



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:25 AM BST

PDB ID : 6KOQ
Title : Mycobacterium tuberculosis initial transcription complex comprising sigma H and 5'-OH RNA of 10 nt
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-08-12
Resolution : 3.35 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	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

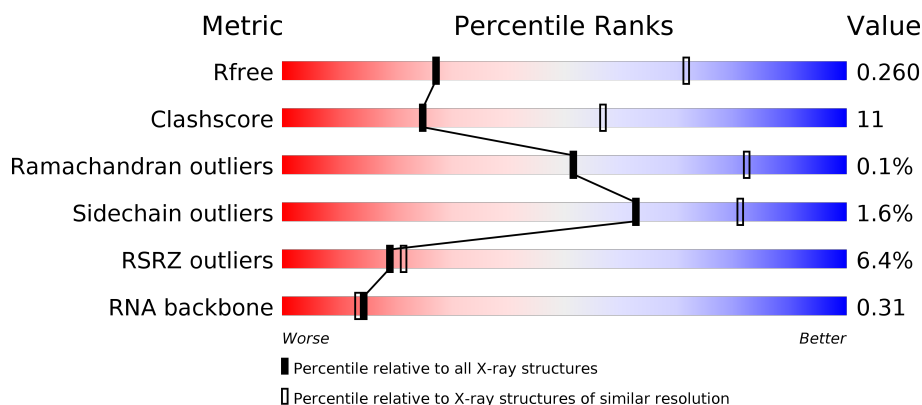
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	368	<div> <div>50%</div> <div>9%</div> <div>41%</div> </div>
1	B	368	<div> <div>5%</div> <div>50%</div> <div>12%</div> <div>38%</div> </div>
2	C	1174	<div> <div>6%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
3	D	1317	<div> <div>4%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	218	
6	G	23	
7	H	21	
8	I	10	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24473 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	217	Total	C	N	O	S	0	0	0
			1632	1029	277	324	2			
1	B	228	Total	C	N	O	S	0	0	0
			1637	1039	278	318	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P9WGZ1
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-20	MET	-	initiating methionine	UNP P9WGZ1
B	-19	GLY	-	expression tag	UNP P9WGZ1
B	-18	HIS	-	expression tag	UNP P9WGZ1
B	-17	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP P9WGZ1
B	-15	HIS	-	expression tag	UNP P9WGZ1
B	-14	HIS	-	expression tag	UNP P9WGZ1
B	-13	HIS	-	expression tag	UNP P9WGZ1
B	-12	HIS	-	expression tag	UNP P9WGZ1
B	-11	HIS	-	expression tag	UNP P9WGZ1
B	-10	HIS	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	SER	-	expression tag	UNP P9WGZ1
B	-7	SER	-	expression tag	UNP P9WGZ1
B	-6	GLY	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	ILE	-	expression tag	UNP P9WGZ1
B	-3	GLU	-	expression tag	UNP P9WGZ1
B	-2	GLY	-	expression tag	UNP P9WGZ1
B	-1	ARG	-	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	1138	Total	C	N	O	S	0	0	0
			8656	5418	1508	1691	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP P9WGY9
C	0	VAL	-	expression tag	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1258	Total	C	N	O	S	0	0	0
			9719	6093	1752	1833	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P9WGY7
D	1	VAL	-	expression tag	UNP P9WGY7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	75	Total	C	N	O	0	0	0
			586	375	96	115			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	148	Total	C	N	O	S	0	0	0
			1137	715	194	223	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P9WGH9
F	0	ALA	-	expression tag	UNP P9WGH9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	23	Total	C	N	O	P	0	0	0
			444	211	77	134	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	21	Total	C	N	O	P	0	0	0
			434	206	82	126	20			

- Molecule 8 is a RNA chain called RNA (5'-R(*UP*CP*AP*CP*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	10	Total	C	N	O	P	0	0	0
			204	93	34	68	9			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

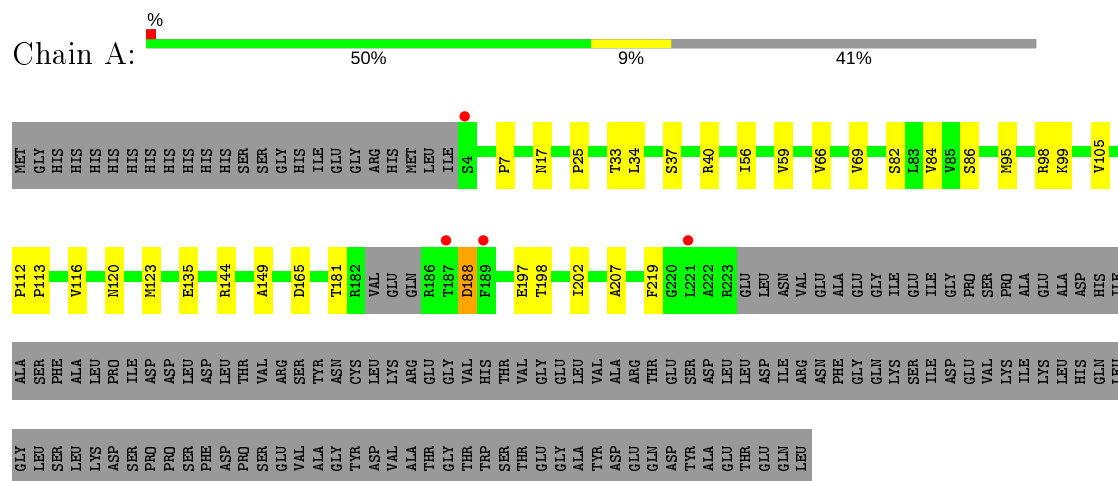
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total 2	O 2	0	0
11	B	1	Total 1	O 1	0	0
11	C	7	Total 7	O 7	0	0
11	D	7	Total 7	O 7	0	0
11	E	1	Total 1	O 1	0	0
11	G	1	Total 1	O 1	0	0
11	H	2	Total 2	O 2	0	0

