



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:34 PM UTC

PDB ID : 6DV9 / pdb_00006dv9
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex(ECF sigma factor L) containing 5nt RNA with 4nt spacer
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on : 2018-06-23
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

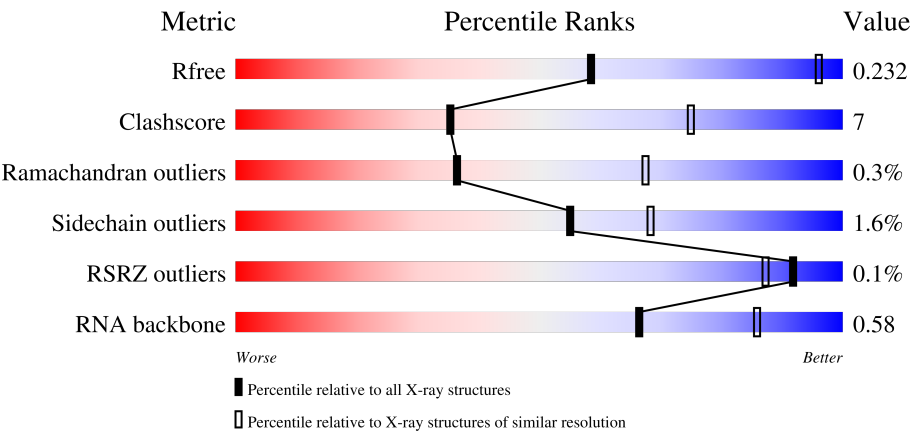
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



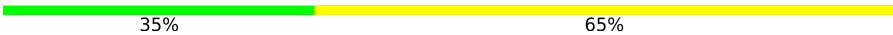
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	359	
1	B	359	
2	C	1178	
3	D	1316	

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Mol	Chain	Length	Quality of chain
4	E	110	 61% 13% 26%
5	F	177	 79% 19% ..
6	I	5	 40% 60%
7	G	17	 35% 65%
8	H	22	 59% 41%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1716	1080	296	338	2			
1	B	233	Total	C	N	O	S	0	0	0
			1733	1094	297	340	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P9WGZ1
A	-10	GLY	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	HIS	-	expression tag	UNP P9WGZ1
A	-7	HIS	-	expression tag	UNP P9WGZ1
A	-6	HIS	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	HIS	-	expression tag	UNP P9WGZ1
A	-3	HIS	-	expression tag	UNP P9WGZ1
A	-2	HIS	-	expression tag	UNP P9WGZ1
A	-1	HIS	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-11	MET	-	initiating methionine	UNP P9WGZ1
B	-10	GLY	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	HIS	-	expression tag	UNP P9WGZ1
B	-7	HIS	-	expression tag	UNP P9WGZ1
B	-6	HIS	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	HIS	-	expression tag	UNP P9WGZ1
B	-3	HIS	-	expression tag	UNP P9WGZ1
B	-2	HIS	-	expression tag	UNP P9WGZ1
B	-1	HIS	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1126	Total	C	N	O	S	0	0	0
			8728	5461	1531	1697	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1265	Total	C	N	O	S	0	0	0
			9895	6195	1794	1866	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	81	Total	C	N	O		0	0	0
			630	403	106	121				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	174	Total	C	N	O	S	0	0	0
			1349	839	256	252	2			

- Molecule 6 is a RNA chain called RNA (5'-R(*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	5	Total	C	N	O	P	0	0	0
			102	47	18	33	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	17	Total	C	N	O	P	0	0	0
			350	166	68	100	16			

- Molecule 8 is a DNA chain called DNA (5'-D(P*CP*GP*TP*GP*TP*CP*AP*GP*AP*GP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	22	Total	C	N	O	P	0	0	0
			452	215	85	131	21			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

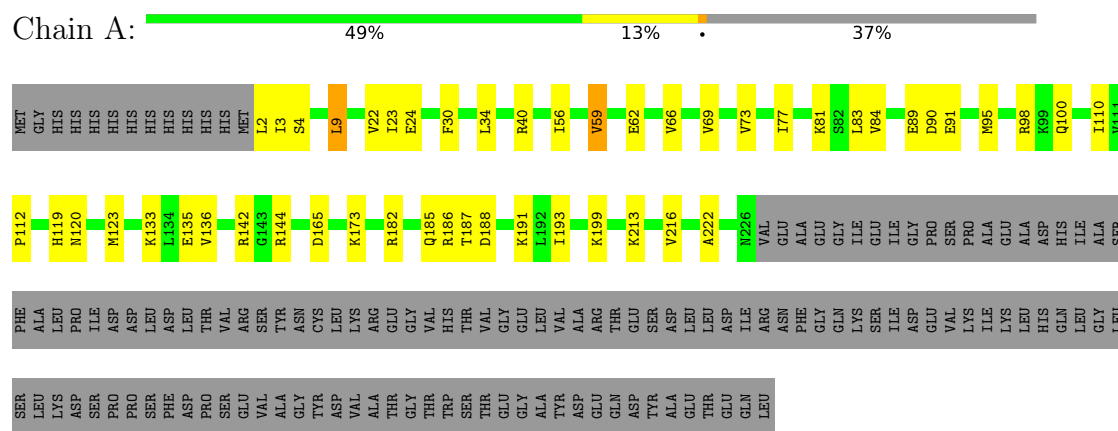
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

