



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:25 PM UTC

PDB ID : 6TYE / pdb_00006tye
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 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

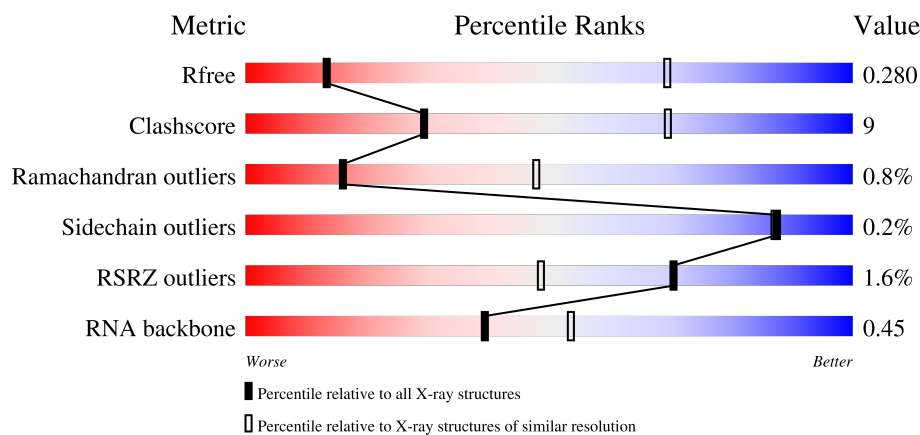
1 Overall quality at a glance

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}	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	F	177	3% 69% 21% 8%
2	G	17	41% 59%
3	H	27	48% 37% 15%
4	I	5	80% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	347	%49%15%35% ..
5	B	347	3%46%20%33% .
6	C	1178	%77%17%5%
7	D	1316	2%79%16% .
8	E	110	2%65%8%26%

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			

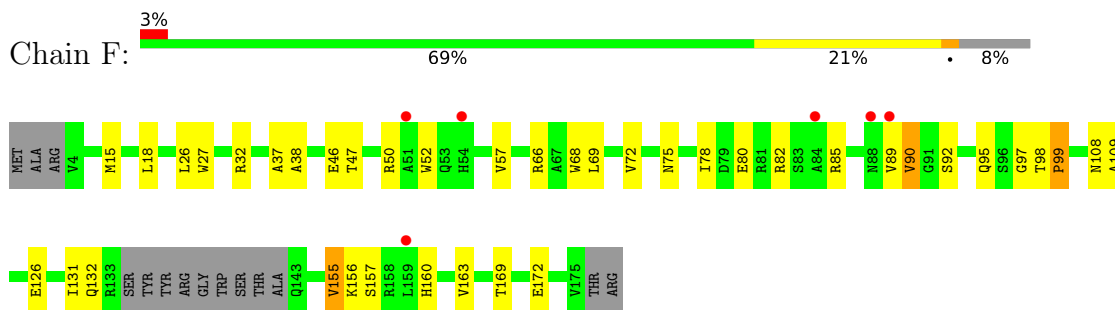
- Molecule 8 is a protein called DNA-directed RNA polymerase subunit omega.

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

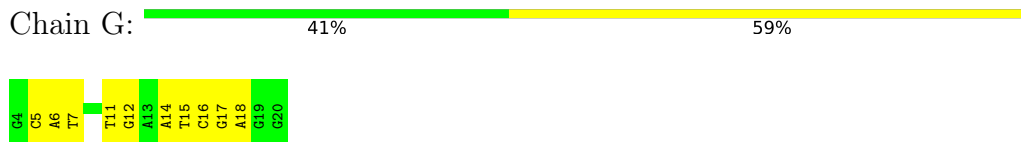
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: RNA polymerase sigma factor



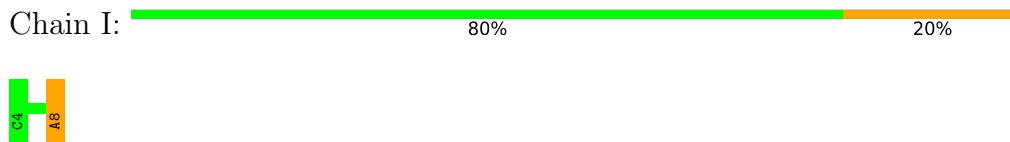
- Molecule 2: DNA (5'-D(*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*AP*TP*CP*GP*AP*GP*G)-3')