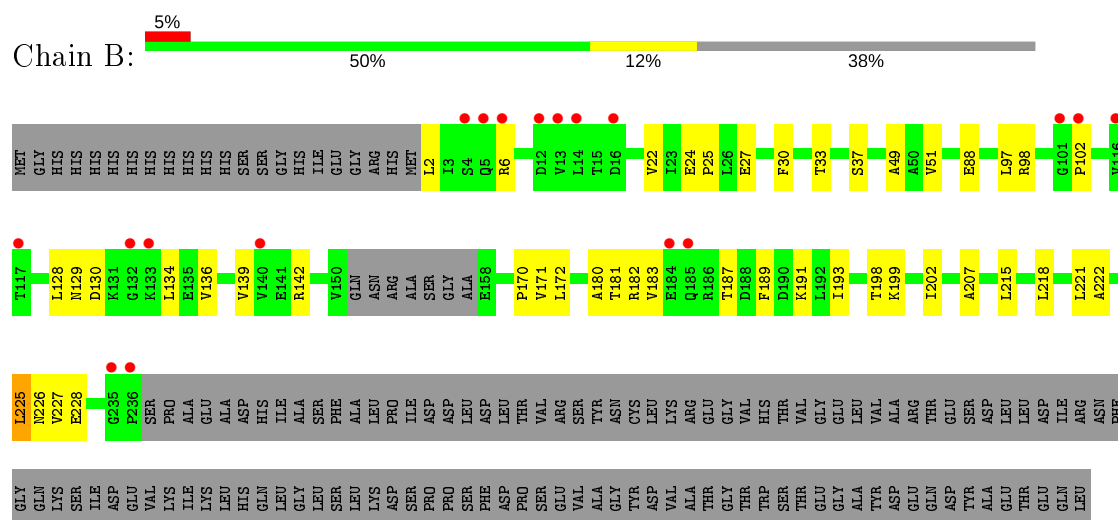
3 Residue-property plots

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.

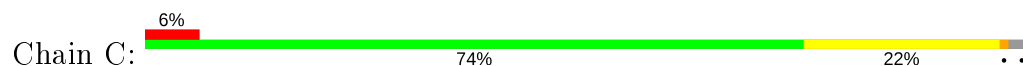
- Molecule 1: DNA-directed RNA polymerase subunit alpha

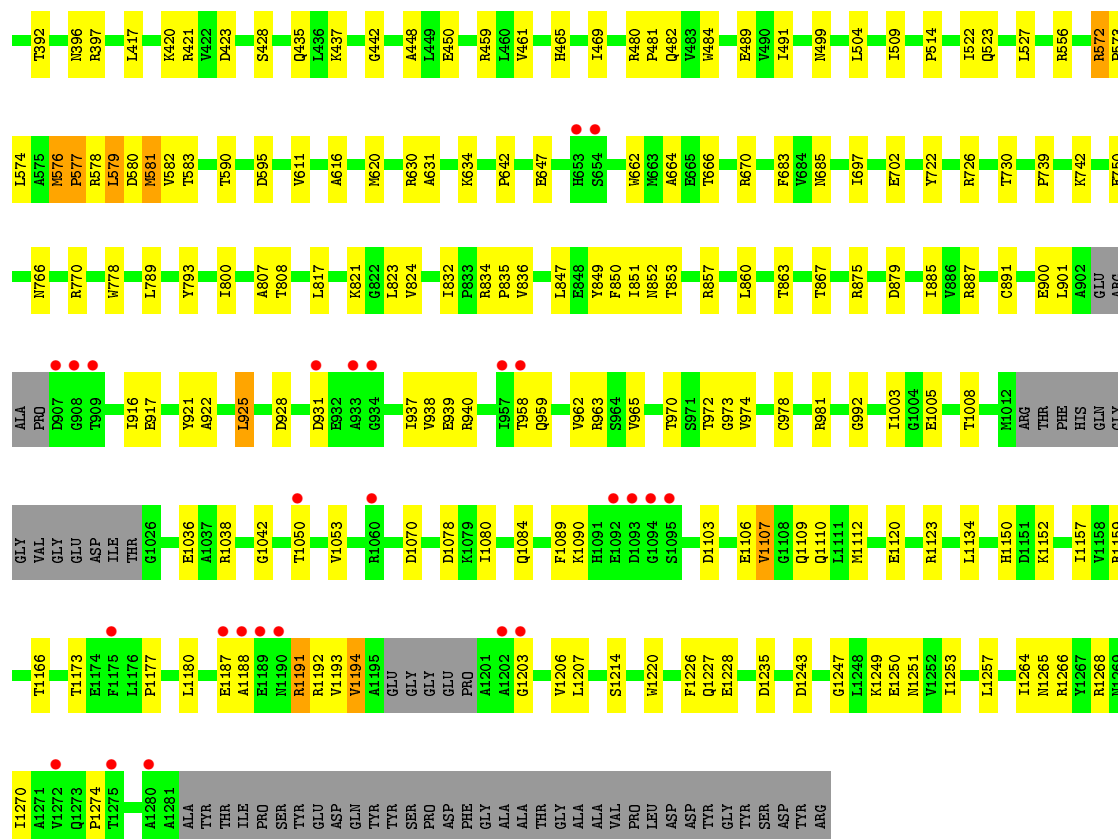


- Molecule 1: DNA-directed RNA polymerase subunit alpha

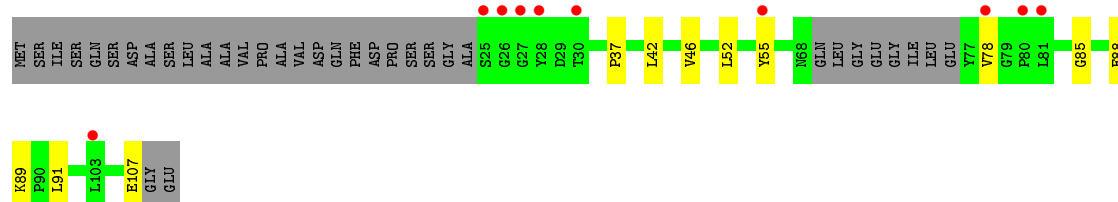


- Molecule 2: DNA-directed RNA polymerase subunit beta

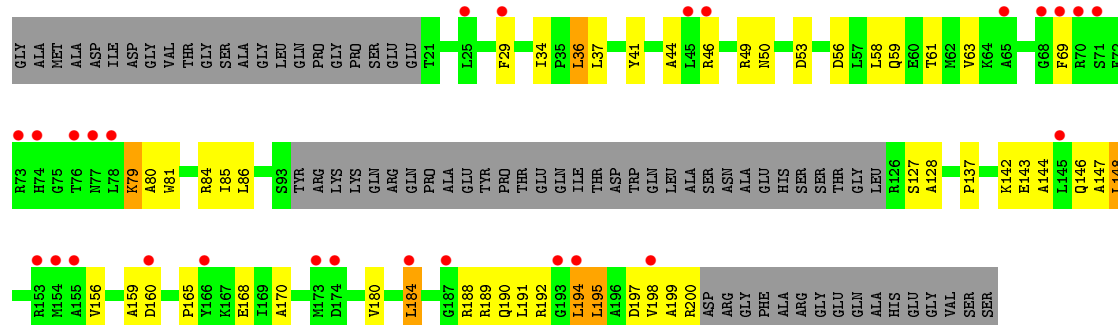




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: ECF RNA polymerase sigma factor SigH