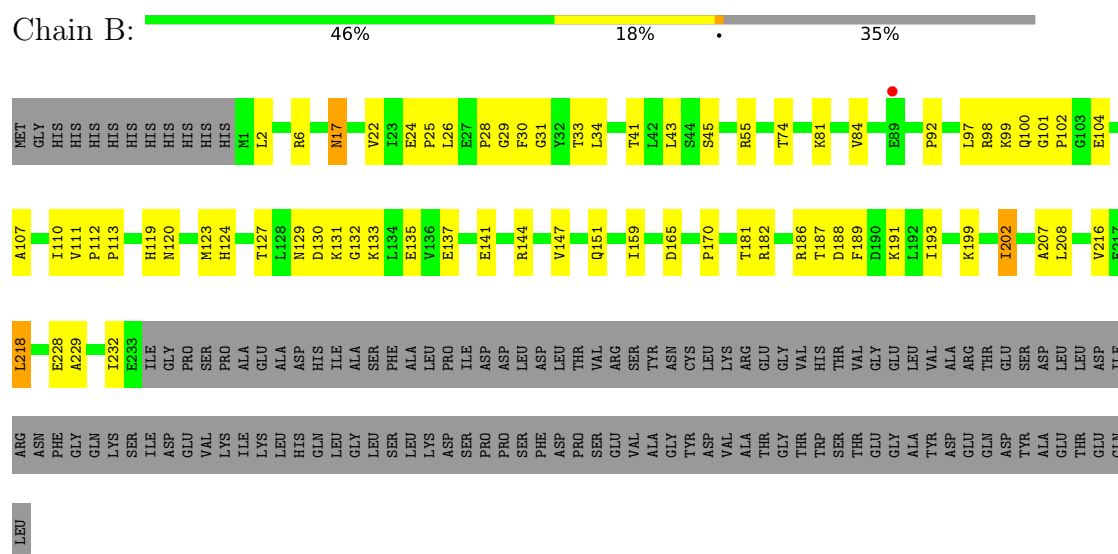
3 Residue-property plots

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.

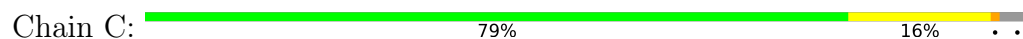
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

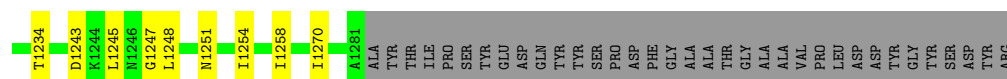


• Molecule 2: DNA-directed RNA polymerase subunit beta

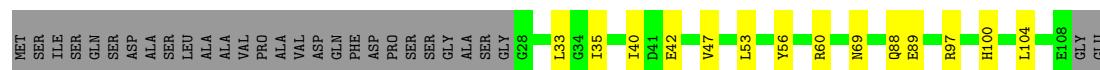




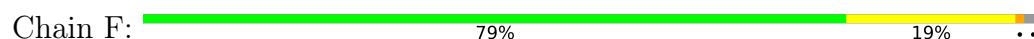
V1098	K961	L746	M541	R389	T128	MET
D1101	V962	V543	R390	P390	R173	LEU
D1103	R963	Q759	R566	S401	K190	T16
V1107	I997	R762	I557	R412	A191	A17
	E1005	W778	L558	R427	D192	E18
L1111	T1008	L789	I565		C201	D19
M1112	Q1009				I20	
E1120	L1010	Y793	P573	V431	L234	S24
Q1131	T1011		L574	Q435	D237	T33
Q1139	MET	T802	A575	L436	E238	I34
	ARG		M576		M239	
Q1139	THR	L817	P577	K445	L240	P41
	PHE		B578	L446	Y241	
Q1145	H15	L823	L579	M447	R242	K50
	GLN		B580			
T1149	GLY	N826	M581	E450	M256	W58
	GLY	P827			E59	
K1152	VAL		L585	K453	Q262	
H1153	GLY	T832		P454	D271	G63
I1154	GLU	P833	L588			
E1155	ASP	R834	T589	M457	K66	K66
V1156	ILE	P835		K458	R67	R67
I1157	THR		P593	R459	V68	V68
V1158	G1026	R841			L290	
			G597	D462	R291	I73
L1162	R1030	Y849	E598	L463	L292	
R1163		P850	P699	R464	L293	E76
K1164	L1034	T851	Q600	H465	K294	
V1165	F1035	R852			Q303	G79
T1166	E1036	T853	P607	K473		
I1167		H854	E608	E477	V313	V82
L1168	G1042		T609			
D1169		G859	G610	E477	P318	R89
	P1045		V611	W484		
T1173	I1046	T863		E488	M327	H94
			L627			
P1177	T1050	T867		R500	R334	L97
	G1051		L633			
M1190	L1055	Q882	K634	H505	T337	T102
V1193	E1056	D890	P642	R506	I104	H103
V1194	D1057			L507	N341	W105
		D907	E647		D342	Y106
A1201	D1089			E518	L343	F107
A1202		L910	R670	Q523	P111	
	S1080	T911		L524	P363	P111
P1205	I1081		M688			S112
V1206	K1082	Y921		H525	I366	R113
	R1083		V713	P526		L114
T1211	Q1084	T927			L374	
	R1085		W723	F532		P122
A1216	L1086	V930		D535	D379	K123
	R1087		W729		A380	D124
W1220		V936	T730		L381	L126
	K1090			D539		K127
			W740	G540	W528	



- Molecule 4: DNA-directed RNA polymerase subunit omega



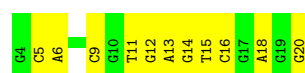
- Molecule 5: ECF RNA polymerase sigma factor SigL



- Molecule 6: RNA (5'-R(*CP*UP*CP*GP*A)-3')