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

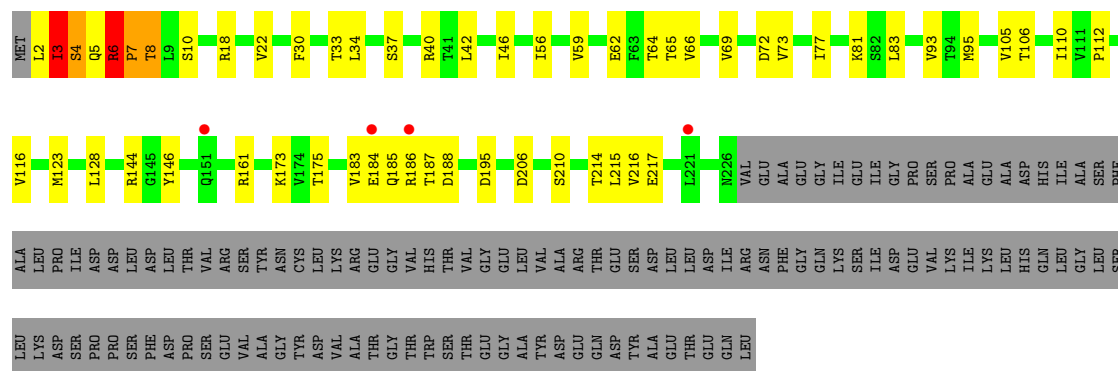


- Molecule 4: RNA (5'-R(P*CP*UP*CP*GP*A)-3')

