



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:56 pm BST

PDB ID : 6TYE
Title : Crystal structure of MTB sigma L transcription initiation complex with 5 nt long RNA primer
Authors : Molodtsov, V.; Ebright, R.H.
Deposited on : 2019-08-08
Resolution : 3.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

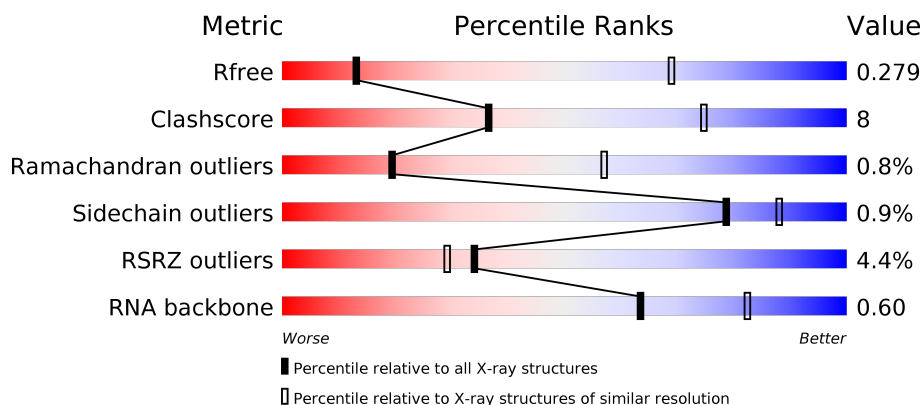
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	F	177	<div> <div>4%</div> <div>71%</div> <div>20%</div> <div>8%</div> </div>
2	G	17	<div> <div>41%</div> <div>59%</div> </div>
3	H	27	<div> <div>11%</div> <div>48%</div> <div>37%</div> <div>15%</div> </div>
4	I	5	<div> <div>20%</div> <div>80%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
5	A	347	<div><div><div>%</div><div><div></div><div>48%</div><div>16%</div><div>35%</div></div></div></div>
5	B	347	<div><div><div>%</div><div><div></div><div>49%</div><div>18%</div><div>33%</div></div></div></div>
6	C	1178	<div><div><div>%</div><div><div></div><div>77%</div><div>17%</div><div>5%</div></div></div></div>
7	D	1316	<div><div><div>8%</div><div><div></div><div>80%</div><div>15%</div><div></div></div></div></div>
8	E	110	<div><div><div>5%</div><div><div></div><div>65%</div><div>8%</div><div>26%</div></div></div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 49194 atoms, of which 24415 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 RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	F	163	Total	C	H	N	O	S	0	0	0
			2516	780	1259	238	237	2			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*AP*TP*CP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	17	Total	C	H	N	O	P	0	0	0
			541	166	192	68	99	16			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	23	Total	C	H	N	O	P	0	0	0
			734	225	259	87	140	23			

- Molecule 4 is a RNA chain called RNA (5'-R(P*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	I	5	Total	C	H	N	O	P	0	0	0
			160	47	55	18	35	5			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	A	225	Total	C	H	N	O	S	0	0	0
			3472	1080	1756	296	338	2			
5	B	232	Total	C	H	N	O	S	0	0	0
			3486	1093	1754	296	341	2			

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	C	1114	Total	C	H	N	O	S	0	0	0
			17219	5411	8576	1512	1681	39			

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	D	1262	Total	C	H	N	O	S	0	0	0
			19814	6182	9942	1790	1860	40			

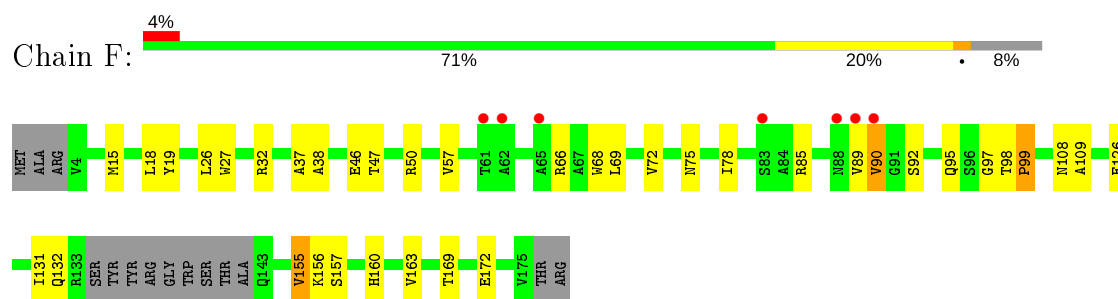
- Molecule 8 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	E	81	Total	C	H	N	O		0	0	0
			1252	403	622	106	121				

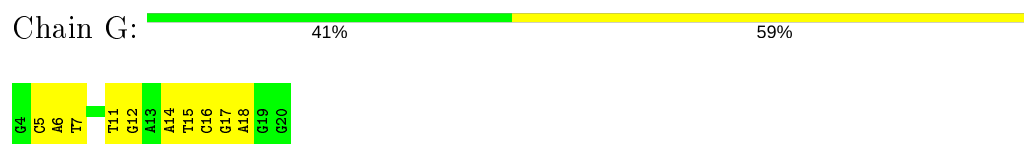
3 Residue-property plots [i](#)

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

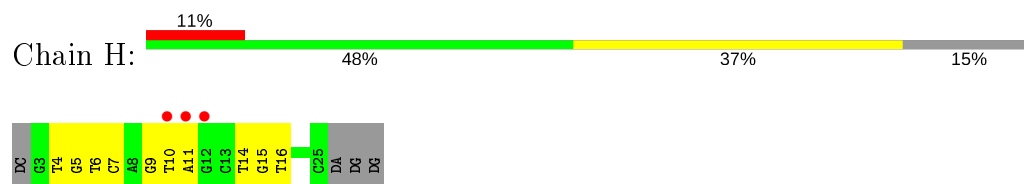
- Molecule 1: RNA polymerase sigma factor



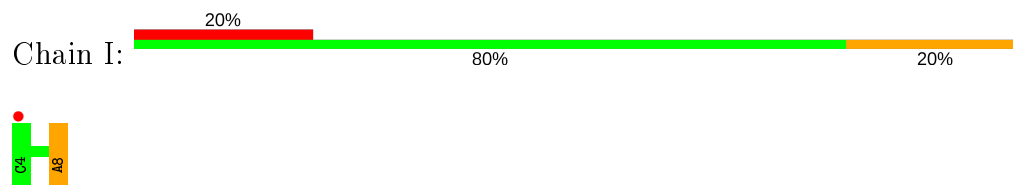
- Molecule 2: DNA (5'-D(*GP*CP*AP*TP*CP*GP*TP*GP*AP*AP*TP*CP*GP*AP*GP*G)-3')