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



- Molecule 8: DNA (5'-D(P*CP*GP*TP*GP*TP*CP*AP*GP*AP*GP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	143.27Å 161.44Å 237.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.47 – 3.80 91.47 – 3.80	Depositor EDS
% Data completeness (in resolution range)	93.6 (91.47-3.80) 95.5 (91.47-3.80)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.78Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.184 , 0.232 0.187 , 0.232	Depositor DCC
R_{free} test set	2618 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24958	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.11	0/1742	0.30	0/2370
1	B	0.12	0/1759	0.34	0/2399
2	C	0.10	0/8887	0.31	0/12048
3	D	0.10	0/10061	0.30	0/13600
4	E	0.11	0/643	0.30	0/877
5	F	0.13	0/1371	0.32	0/1865
6	I	0.07	0/113	0.18	0/174
7	G	0.18	0/393	0.40	0/606
8	H	0.21	0/507	0.46	0/782
All	All	0.11	0/25476	0.31	0/34721

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1716	0	1756	36	0
1	B	1733	0	1752	47	0
2	C	8728	0	8655	123	0
3	D	9895	0	9953	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	630	0	622	11	0
5	F	1349	0	1344	24	0
6	I	102	0	55	2	0
7	G	350	0	192	10	0
8	H	452	0	249	10	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	24958	0	24578	362	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 7.

