HIS
2	C	1288	GLN
2	C	1313	HIS
2	C	1314	GLN
3	D	200	GLN
3	D	232	ASN
3	D	365	GLN
3	D	435	GLN
3	D	465	GLN
3	D	495	ASN
3	D	560	ASN
3	D	680	ASN
3	D	702	GLN
3	D	716	GLN
3	D	736	GLN
3	D	805	GLN
3	D	907	HIS
3	D	929	GLN
3	D	1010	GLN
3	D	1218	HIS
3	D	1244	GLN
3	D	1268	ASN
5	F	396	ASN
5	F	579	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	231/239 (96%)	0.35	25 (10%) 5 4	138, 193, 227, 277	0
1	B	218/239 (91%)	-0.13	4 (1%) 68 56	133, 191, 230, 261	0
2	C	1335/1342 (99%)	-0.11	32 (2%) 59 45	93, 170, 229, 271	0
3	D	1236/1409 (87%)	0.02	46 (3%) 41 29	99, 176, 247, 304	0
4	E	79/91 (86%)	0.27	7 (8%) 9 6	144, 183, 238, 268	0
5	F	318/612 (51%)	0.00	10 (3%) 49 35	128, 190, 250, 265	0
6	M	21/21 (100%)	0.18	2 (9%) 8 5	151, 194, 226, 257	0
7	N	29/29 (100%)	-0.82	0 100 100	139, 222, 253, 255	0
8	T	24/24 (100%)	-0.81	0 100 100	125, 223, 249, 259	0
All	All	3491/4006 (87%)	-0.02	126 (3%) 42 31	93, 179, 240, 304	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	476	ARG	10.1
2	C	243	PRO	9.6
1	A	89	ALA	9.3
1	A	90	VAL	7.5
2	C	230	PHE	6.5
5	F	136	GLU	5.4
3	D	676	GLY	5.2
1	A	88	LEU	5.0
1	A	25	LYS	4.8
3	D	1165	PHE	4.7
2	C	241	LEU	4.5
5	F	265	GLN	4.4
2	C	172	TYR	4.4
3	D	1198	VAL	4.2
4	E	38	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
5	F	111	LEU	4.1
3	D	155	GLU	4.1
3	D	1276	GLU	4.1
3	D	675	ALA	3.9
3	D	1166	GLY	3.8
5	F	477	GLU	3.7
2	C	333	ILE	3.7
1	A	100	LEU	3.7
3	D	1006	GLY	3.7
3	D	741	ALA	3.6
1	A	174	ASP	3.6
1	A	16	ILE	3.4
2	C	258	ASN	3.3
1	A	144	ILE	3.3
3	D	712	GLN	3.3
3	D	960	LEU	3.3
3	D	154	LEU	3.2
3	D	958	ILE	3.2
1	A	24	ALA	3.2
3	D	743	MET	3.2
3	D	174	ASP	3.1
2	C	207	THR	3.1
3	D	645	VAL	3.1
6	M	14	GLY	3.1
2	C	314	ASN	3.1
1	A	85	LEU	3.1
1	A	98	VAL	3.1
2	C	239	MET	3.0
2	C	317	LEU	3.0
2	C	783	LEU	3.0
6	M	13	ILE	3.0
3	D	1200	GLU	3.0
3	D	1274	PHE	3.0
3	D	677	GLU	3.0
1	A	15	ASP	2.9
1	A	143	ARG	2.9
3	D	1204	VAL	2.9
2	C	232	ILE	2.9
5	F	480	PRO	2.8
4	E	39	VAL	2.8
2	C	184	LEU	2.8
3	D	1210	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	246	LEU	2.7
4	E	59	ILE	2.7
5	F	475	GLY	2.7
3	D	1280	VAL	2.7
5	F	135	ALA	2.7
1	A	173	VAL	2.7
1	A	29	GLU	2.7
2	C	492	MET	2.7
2	C	292	ILE	2.7
3	D	178	ALA	2.6
1	A	193	GLU	2.6
5	F	489	MET	2.5
1	A	99	ILE	2.5
3	D	1174	ARG	2.5
1	A	58	GLU	2.5
2	C	231	GLU	2.5
2	C	245	ARG	2.5
4	E	72	GLN	2.5
1	A	26	VAL	2.5
3	D	213	LYS	2.5
1	B	172	LEU	2.4
1	A	160	HIS	2.4
2	C	171	LEU	2.4
1	A	172	LEU	2.4
2	C	1261	GLY	2.4
3	D	1172	LYS	2.4
2	C	311	CYS	2.4
1	B	98	VAL	2.4
3	D	165	TYR	2.4
3	D	160	LEU	2.4
2	C	942	ASP	2.3
3	D	146	VAL	2.3
3	D	1005	LYS	2.3
2	C	316	GLU	2.3
3	D	221	ILE	2.3
3	D	1171	GLY	2.3
3	D	176	PHE	2.3
1	A	162	GLU	2.3
3	D	216	LYS	2.3
2	C	604	HIS	2.3
3	D	1201	GLY	2.3
3	D	1195	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	35	LYS	2.2
3	D	1212	ASP	2.2
3	D	1285	VAL	2.2
3	D	1160	SER	2.2
2	C	186	PHE	2.2
2	C	1025	PHE	2.2
2	C	332	ARG	2.2
3	D	685	ILE	2.2
2	C	194	LEU	2.1
4	E	77	ALA	2.1
1	B	95	LYS	2.1
3	D	1289	ASN	2.1
2	C	429	MET	2.1
3	D	1241	TYR	2.1
4	E	80	LEU	2.1
1	A	161	SER	2.1
1	B	196	THR	2.1
3	D	145	VAL	2.1
2	C	224	PHE	2.1
1	A	200	LYS	2.1
3	D	1196	LEU	2.1
5	F	470	MET	2.1
1	A	163	GLU	2.1
2	C	294	GLY	2.1
2	C	1149	TYR	2.0
3	D	690	ASN	2.0
3	D	136	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MG	D	1501	1/1	0.95	0.25	83,83,83,83	0
10	ZN	D	1503	1/1	0.96	0.21	185,185,185,185	0
10	ZN	D	1502	1/1	0.98	0.12	162,162,162,162	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.