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

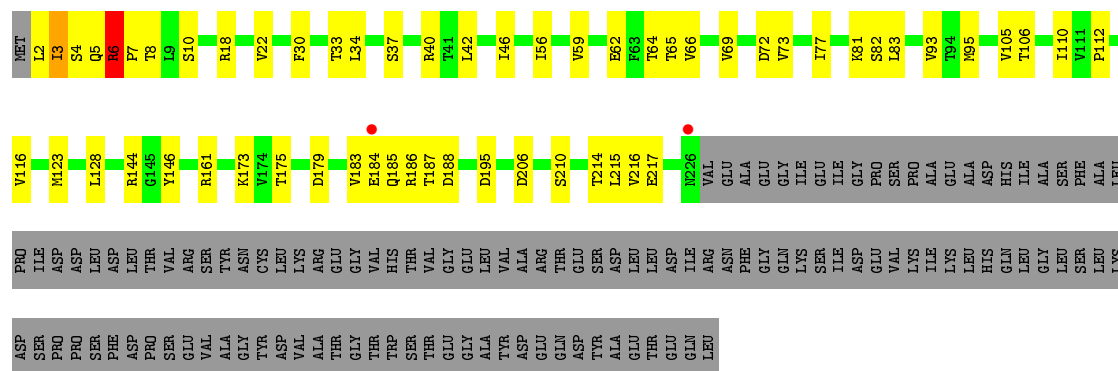


- Molecule 4: RNA (5'-R(P*CP*UP*CP*GP*A)-3')

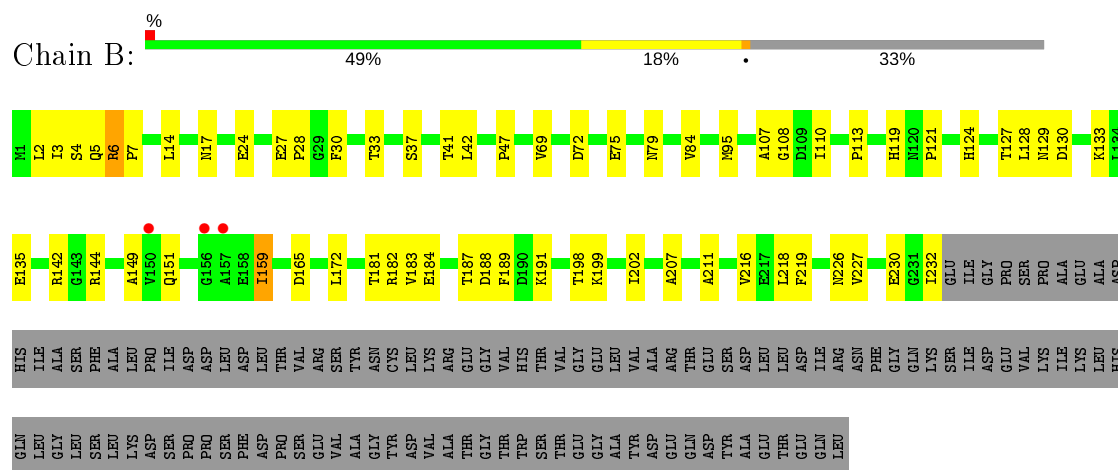


- Molecule 5: DNA-directed RNA polymerase subunit alpha

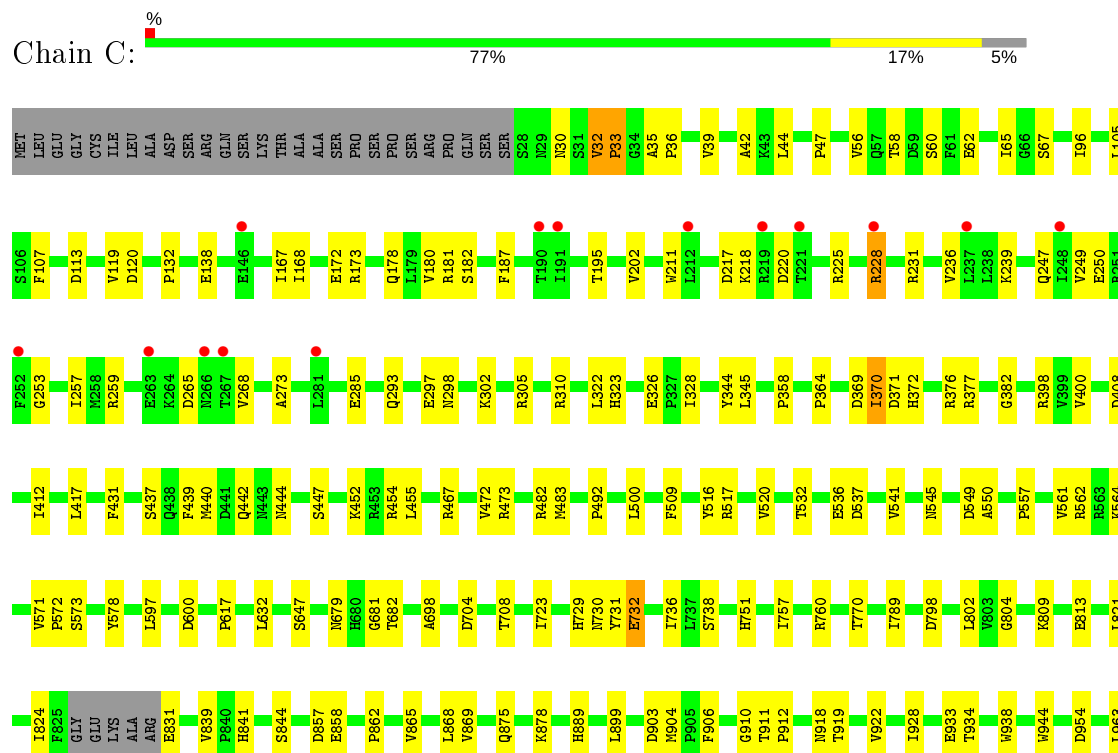


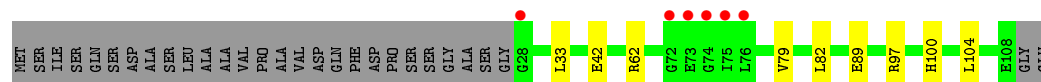


• Molecule 5: DNA-directed RNA polymerase subunit alpha



• Molecule 6: DNA-directed RNA polymerase subunit beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	129.53Å 158.52Å 214.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 3.79 48.02 – 3.79	Depositor EDS
% Data completeness (in resolution range)	96.1 (48.02-3.79) 96.1 (48.02-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.16 _3549	Depositor
R, R_{free}	0.235 , 0.279 0.235 , 0.279	Depositor DCC
R_{free} test set	1904 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	49194	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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 [i](#)

5.1 Standard geometry [i](#)

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	F	0.26	0/1274	0.46	0/1731
2	G	0.59	0/392	0.90	0/604
3	H	0.59	0/532	0.96	0/820
4	I	0.29	0/116	1.00	0/178
5	A	0.32	0/1742	0.57	0/2370
5	B	0.27	0/1758	0.52	0/2397
6	C	0.26	0/8801	0.45	0/11933
7	D	0.27	0/10038	0.45	0/13568
8	E	0.25	0/643	0.41	0/877
All	All	0.29	0/25296	0.50	0/34478

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 [i](#)

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	F	1257	1259	1259	25	0
2	G	349	192	192	8	0
3	H	475	259	260	16	0
4	I	105	55	55	2	0
5	A	1716	1756	1756	47	0
5	B	1732	1754	1754	48	0
6	C	8643	8576	8575	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	9872	9942	9942	151	0
8	E	630	622	622	7	0
All	All	24779	24415	24415	389	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 8.