All (362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HE	1:B:33:THR:HG22	1.31	0.95
3:D:334:ARG:HD3	5:F:90:VAL:HG21	1.54	0.90
2:C:1024:THR:H	3:D:730:THR:HG21	1.48	0.79
2:C:593:MET:HA	2:C:628:THR:HG21	1.66	0.77
1:A:4:SER:HB3	1:B:144:ARG:HH12	1.51	0.74
2:C:541:VAL:HG12	2:C:578:TYR:HB2	1.69	0.73
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.72	0.72
3:D:832:ILE:HG22	3:D:834:ARG:H	1.55	0.72
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.74	0.70
2:C:558:ARG:HB3	2:C:570:TYR:HB3	1.71	0.70
5:F:50:ARG:NH1	8:H:6:DT:O4	2.26	0.69
2:C:458:LEU:HD21	2:C:496:LEU:HD13	1.74	0.69
3:D:363:PRO:HG2	5:F:15:MET:HG3	1.76	0.68
3:D:1055:LEU:H	3:D:1101:ASP:HB3	1.60	0.67
3:D:436:LEU:HD11	3:D:523:GLN:HB3	1.75	0.67
2:C:928:ILE:HD11	3:D:817:LEU:HD11	1.77	0.67
3:D:1248:LEU:HD22	3:D:1258:ILE:HB	1.77	0.66
2:C:104:SER:HB3	2:C:140:ILE:HB	1.76	0.66
3:D:827:PRO:HD3	3:D:854:HIS:HB3	1.78	0.66
3:D:50:LYS:HE2	3:D:79:GLY:HA3	1.76	0.66
3:D:454:PRO:HA	3:D:457:MET:HE2	1.78	0.65
2:C:113:ASP:HB3	2:C:132:PRO:HG2	1.78	0.65
2:C:1104:GLU:OE1	5:F:113:ARG:NH1	2.30	0.65
3:D:366:ILE:HD11	5:F:15:MET:HE2	1.78	0.65
5:F:124:SER:HG	5:F:127:HIS:HD1	1.44	0.65
2:C:401:ARG:HA	2:C:404:MET:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.79	0.64
3:D:1045:PRO:HG2	3:D:1111:LEU:HB2	1.81	0.63
2:C:1052:ILE:O	3:D:89:ARG:NH1	2.32	0.63
5:F:124:SER:OG	5:F:127:HIS:ND1	2.30	0.63
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.80	0.63
1:A:186:ARG:HG3	1:A:187:THR:HG23	1.81	0.62
1:A:83:LEU:HA	1:A:123:MET:HE1	1.81	0.62
3:D:337:THR:OG1	3:D:341:ASN:ND2	2.29	0.61
1:B:84:VAL:HG12	1:B:199:LYS:HD2	1.83	0.61
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.81	0.61
1:B:81:LYS:HD3	1:B:165:ASP:HB2	1.81	0.61
3:D:907:ASP:OD1	3:D:907:ASP:N	2.30	0.60
2:C:536:GLU:OE2	2:C:562:ARG:NH2	2.33	0.60
2:C:982:GLU:HG3	3:D:841:ARG:HH12	1.66	0.60
2:C:473:ARG:NH2	2:C:492:PRO:O	2.35	0.59
2:C:57:GLN:HG3	2:C:452:LYS:HB3	1.85	0.59
3:D:535:ASP:OD1	3:D:535:ASP:N	2.34	0.59
2:C:926:MET:HE1	3:D:817:LEU:HA	1.84	0.58
2:C:686:GLN:HA	2:C:705:GLY:HA2	1.85	0.58
2:C:732:GLU:HB3	3:D:579:LEU:HD12	1.85	0.58
2:C:47:PRO:HG2	2:C:581:VAL:HG13	1.85	0.58
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.68	0.58
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.86	0.58
3:D:16:THR:HG22	3:D:18:GLU:H	1.69	0.58
3:D:1042:GLY:O	3:D:1083:ARG:NH2	2.34	0.58
1:A:95:MET:HE3	1:A:110:ILE:HG21	1.84	0.58
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.35	0.57
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.86	0.57
2:C:234:VAL:HG12	2:C:261:THR:HG21	1.87	0.57
1:A:188:ASP:OD2	1:B:151:GLN:NE2	2.35	0.57
3:D:1083:ARG:HD2	3:D:1112:MET:HE3	1.87	0.57
3:D:1270:ILE:HD13	4:E:56:TYR:HE2	1.69	0.57
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.32	0.57
1:B:187:THR:HG22	3:D:518:GLU:HG2	1.86	0.56
2:C:446:LEU:HD13	2:C:593:MET:HE1	1.87	0.56
2:C:853:PHE:HD2	2:C:868:LEU:HD23	1.71	0.56
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.87	0.56
2:C:190:THR:HG23	2:C:199:LEU:HB2	1.87	0.56
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.87	0.56
3:D:1173:THR:HG22	3:D:1193:VAL:HG21	1.87	0.56
2:C:848:ILE:HD13	2:C:874:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.87	0.56
3:D:1045:PRO:HB2	3:D:1111:LEU:HD12	1.88	0.56
5:F:140:SER:HB3	5:F:143:GLN:HG3	1.88	0.56
1:B:55:ARG:NH2	1:B:137:GLU:OE1	2.38	0.55
2:C:168:ILE:HB	2:C:173:ARG:HD2	1.87	0.55
2:C:590:ALA:HA	2:C:593:MET:HE3	1.87	0.55
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.88	0.55
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.89	0.55
1:B:84:VAL:HG23	1:B:119:HIS:HB2	1.88	0.55
3:D:1139:GLN:NE2	3:D:1149:ILE:O	2.40	0.55
1:A:40:ARG:NE	1:B:33:THR:HG22	2.13	0.55
2:C:32:VAL:H	2:C:33:PRO:HD3	1.72	0.55
2:C:93:LEU:HD11	2:C:96:ILE:HD11	1.88	0.55
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.89	0.55
2:C:628:THR:HG23	2:C:630:MET:H	1.70	0.55
1:A:56:ILE:HG12	1:A:136:VAL:HG22	1.89	0.55
1:B:24:GLU:HB2	1:B:191:LYS:HG3	1.88	0.55
1:B:100:GLN:HG3	1:B:133:LYS:HB2	1.89	0.54
3:D:597:GLY:HA3	3:D:627:LEU:HA	1.89	0.54
3:D:557:ILE:HG23	4:E:40:ILE:HD11	1.90	0.54
2:C:592:ALA:HA	2:C:976:VAL:HG21	1.90	0.54
2:C:607:MET:SD	2:C:892:LYS:NZ	2.81	0.54
7:G:12:DG:H2'	7:G:13:DA:C8	2.43	0.54
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.44	0.53