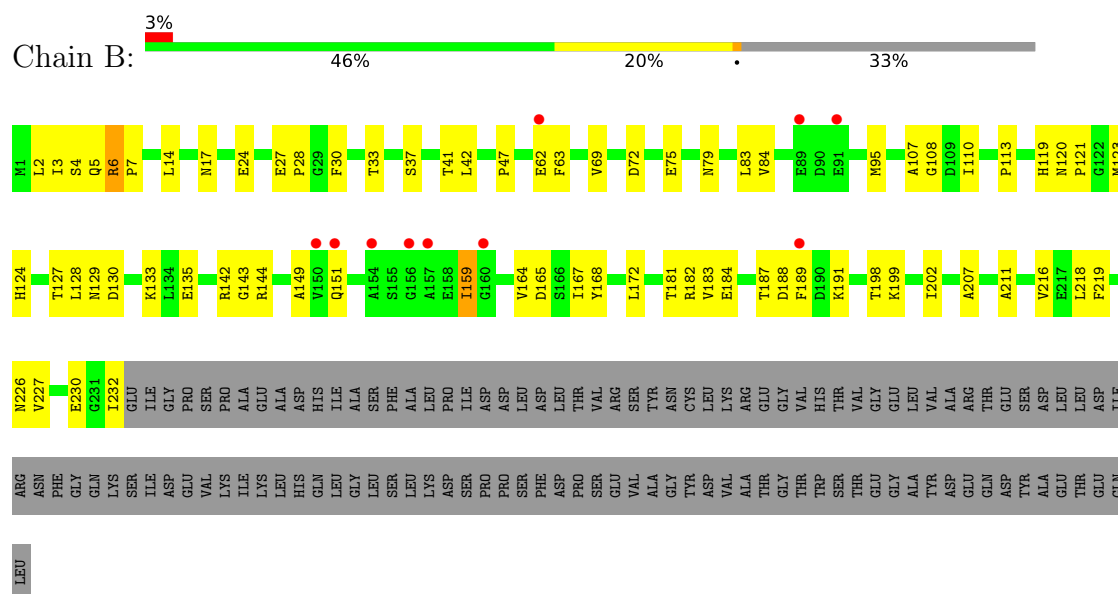


- Molecule 5: DNA-directed RNA polymerase subunit alpha

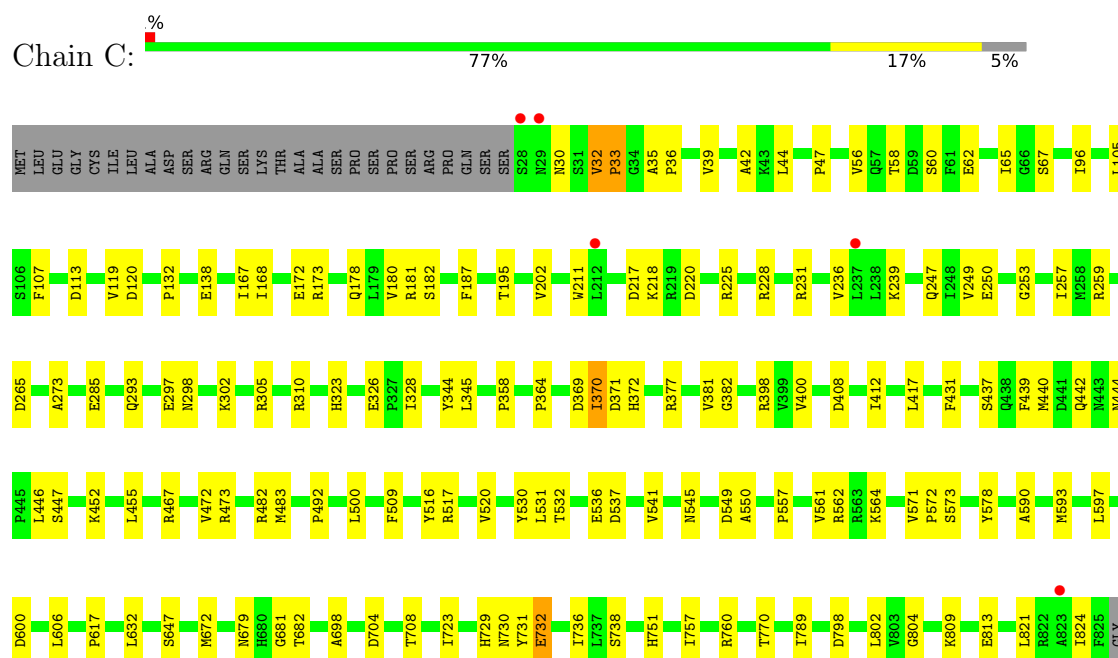


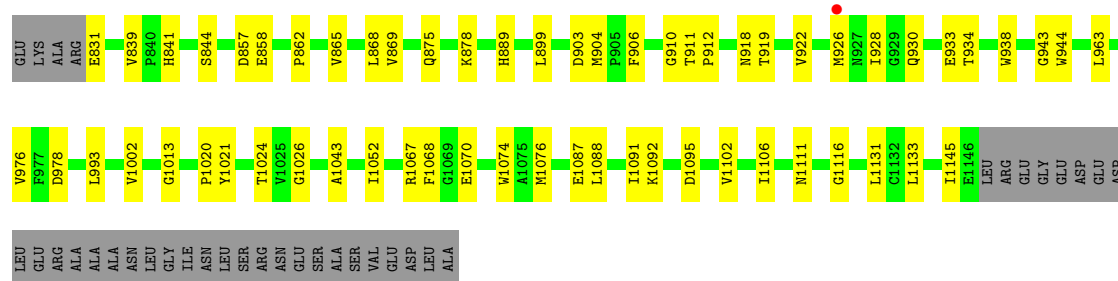


• Molecule 5: DNA-directed RNA polymerase subunit alpha

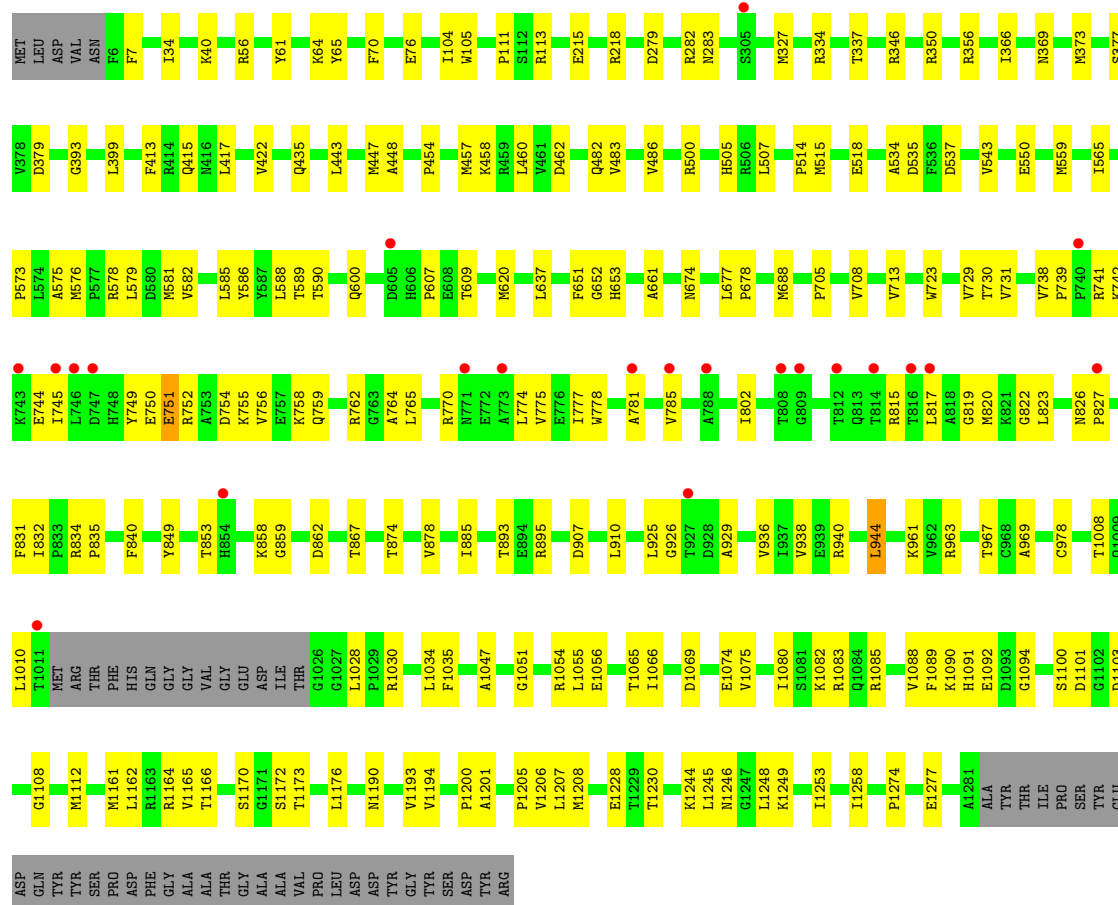
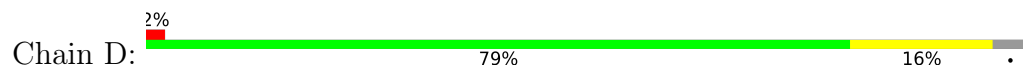