All (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:40:ARG:HE	5:B:33:THR:HG22	1.31	0.94
7:D:745:ILE:HG21	7:D:785:VAL:HG22	1.55	0.86
6:C:1024:THR:H	7:D:730:THR:HG21	1.41	0.84
3:H:14:DT:OP1	6:C:467:ARG:NH1	2.10	0.84
7:D:832:ILE:HG22	7:D:834:ARG:H	1.42	0.84
7:D:1248:LEU:HD23	7:D:1258:ILE:HB	1.58	0.82
6:C:119:VAL:HG23	6:C:167:ILE:CD1	2.11	0.80
1:F:126:GLU:N	1:F:126:GLU:OE1	2.15	0.79
3:H:15:DG:OP2	6:C:181:ARG:NH1	2.15	0.79
6:C:944:TRP:NE1	6:C:963:LEU:O	2.19	0.75
7:D:1054:ARG:NE	7:D:1056:GLU:OE2	2.21	0.74
6:C:236:VAL:HG13	6:C:273:ALA:HB1	1.70	0.73
7:D:1054:ARG:HD3	7:D:1065:THR:HB	1.71	0.73
1:F:50:ARG:NH1	3:H:4:DT:O4	2.22	0.72
6:C:1087:GLU:HG3	6:C:1091:ILE:HD11	1.71	0.71
6:C:536:GLU:OE2	6:C:562:ARG:NH2	2.22	0.71
7:D:674:ASN:HA	7:D:677:LEU:HD21	1.73	0.69
7:D:677:LEU:H	7:D:677:LEU:HD23	1.57	0.69
7:D:279:ASP:OD1	7:D:282:ARG:NH1	2.26	0.69
6:C:323:HIS:ND1	6:C:326:GLU:OE1	2.26	0.68
5:A:40:ARG:NE	5:B:33:THR:HG22	2.06	0.68
3:H:9:DG:N2	6:C:285:GLU:OE1	2.27	0.68
7:D:926:GLY:N	7:D:961:LYS:O	2.24	0.68
7:D:585:LEU:O	7:D:589:THR:OG1	2.12	0.67
7:D:751:GLU:HG3	7:D:752:ARG:N	2.10	0.67
6:C:444:ASN:O	6:C:447:SER:OG	2.13	0.67
6:C:310:ARG:NH1	6:C:328:ILE:O	2.28	0.66
8:E:42:GLU:OE1	8:E:100:HIS:NE2	2.29	0.66
1:F:46:GLU:OE2	7:D:356:ARG:NH2	2.29	0.65
7:D:550:GLU:OE2	7:D:550:GLU:N	2.28	0.65
6:C:239:LYS:NZ	6:C:265:ASP:OD2	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:723:ILE:O	7:D:730:THR:HG23	1.97	0.64
5:A:206:ASP:OD1	5:B:226:ASN:ND2	2.32	0.63
7:D:749:TYR:CG	7:D:781:ALA:HB2	2.34	0.63
7:D:895:ARG:HB2	7:D:967:THR:HB	1.80	0.63
6:C:65:ILE:HD11	6:C:67:SER:HB3	1.80	0.63
7:D:774:LEU:HA	7:D:777:ILE:HD12	1.81	0.62
6:C:172:GLU:OE1	6:C:442:GLN:NE2	2.32	0.62
5:A:37:SER:OG	5:B:37:SER:OG	2.18	0.62
5:A:18:ARG:NH1	5:A:195:ASP:OD2	2.33	0.61
7:D:1166:THR:HB	7:D:1206:VAL:HG21	1.81	0.61
5:A:2:LEU:HD12	5:B:142:ARG:O	2.02	0.60
7:D:460:LEU:HD11	7:D:483:VAL:HG12	1.82	0.60
5:A:56:ILE:HB	5:A:59:VAL:HG22	1.84	0.59
7:D:588:LEU:HD23	7:D:723:TRP:CD1	2.38	0.59
6:C:113:ASP:HB3	6:C:132:PRO:HG2	1.86	0.58
6:C:731:TYR:OH	7:D:578:ARG:NH1	2.36	0.58
5:B:69:VAL:HG12	5:B:128:LEU:HD23	1.85	0.58
6:C:561:VAL:HG21	6:C:571:VAL:CG1	2.33	0.58
6:C:119:VAL:HG23	6:C:167:ILE:HD11	1.85	0.58
7:D:858:LYS:O	7:D:862:ASP:OD1	2.22	0.58
6:C:217:ASP:OD2	6:C:231:ARG:NH2	2.37	0.58
7:D:885:ILE:HD11	7:D:1248:LEU:HD11	1.86	0.58
7:D:1244:LYS:O	7:D:1246:ASN:N	2.37	0.57
6:C:1067:ARG:NH2	7:D:415:GLN:O	2.38	0.57
7:D:435:GLN:OE1	7:D:435:GLN:N	2.35	0.57
6:C:944:TRP:CA	6:C:993:LEU:HD13	2.35	0.57
7:D:781:ALA:O	7:D:785:VAL:HG23	2.04	0.57
6:C:944:TRP:N	6:C:993:LEU:HD13	2.19	0.56
6:C:1095:ASP:OD2	6:C:1116:GLY:N	2.33	0.56
7:D:741:ARG:HB3	7:D:744:GLU:HB2	1.88	0.56
5:A:40:ARG:NH1	6:C:903:ASP:OD1	2.38	0.56
1:F:68:TRP:O	1:F:72:VAL:HG23	2.06	0.56
7:D:756:VAL:HG13	7:D:765:LEU:HD12	1.87	0.56
6:C:173:ARG:NH1	6:C:437:SER:O	2.39	0.56
5:A:42:LEU:HD23	5:A:46:ILE:HD11	1.88	0.56
6:C:377:ARG:NE	6:C:509:PHE:O	2.33	0.55
5:A:183:VAL:O	5:A:185:GLN:N	2.39	0.55
5:A:105:VAL:HG23	5:A:128:LEU:HD13	1.89	0.54
7:D:926:GLY:C	7:D:940:ARG:HD2	2.27	0.54
7:D:1170:SER:OG	7:D:1173:THR:O	2.25	0.54
7:D:750:GLU:OE2	7:D:834:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:214:THR:OG1	5:B:230:GLU:HG3	2.07	0.54
6:C:369:ASP:O	6:C:370:ILE:HG12	2.07	0.54
7:D:738:VAL:HG22	7:D:739:PRO:HD2	1.89	0.54
6:C:541:VAL:HG12	6:C:578:TYR:HB2	1.90	0.53
1:F:163:VAL:HG13	6:C:824:ILE:HG22	1.91	0.53
5:A:2:LEU:O	5:A:2:LEU:HD12	2.09	0.53
6:C:60:SER:OG	6:C:382:GLY:N	2.41	0.53
5:B:84:VAL:HG12	5:B:199:LYS:HD2	1.90	0.53
7:D:500:ARG:HD2	7:D:534:ALA:HB2	1.91	0.53
4:I:8:A:O2'	7:D:500:ARG:NH2	2.41	0.53
6:C:1088:LEU:HD22	7:D:422:VAL:HG11	1.91	0.53
7:D:1030:ARG:NH2	7:D:1034:LEU:HD21	2.24	0.53
2:G:5:DC:H2''	2:G:6:DA:C8	2.44	0.53
5:B:75:GLU:O	5:B:79:ASN:ND2	2.42	0.52
7:D:752:ARG:HB2	7:D:777:ILE:CG2	2.39	0.52
6:C:600:ASP:OD2	6:C:889:HIS:ND1	2.36	0.52
1:F:90:VAL:HG21	7:D:334:ARG:HB3	1.92	0.52
6:C:168:ILE:HG12	6:C:431:PHE:HB3	1.90	0.52
6:C:549:ASP:OD1	6:C:550:ALA:N	2.42	0.52
5:A:185:GLN:HG2	5:A:186:ARG:H	1.75	0.52
6:C:809:LYS:HE2	6:C:813:GLU:HB2	1.91	0.52
7:D:458:LYS:NZ	7:D:462:ASP:OD2	2.39	0.52
6:C:293:GLN:NE2	6:C:297:GLU:OE2	2.41	0.51
2:G:11:DT:H2'	2:G:12:DG:C8	2.45	0.51
6:C:473:ARG:NH2	6:C:492:PRO:O	2.43	0.51
6:C:253:GLY:HA2	6:C:259:ARG:HE	1.75	0.51
6:C:30:ASN:HB3	6:C:632:LEU:HD23	1.92	0.51
6:C:228:ARG:O	6:C:228:ARG:HG3	2.11	0.51
7:D:482:GLN:N	7:D:482:GLN:OE1	2.38	0.51
7:D:752:ARG:HG2	7:D:755:LYS:HD3	1.93	0.51
5:B:107:ALA:O	5:B:110:ILE:HG22	2.11	0.51
7:D:1274:PRO:HB3	8:E:82:LEU:HD11	1.92	0.51
7:D:756:VAL:HG11	7:D:770:ARG:HG3	1.93	0.51
5:B:133:LYS:NZ	5:B:135:GLU:OE2	2.31	0.51
5:B:6:ARG:N	5:B:7:PRO:CD	2.74	0.51
1:F:92:SER:HA	7:D:337:THR:O	2.10	0.51
7:D:1085:ARG:HA	7:D:1112:MET:HA	1.93	0.51
7:D:742:LYS:NZ	7:D:819:GLY:O	2.30	0.51
6:C:168:ILE:HB	6:C:173:ARG:HD2	1.92	0.50
5:A:56:ILE:HB	5:A:59:VAL:CG2	2.41	0.50
5:B:202:ILE:O	5:B:202:ILE:HD12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:30:PHE:HA	5:B:33:THR:HG23	1.93	0.50
7:D:1172:SER:HB3	7:D:1193:VAL:HG11	1.93	0.50
7:D:729:VAL:HG11	7:D:802:ILE:HD11	1.93	0.50
7:D:752:ARG:O	7:D:777:ILE:HD13	2.11	0.50
6:C:889:HIS:NE2	6:C:933:GLU:OE2	2.44	0.50
5:B:95:MET:HE3	5:B:110:ILE:HD11	1.92	0.50
6:C:857:ASP:O	6:C:858:GLU:HG2	2.11	0.50
7:D:677:LEU:HB2	7:D:678:PRO:HD2	1.93	0.50
5:A:62:GLU:O	5:A:73:VAL:HB	2.12	0.50
7:D:575:ALA:O	7:D:713:VAL:HG21	2.10	0.50
7:D:895:ARG:CB	7:D:967:THR:HB	2.41	0.50
5:A:188:ASP:OD2	5:B:151:GLN:NE2	2.33	0.50
7:D:759:GLN:HG2	7:D:764:ALA:HB3	1.92	0.50
1:F:92:SER:HB2	1:F:95:GLN:HB2	1.94	0.50
7:D:1162:LEU:HD23	7:D:1207:LEU:HA	1.92	0.50
7:D:579:LEU:O	7:D:582:VAL:HG12	2.12	0.50
6:C:1145:ILE:HD11	7:D:7:PHE:HB3	1.94	0.50
5:B:202:ILE:HD13	5:B:207:ALA:HB2	1.93	0.49
1:F:18:LEU:HD12	1:F:18:LEU:C	2.33	0.49
7:D:215:GLU:OE1	7:D:218:ARG:NH1	2.45	0.49
6:C:647:SER:OG	6:C:698:ALA:N	2.45	0.49
7:D:1055:LEU:HB3	7:D:1101:ASP:HB3	1.94	0.49
6:C:32:VAL:HG13	6:C:33:PRO:HD3	1.93	0.49
7:D:759:GLN:O	7:D:765:LEU:N	2.44	0.49
7:D:778:TRP:O	7:D:781:ALA:HB3	2.13	0.49
5:B:84:VAL:HG23	5:B:119:HIS:HB2	1.95	0.49
7:D:40:LYS:HB3	7:D:61:TYR:HE1	1.77	0.49
3:H:10:DT:H2'	3:H:11:DA:C8	2.47	0.49
5:A:34:LEU:HD11	5:B:218:LEU:HD13	1.95	0.49
2:G:11:DT:H4'	7:D:1228:GLU:HG2	1.95	0.49
7:D:758:LYS:O	7:D:762:ARG:HG2	2.13	0.49
6:C:1145:ILE:CD1	7:D:7:PHE:HB3	2.43	0.49
3:H:14:DT:H4'	3:H:15:DG:O5'	2.12	0.49
6:C:934:THR:HG22	6:C:1026:GLY:HA3	1.94	0.48
7:D:1088:VAL:O	7:D:1090:LYS:N	2.46	0.48
1:F:169:THR:O	1:F:172:GLU:HB2	2.13	0.48
5:A:66:VAL:O	5:A:69:VAL:HG22	2.13	0.48
6:C:119:VAL:HG23	6:C:167:ILE:HD12	1.92	0.48
7:D:505:HIS:CE1	7:D:507:LEU:HB2	2.48	0.48
5:A:175:THR:HB	6:C:910:GLY:HA3	1.95	0.48
6:C:202:VAL:HG21	6:C:345:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:561:VAL:HG21	6:C:571:VAL:HG12	1.94	0.48
6:C:239:LYS:HZ2	6:C:268:VAL:HA	1.79	0.48
3:H:14:DT:H5'	3:H:15:DG:OP1	2.13	0.48
5:A:210:SER:O	5:A:214:THR:OG1	2.29	0.48
6:C:1043:ALA:HB2	7:D:447:MET:HG2	1.96	0.48
7:D:105:TRP:CZ2	7:D:1230:THR:HG22	2.48	0.48
7:D:369:ASN:O	7:D:373:MET:HG3	2.14	0.48
6:C:928:ILE:HD11	7:D:817:LEU:HD21	1.96	0.48
6:C:178:GLN:HG2	6:C:180:VAL:HG13	1.96	0.47
6:C:220:ASP:HB3	6:C:257:ILE:HG22	1.97	0.47
6:C:44:LEU:HD11	6:C:545:ASN:HA	1.95	0.47
2:G:15:DT:H73	4:I:8:A:N1	2.29	0.47
7:D:283:ASN:ND2	7:D:283:ASN:O	2.48	0.47
5:B:172:LEU:HD11	5:B:199:LYS:HG2	1.96	0.47
6:C:482:ARG:NH2	6:C:532:THR:O	2.47	0.47
6:C:187:PHE:HD2	6:C:202:VAL:HG22	1.80	0.47
8:E:89:GLU:OE2	8:E:97:ARG:NH1	2.47	0.47
3:H:14:DT:H73	6:C:228:ARG:HD3	1.96	0.47
7:D:1055:LEU:HD22	7:D:1100:SER:HA	1.95	0.47
6:C:120:ASP:N	6:C:120:ASP:OD1	2.48	0.47
1:F:85:ARG:CZ	1:F:89:VAL:HG21	2.45	0.47
2:G:14:DA:H2'	2:G:15:DT:O2	2.15	0.47
7:D:393:GLY:HA3	7:D:399:LEU:HD21	1.97	0.47
6:C:813:GLU:OE2	7:D:56:ARG:HD3	2.15	0.47
7:D:752:ARG:HB2	7:D:777:ILE:HG23	1.96	0.47
6:C:369:ASP:C	6:C:371:ASP:H	2.17	0.47
6:C:557:PRO:O	6:C:573:SER:N	2.47	0.47
6:C:899:LEU:HB2	6:C:904:MET:HE1	1.97	0.47
7:D:756:VAL:HG13	7:D:765:LEU:CD1	2.45	0.47
7:D:752:ARG:C	7:D:777:ILE:HD13	2.36	0.47
1:F:57:VAL:HG13	3:H:5:DG:C2	2.49	0.47
6:C:298:ASN:HA	6:C:302:LYS:HB2	1.97	0.46
7:D:751:GLU:O	7:D:754:ASP:N	2.48	0.46
7:D:849:TYR:O	7:D:853:THR:HG23	2.15	0.46
7:D:651:PHE:O	7:D:653:HIS:N	2.47	0.46
6:C:195:THR:HG21	6:C:218:LYS:HD2	1.96	0.46
8:E:33:LEU:H	8:E:33:LEU:HD23	1.81	0.46
7:D:586:TYR:O	7:D:590:THR:OG1	2.33	0.46
7:D:674:ASN:HA	7:D:677:LEU:CD2	2.43	0.46
6:C:439:PHE:CZ	6:C:679:ASN:HB3	2.51	0.46
7:D:745:ILE:CG2	7:D:785:VAL:HG22	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:929:ALA:HB3	7:D:938:VAL:H	1.81	0.46
5:A:144:ARG:NH2	5:B:27:GLU:OE2	2.48	0.46
3:H:9:DG:N1	6:C:285:GLU:OE2	2.49	0.46