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.90	0.53
1:B:182:ARG:NH1	3:D:488:GLU:HG2	2.24	0.53
2:C:217:ASP:OD2	2:C:231:ARG:NH2	2.42	0.53
3:D:1080:ILE:HG22	3:D:1082:LYS:H	1.73	0.53
1:A:22:VAL:HG12	1:A:193:ILE:HG12	1.90	0.53
2:C:83:VAL:HG13	2:C:87:GLU:HB2	1.91	0.53
1:A:34:LEU:HD11	1:B:218:LEU:HD13	1.90	0.53
1:B:228:GLU:HG2	1:B:229:ALA:H	1.73	0.53
7:G:20:DG:H5''	7:G:20:DG:H8	1.74	0.53
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.91	0.53
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.40	0.53
7:G:11:DT:H2'	7:G:12:DG:C8	2.44	0.53
4:E:89:GLU:OE2	4:E:97:ARG:NH1	2.42	0.53
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.44	0.52
5:F:32:ARG:HB2	8:H:11:DG:H4'	1.90	0.52
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.24	0.52
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLN:HB2	2:C:679:ASN:HB2	1.92	0.52
2:C:795:GLU:HG2	2:C:846:LYS:HG2	1.90	0.52
2:C:185:VAL:HG23	2:C:316:VAL:HG22	1.92	0.52
1:A:84:VAL:HG13	1:A:119:HIS:HB2	1.92	0.52
1:B:17:ASN:OD1	1:B:17:ASN:N	2.41	0.52
2:C:731:TYR:OH	3:D:578:ARG:NH1	2.43	0.52
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.75	0.51
3:D:578:ARG:H	3:D:581:MET:HE3	1.75	0.51
5:F:88:ASN:O	5:F:90:VAL:N	2.42	0.51
3:D:97:LEU:HD22	3:D:374:LEU:HD21	1.91	0.51
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.75	0.51
3:D:729:VAL:HG11	3:D:802:ILE:HD11	1.93	0.51
3:D:1167:ILE:HB	3:D:1177:PRO:HA	1.91	0.51
3:D:826:ASN:HB3	3:D:832:ILE:HD11	1.91	0.51
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.92	0.51
7:G:5:DC:H2"	7:G:6:DA:C8	2.45	0.51
3:D:34:ILE:HA	3:D:41:PRO:HA	1.92	0.51
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.93	0.51
2:C:122:CYS:HA	2:C:127:MET:HG3	1.93	0.51
2:C:522:GLY:O	2:C:553:ARG:HA	2.11	0.51
5:F:170:LEU:HD13	5:F:175:VAL:HG11	1.92	0.51
2:C:455:LEU:HD12	2:C:483:MET:HG3	1.93	0.51
2:C:549:ASP:OD1	2:C:550:ALA:N	2.44	0.51
1:B:129:ASN:OD1	1:B:130:ASP:N	2.42	0.50
2:C:751:HIS:CD2	2:C:877:ARG:HD2	2.45	0.50
3:D:789:LEU:HD22	3:D:793:TYR:HE2	1.76	0.50
2:C:450:THR:HG21	2:C:613:ARG:HD2	1.93	0.50
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.77	0.50
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.46	0.50
3:D:435:GLN:OE1	3:D:435:GLN:N	2.44	0.50
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.93	0.50
3:D:927:THR:HB	3:D:961:LYS:HB3	1.92	0.50
2:C:298:ASN:HA	2:C:302:LYS:HB2	1.94	0.49
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.45	0.49
1:A:98:ARG:HG3	1:A:135:GLU:HG3	1.94	0.49
4:E:42:GLU:OE1	4:E:100:HIS:NE2	2.42	0.49
3:D:573:PRO:HB2	3:D:576:MET:HE2	1.94	0.49
5:F:75:ASN:ND2	8:H:6:DT:O2	2.46	0.49
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.94	0.49
3:D:459:ARG:HH22	4:E:88:GLN:HG2	1.78	0.49
1:B:202:ILE:HD13	1:B:207:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:CZ	3:D:488:GLU:HG2	2.43	0.49
3:D:834:ARG:HD2	3:D:835:PRO:HD2	1.94	0.49
3:D:63:GLY:HA2	3:D:66:LYS:HE2	1.95	0.49
1:B:97:LEU:HB2	1:B:110:ILE:HG13	1.95	0.48
3:D:473:LYS:NZ	3:D:477:GLU:OE2	2.35	0.48
3:D:588:LEU:HD23	3:D:723:TRP:CD1	2.48	0.48
1:A:59:VAL:HG11	1:A:73:VAL:HG21	1.95	0.48
3:D:1166:THR:HB	3:D:1206:VAL:HG21	1.96	0.48
1:A:9:LEU:HB2	1:A:23:ILE:HG12	1.96	0.48
1:A:216:VAL:HG13	1:B:216:VAL:HG13	1.95	0.48
2:C:450:THR:HG22	2:C:454:ARG:HE	1.77	0.48
3:D:271:ASP:OD1	3:D:303:GLN:NE2	2.44	0.48
5:F:51:ALA:HB1	5:F:58:ILE:HD11	1.95	0.48
1:B:28:PRO:HD3	1:B:189:PHE:HA	1.95	0.48
3:D:458:LYS:NZ	3:D:462:ASP:OD2	2.44	0.48
3:D:859:GLY:O	3:D:863:THR:OG1	2.31	0.48
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.94	0.48
2:C:731:TYR:CE1	3:D:579:LEU:HB2	2.49	0.48
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.46	0.48
4:E:33:LEU:HD23	4:E:33:LEU:H	1.79	0.48
7:G:9:DC:O2	8:H:20:DG:N2	2.44	0.48
2:C:1060:LYS:N	7:G:18:DA:OP1	2.46	0.47
3:D:500:ARG:HB2	3:D:541:MET:HG2	1.96	0.47
3:D:59:GLU:HG2	3:D:66:LYS:HD3	1.96	0.47
7:G:14:DG:H8	7:G:14:DG:H5'	1.80	0.47
2:C:960:PRO:HD2	2:C:963:LEU:HD22	1.96	0.47
2:C:120:ASP:OD1	2:C:120:ASP:N	2.47	0.47
2:C:412:ILE:HD13	2:C:417:LEU:HD21	1.97	0.47
2:C:463:LEU:HD13	2:C:468:ALA:HB2	1.96	0.47
2:C:737:LEU:HG	2:C:895:ILE:HD12	1.95	0.47
3:D:122:PRO:HG2	8:H:23:DT:H3'	1.97	0.47
3:D:556:ARG:HG3	4:E:35:ILE:HD11	1.96	0.47
1:A:100:GLN:HG3	1:A:133:LYS:HB2	1.97	0.47
1:B:98:ARG:HG2	1:B:135:GLU:HG2	1.97	0.47