• Molecule 6: DNA-directed RNA polymerase subunit beta

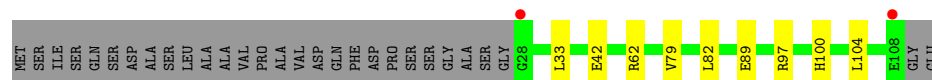




• Molecule 7: DNA-directed RNA polymerase subunit beta'



• Molecule 8: DNA-directed RNA polymerase subunit omega



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) 96.0 (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 0.236 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (4.28%)	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)	0.33 , 44.7	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	0.88	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	0.18	0/1274	0.39	0/1731
2	G	0.24	0/392	0.49	0/604
3	H	0.23	0/532	0.49	0/820
4	I	0.17	0/116	0.40	0/178
5	A	0.33	0/1742	0.59	4/2370 (0.2%)
5	B	0.17	0/1758	0.45	0/2397
6	C	0.14	0/8801	0.33	0/11933
7	D	0.16	0/10038	0.35	0/13568
8	E	0.13	0/643	0.30	0/877
All	All	0.18	0/25296	0.38	4/34478 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	7	PRO	N-CA-C	7.31	121.45	111.22
5	A	4	SER	N-CA-C	6.42	118.61	110.33
5	A	3	ILE	CB-CA-C	5.66	119.17	110.91
5	A	8	THR	CB-CA-C	-5.22	99.05	109.33

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	27	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	45	0
5	B	1732	1754	1754	56	0
6	C	8643	8576	8575	158	0
7	D	9872	9942	9942	170	0
8	E	630	622	622	7	0
All	All	24779	24415	24415	422	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 9.