7:D:588:LEU:HD12	7:D:589:THR:N	2.30	0.46
6:C:1111:ASN:HB3	8:E:62:ARG:NH1	2.31	0.46
3:H:14:DT:H3'	6:C:211:TRP:HZ3	1.81	0.46
6:C:1087:GLU:HG2	6:C:1092:LYS:HG3	1.97	0.46
6:C:35:ALA:HB1	6:C:36:PRO:HD2	1.96	0.46
1:F:38:ALA:HB1	7:D:346:ARG:HD3	1.98	0.46
3:H:6:DT:H3'	3:H:7:DC:H5''	1.98	0.46
5:A:93:VAL:HG11	5:A:116:VAL:CG1	2.46	0.45
6:C:906:PHE:HA	6:C:912:PRO:HA	1.98	0.45
7:D:1051:GLY:HA2	7:D:1069:ASP:HB2	1.96	0.45
7:D:775:VAL:HG22	7:D:831:PHE:HB2	1.98	0.45
6:C:704:ASP:HB2	6:C:708:THR:CG2	2.45	0.45
7:D:874:THR:O	7:D:878:VAL:HG23	2.16	0.45
5:A:10:SER:OG	5:A:22:VAL:HG23	2.17	0.45
6:C:802:LEU:HD11	6:C:839:VAL:HG22	1.97	0.45
7:D:1065:THR:HG22	7:D:1066:ILE:N	2.31	0.45
7:D:1190:ASN:ND2	7:D:1201:ALA:O	2.45	0.45
7:D:600:GLN:HB2	7:D:609:THR:HB	1.97	0.45
7:D:910:LEU:O	7:D:910:LEU:HD12	2.17	0.45
7:D:925:LEU:HD22	7:D:938:VAL:HG12	1.98	0.45
5:B:108:GLY:N	5:B:121:PRO:O	2.49	0.45
5:B:129:ASN:OD1	5:B:130:ASP:N	2.41	0.45
6:C:1102:VAL:O	6:C:1106:ILE:HG13	2.17	0.45
6:C:862:PRO:HG2	6:C:865:VAL:HG21	1.99	0.45
5:B:47:PRO:HA	5:B:144:ARG:HG2	1.98	0.45
6:C:821:LEU:HA	6:C:824:ILE:HG12	1.98	0.45
2:G:15:DT:H2'	2:G:16:DC:C6	2.51	0.45
5:A:186:ARG:HG3	5:A:187:THR:HG23	1.99	0.45
6:C:47:PRO:HG3	6:C:517:ARG:HD2	1.99	0.45
7:D:778:TRP:HB2	7:D:823:LEU:HD11	1.99	0.45
6:C:571:VAL:HG22	6:C:572:PRO:HD2	1.99	0.45
6:C:770:THR:N	6:C:804:GLY:O	2.47	0.45
6:C:899:LEU:HB2	6:C:904:MET:CE	2.46	0.45
7:D:104:ILE:HD12	7:D:379:ASP:HB3	1.98	0.45
5:B:181:THR:O	5:B:189:PHE:HB2	2.16	0.45
5:B:149:ALA:HB2	5:B:165:ASP:N	2.31	0.44
6:C:32:VAL:H	6:C:33:PRO:HD3	1.81	0.44
6:C:760:ARG:HG2	6:C:865:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:1065:THR:HA	7:D:1075:VAL:O	2.17	0.44
7:D:926:GLY:CA	7:D:940:ARG:HD2	2.47	0.44
1:F:27:TRP:HZ2	1:F:37:ALA:HB1	1.82	0.44
5:B:124:HIS:CE1	5:B:127:THR:HG23	2.52	0.44
6:C:516:TYR:OH	6:C:536:GLU:OE1	2.33	0.44
6:C:729:HIS:HB2	6:C:736:ILE:HD11	1.98	0.44
5:A:77:ILE:O	5:A:81:LYS:HG3	2.17	0.44
5:A:173:LYS:NZ	6:C:911:THR:HG22	2.33	0.44
6:C:938:TRP:CD1	6:C:1002:VAL:HG21	2.52	0.44
7:D:752:ARG:HB3	7:D:777:ILE:HD13	1.99	0.44
1:F:32:ARG:CB	6:C:398:ARG:HH12	2.31	0.44
6:C:732:GLU:O	6:C:732:GLU:HG3	2.17	0.44
6:C:738:SER:HA	6:C:904:MET:CE	2.47	0.44
7:D:859:GLY:O	7:D:862:ASP:OD1	2.35	0.44
6:C:1068:PHE:HZ	6:C:1076:MET:HG2	1.83	0.44
5:A:3:ILE:HA	5:A:3:ILE:HD12	1.87	0.44
6:C:225:ARG:NH2	6:C:228:ARG:O	2.51	0.44
5:B:95:MET:HG2	5:B:113:PRO:HD2	1.98	0.44
6:C:187:PHE:CD2	6:C:202:VAL:HG22	2.53	0.44
6:C:944:TRP:CA	6:C:993:LEU:CD1	2.96	0.44
5:A:106:THR:HA	5:A:123:MET:O	2.17	0.44
7:D:65:TYR:HD1	7:D:70:PHE:CG	2.36	0.44
7:D:64:LYS:NZ	7:D:76:GLU:OE2	2.35	0.44
6:C:571:VAL:CG2	6:C:572:PRO:HD2	2.48	0.43
7:D:1249:LYS:O	7:D:1253:ILE:HG13	2.18	0.43
7:D:826:ASN:HB3	7:D:832:ILE:HD11	1.99	0.43
6:C:1020:PRO:HB2	6:C:1021:TYR:CD1	2.53	0.43
6:C:1091:ILE:HB	6:C:1102:VAL:HG21	1.98	0.43
6:C:225:ARG:HH12	6:C:228:ARG:HA	1.83	0.43
5:B:187:THR:HG22	7:D:518:GLU:HG2	2.00	0.43
7:D:588:LEU:CD1	7:D:589:THR:HG23	2.48	0.43
7:D:893:THR:HG21	7:D:969:ALA:HB3	1.99	0.43
1:F:155:VAL:O	1:F:156:LYS:C	2.57	0.43
1:F:75:ASN:O	1:F:78:ILE:HG22	2.18	0.43
6:C:597:LEU:HD23	6:C:976:VAL:HG11	2.00	0.43
6:C:844:SER:O	6:C:875:GLN:HB3	2.17	0.43
6:C:730:ASN:O	6:C:918:ASN:HB2	2.18	0.43
1:F:98:THR:HG23	1:F:99:PRO:HD2	2.01	0.43
6:C:32:VAL:CG1	6:C:33:PRO:HD3	2.48	0.43
7:D:1194:VAL:HG23	7:D:1200:PRO:HB3	2.00	0.43
7:D:749:TYR:CZ	7:D:781:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:867:THR:HG22	7:D:1008:THR:HG23	2.00	0.43
7:D:929:ALA:O	7:D:936:VAL:HA	2.18	0.43
2:G:7:DT:OP1	6:C:218:LYS:HE2	2.17	0.43
5:B:183:VAL:HG13	5:B:184:GLU:N	2.34	0.43
5:B:42:LEU:HD23	5:B:211:ALA:HB2	2.00	0.43
6:C:1052:ILE:HD12	6:C:1052:ILE:H	1.83	0.43
5:B:28:PRO:HG3	5:B:188:ASP:C	2.39	0.43
6:C:249:VAL:HG13	6:C:259:ARG:NE	2.33	0.43
6:C:42:ALA:HA	6:C:978:ASP:OD2	2.19	0.43
7:D:775:VAL:CG2	7:D:831:PHE:HB2	2.48	0.43
7:D:1090:LYS:HG2	7:D:1091:HIS:N	2.32	0.43
7:D:443:LEU:HD13	7:D:448:ALA:HB2	2.00	0.43
5:A:82:SER:C	5:A:123:MET:HE1	2.39	0.43
5:B:24:GLU:HB2	5:B:191:LYS:HG3	1.99	0.43
7:D:637:LEU:O	7:D:661:ALA:HA	2.18	0.43
7:D:815:ARG:NH1	7:D:820:MET:O	2.51	0.43
5:B:3:ILE:HG22	5:B:4:SER:N	2.33	0.43
6:C:96:ILE:HD11	6:C:107:PHE:HE2	1.83	0.43
5:A:217:GLU:HG2	5:B:232:ILE:HA	2.01	0.43
5:B:182:ARG:HB3	5:B:187:THR:HA	2.00	0.43
7:D:350:ARG:HD2	7:D:377:SER:OG	2.19	0.43
7:D:565:ILE:HG23	7:D:575:ALA:HB3	2.01	0.43
6:C:455:LEU:HD12	6:C:483:MET:HG3	2.00	0.42
6:C:681:GLY:O	6:C:751:HIS:HA	2.19	0.42
7:D:1065:THR:HG21	7:D:1074:GLU:HB3	2.01	0.42
6:C:372:HIS:NE2	6:C:537:ASP:OD2	2.52	0.42
7:D:535:ASP:OD1	7:D:537:ASP:OD1	2.37	0.42
7:D:111:PRO:O	7:D:113:ARG:NH1	2.52	0.42
5:B:5:GLN:O	5:B:6:ARG:CB	2.68	0.42
6:C:400:VAL:HG22	6:C:417:LEU:O	2.19	0.42
7:D:1047:ALA:O	7:D:1108:GLY:N	2.31	0.42
6:C:1131:LEU:HD13	7:D:105:TRP:CH2	2.54	0.42
5:A:215:LEU:HD13	5:B:219:PHE:CE1	2.55	0.42
6:C:757:ILE:O	6:C:868:LEU:HD12	2.19	0.42
1:F:26:LEU:HD21	1:F:47:THR:HG21	2.02	0.42
5:A:216:VAL:HG13	5:B:216:VAL:HG13	2.02	0.42
6:C:561:VAL:CG2	6:C:571:VAL:HG12	2.50	0.42
7:D:1176:LEU:HD12	7:D:1176:LEU:H	1.85	0.42
5:A:95:MET:HE3	5:A:110:ILE:HG21	2.02	0.42
5:A:83:LEU:HA	5:A:123:MET:HE1	2.02	0.42
5:B:17:ASN:OD1	5:B:17:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:408:ASP:O	6:C:412:ILE:HG13	2.20	0.42
6:C:56:VAL:HG21	6:C:500:LEU:HD22	2.01	0.42
6:C:789:ILE:HD12	6:C:869:VAL:HG11	2.01	0.42
7:D:1274:PRO:HA	8:E:104:LEU:HD23	2.01	0.42
5:A:72:ASP:N	5:A:72:ASP:OD1	2.49	0.42
7:D:826:ASN:HB2	7:D:827:PRO:CD	2.49	0.42
5:A:82:SER:O	5:A:123:MET:HE1	2.20	0.42
6:C:344:TYR:OH	6:C:364:PRO:O	2.26	0.42
6:C:919:THR:CG2	7:D:731:VAL:HG23	2.49	0.42
7:D:925:LEU:HD11	7:D:944:LEU:HD21	2.02	0.42
1:F:108:ASN:O	1:F:109:ALA:C	2.58	0.42
1:F:66:ARG:HA	1:F:69:LEU:HD12	2.01	0.42
5:B:159:ILE:HG13	5:B:159:ILE:O	2.20	0.42
6:C:831:GLU:OE1	6:C:831:GLU:N	2.53	0.41
6:C:798:ASP:HB2	6:C:841:HIS:HA	2.01	0.41
7:D:1277:GLU:N	7:D:1277:GLU:OE1	2.41	0.41
5:A:30:PHE:HE2	5:B:41:THR:HA	1.84	0.41
6:C:944:TRP:HA	6:C:993:LEU:HD13	2.02	0.41
7:D:460:LEU:HD23	7:D:486:VAL:HG21	2.01	0.41
7:D:963:ARG:HB3	7:D:978:CYS:HA	2.01	0.41
5:A:146:TYR:OH	6:C:878:LYS:HE2	2.20	0.41
7:D:1090:LYS:HB3	7:D:1092:GLU:HG2	2.03	0.41
7:D:413:PHE:HA	7:D:417:LEU:HD12	2.02	0.41
2:G:17:DG:H2''	2:G:18:DA:H5'	2.02	0.41
6:C:440:MET:HE3	6:C:452:LYS:HE3	2.02	0.41
3:H:16:DT:H5'	6:C:467:ARG:HG3	2.02	0.41
7:D:589:THR:HG21	7:D:688:MET:HG2	2.01	0.41
7:D:907:ASP:N	7:D:907:ASP:OD1	2.47	0.41
5:A:40:ARG:NH2	6:C:1013:GLY:O	2.49	0.41
7:D:756:VAL:HB	7:D:774:LEU:HD21	2.01	0.41
6:C:1133:LEU:HD11	7:D:105:TRP:HZ3	1.85	0.41
5:A:6:ARG:HH21	5:A:6:ARG:HB3	1.85	0.41
3:H:15:DG:H2''	6:C:467:ARG:HG2	2.03	0.41
6:C:617:PRO:CG	6:C:682:THR:HB	2.51	0.41
7:D:350:ARG:NH1	7:D:373:MET:HB3	2.36	0.41
1:F:15:MET:CE	7:D:366:ILE:HD11	2.50	0.41
1:F:131:ILE:HD12	1:F:132:GLN:N	2.36	0.41
5:A:112:PRO:CB	5:A:116:VAL:HG23	2.51	0.41
6:C:39:VAL:HG12	6:C:963:LEU:HD11	2.03	0.41
7:D:1092:GLU:HG3	7:D:1094:GLY:H	1.86	0.41
7:D:752:ARG:HB3	7:D:777:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:14:LEU:N	5:B:14:LEU:HD22	2.36	0.41
6:C:247:GLN:O	6:C:250:GLU:HB3	2.21	0.41
6:C:58:THR:O	6:C:62:GLU:HG3	2.20	0.41
7:D:1165:VAL:HG12	7:D:1205:PRO:HA	2.02	0.41
5:A:4:SER:HB3	5:B:144:ARG:HH12	1.86	0.41
5:B:198:THR:OG1	5:B:199:LYS:N	2.54	0.41
5:B:95:MET:HG2	5:B:113:PRO:CD	2.51	0.41
6:C:105:LEU:HD12	6:C:138:GLU:O	2.21	0.41
3:H:15:DG:N2	6:C:472:VAL:HG22	2.36	0.41
7:D:1010:LEU:HD13	7:D:1028:LEU:HB2	2.03	0.41
5:A:161:ARG:HB2	5:A:161:ARG:NH1	2.36	0.40
5:A:33:THR:HG21	5:B:37:SER:HA	2.03	0.40
1:F:89:VAL:O	1:F:89:VAL:HG22	2.20	0.40
5:B:72:ASP:OD1	5:B:72:ASP:N	2.53	0.40
6:C:119:VAL:HG13	6:C:120:ASP:N	2.36	0.40
6:C:944:TRP:HA	6:C:993:LEU:CD1	2.50	0.40
7:D:1090:LYS:HE2	7:D:1103:ASP:HA	2.03	0.40
7:D:1274:PRO:CG	8:E:79:VAL:HG21	2.51	0.40
7:D:705:PRO:HG2	7:D:708:VAL:HG23	2.04	0.40
7:D:752:ARG:HB2	7:D:777:ILE:HG21	2.04	0.40
3:H:9:DG:N3	3:H:9:DG:H2'	2.35	0.40
5:A:30:PHE:CE1	5:A:34:LEU:HG	2.56	0.40
5:A:64:THR:OG1	5:A:65:THR:N	2.54	0.40
6:C:305:ARG:HA	6:C:305:ARG:HD2	1.90	0.40
6:C:182:SER:HB2	6:C:377:ARG:HB2	2.04	0.40
1:F:157:SER:O	1:F:160:HIS:N	2.54	0.40
6:C:1070:GLU:HG2	6:C:1074:TRP:CE2	2.57	0.40
7:D:1080:ILE:HG22	7:D:1082:LYS:H	1.86	0.40
7:D:778:TRP:CE2	7:D:835:PRO:HG3	2.56	0.40
6:C:442:GLN:HB2	6:C:679:ASN:HB2	2.02	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	F	159/177 (90%)	134 (84%)	21 (13%)	4 (2%)	5	36
5	A	223/347 (64%)	210 (94%)	10 (4%)	3 (1%)	12	48
5	B	230/347 (66%)	214 (93%)	12 (5%)	4 (2%)	9	43
6	C	1110/1178 (94%)	1041 (94%)	61 (6%)	8 (1%)	22	60
7	D	1258/1316 (96%)	1189 (94%)	63 (5%)	6 (0%)	29	66
8	E	79/110 (72%)	73 (92%)	6 (8%)	0	100	100
All	All	3059/3475 (88%)	2861 (94%)	173 (6%)	25 (1%)	19	57