1:B:107:ALA:HB2	1:B:123:MET:HE2	1.96	0.47
2:C:1045:SER:HB3	3:D:450:GLU:O	2.14	0.47
3:D:585:LEU:O	3:D:589:THR:OG1	2.31	0.47
3:D:73:ILE:O	3:D:82:VAL:HG22	2.15	0.47
3:D:500:ARG:NH1	3:D:532:PHE:O	2.48	0.47
2:C:288:THR:HG22	2:C:290:GLU:H	1.80	0.46
3:D:291:ARG:NH2	8:H:24:DG:O6	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:589:THR:HG21	3:D:688:MET:HG2	1.97	0.46
2:C:1109:GLY:O	4:E:69:ASN:ND2	2.49	0.46
3:D:1131:GLN:HE21	3:D:1162:LEU:HD12	1.80	0.46
5:F:66:ARG:HD3	5:F:70:PHE:HE2	1.81	0.46
1:A:3:ILE:HD12	1:A:3:ILE:HA	1.85	0.46
3:D:447:MET:HE1	3:D:543:VAL:HG21	1.97	0.46
3:D:867:THR:HG22	3:D:1008:THR:HG23	1.97	0.46
1:A:30:PHE:HE1	1:B:41:THR:HA	1.80	0.46
2:C:572:PRO:HG2	2:C:575:GLU:HB2	1.97	0.46
2:C:615:ALA:HB3	2:C:715:LEU:HD22	1.97	0.46
2:C:1108:LYS:HE3	5:F:114:LEU:HD22	1.97	0.46
1:A:62:GLU:HG2	1:A:77:ILE:HD12	1.96	0.46
2:C:56:VAL:HG21	2:C:500:LEU:HD22	1.98	0.46
3:D:1055:LEU:HB3	3:D:1101:ASP:HB3	1.98	0.46
8:H:13:DG:H2''	8:H:14:DT:OP1	2.16	0.46
3:D:611:VAL:HG22	3:D:634:LYS:HB2	1.98	0.46
1:B:24:GLU:HA	1:B:25:PRO:HA	1.71	0.46
2:C:58:THR:O	2:C:62:GLU:HG3	2.16	0.46
3:D:128:ILE:HD11	3:D:234:LEU:HD11	1.97	0.46
2:C:115:VAL:HG11	2:C:129:TYR:CZ	2.51	0.45
2:C:236:VAL:HG13	2:C:273:ALA:HB1	1.97	0.45
1:B:74:THR:HG21	3:D:608:GLU:HB2	1.98	0.45
2:C:896:GLY:HA2	3:D:431:VAL:HG13	1.99	0.45
1:A:213:LYS:HG2	1:B:232:ILE:HD11	1.98	0.45
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.80	0.45
3:D:363:PRO:HD3	5:F:52:TRP:CE2	2.51	0.45
3:D:1190:ASN:ND2	3:D:1201:ALA:O	2.47	0.45
7:G:12:DG:H2'	7:G:13:DA:H8	1.79	0.45
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.24	0.45
3:D:105:TRP:CZ2	3:D:1230:THR:HG22	2.52	0.45
1:A:173:LYS:HE3	1:A:173:LYS:HB2	1.84	0.45
1:B:45:SER:HA	1:B:144:ARG:HD2	1.99	0.45
1:B:84:VAL:HG22	1:B:120:ASN:CG	2.42	0.45
2:C:446:LEU:HB2	2:C:713:MET:HE2	1.98	0.45
3:D:337:THR:O	5:F:92:SER:HA	2.17	0.45
2:C:891:ASN:OD1	2:C:891:ASN:N	2.45	0.45
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.82	0.45
3:D:111:PRO:O	3:D:113:ARG:NH1	2.50	0.45
2:C:214:PHE:CD1	2:C:224:VAL:HB	2.52	0.44
3:D:389:ARG:HA	3:D:390:PRO:HD3	1.86	0.44
2:C:1067:ARG:NH1	7:G:16:DC:OP1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1127:GLU:OE2	3:D:412:ARG:NH2	2.41	0.44
5:F:88:ASN:C	5:F:90:VAL:H	2.26	0.44
1:A:89:GLU:HB3	1:A:91:GLU:HG2	2.00	0.44
3:D:588:LEU:HD12	3:D:589:THR:HG23	1.99	0.44
8:H:10:DA:H2''	8:H:11:DG:OP1	2.17	0.44
1:B:33:THR:OG1	1:B:34:LEU:N	2.51	0.44
3:D:600:GLN:HB2	3:D:609:THR:HB	1.98	0.44
2:C:32:VAL:H	2:C:33:PRO:CD	2.30	0.44
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.98	0.44
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.45	0.44
2:C:927:ASN:O	2:C:930:GLN:HG2	2.17	0.44
2:C:982:GLU:HG3	3:D:841:ARG:NH1	2.32	0.44
3:D:642:PRO:HG2	3:D:647:GLU:HB2	2.00	0.44
3:D:1046:ILE:HD11	3:D:1120:GLU:HB3	1.98	0.44
2:C:742:VAL:HG13	2:C:878:LYS:HD3	2.00	0.44
2:C:1146:GLU:H	2:C:1146:GLU:HG2	1.60	0.44
3:D:539:ASP:OD2	6:I:7:A:O2'	2.36	0.44
1:B:22:VAL:HG12	1:B:193:ILE:HG12	2.00	0.43
1:B:28:PRO:HB3	1:B:188:ASP:O	2.18	0.43
1:A:185:GLN:HG2	1:A:186:ARG:H	1.83	0.43
2:C:976:VAL:C	2:C:978:ASP:H	2.26	0.43
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.18	0.43
1:B:181:THR:O	1:B:189:PHE:HB2	2.18	0.43
2:C:206:PRO:HD2	2:C:211:TRP:CD1	2.53	0.43
1:A:144:ARG:HH12	1:B:2:LEU:HB2	1.83	0.43
2:C:442:GLN:H	2:C:680:HIS:CD2	2.35	0.43
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.83	0.43
1:A:90:ASP:OD1	1:A:142:ARG:HD3	2.17	0.43
1:B:30:PHE:O	1:B:33:THR:N	2.50	0.43
2:C:370:ILE:HD12	2:C:370:ILE:HA	1.67	0.43
2:C:705:GLY:O	2:C:708:THR:OG1	2.36	0.43
1:B:30:PHE:HA	1:B:33:THR:HG23	1.99	0.43
3:D:105:TRP:HB3	3:D:1234:THR:HG22	2.01	0.43
3:D:282:ARG:HE	3:D:282:ARG:HB2	1.65	0.43
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.99	0.43
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.53	0.43
3:D:823:LEU:HD23	3:D:835:PRO:HB3	2.01	0.43
4:E:47:VAL:HG23	4:E:56:TYR:CE1	2.54	0.43
2:C:723:ILE:O	3:D:730:THR:HG23	2.19	0.43
3:D:759:GLN:HE21	3:D:762:ARG:HH21	1.66	0.43
1:B:112:PRO:HA	1:B:113:PRO:HD2	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1042:HIS:HE1	2:C:1063:PHE:HD1	1.66	0.43
3:D:294:LYS:HB2	3:D:294:LYS:HE3	1.91	0.43
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.83	0.43