All (422) 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
5:B:167:ILE:HG23	7:D:620:MET:HE1	1.63	0.78
6:C:926:MET:HE1	7:D:817:LEU:HA	1.66	0.77
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
5:B:95:MET:HE3	5:B:110:ILE:HD11	1.72	0.72
7:D:454:PRO:HA	7:D:457:MET:HE2	1.71	0.72
6:C:536:GLU:OE2	6:C:562:ARG:NH2	2.22	0.71
6:C:1087:GLU:HG3	6:C:1091:ILE:HD11	1.71	0.71
6:C:899:LEU:HB2	6:C:904:MET:HE1	1.72	0.70
7:D:573:PRO:HB2	7:D:576:MET:HE2	1.74	0.70
7:D:674:ASN:HA	7:D:677:LEU:HD21	1.73	0.69
7:D:677:LEU:HD23	7:D:677:LEU:H	1.57	0.69
7:D:279:ASP:OD1	7:D:282:ARG:NH1	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:323:HIS:ND1	6:C:326:GLU:OE1	2.26	0.68
3:H:9:DG:N2	6:C:285:GLU:OE1	2.27	0.68
5:A:40:ARG:NE	5:B:33:THR:HG22	2.06	0.68
7:D:926:GLY:N	7:D:961:LYS:O	2.24	0.68
6:C:239:LYS:NZ	6:C:265:ASP:OD2	2.25	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
5:A:83:LEU:HA	5:A:123:MET:HE1	1.77	0.65
6:C:1076:MET:HE1	7:D:559:MET:CE	2.25	0.65
1:F:46:GLU:OE2	7:D:356:ARG:NH2	2.29	0.65
7:D:550:GLU:N	7:D:550:GLU:OE2	2.28	0.65
7:D:447:MET:HE1	7:D:543:VAL:HG21	1.79	0.64
7:D:578:ARG:H	7:D:581:MET:HE3	1.62	0.64
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
5:B:133:LYS:NZ	5:B:135:GLU:OE2	2.31	0.63
6:C:65:ILE:HD11	6:C:67:SER:HB3	1.80	0.63
6:C:440:MET:HE3	6:C:452:LYS:HE3	1.81	0.62
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
7:D:926:GLY:C	7:D:940:ARG:HD2	2.27	0.59
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
5:A:95:MET:HE3	5:A:110:ILE:HG21	1.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:885:ILE:HD11	7:D:1248:LEU:HD11	1.86	0.58
6:C:738:SER:HA	6:C:904:MET:HE3	1.86	0.57
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:N	7:D:435:GLN:OE1	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
1:F:18:LEU:C	1:F:18:LEU:HD12	2.33	0.54
5:B:83:LEU:HB2	5:B:123:MET:HE1	1.89	0.54
7:D:750:GLU:OE2	7:D:834:ARG:NH1	2.40	0.54
7:D:1170:SER:OG	7:D:1173:THR:O	2.25	0.54
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
1:F:163:VAL:HG13	6:C:824:ILE:HG22	1.91	0.53
6:C:541:VAL:HG12	6:C:578:TYR:HB2	1.90	0.53
5:A:2:LEU:HD12	5:A:2:LEU:O	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:1076:MET:HE1	7:D:559:MET:HE1	1.89	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
7:D:34:ILE:HD13	7:D:327:MET:HE3	1.91	0.52
1:F:90:VAL:HG21	7:D:334:ARG:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:11:DT:H2'	2:G:12:DG:C8	2.45	0.51
6:C:293:GLN:NE2	6:C:297:GLU:OE2	2.41	0.51
6:C:473:ARG:NH2	6:C:492:PRO:O	2.43	0.51
6:C:30:ASN:HB3	6:C:632:LEU:HD23	1.92	0.51
6:C:253:GLY:HA2	6:C:259:ARG:HE	1.75	0.51
6:C:369:ASP:C	6:C:371:ASP:H	2.17	0.51
5:B:167:ILE:CG2	7:D:620:MET:HE1	2.39	0.51
7:D:482:GLN:OE1	7:D:482:GLN:N	2.38	0.51
7:D:752:ARG:HG2	7:D:755:LYS:HD3	1.93	0.51
7:D:1164:ARG:HB2	7:D:1208:MET:HE2	1.93	0.51
5:B:107:ALA:O	5:B:110:ILE:HG22	2.11	0.51
7:D:752:ARG:C	7:D:777:ILE:HD13	2.36	0.51
7:D:756:VAL:HG11	7:D:770:ARG:HG3	1.93	0.51
7:D:1274:PRO:HB3	8:E:82:LEU:HD11	1.92	0.51
1:F:92:SER:HA	7:D:337:THR:O	2.10	0.51
5:B:6:ARG:N	5:B:7:PRO:CD	2.74	0.51
6:C:228:ARG:O	6:C:228:ARG:HG3	2.11	0.51
7:D:742:LYS:NZ	7:D:819:GLY:O	2.30	0.51
7:D:1085:ARG:HA	7:D:1112:MET:HA	1.93	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:30:PHE:HA	5:B:33:THR:HG23	1.93	0.50
5:B:202:ILE:HD12	5:B:202:ILE:O	2.10	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
7:D:1172:SER:HB3	7:D:1193:VAL:HG11	1.93	0.50
6:C:889:HIS:NE2	6:C:933:GLU:OE2	2.44	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
1:F:92:SER:HB2	1:F:95:GLN:HB2	1.94	0.50
5:A:188:ASP:OD2	5:B:151:GLN:NE2	2.33	0.50
7:D:458:LYS:NZ	7:D:462:ASP:OD2	2.39	0.50
7:D:759:GLN:HG2	7:D:764:ALA:HB3	1.92	0.50
7:D:579:LEU:O	7:D:582:VAL:HG12	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:1162:LEU:HD23	7:D:1207:LEU:HA	1.92	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
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
2:G:11:DT:H4'	7:D:1228:GLU:HG2	1.95	0.49
5:A:34:LEU:HD11	5:B:218:LEU:HD13	1.95	0.49
3:H:14:DT:H4'	3:H:15:DG:O5'	2.12	0.49
6:C:1145:ILE:CD1	7:D:7:PHE:HB3	2.43	0.49
7:D:758:LYS:O	7:D:762:ARG:HG2	2.13	0.49