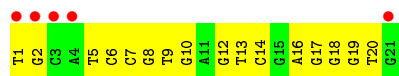
- Molecule 6: DNA (5'-D(*TP*TP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3')

Chain G: 



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

Chain H: 



- Molecule 8: RNA (5'-R(*UP*CP*AP*CP*CP*CP*UP*CP*GP*A)-3')

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.85Å 161.10Å 129.55Å 90.00° 117.44° 90.00°	Depositor
Resolution (Å)	36.51 – 3.35 36.55 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (36.51-3.35) 97.2 (36.55-3.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.221 , 0.260 0.221 , 0.260	Depositor DCC
R_{free} test set	2395 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24473	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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	0.26	0/1657	0.46	0/2256
1	B	0.33	0/1663	0.50	0/2275
2	C	0.27	0/8815	0.46	0/11982
3	D	0.29	0/9880	0.45	3/13377 (0.0%)
4	E	0.24	0/598	0.45	0/815
5	F	0.27	0/1155	0.44	0/1568
6	G	0.48	0/497	0.90	0/765
7	H	0.50	0/487	0.89	0/752
8	I	0.35	0/226	0.97	0/349
All	All	0.29	0/24978	0.49	3/34139 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	574	LEU	N-CA-C	-5.59	95.91	111.00
3	D	572	ARG	C-N-CD	5.46	139.87	128.40
3	D	576	MET	C-N-CD	5.21	139.34	128.40

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	1632	0	1654	23	0
1	B	1637	0	1607	32	0
2	C	8656	0	8438	197	0
3	D	9719	0	9680	214	0
4	E	586	0	576	8	0
5	F	1137	0	1088	55	0
6	G	444	0	245	43	0
7	H	434	0	238	17	0
8	I	204	0	110	7	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	7	0	0	0	0
11	D	7	0	0	1	0
11	E	1	0	0	0	0
11	G	1	0	0	0	0
11	H	2	0	0	0	0
All	All	24473	0	23636	519	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 11.