3:D:1101:ASP:N	3:D:1101:ASP:OD1	2.52	0.43
2:C:181:ARG:HH22	2:C:203:LYS:HD2	1.83	0.43
3:D:598:GLU:HG2	3:D:599:TYR:H	1.83	0.43
7:G:14:DG:H2'	7:G:15:DT:C6	2.54	0.43
2:C:119:VAL:HG13	2:C:167:ILE:HD11	2.01	0.43
2:C:906:PHE:HA	2:C:912:PRO:HA	2.00	0.43
3:D:384:ASN:H	3:D:401:SER:HB3	1.83	0.43
3:D:575:ALA:O	3:D:713:VAL:HG21	2.18	0.43
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	2.01	0.43
3:D:1090:LYS:HE2	3:D:1103:ASP:HA	1.99	0.43
2:C:445:PRO:HD2	2:C:707:CYS:HB2	2.00	0.42
2:C:853:PHE:HB2	2:C:868:LEU:HB3	2.01	0.42
5:F:170:LEU:HD22	5:F:175:VAL:HG21	2.01	0.42
3:D:173:ARG:HH21	3:D:201:GLY:HA2	1.83	0.42
2:C:624:PRO:HB3	2:C:1029:TYR:CG	2.54	0.42
3:D:445:LYS:HB3	3:D:484:TRP:CZ3	2.54	0.42
3:D:589:THR:HG22	3:D:670:ARG:HG2	2.01	0.42
1:A:182:ARG:HA	1:A:182:ARG:HD2	1.88	0.42
1:B:101:GLY:N	1:B:132:GLY:O	2.53	0.42
3:D:290:LEU:HA	3:D:293:LEU:HD12	2.01	0.42
1:A:222:ALA:HB1	1:B:208:LEU:HG	2.00	0.42
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.55	0.42
3:D:505:HIS:ND1	3:D:1005:GLU:HG3	2.35	0.42
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.16	0.42
2:C:96:ILE:O	2:C:104:SER:HA	2.19	0.42
2:C:38:ARG:HA	2:C:971:ILE:HG13	2.02	0.42
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.83	0.42
3:D:33:THR:HB	3:D:327:MET:HE1	2.02	0.42
1:B:182:ARG:HA	1:B:186:ARG:O	2.20	0.42
3:D:431:VAL:O	3:D:523:GLN:HA	2.19	0.42
5:F:57:VAL:HG21	5:F:68:TRP:CE2	2.55	0.42
1:B:99:LYS:NZ	1:B:104:GLU:O	2.48	0.42
2:C:202:VAL:HG21	2:C:345:LEU:HB2	2.02	0.42
3:D:76:GLU:CD	3:D:76:GLU:H	2.28	0.42
3:D:1030:ARG:NH2	3:D:1034:LEU:HD21	2.35	0.42
3:D:123:LYS:HE3	3:D:127:LYS:HE2	2.02	0.41
3:D:1010:LEU:HD23	3:D:1145:GLN:HG3	2.02	0.41
5:F:81:ARG:HA	5:F:85:ARG:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LEU:HD12	1:B:31:GLY:HA2	2.02	0.41
2:C:227:ASP:O	2:C:228:ARG:HG2	2.20	0.41
2:C:441:ASP:HA	2:C:680:HIS:NE2	2.36	0.41
3:D:20:ILE:HG23	3:D:318:PRO:HB3	2.02	0.41
3:D:1055:LEU:HD11	3:D:1057:ASP:HB3	2.02	0.41
1:A:40:ARG:NH2	2:C:903:ASP:OD1	2.50	0.41
1:A:95:MET:HG2	1:A:112:PRO:HA	2.02	0.41
3:D:24:SER:HB2	3:D:94:HIS:HB3	2.03	0.41
3:D:262:GLN:HB2	3:D:313:VAL:HG11	2.03	0.41
2:C:680:HIS:O	2:C:1034:HIS:HE1	2.04	0.41
2:C:831:GLU:H	2:C:831:GLU:CD	2.28	0.41
2:C:1072:GLU:OE2	2:C:1072:GLU:N	2.52	0.41
3:D:111:PRO:HB3	8:H:22:DA:H5''	2.01	0.41
3:D:1247:GLY:H	3:D:1251:ASN:HD21	1.69	0.41
3:D:851:ILE:HA	3:D:854:HIS:HD2	1.86	0.41
3:D:1050:THR:HB	3:D:1107:VAL:N	2.36	0.41
1:A:84:VAL:HG21	1:A:199:LYS:O	2.20	0.41
2:C:344:TYR:OH	2:C:364:PRO:O	2.26	0.41
2:C:94:SER:HA	2:C:95:PRO:HA	1.76	0.41
3:D:453:LYS:O	3:D:457:MET:HG3	2.21	0.41
1:A:66:VAL:O	1:A:69:VAL:HG22	2.20	0.41
1:B:102:PRO:HD3	1:B:131:LYS:H	1.85	0.41
2:C:732:GLU:HB3	3:D:579:LEU:CD1	2.49	0.41
2:C:824:ILE:HA	5:F:163:VAL:HG13	2.02	0.41
3:D:58:TRP:CE2	3:D:68:VAL:HG13	2.56	0.41
3:D:237:ASP:HB3	3:D:240:LEU:HB3	2.03	0.41
3:D:1036:GLU:CD	3:D:1211:THR:HG1	2.29	0.41
3:D:1154:ILE:O	3:D:1158:VAL:HG23	2.21	0.41
4:E:60:ARG:HG2	4:E:104:LEU:HD11	2.02	0.41
5:F:82:ARG:HB3	5:F:83:SER:H	1.72	0.41
2:C:993:LEU:HG	2:C:994:PRO:HD2	2.02	0.41
3:D:849:TYR:O	3:D:853:THR:HG23	2.21	0.41
1:A:84:VAL:HG12	1:A:120:ASN:ND2	2.35	0.40
2:C:172:GLU:OE1	2:C:442:GLN:NE2	2.54	0.40
2:C:720:LEU:HD23	2:C:913:VAL:HA	2.02	0.40
3:D:627:LEU:HD21	3:D:633:ILE:HD13	2.03	0.40
3:D:238:GLU:HG2	3:D:242:ARG:HH22	1.86	0.40
5:F:131:ILE:H	5:F:131:ILE:HG13	1.72	0.40
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.87	0.40
2:C:211:TRP:CZ3	8:H:14:DT:H2'	2.56	0.40
2:C:465:ARG:NH2	6:I:4:U:OP2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:ALA:HB1	2:C:36:PRO:HD2	2.02	0.40
3:D:114:LEU:HB3	3:D:125:LEU:HD21	2.03	0.40
3:D:742:LYS:HE2	3:D:746:LEU:HD11	2.02	0.40
1:A:24:GLU:OE1	1:A:191:LYS:HD3	2.22	0.40
2:C:282:ARG:HD2	2:C:295:LEU:HD22	2.03	0.40
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.56	0.40
2:C:588:SER:OG	2:C:589:VAL:N	2.55	0.40
3:D:525:HIS:HA	3:D:526:PRO:HD3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/359 (62%)	217 (97%)	6 (3%)	0	100	100
1	B	231/359 (64%)	212 (92%)	17 (7%)	2 (1%)	14	45
2	C	1124/1178 (95%)	1069 (95%)	50 (4%)	5 (0%)	30	62
3	D	1261/1316 (96%)	1202 (95%)	57 (4%)	2 (0%)	43	73
4	E	79/110 (72%)	75 (95%)	4 (5%)	0	100	100
5	F	172/177 (97%)	168 (98%)	3 (2%)	1 (1%)	21	54
All	All	3090/3499 (88%)	2943 (95%)	137 (4%)	10 (0%)	36	67