1:F:169:THR:O	1:F:172:GLU:HB2	2.13	0.48
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
5:A:66:VAL:O	5:A:69:VAL:HG22	2.13	0.48
1:F:155:VAL:O	1:F:156:LYS:C	2.57	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
6:C:561:VAL:HG21	6:C:571:VAL:HG12	1.94	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
5:B:28:PRO:HG3	5:B:188:ASP:C	2.39	0.48
6:C:1043:ALA:HB2	7:D:447:MET:HG2	1.96	0.48
7:D:820:MET:HE2	7:D:822:GLY:HA2	1.96	0.48
6:C:928:ILE:HD11	7:D:817:LEU:HD21	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:178:GLN:HG2	6:C:180:VAL:HG13	1.96	0.47
2:G:15:DT:H73	4:I:8:A:N1	2.29	0.47
6:C:44:LEU:HD11	6:C:545:ASN:HA	1.95	0.47
6:C:220:ASP:HB3	6:C:257:ILE:HG22	1.97	0.47
7:D:283:ASN:O	7:D:283:ASN:ND2	2.48	0.47
5:B:172:LEU:HD11	5:B:199:LYS:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:C:120:ASP:OD1	6:C:120:ASP:N	2.48	0.47
6:C:813:GLU:OE2	7:D:56:ARG:HD3	2.15	0.47
7:D:393:GLY:HA3	7:D:399:LEU:HD21	1.97	0.47
7:D:752:ARG:HB2	7:D:777:ILE:HG23	1.96	0.47
1:F:57:VAL:HG13	3:H:5:DG:C2	2.49	0.47
6:C:557:PRO:O	6:C:573:SER:N	2.47	0.47
7:D:756:VAL:HG13	7:D:765:LEU:CD1	2.45	0.47
1:F:108:ASN:O	1:F:109:ALA:C	2.58	0.46
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:HD23	8:E:33:LEU:H	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
7:D:929:ALA:HB3	7:D:938:VAL:H	1.81	0.46
3:H:9:DG:N1	6:C:285:GLU:OE2	2.49	0.46
5:A:144:ARG:NH2	5:B:27:GLU:OE2	2.48	0.46
7:D:588:LEU:HD12	7:D:589:THR:N	2.30	0.46
3:H:14:DT:H3'	6:C:211:TRP:HZ3	1.81	0.46
6:C:1111:ASN:HB3	8:E:62:ARG:NH1	2.31	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
6:C:35:ALA:HB1	6:C:36:PRO:HD2	1.96	0.46
6:C:1087:GLU:HG2	6:C:1092:LYS:HG3	1.97	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:775:VAL:HG22	7:D:831:PHE:HB2	1.98	0.45
7:D:1051:GLY:HA2	7:D:1069:ASP:HB2	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:600:GLN:HB2	7:D:609:THR:HB	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:910:LEU:HD12	7:D:910:LEU:O	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:862:PRO:HG2	6:C:865:VAL:HG21	1.99	0.45
6:C:1102:VAL:O	6:C:1106:ILE:HG13	2.17	0.45
2:G:15:DT:H2'	2:G:16:DC:C6	2.51	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
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
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
1:F:27:TRP:HZ2	1:F:37:ALA:HB1	1.82	0.44
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
7:D:926:GLY:CA	7:D:940:ARG:HD2	2.47	0.44
7:D:1065:THR:HA	7:D:1075:VAL:O	2.17	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
1:F:15:MET:HE2	1:F:52:TRP:HB2	2.00	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
5:B:84:VAL:HG22	5:B:120:ASN:CG	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3:ILE:HD12	5:A:3:ILE:HA	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
7:D:34:ILE:HG23	7:D:327:MET:HE1	1.99	0.44
5:A:106:THR:HA	5:A:123:MET:O	2.17	0.44
7:D:64:LYS:NZ	7:D:76:GLU:OE2	2.35	0.44
7:D:65:TYR:HD1	7:D:70:PHE:CG	2.36	0.44
6:C:167:ILE:C	6:C:168:ILE:HD12	2.43	0.43
6:C:571:VAL:CG2	6:C:572:PRO:HD2	2.48	0.43
7:D:826:ASN:HB3	7:D:832:ILE:HD11	1.99	0.43
7:D:1249:LYS:O	7:D:1253:ILE:HG13	2.18	0.43
1:F:75:ASN:O	1:F:78:ILE:HG22	2.18	0.43
5:B:187:THR:HG22	7:D:518:GLU:HG2	2.00	0.43
6:C:225:ARG:HH12	6:C:228:ARG:HA	1.83	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
7:D:514:PRO:O	7:D:515:MET:HE2	2.17	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:98:THR:HG23	1:F:99:PRO:HD2	2.01	0.43
6:C:597:LEU:HD23	6:C:976:VAL:HG11	2.00	0.43
6:C:730:ASN:O	6:C:918:ASN:HB2	2.18	0.43
6:C:844:SER:O	6:C:875:GLN:HB3	2.17	0.43
2:G:7:DT:OP1	6:C:218:LYS:HE2	2.17	0.43
6:C:32:VAL:CG1	6:C:33:PRO:HD3	2.48	0.43
7:D:749:TYR:CZ	7:D:781:ALA:HA	2.53	0.43
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
7:D:1194:VAL:HG23	7:D:1200:PRO:HB3	2.00	0.43
5:B:42:LEU:HD23	5:B:211:ALA:HB2	2.00	0.43
5:B:183:VAL:HG13	5:B:184:GLU:N	2.34	0.43
6:C:1052:ILE:HD12	6:C:1052:ILE:H	1.83	0.43
6:C:42:ALA:HA	6:C:978:ASP:OD2	2.19	0.43
6:C:249:VAL:HG13	6:C:259:ARG:NE	2.33	0.43
7:D:775:VAL:CG2	7:D:831:PHE:HB2	2.48	0.43
7:D:443:LEU:HD13	7:D:448:ALA:HB2	2.00	0.43