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	184	GLU
5	B	6	ARG
5	B	159	ILE
6	C	370	ILE
1	F	90	VAL
6	C	732	GLU
7	D	944	LEU
7	D	1089	PHE
7	D	1245	LEU
6	C	32	VAL
1	F	97	GLY
5	B	2	LEU
5	B	227	VAL
6	C	33	PRO
6	C	564	LYS
6	C	922	VAL
7	D	607	PRO
7	D	652	GLY
5	A	5	GLN
7	D	751	GLU
1	F	99	PRO
1	F	155	VAL
5	A	6	ARG
6	C	358	PRO
6	C	520	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	F	125/136 (92%)	124 (99%)	1 (1%)	81	89
5	A	194/297 (65%)	189 (97%)	5 (3%)	46	69
5	B	191/297 (64%)	191 (100%)	0	100	100
6	C	945/998 (95%)	940 (100%)	5 (0%)	88	94
7	D	1047/1095 (96%)	1035 (99%)	12 (1%)	73	85
8	E	66/90 (73%)	66 (100%)	0	100	100
All	All	2568/2913 (88%)	2545 (99%)	23 (1%)	78	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	19	TYR
5	A	3	ILE
5	A	6	ARG
5	A	7	PRO
5	A	8	THR
5	A	179	ASP
6	C	228	ARG
6	C	322	LEU
6	C	376	ARG
6	C	454	ARG
6	C	954	ASP
7	D	279	ASP
7	D	283	ASN
7	D	359	ASP
7	D	443	LEU
7	D	459	ARG
7	D	539	ASP
7	D	578	ARG
7	D	588	LEU
7	D	804	ASP
7	D	1069	ASP
7	D	1240	CYS