All (519) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:80:ALA:CB	6:G:3:DG:H5''	1.49	1.38
5:F:80:ALA:HB1	6:G:3:DG:C5'	1.69	1.20
3:D:1188:ALA:HA	3:D:1191:ARG:CD	1.78	1.13
3:D:60:CYS:HB2	3:D:78:CYS:SG	1.89	1.11
3:D:1188:ALA:HA	3:D:1191:ARG:HD2	1.33	1.08
6:G:2:DT:H2''	6:G:3:DG:OP2	1.49	1.06
3:D:1188:ALA:HA	3:D:1191:ARG:CG	1.87	1.04
3:D:579:LEU:HB3	3:D:807:ALA:O	1.58	1.02
3:D:527:LEU:CD2	3:D:581:MET:CE	2.38	1.01
3:D:527:LEU:HD23	3:D:581:MET:CE	1.92	1.00
2:C:70:GLU:N	2:C:70:GLU:OE1	1.95	1.00
3:D:527:LEU:CD2	3:D:581:MET:HE3	1.94	0.97
3:D:1188:ALA:O	3:D:1191:ARG:HG3	1.65	0.96
3:D:580:ASP:O	3:D:583:THR:HG22	1.65	0.96
5:F:80:ALA:CB	6:G:3:DG:C5'	2.34	0.95
5:F:197:ASP:OD1	5:F:198:VAL:N	1.99	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:HD21	3:D:581:MET:HE3	1.47	0.94
3:D:527:LEU:CD2	3:D:581:MET:HE1	2.03	0.87
3:D:527:LEU:HD23	3:D:581:MET:HE1	1.52	0.86
2:C:317:HIS:HB3	2:C:321:PRO:HG2	1.57	0.86
3:D:1188:ALA:O	3:D:1191:ARG:CG	2.24	0.86
6:G:7:DG:C6	6:G:8:DA:N6	2.45	0.85
3:D:75:CYS:HB3	3:D:78:CYS:SG	2.16	0.85
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.58	0.85
3:D:527:LEU:HD21	3:D:581:MET:CE	2.05	0.84
3:D:578:ARG:O	3:D:582:VAL:HG23	1.78	0.84
2:C:541:PRO:HG3	2:C:550:GLU:HG2	1.60	0.83
2:C:1018:THR:H	3:D:730:THR:HG21	1.47	0.79
6:G:7:DG:C5	6:G:8:DA:N6	2.50	0.79
7:H:19:DG:H1	8:I:4:C:H42	1.30	0.79
3:D:576:MET:CG	3:D:697:ILE:HD12	2.12	0.79
2:C:93:PHE:CE2	6:G:4:DT:C5'	2.67	0.78
2:C:806:THR:HG21	3:D:56:ARG:HD3	1.66	0.77
3:D:1188:ALA:CA	3:D:1191:ARG:CG	2.63	0.77
3:D:67:ARG:HG3	3:D:69:ARG:H	1.50	0.77
5:F:81:TRP:HE1	6:G:1:DT:H3'	1.51	0.76
6:G:2:DT:C2'	6:G:3:DG:OP2	2.29	0.76
1:B:226:ASN:O	1:B:228:GLU:HG2	1.86	0.76
3:D:1188:ALA:HA	3:D:1191:ARG:HG2	1.67	0.75
5:F:46:ARG:NH2	6:G:6:DG:O5'	2.20	0.75
5:F:191:LEU:CD2	5:F:195:LEU:HD21	2.17	0.74
2:C:151:PHE:HE1	2:C:383:ILE:HD11	1.53	0.74
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.70	0.74
2:C:752:ASP:HB3	2:C:862:LEU:HD23	1.68	0.74
1:B:218:LEU:O	1:B:221:LEU:HB2	1.88	0.73
3:D:576:MET:HG3	3:D:697:ILE:HD12	1.70	0.73
6:G:4:DT:H4'	6:G:5:DG:OP1	1.89	0.73
5:F:36:LEU:HD11	5:F:79:LYS:HD2	1.71	0.72
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.69	0.72
2:C:67:SER:O	2:C:71:ARG:HG2	1.89	0.72
2:C:389:ARG:HD3	5:F:49:ARG:HH12	1.55	0.71
2:C:1129:VAL:HG12	3:D:12:ILE:HG22	1.71	0.70
2:C:557:ARG:HB2	2:C:561:GLU:O	1.89	0.70
7:H:19:DG:H1	8:I:4:C:N4	1.88	0.70
3:D:1188:ALA:CA	3:D:1191:ARG:HG2	2.22	0.70
2:C:93:PHE:CE2	6:G:4:DT:H5''	2.27	0.70
3:D:1188:ALA:CA	3:D:1191:ARG:HD2	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:572:ARG:HG2	3:D:572:ARG:HH11	1.56	0.70
3:D:577:PRO:HA	3:D:581:MET:HE3	1.74	0.69
3:D:293:LEU:HD21	3:D:1177:PRO:HG2	1.74	0.69
2:C:1038:ARG:NH2	3:D:423:ASP:OD1	2.22	0.69
3:D:579:LEU:CD1	3:D:580:ASP:H	2.06	0.69
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.26	0.68
5:F:80:ALA:HB1	6:G:3:DG:H5''	0.73	0.68
3:D:834:ARG:HD3	3:D:835:PRO:HD2	1.75	0.68
2:C:1145:GLU:HB3	3:D:84:ARG:HH11	1.57	0.68
3:D:1050:THR:HG23	3:D:1107:VAL:HG13	1.75	0.68
6:G:3:DG:P	6:G:3:DG:H3'	2.34	0.68
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.75	0.68
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.26	0.68
3:D:579:LEU:HD12	3:D:579:LEU:N	2.08	0.67
2:C:201:SER:HB3	2:C:303:ALA:HB2	1.76	0.67
3:D:1193:VAL:C	3:D:1194:VAL:HG23	2.15	0.67
3:D:963:ARG:NH1	3:D:978:CYS:SG	2.68	0.67
2:C:179:VAL:HG12	2:C:198:VAL:HG22	1.77	0.66
5:F:147:ALA:HB3	5:F:194:LEU:CD1	2.25	0.66
3:D:579:LEU:HD13	3:D:580:ASP:H	1.59	0.66
2:C:62:PRO:O	2:C:66:GLU:HG2	1.96	0.65
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.79	0.65
2:C:1131:VAL:HG21	2:C:1141:LEU:HD13	1.79	0.65
2:C:554:LEU:HD12	2:C:563:GLU:O	1.96	0.65
3:D:576:MET:HG2	3:D:697:ILE:HD12	1.78	0.65
2:C:922:ILE:HD12	3:D:817:LEU:HD21	1.78	0.65
5:F:184:LEU:HD13	5:F:188:ARG:HD2	1.77	0.65
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.30	0.65
2:C:44:VAL:O	2:C:627:ARG:NH2	2.30	0.65
3:D:1120:GLU:OE2	3:D:1123:ARG:NH2	2.30	0.64
5:F:80:ALA:HB3	6:G:3:DG:C5'	2.25	0.64
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.79	0.64