7:D:1090:LYS:HG2	7:D:1091:HIS:N	2.32	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:149:ALA:HB2	5:B:164:VAL:C	2.43	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
6:C:1131:LEU:HD13	7:D:105:TRP:CH2	2.54	0.42
7:D:1047:ALA:O	7:D:1108:GLY:N	2.31	0.42
1:F:26:LEU:HD21	1:F:47:THR:HG21	2.02	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
7:D:447:MET:HE1	7:D:543:VAL:CG2	2.48	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:H	7:D:1176:LEU:HD12	1.85	0.42
5:B:17:ASN:OD1	5:B:17:ASN:N	2.53	0.42
6:C:56:VAL:HG21	6:C:500:LEU:HD22	2.01	0.42
6:C:408:ASP:O	6:C:412:ILE:HG13	2.20	0.42
6:C:789:ILE:HD12	6:C:869:VAL:HG11	2.01	0.42
7:D:1083:ARG:HD2	7:D:1112:MET:HE3	2.02	0.42
7:D:1274:PRO:HA	8:E:104:LEU:HD23	2.01	0.42
5:A:72:ASP:OD1	5:A:72:ASP:N	2.49	0.42
7:D:826:ASN:HB2	7:D:827:PRO:CD	2.49	0.42
1:F:66:ARG:HA	1:F:69:LEU:HD12	2.01	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
5:B:159:ILE:O	5:B:159:ILE:HG13	2.20	0.42
6:C:606:LEU:HD23	6:C:606:LEU:C	2.45	0.42
6:C:1076:MET:HE1	7:D:559:MET:HE3	2.01	0.42
6:C:798:ASP:HB2	6:C:841:HIS:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:831:GLU:OE1	6:C:831:GLU:N	2.53	0.41
7:D:1277:GLU:OE1	7:D:1277:GLU:N	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
2:G:17:DG:H2''	2:G:18:DA:H5'	2.02	0.41
5:A:146:TYR:OH	6:C:878:LYS:HE2	2.20	0.41
7:D:413:PHE:HA	7:D:417:LEU:HD12	2.02	0.41
7:D:1090:LYS:HB3	7:D:1092:GLU:HG2	2.03	0.41
3:H:16:DT:H5'	6:C:467:ARG:HG3	2.02	0.41
6:C:926:MET:HE2	7:D:840:PHE:CD2	2.56	0.41
7:D:589:THR:HG21	7:D:688:MET:HG2	2.01	0.41
7:D:907:ASP:OD1	7:D:907:ASP:N	2.47	0.41
5:A:40:ARG:NH2	6:C:1013:GLY:O	2.49	0.41
5:B:62:GLU:O	5:B:63:PHE:C	2.62	0.41
5:B:202:ILE:HD12	5:B:202:ILE:C	2.45	0.41
7:D:756:VAL:HB	7:D:774:LEU:HD21	2.01	0.41
6:C:381:VAL:O	6:C:382:GLY:C	2.64	0.41
6:C:943:GLY:C	6:C:993:LEU:HD13	2.46	0.41
6:C:1133:LEU:HD11	7:D:105:TRP:HZ3	1.85	0.41
1:F:15:MET:CE	7:D:366:ILE:HD11	2.50	0.41
1:F:80:GLU:C	1:F:82:ARG:H	2.28	0.41
1:F:131:ILE:HD12	1:F:132:GLN:N	2.36	0.41
3:H:15:DG:H2''	6:C:467:ARG:HG2	2.03	0.41
5:A:6:ARG:HH21	5:A:6:ARG:HB3	1.85	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
5:A:112:PRO:CB	5:A:116:VAL:HG23	2.51	0.41
5:B:14:LEU:N	5:B:14:LEU:HD22	2.36	0.41
5:B:143:GLY:C	5:B:168:TYR:HB3	2.45	0.41
6:C:39:VAL:HG12	6:C:963:LEU:HD11	2.03	0.41
6:C:58:THR:O	6:C:62:GLU:HG3	2.20	0.41
6:C:247:GLN:O	6:C:250:GLU:HB3	2.21	0.41
7:D:752:ARG:HB3	7:D:777:ILE:CD1	2.51	0.41
7:D:1035:PHE:O	7:D:1161:MET:HE3	2.21	0.41
7:D:1092:GLU:HG3	7:D:1094:GLY:H	1.86	0.41
7:D:1165:VAL:HG12	7:D:1205:PRO:HA	2.02	0.41
3:H:15:DG:N2	6:C:472:VAL:HG22	2.36	0.41
5:A:4:SER:HB3	5:B:144:ARG:HH12	1.86	0.41
5:B:95:MET:HG2	5:B:113:PRO:CD	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:198:THR:OG1	5:B:199:LYS:N	2.54	0.41
6:C:105:LEU:HD12	6:C:138:GLU:O	2.21	0.41
6:C:530:TYR:C	6:C:531:LEU:HD12	2.45	0.41
6:C:590:ALA:HA	6:C:593:MET:HE3	2.02	0.41
7:D:1010:LEU:HD13	7:D:1028:LEU:HB2	2.03	0.41
1:F:89:VAL:HG22	1:F:89:VAL:O	2.20	0.40
5:A:33:THR:HG21	5:B:37:SER:HA	2.03	0.40
5:A:161:ARG:HB2	5:A:161:ARG:NH1	2.36	0.40
3:H:9:DG:N3	3:H:9:DG:H2'	2.35	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: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
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
1:F:157:SER:O	1:F:160:HIS:N	2.54	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:182:SER:HB2	6:C:377:ARG:HB2	2.04	0.40
6:C:305:ARG:HD2	6:C:305:ARG:HA	1.90	0.40
6:C:930:GLN:O	6:C:934:THR:OG1	2.38	0.40
6:C:446:LEU:HD13	6:C:593:MET:HE1	2.04	0.40
6:C:1070:GLU:HG2	6:C:1074:TRP:CE2	2.57	0.40
7:D:778:TRP:CE2	7:D:835:PRO:HG3	2.56	0.40
7:D:1080:ILE:HG22	7:D:1082:LYS:H	1.86	0.40
6:C:442:GLN:HB2	6:C:679:ASN:HB2	2.02	0.40
6:C:672:MET:HE2	6:C:672:MET:HA	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	F	159/177 (90%)	134 (84%)	21 (13%)	4 (2%)	4	28
5	A	223/347 (64%)	210 (94%)	10 (4%)	3 (1%)	9	38
5	B	230/347 (66%)	214 (93%)	12 (5%)	4 (2%)	7	34
6	C	1110/1178 (94%)	1041 (94%)	61 (6%)	8 (1%)	18	51
7	D	1258/1316 (96%)	1189 (94%)	63 (5%)	6 (0%)	24	57
8	E	79/110 (72%)	73 (92%)	6 (8%)	0	100	100
All	All	3059/3475 (88%)	2861 (94%)	173 (6%)	25 (1%)	16	48