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	ARG
2	C	370	ILE
1	B	159	ILE
2	C	732	GLU

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Mol	Chain	Res	Type
3	D	593	PRO
2	C	32	VAL
3	D	607	PRO
2	C	922	VAL
2	C	520	VAL
5	F	89	VAL

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	194/308 (63%)	191 (98%)	3 (2%)	57	69
1	B	190/308 (62%)	184 (97%)	6 (3%)	34	56
2	C	951/998 (95%)	935 (98%)	16 (2%)	53	67
3	D	1050/1095 (96%)	1039 (99%)	11 (1%)	68	74
4	E	66/90 (73%)	66 (100%)	0	100	100
5	F	133/136 (98%)	127 (96%)	6 (4%)	24	48
All	All	2584/2935 (88%)	2542 (98%)	42 (2%)	55	68

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	9	LEU
1	A	59	VAL
1	B	17	ASN
1	B	43	LEU
1	B	111	VAL
1	B	147	VAL
1	B	202	ILE
1	B	218	LEU
2	C	39	VAL
2	C	80	VAL
2	C	115	VAL

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Mol	Chain	Res	Type
2	C	224	VAL
2	C	322	LEU
2	C	363	VAL
2	C	370	ILE
2	C	373	PHE
2	C	409	VAL
2	C	435	GLN
2	C	506	VAL
2	C	571	VAL
2	C	875	GLN
2	C	1057	LEU
2	C	1090	THR
2	C	1146	GLU
3	D	82	VAL
3	D	256	MET
3	D	427	ARG
3	D	431	VAL
3	D	535	ASP
3	D	578	ARG
3	D	907	ASP
3	D	910	LEU
3	D	911	ILE
3	D	1009	GLN
3	D	1194	VAL
5	F	31	LEU
5	F	56	GLU
5	F	60	ASP
5	F	85	ARG
5	F	86	PHE
5	F	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	37	ASN
2	C	142	ASN
2	C	178	GLN
2	C	200	HIS
2	C	349	HIS
2	C	386	GLN
2	C	388	GLN
2	C	435	GLN

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Mol	Chain	Res	Type
2	C	700	GLN
2	C	918	ASN
2	C	1066	GLN
3	D	262	GLN
3	D	759	GLN
3	D	767	HIS
3	D	882	GLN
3	D	1001	GLN
3	D	1109	GLN
5	F	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	I	5	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	225/359 (62%)	-0.44	0 100 100	54, 84, 147, 174	0
1	B	233/359 (64%)	-0.28	1 (0%) 88 74	62, 104, 156, 206	0
2	C	1126/1178 (95%)	-0.36	3 (0%) 90 78	51, 95, 169, 212	0
3	D	1265/1316 (96%)	-0.40	0 100 100	48, 101, 187, 239	0
4	E	81/110 (73%)	-0.47	0 100 100	95, 121, 191, 210	0
5	F	174/177 (98%)	-0.35	0 100 100	62, 115, 182, 225	0
6	I	5/5 (100%)	-0.13	0 100 100	120, 131, 144, 156	0
7	G	17/17 (100%)	0.05	0 100 100	121, 141, 179, 180	0
8	H	22/22 (100%)	0.07	0 100 100	135, 177, 224, 228	0
All	All	3148/3543 (88%)	-0.37	4 (0%) 92 87	48, 100, 178, 239	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	979	GLY	2.6
2	C	492	PRO	2.6
1	B	89	GLU	2.2
2	C	325	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	D	1401	1/1	0.99	0.04	90,90,90,90	0
10	ZN	D	1402	1/1	1.00	0.06	184,184,184,184	0
10	ZN	D	1403	1/1	1.00	0.04	137,137,137,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.