2:C:365:ASP:OD1	6:G:12:DG:N2	2.24	0.64
3:D:875:ARG:NH2	3:D:1226:PHE:O	2.31	0.64
3:D:100:PRO:HD2	3:D:259:GLU:HG3	1.80	0.64
3:D:392:THR:HB	3:D:396:ASN:HA	1.79	0.63
6:G:7:DG:OP2	6:G:7:DG:H8	1.80	0.63
8:I:2:C:H2'	8:I:3:A:H8	1.62	0.63
3:D:670:ARG:NH1	3:D:685:ASN:OD1	2.30	0.63
3:D:116:TYR:O	3:D:295:ARG:NH1	2.32	0.62
2:C:307:ARG:NH1	2:C:326:THR:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:ALA:HB3	5:F:194:LEU:HD11	1.81	0.62
3:D:417:LEU:HD23	3:D:1253:ILE:HG23	1.81	0.61
2:C:1134:SER:HA	3:D:8:ASP:HB2	1.81	0.61
3:D:1227:GLN:HG2	3:D:1228:GLU:HG3	1.81	0.61
8:I:2:C:H2'	8:I:3:A:C8	2.35	0.61
3:D:1188:ALA:C	3:D:1191:ARG:HG2	2.21	0.61
6:G:8:DA:H2"	6:G:9:DG:H5"	1.82	0.61
2:C:622:THR:HG23	2:C:969:PRO:HA	1.83	0.61
3:D:459:ARG:NE	3:D:489:GLU:OE2	2.34	0.60
2:C:671:ARG:HE	2:C:747:GLU:HA	1.65	0.60
3:D:1110:GLN:NE2	3:D:1112:MET:O	2.32	0.60
3:D:879:ASP:OD1	3:D:1249:LYS:NZ	2.33	0.60
3:D:1187:GLU:O	3:D:1191:ARG:HG2	2.02	0.60
6:G:12:DG:H2"	6:G:13:DT:H5"	1.82	0.60
1:A:98:ARG:HG3	1:A:135:GLU:HG3	1.83	0.60
1:B:227:VAL:HG13	1:B:227:VAL:O	2.01	0.60
5:F:41:TYR:HB2	5:F:58:LEU:HD22	1.84	0.60
1:B:171:VAL:HA	1:B:198:THR:HA	1.84	0.60
2:C:276:ARG:HD3	2:C:279:GLU:HB2	1.84	0.59
2:C:541:PRO:HB2	2:C:549:VAL:HG12	1.84	0.59
3:D:1193:VAL:O	3:D:1194:VAL:HG23	2.02	0.59
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.84	0.59
2:C:445:HIS:HA	2:C:448:ARG:HG2	1.84	0.59
3:D:504:LEU:HB3	3:D:1005:GLU:HG2	1.85	0.59
5:F:198:VAL:O	5:F:198:VAL:HG12	2.02	0.59
5:F:170:ALA:HA	5:F:180:VAL:HG21	1.84	0.58
2:C:882:ARG:NH2	2:C:927:GLU:OE1	2.33	0.58
2:C:71:ARG:HD2	2:C:71:ARG:N	2.19	0.58
1:A:40:ARG:HE	1:B:33:THR:HG22	1.68	0.58
2:C:26:VAL:HG11	2:C:626:LEU:HD11	1.86	0.58
4:E:42:LEU:HB3	4:E:52:LEU:HD11	1.86	0.58
6:G:3:DG:H4'	6:G:4:DT:OP2	2.04	0.58
3:D:1250:GLU:OE1	3:D:1250:GLU:N	2.31	0.58
3:D:1270:ILE:HG12	4:E:107:GLU:HA	1.86	0.58
2:C:1146:ASP:OD1	3:D:71:LYS:NZ	2.36	0.58
2:C:699:GLY:N	2:C:702:THR:OG1	2.33	0.57
2:C:193:LEU:HB2	2:C:210:VAL:HG23	1.85	0.57
3:D:1166:THR:O	3:D:1203:GLY:HA2	2.04	0.57
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.39	0.57
2:C:305:VAL:HG22	2:C:503:PHE:HD1	1.69	0.57
2:C:172:GLN:OE1	2:C:373:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:383:ILE:HG13	2:C:421:ILE:HD11	1.87	0.57
2:C:805:GLU:HA	2:C:808:LEU:HB2	1.87	0.57
3:D:726:ARG:NH1	11:D:2101:HOH:O	2.37	0.57
3:D:925:LEU:HD13	3:D:928:ASP:HA	1.86	0.57
3:D:61:TYR:HB3	3:D:78:CYS:HB2	1.85	0.56
2:C:382:GLN:HG2	2:C:424:PHE:HB2	1.86	0.56
2:C:725:TYR:HE1	3:D:579:LEU:CD1	2.18	0.56
2:C:461:ARG:NH1	6:G:11:DT:O4'	2.37	0.56
3:D:1188:ALA:C	3:D:1191:ARG:CG	2.72	0.56
3:D:885:ILE:HD11	3:D:887:ARG:HE	1.70	0.56
3:D:1173:THR:HB	3:D:1193:VAL:HG21	1.88	0.56
3:D:1188:ALA:O	3:D:1191:ARG:HG2	2.03	0.56
2:C:625:GLU:OE1	2:C:625:GLU:N	2.32	0.56
2:C:942:ALA:HA	2:C:945:GLY:HA3	1.87	0.56
2:C:272:TYR:OH	2:C:276:ARG:NH1	2.38	0.56
2:C:882:ARG:HG2	2:C:1025:MET:HE3	1.87	0.55
3:D:41:PRO:HG2	3:D:49:GLU:HG3	1.87	0.55
5:F:191:LEU:O	5:F:195:LEU:HD23	2.06	0.55
1:B:172:LEU:HD11	1:B:199:LYS:HG3	1.88	0.55
2:C:1081:GLU:HG3	2:C:1085:ILE:HD11	1.87	0.55
2:C:69:ALA:HB3	2:C:70:GLU:OE1	2.07	0.55
1:A:181:THR:O	1:A:188:ASP:HA	2.06	0.55
6:G:10:DC:H2''	6:G:11:DT:H3'	1.87	0.55
1:B:182:ARG:CB	1:B:189:PHE:H	2.20	0.55
2:C:542:ILE:HG23	2:C:546:GLY:HA2	1.89	0.55
2:C:669:PHE:N	2:C:679:ASN:OD1	2.38	0.55
1:B:226:ASN:O	1:B:227:VAL:HG12	2.07	0.55
5:F:46:ARG:HH22	6:G:6:DG:P	2.29	0.55
5:F:142:LYS:O	5:F:146:GLN:HG3	2.07	0.55
3:D:579:LEU:HD13	3:D:580:ASP:N	2.21	0.55
4:E:46:VAL:HG21	4:E:52:LEU:HG	1.88	0.55
2:C:105:ARG:NH2	2:C:130:THR:OG1	2.39	0.54
2:C:714:LEU:HD23	2:C:907:VAL:HA	1.88	0.54
3:D:75:CYS:CB	3:D:78:CYS:SG	2.88	0.54
2:C:657:ASP:OD2	2:C:689:ARG:NH2	2.41	0.54
3:D:499:ASN:HB2	3:D:509:ILE:HG12	1.89	0.54
1:B:129:ASN:OD1	1:B:130:ASP:N	2.38	0.54
1:A:40:ARG:NH2	2:C:1007:GLY:O	2.40	0.54
2:C:629:ALA:HB2	2:C:707:MET:HG2	1.90	0.54
3:D:24:SER:OG	3:D:26:GLY:O	2.26	0.54
5:F:36:LEU:HG	5:F:79:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:893:LEU:HB2	2:C:898:MET:HE2	1.90	0.53
3:D:900:GLU:O	3:D:959:GLN:HA	2.08	0.53