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%)	125 (100%)	0	100	100
5	A	194/297 (65%)	190 (98%)	4 (2%)	47	64
5	B	191/297 (64%)	191 (100%)	0	100	100
6	C	945/998 (95%)	945 (100%)	0	100	100
7	D	1047/1095 (96%)	1047 (100%)	0	100	100
8	E	66/90 (73%)	66 (100%)	0	100	100
All	All	2568/2913 (88%)	2564 (100%)	4 (0%)	87	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ILE
5	A	6	ARG
5	A	7	PRO
5	A	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	95	GLN
1	F	101	GLN
1	F	132	GLN
5	A	36	ASN
6	C	419	ASN
6	C	680	HIS
6	C	755	HIS
6	C	930	GLN
6	C	1054	GLN
6	C	1066	GLN
6	C	1111	ASN
7	D	262	GLN
7	D	283	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	564	ASN

5.3.3 RNA [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	F	163/177 (92%)	0.58	6 (3%) 45 31	68, 135, 176, 203	0
2	G	17/17 (100%)	0.46	0 100 100	60, 83, 143, 152	0
3	H	23/27 (85%)	0.79	0 100 100	88, 144, 192, 204	0
4	I	5/5 (100%)	0.60	0 100 100	68, 72, 78, 118	0
5	A	225/347 (64%)	0.15	4 (1%) 67 46	48, 76, 121, 155	0
5	B	232/347 (66%)	0.45	10 (4%) 40 28	54, 94, 134, 167	0
6	C	1114/1178 (94%)	0.13	6 (0%) 87 71	29, 69, 150, 187	0
7	D	1262/1316 (95%)	0.26	22 (1%) 69 47	28, 82, 209, 295	0
8	E	81/110 (73%)	0.16	2 (2%) 58 40	58, 89, 146, 172	0
All	All	3122/3524 (88%)	0.24	50 (1%) 70 48	28, 81, 167, 295	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	157	ALA	4.8
1	F	88	ASN	4.2
7	D	605	ASP	4.2
5	B	150	VAL	4.1
6	C	237	LEU	4.1
7	D	745	ILE	4.0
5	B	89	GLU	3.7
5	A	186	ARG	3.6
7	D	814	THR	3.5
7	D	809	GLY	3.4
5	B	160	GLY	3.4
5	B	154	ALA	3.3
7	D	817	LEU	3.3
7	D	816	THR	3.1
8	E	108	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	D	746	LEU	2.9
7	D	771	ASN	2.8
1	F	159	LEU	2.8
7	D	827	PRO	2.7
7	D	785	VAL	2.7
5	B	62	GLU	2.7
7	D	854	HIS	2.6
7	D	747	ASP	2.6
6	C	29	ASN	2.6
5	A	184	GLU	2.5
5	A	151	GLN	2.5
7	D	788	ALA	2.5
6	C	212	LEU	2.4
5	B	91	GLU	2.4
8	E	28	GLY	2.4
5	B	151	GLN	2.4
6	C	823	ALA	2.4
7	D	740	PRO	2.4
7	D	927	THR	2.4
7	D	773	ALA	2.3
7	D	781	ALA	2.3
1	F	84	ALA	2.3
7	D	305	SER	2.3
7	D	743	LYS	2.3
7	D	812	THR	2.2
7	D	808	THR	2.2
6	C	926	MET	2.2
1	F	89	VAL	2.2
5	B	156	GLY	2.2
1	F	54	HIS	2.1
1	F	51	ALA	2.1
6	C	28	SER	2.1
5	A	221	LEU	2.1
5	B	189	PHE	2.0
7	D	1011	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.