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Mol	Chain	Res	Type
7	D	1250	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	I	8	A

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	F	163/177 (92%)	0.43	7 (4%) 35 30	60, 123, 162, 182	0
2	G	17/17 (100%)	-0.20	0 100 100	56, 75, 132, 142	0
3	H	23/27 (85%)	0.64	3 (13%) 3 4	83, 133, 182, 189	0
4	I	5/5 (100%)	0.65	1 (20%) 1 1	62, 67, 74, 115	0
5	A	225/347 (64%)	-0.12	2 (0%) 84 79	44, 69, 108, 136	0
5	B	232/347 (66%)	0.13	3 (1%) 77 70	49, 85, 122, 151	0
6	C	1114/1178 (94%)	-0.05	15 (1%) 77 70	27, 61, 137, 171	0
7	D	1262/1316 (95%)	0.25	101 (8%) 12 10	26, 73, 193, 275	0
8	E	81/110 (73%)	0.04	6 (7%) 14 11	53, 80, 135, 159	0
All	All	3122/3524 (88%)	0.11	138 (4%) 34 29	26, 73, 152, 275	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	D	814	THR	9.1
7	D	763	GLY	8.9
7	D	761	GLN	8.6
7	D	828	LYS	8.3
7	D	776	GLU	7.8
7	D	764	ALA	7.5
7	D	829	GLY	7.5
7	D	771	ASN	7.3
7	D	830	GLU	6.7
7	D	810	ASN	6.4
7	D	809	GLY	6.2
7	D	773	ALA	6.1
7	D	780	GLU	6.0
7	D	767	HIS	5.6
7	D	816	THR	5.6