2:C:622:THR:HG22	2:C:623:GLY:H	1.72	0.53
3:D:577:PRO:HB3	3:D:581:MET:HB2	1.90	0.53
4:E:37:PRO:HG2	4:E:42:LEU:HD11	1.90	0.53
2:C:818:ILE:HG21	5:F:191:LEU:HD22	1.91	0.53
3:D:137:THR:HG21	3:D:263:LYS:HD2	1.90	0.53
3:D:750:GLU:OE2	3:D:834:ARG:NH2	2.41	0.53
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.89	0.53
2:C:328:THR:N	2:C:331:ASP:OD2	2.33	0.53
3:D:1050:THR:HG22	3:D:1106:GLU:HA	1.90	0.53
2:C:1132:LEU:HD21	3:D:11:ARG:HH12	1.74	0.53
3:D:611:VAL:HG12	3:D:634:LYS:HB2	1.90	0.53
5:F:81:TRP:CE2	5:F:85:ILE:HD11	2.44	0.53
7:H:7:DC:H2''	7:H:8:DG:C8	2.43	0.53
2:C:196:VAL:HG13	2:C:208:PHE:HB2	1.91	0.52
2:C:1111:ILE:HD13	3:D:3:ASP:HB2	1.90	0.52
2:C:320:GLU:N	2:C:321:PRO:HD3	2.24	0.52
5:F:44:ALA:HB2	5:F:86:LEU:HD11	1.91	0.52
3:D:386:ARG:NH2	7:H:9:DT:OP1	2.42	0.52
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.90	0.52
2:C:929:HIS:HB3	2:C:983:LEU:HD21	1.90	0.52
3:D:891:CYS:SG	3:D:970:THR:HG23	2.49	0.52
5:F:144:ALA:O	5:F:194:LEU:HD12	2.09	0.52
1:A:84:VAL:HG12	1:A:120:ASN:ND2	2.25	0.52
2:C:732:SER:HA	2:C:898:MET:HE3	1.90	0.52
3:D:579:LEU:CD1	3:D:580:ASP:N	2.73	0.52
2:C:168:VAL:HG11	2:C:446:LYS:HA	1.91	0.52
2:C:510:TYR:HB3	2:C:572:TYR:HB3	1.92	0.52
2:C:480:ILE:HD11	3:D:849:TYR:HE1	1.75	0.52
1:B:183:VAL:O	1:B:187:THR:N	2.37	0.52
3:D:97:LEU:HD11	3:D:317:VAL:HG23	1.92	0.52
6:G:18:DG:H2'	6:G:19:DA:C8	2.44	0.52
2:C:556:ARG:HG3	3:D:847:LEU:HD21	1.92	0.52
3:D:572:ARG:CG	3:D:572:ARG:HH11	2.22	0.51
8:I:4:C:O2	8:I:4:C:H2'	2.09	0.51
1:A:34:LEU:HD11	1:B:218:LEU:HD13	1.92	0.51
2:C:1082:LEU:HD23	2:C:1086:LYS:HD2	1.93	0.51
3:D:480:ARG:NH1	3:D:482:GLN:OE1	2.43	0.51
3:D:128:ILE:HD11	3:D:234:LEU:HD11	1.93	0.51
2:C:433:PHE:CE2	7:H:18:DG:H4'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:722:TYR:O	3:D:726:ARG:HG2	2.10	0.51
1:B:102:PRO:HA	1:B:128:LEU:O	2.11	0.51
1:B:202:ILE:HD13	1:B:207:ALA:HB2	1.91	0.51
5:F:61:THR:HG23	5:F:85:ILE:HG22	1.93	0.51
2:C:557:ARG:O	2:C:560:GLY:N	2.44	0.51
5:F:191:LEU:HG	5:F:195:LEU:HD21	1.93	0.51
2:C:1061:ARG:HA	3:D:421:ARG:HA	1.93	0.50
3:D:1180:LEU:HD22	3:D:1206:VAL:HG21	1.92	0.50
5:F:29:PHE:HB2	5:F:69:PHE:CE2	2.47	0.50
1:A:112:PRO:HB2	1:A:116:VAL:HG23	1.93	0.50
2:C:435:ASP:HA	2:C:674:HIS:NE2	2.26	0.50
3:D:922:ALA:HA	3:D:981:ARG:HD3	1.91	0.50
2:C:233:LYS:HZ2	2:C:262:VAL:HA	1.76	0.50
2:C:479:PRO:O	3:D:857:ARG:NH2	2.40	0.50
2:C:554:LEU:HG	3:D:847:LEU:HD13	1.92	0.50
3:D:1134:LEU:HD11	3:D:1207:LEU:HD21	1.92	0.50
3:D:832:ILE:HD12	3:D:851:ILE:HG23	1.93	0.50
2:C:1084:THR:OG1	2:C:1109:PRO:HB3	2.12	0.50
3:D:242:ARG:HA	3:D:245:VAL:HG22	1.93	0.50
5:F:189:ARG:HA	5:F:192:ARG:HD2	1.93	0.50
2:C:899:PRO:HB3	2:C:1013:PHE:HE2	1.76	0.50
2:C:776:ALA:O	2:C:785:ARG:NH2	2.45	0.50
3:D:327:MET:HG3	3:D:337:THR:HG22	1.93	0.50
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.47	0.50
3:D:992:GLY:HA2	3:D:1264:ILE:HD12	1.93	0.50
2:C:194:HIS:ND1	2:C:342:LEU:HG	2.27	0.50
3:D:642:PRO:HG2	3:D:647:GLU:HB2	1.93	0.50
3:D:328:VAL:HG11	8:I:1:U:H3	1.76	0.50
2:C:74:VAL:HG13	2:C:75:ASN:N	2.27	0.49
3:D:579:LEU:HD12	3:D:579:LEU:H	1.77	0.49
2:C:134:ILE:HG12	2:C:141:ILE:HG12	1.94	0.49
3:D:937:ILE:HG13	3:D:938:VAL:HG23	1.94	0.49
7:H:12:DG:H2'	7:H:13:DT:C6	2.48	0.49
2:C:1130:GLU:OE1	3:D:11:ARG:NH2	2.40	0.49
2:C:314:LEU:HB2	2:C:316:LEU:HD23	1.94	0.49
2:C:554:LEU:HD11	2:C:562:VAL:HB	1.95	0.49
3:D:702:GLU:OE2	3:D:981:ARG:NH2	2.45	0.49
2:C:1040:THR:HG22	5:F:127:SER:HB2	1.94	0.49
2:C:191:LYS:NZ	2:C:212:LYS:O	2.39	0.49
2:C:895:VAL:HG22	2:C:906:PRO:HG2	1.93	0.49
2:C:467:ARG:HB3	2:C:489:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1265:ASN:OD1	3:D:1268:ARG:NH1	2.38	0.49
2:C:481:GLU:OE2	2:C:607:ARG:NH2	2.46	0.49
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.48	0.49
6:G:4:DT:H2''	6:G:5:DG:O5'	2.13	0.49
1:A:37:SER:OG	1:B:37:SER:OG	2.27	0.49
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.95	0.49
2:C:898:MET:HG2	2:C:907:VAL:O	2.13	0.49
5:F:197:ASP:O	5:F:200:ARG:N	2.45	0.49
2:C:391:GLU:OE2	2:C:395:ARG:NH2	2.46	0.49
7:H:16:DA:H2'	7:H:17:DG:C8	2.48	0.49
7:H:5:DT:H2''	7:H:6:DC:C6	2.48	0.48