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Mol	Chain	Res	Type	RSRZ
7	D	768	ASP	5.4
7	D	833	PRO	5.2
7	D	826	ASN	5.1
7	D	817	LEU	5.1
7	D	757	GLU	4.9
7	D	811	PHE	4.8
7	D	740	PRO	4.7
7	D	762	ARG	4.7
7	D	753	ALA	4.6
7	D	827	PRO	4.5
7	D	755	LYS	4.5
7	D	813	GLN	4.4
1	F	89	VAL	4.3
7	D	1082	LYS	4.3
6	C	267	THR	4.2
7	D	742	LYS	4.2
7	D	760	PHE	4.2
7	D	1281	ALA	4.1
7	D	653	HIS	4.1
7	D	818	ALA	4.0
7	D	770	ARG	3.9
7	D	1096	GLU	3.9
7	D	785	VAL	3.8
7	D	747	ASP	3.8
3	H	12	DG	3.8
7	D	787	GLN	3.8
7	D	819	GLY	3.7
7	D	825	THR	3.7
6	C	219	ARG	3.7
7	D	754	ASP	3.6
7	D	759	GLN	3.5
6	C	237	LEU	3.5
7	D	786	GLY	3.5
8	E	28	GLY	3.5
7	D	1087	ARG	3.5
7	D	1095	SER	3.4
7	D	775	VAL	3.4
7	D	815	ARG	3.4
7	D	779	LYS	3.4
7	D	741	ARG	3.3
7	D	758	LYS	3.3
7	D	820	MET	3.2

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Mol	Chain	Res	Type	RSRZ
7	D	756	VAL	3.2
7	D	1280	ALA	3.1
7	D	781	ALA	3.0
7	D	750	GLU	2.9
7	D	772	GLU	2.8
7	D	744	GLU	2.8
1	F	90	VAL	2.8
6	C	266	ASN	2.8
7	D	793	TYR	2.8
6	C	248	ILE	2.7
1	F	62	ALA	2.7
7	D	743	LYS	2.7
6	C	221	THR	2.7
7	D	82	VAL	2.7
7	D	769	GLU	2.7
1	F	88	ASN	2.7
8	E	73	GLU	2.7
5	B	157	ALA	2.6
7	D	1078	ASP	2.6
7	D	796	ASP	2.6
7	D	766	ASN	2.6
7	D	1104	HIS	2.5
3	H	11	DA	2.5
7	D	835	PRO	2.5
7	D	794	PRO	2.5
7	D	1026	GLY	2.5
7	D	752	ARG	2.4
7	D	774	LEU	2.4
7	D	808	THR	2.4
7	D	788	ALA	2.4
7	D	746	LEU	2.4
7	D	831	PHE	2.4
7	D	83	THR	2.4
7	D	737	LEU	2.4
7	D	649	GLU	2.3
6	C	212	LEU	2.3
7	D	765	LEU	2.3
8	E	76	LEU	2.3
6	C	228	ARG	2.3
7	D	1105	VAL	2.3
7	D	1069	ASP	2.3
5	A	226	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
7	D	824	VAL	2.3
6	C	191	ILE	2.3
7	D	1200	PRO	2.3
6	C	1146	GLU	2.3
7	D	250	GLU	2.3
6	C	146	GLU	2.3
7	D	834	ARG	2.2
7	D	1074	GLU	2.2
7	D	1089	PHE	2.2
7	D	797	ASN	2.2
7	D	1199	GLU	2.2
7	D	782	THR	2.2
7	D	789	LEU	2.2
5	A	184	GLU	2.2
7	D	832	ILE	2.2
6	C	252	PHE	2.2
8	E	74	GLY	2.2
5	B	156	GLY	2.2
7	D	812	THR	2.2
7	D	807	ALA	2.2
7	D	1091	HIS	2.2
5	B	150	VAL	2.2
6	C	281	LEU	2.1
7	D	1057	ASP	2.1
7	D	334	ARG	2.1
7	D	1059	GLU	2.1
8	E	72	GLY	2.1
1	F	83	SER	2.1
6	C	263	GLU	2.1
4	I	4	C	2.1
1	F	61	THR	2.1
1	F	65	ALA	2.1
7	D	1093	ASP	2.1
7	D	37	ARG	2.1
8	E	75	ILE	2.0
7	D	784	GLU	2.0
6	C	190	THR	2.0
3	H	10	DT	2.0
7	D	1061	PHE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.