2:C:270:ASP:HA	2:C:273:ARG:HG2	1.95	0.48
2:C:1140:GLU:OE1	2:C:1141:LEU:N	2.46	0.48
2:C:198:VAL:HB	2:C:206:LEU:HB3	1.95	0.48
3:D:556:ARG:HD3	4:E:91:LEU:HD22	1.95	0.48
2:C:1040:THR:HG21	5:F:128:ALA:HB3	1.95	0.48
2:C:803:LYS:HG2	2:C:805:GLU:H	1.77	0.48
3:D:1089:PHE:O	3:D:1109:GLN:NE2	2.45	0.48
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.95	0.48
1:A:197:GLU:OE1	2:C:990:ARG:NH2	2.27	0.48
2:C:93:PHE:CE2	6:G:4:DT:C4'	2.97	0.48
2:C:1088:ASP:HB3	2:C:1112:PRO:HA	1.96	0.48
2:C:652:ILE:HD13	2:C:696:ILE:HG22	1.96	0.48
3:D:47:PHE:O	3:D:88:ARG:NH2	2.46	0.48
5:F:191:LEU:HG	5:F:195:LEU:CD2	2.44	0.48
7:H:12:DG:H2'	7:H:13:DT:H6	1.79	0.48
1:B:222:ALA:O	1:B:225:LEU:HB2	2.14	0.48
2:C:237:TRP:HB3	2:C:242:ILE:HG23	1.96	0.48
3:D:1264:ILE:HG22	3:D:1266:ARG:H	1.78	0.48
3:D:219:LEU:HA	3:D:222:ILE:HD12	1.96	0.48
2:C:717:ILE:O	3:D:730:THR:HG23	2.14	0.48
5:F:59:GLN:O	5:F:63:VAL:HG23	2.12	0.48
3:D:1193:VAL:HG12	3:D:1194:VAL:N	2.29	0.48
3:D:230:ALA:N	3:D:233:GLN:OE1	2.45	0.48
3:D:582:VAL:O	3:D:583:THR:C	2.51	0.48
2:C:508:THR:HG22	2:C:579:GLN:HE21	1.78	0.47
2:C:93:PHE:CG	6:G:5:DG:OP1	2.67	0.47
2:C:1005:PHE:HA	2:C:1012:PRO:HA	1.97	0.47
2:C:756:THR:N	2:C:759:GLY:O	2.45	0.47
3:D:141:GLU:OE1	3:D:144:ARG:NH2	2.46	0.47
5:F:191:LEU:HD23	5:F:195:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ALA:HA	1:B:189:PHE:O	2.13	0.47
7:H:1:DT:H1'	7:H:2:DG:N7	2.30	0.47
7:H:7:DC:H2''	7:H:8:DG:H8	1.79	0.47
5:F:34:ILE:HA	5:F:37:LEU:HD13	1.95	0.47
3:D:269:ASP:HB3	3:D:272:ALA:HB3	1.95	0.47
3:D:367:VAL:HG12	3:D:371:LYS:HE3	1.97	0.47
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.96	0.47
3:D:925:LEU:HA	3:D:962:VAL:HG12	1.96	0.47
2:C:576:SER:OG	2:C:577:PRO:O	2.32	0.47
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.80	0.47
3:D:1257:LEU:HD23	3:D:1268:ARG:HD3	1.95	0.47
5:F:50:ASN:ND2	5:F:53:ASP:OD1	2.44	0.47
5:F:80:ALA:CB	6:G:3:DG:C4'	2.93	0.47
2:C:1039:SER:HB3	3:D:450:GLU:O	2.14	0.47
2:C:238:THR:O	2:C:242:ILE:HG12	2.15	0.47
3:D:940:ARG:HH12	3:D:963:ARG:HH21	1.62	0.47
5:F:156:VAL:O	5:F:160:ASP:HB2	2.14	0.47
2:C:1029:HIS:HB3	2:C:1034:LYS:HE2	1.96	0.47
2:C:120:ASP:HA	2:C:164:GLY:HA3	1.97	0.47
2:C:135:ASN:O	2:C:139:GLY:N	2.47	0.47
2:C:1146:ASP:HA	2:C:1149:LEU:HD13	1.97	0.46
3:D:931:ASP:OD1	3:D:931:ASP:N	2.47	0.46
5:F:148:LEU:HD11	5:F:190:GLN:HB3	1.97	0.46
1:B:49:ALA:HA	1:B:142:ARG:HA	1.97	0.46
1:B:30:PHE:HA	1:B:33:THR:OG1	2.15	0.46
2:C:74:VAL:O	2:C:76:PRO:HD3	2.16	0.46
5:F:165:PRO:HG2	5:F:168:GLU:HB2	1.96	0.46
2:C:1090:THR:HG22	2:C:1093:ARG:HH21	1.80	0.46
2:C:534:VAL:CG2	2:C:555:VAL:HG21	2.45	0.46
2:C:605:MET:HE3	2:C:886:LYS:HD3	1.98	0.46
3:D:973:GLY:O	3:D:1159:ARG:NH2	2.48	0.46
1:B:97:LEU:HB3	1:B:136:VAL:HG13	1.97	0.46
2:C:856:PRO:HG2	2:C:859:VAL:HG21	1.96	0.46
7:H:16:DA:H2'	7:H:17:DG:H8	1.80	0.46
1:A:95:MET:HG2	1:A:113:PRO:HD2	1.98	0.46
2:C:698:ASP:OD2	2:C:704:ASP:N	2.41	0.46
3:D:100:PRO:HG3	3:D:315:ASP:OD1	2.16	0.46
3:D:45:GLY:H	3:D:48:CYS:HB2	1.81	0.46
6:G:9:DG:H2''	6:G:10:DC:C6	2.51	0.46
2:C:103:ASP:O	2:C:129:VAL:HA	2.15	0.46
2:C:355:VAL:HG22	2:C:356:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:PHE:CD2	6:G:4:DT:H4'	2.51	0.46
2:C:803:LYS:HE3	2:C:827:ARG:HB3	1.96	0.46
3:D:1227:GLN:HG3	7:H:10:DG:H5''	1.96	0.46
2:C:605:MET:HE1	2:C:886:LYS:HB3	1.99	0.45
3:D:52:PHE:CD1	3:D:322:PRO:HD3	2.51	0.45
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.98	0.45
2:C:644:ILE:HG21	2:C:647:VAL:HG23	1.98	0.45
3:D:481:PRO:HA	3:D:484:TRP:CD1	2.52	0.45
5:F:36:LEU:HA	5:F:36:LEU:HD13	1.75	0.45
2:C:540:SER:HB3	2:C:548:PHE:HE1	1.81	0.45
2:C:893:LEU:HB2	2:C:898:MET:CE	2.47	0.45
3:D:127:LYS:HA	3:D:132:ALA:HB3	1.97	0.45
3:D:448:ALA:HB1	3:D:491:ILE:HD11	1.98	0.45
3:D:616:ALA:O	3:D:620:MET:HG3	2.17	0.45
6:G:11:DT:H2''	6:G:12:DG:OP2	2.15	0.45
2:C:929:HIS:HB2	2:C:979:LEU:HD21	1.98	0.45
2:C:557:ARG:C	2:C:560:GLY:H	2.20	0.45
2:C:873:ILE:HA	2:C:873:ILE:HD12	1.82	0.45
3:D:1036:GLU:HB3	3:D:1038:ARG:HG3	1.98	0.45
1:A:219:PHE:CE1	1:B:215:LEU:HD13	2.51	0.45
3:D:849:TYR:O	3:D:853:THR:HG23	2.16	0.45
2:C:1001:LYS:HA	2:C:1018:THR:HA	1.99	0.45
2:C:80:LEU:O	2:C:84:LEU:HG	2.17	0.45
3:D:867:THR:HA	3:D:1008:THR:HG22	1.99	0.45
1:B:181:THR:HG21	1:B:191:LYS:HD3	1.99	0.44
2:C:272:TYR:CZ	2:C:276:ARG:HD2	2.52	0.44
2:C:713:LEU:HD13	2:C:1024:ILE:HB	1.99	0.44
3:D:27:GLU:HB2	3:D:94:HIS:CE1	2.52	0.44
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.52	0.44
6:G:17:DG:H2''	6:G:18:DG:C8	2.53	0.44
1:B:6:ARG:O	1:B:25:PRO:HD2	2.18	0.44
2:C:1047:THR:HG23	2:C:1049:GLN:H	1.83	0.44
2:C:501:ASN:HB3	2:C:505:PHE:H	1.82	0.44
3:D:461:VAL:HG21	3:D:469:ILE:HD12	2.00	0.44
2:C:813:ARG:HD2	3:D:67:ARG:HH12	1.83	0.44
5:F:191:LEU:CG	5:F:195:LEU:HD21	2.48	0.44
2:C:652:ILE:HD11	2:C:682:PRO:HB3	2.00	0.44
2:C:87:LEU:HD11	2:C:391:GLU:HB2	2.00	0.44
2:C:393:VAL:HG11	2:C:413:ASN:HB3	2.00	0.44
2:C:93:PHE:CE2	6:G:4:DT:H5'	2.50	0.44
3:D:1090:LYS:HA	3:D:1109:GLN:HE22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:ILE:HG23	3:D:514:PRO:HG2	2.00	0.44
3:D:778:TRP:HB2	3:D:823:LEU:HD21	1.99	0.44
7:H:1:DT:H4'	7:H:2:DG:H5'	1.99	0.44
2:C:235:LEU:HA	2:C:235:LEU:HD23	1.83	0.44
7:H:19:DG:H2''	7:H:20:DT:H5'	1.99	0.44
2:C:185:ILE:HG22	2:C:186:ASP:H	1.82	0.44
5:F:159:ALA:HB3	5:F:184:LEU:HD21	2.00	0.44
1:B:98:ARG:HA	1:B:134:LEU:O	2.17	0.43
3:D:1003:ILE:HD12	3:D:1157:ILE:HG13	1.99	0.43
6:G:3:DG:C3'	6:G:3:DG:P	3.03	0.43
3:D:821:LYS:HB3	3:D:836:VAL:HB	2.00	0.43
2:C:181:PHE:CD2	2:C:196:VAL:HB	2.53	0.43
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.33	0.43
5:F:198:VAL:O	5:F:199:ALA:HB3	2.18	0.43
2:C:407:THR:HG23	2:C:410:THR:H	1.83	0.43
3:D:428:SER:HB3	3:D:522:ILE:HG13	2.00	0.43
5:F:81:TRP:O	5:F:85:ILE:HG13	2.19	0.43
6:G:7:DG:C6	6:G:8:DA:C6	3.06	0.43
3:D:191:ALA:O	3:D:195:ARG:HB2	2.18	0.43
2:C:221:ASP:N	2:C:221:ASP:OD1	2.52	0.43
2:C:725:TYR:CE1	3:D:579:LEU:CD1	3.00	0.43
2:C:715:VAL:HA	2:C:909:ILE:O	2.19	0.43
2:C:946:VAL:HG23	2:C:946:VAL:O	2.19	0.43
3:D:71:LYS:HE3	3:D:71:LYS:HB2	1.80	0.43
3:D:850:PHE:O	3:D:853:THR:OG1	2.32	0.43
3:D:965:VAL:HG13	3:D:974:VAL:HG11	2.00	0.43
2:C:461:ARG:HA	6:G:13:DT:H5'	2.01	0.43
3:D:937:ILE:HG23	3:D:938:VAL:H	1.84	0.43
2:C:750:GLU:HG3	2:C:862:LEU:HD21	2.01	0.43
2:C:448:ARG:HA	2:C:448:ARG:HD2	1.74	0.42
3:D:579:LEU:HD12	3:D:580:ASP:H	1.80	0.42
5:F:191:LEU:HD21	5:F:195:LEU:HD21	1.98	0.42
2:C:144:GLN:HE22	2:C:409:GLN:HB2	1.84	0.42
2:C:626:LEU:O	2:C:630:ILE:HG23	2.19	0.42
3:D:579:LEU:O	3:D:807:ALA:HB1	2.20	0.42
3:D:437:LYS:HD3	3:D:437:LYS:HA	1.75	0.42
3:D:23:TRP:HB3	3:D:92:MET:HE3	2.00	0.42
2:C:93:PHE:CZ	6:G:4:DT:C5'	3.02	0.42
2:C:1132:LEU:HD21	3:D:11:ARG:NH1	2.34	0.42
2:C:542:ILE:HG22	2:C:543:ASP:O	2.19	0.42
3:D:465:HIS:CD2	3:D:482:GLN:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:347:THR:O	2:C:358:PRO:HA	2.18	0.42
3:D:133:ALA:HB2	3:D:236:VAL:HG13	2.01	0.42
3:D:320:ILE:HG21	3:D:340:LEU:HD23	2.02	0.42
3:D:793:TYR:HB3	3:D:800:ILE:HG13	2.01	0.42
2:C:918:ARG:NH1	3:D:808:THR:OG1	2.53	0.42
4:E:85:GLY:HA3	4:E:88:GLU:HG3	2.00	0.42
5:F:80:ALA:CB	6:G:3:DG:H4'	2.48	0.42
2:C:93:PHE:CZ	6:G:4:DT:H5'	2.54	0.42
2:C:276:ARG:CD	2:C:279:GLU:HB2	2.48	0.42
2:C:509:PRO:HB2	2:C:575:VAL:HG11	2.02	0.42
3:D:177:LEU:HD21	3:D:198:ARG:HA	2.01	0.42
2:C:626:LEU:HD22	2:C:705:GLY:O	2.19	0.42
3:D:590:THR:HG21	3:D:630:ARG:HH21	1.85	0.42
5:F:191:LEU:O	5:F:195:LEU:CD2	2.68	0.42
2:C:172:GLN:O	2:C:372:LEU:HA	2.20	0.42
2:C:303:ALA:HB3	2:C:306:GLY:H	1.84	0.42
2:C:315:GLY:O	2:C:355:VAL:HG12	2.20	0.42
2:C:389:ARG:HD3	5:F:49:ARG:NH1	2.29	0.42
2:C:806:THR:OG1	3:D:56:ARG:NH1	2.53	0.42
3:D:67:ARG:HA	3:D:67:ARG:HD3	1.88	0.42
1:A:82:SER:C	1:A:123:MET:HE1	2.40	0.41
2:C:325:SER:OG	2:C:325:SER:O	2.38	0.41
3:D:1042:GLY:O	3:D:1084:GLN:NE2	2.53	0.41
3:D:925:LEU:HD12	3:D:938:VAL:HG12	2.02	0.41
4:E:89:LYS:HE3	4:E:89:LYS:HB3	1.92	0.41
1:B:51:VAL:HA	1:B:139:VAL:O	2.19	0.41
3:D:1150:HIS:ND1	3:D:1152:LYS:HG2	2.36	0.41
2:C:259:ASP:OD1	2:C:260:ASN:N	2.53	0.41
3:D:325:ARG:HD2	3:D:341:ASN:OD1	2.21	0.41
3:D:353:ARG:HH22	5:F:56:ASP:HB3	1.85	0.41
2:C:1155:ASN:HB3	5:F:137:PRO:HB3	2.01	0.41
7:H:13:DT:H2'	7:H:14:DC:H6	1.86	0.41
2:C:1011:GLU:HG2	2:C:1011:GLU:H	1.62	0.41
2:C:314:LEU:HD13	2:C:334:ALA:HB3	2.02	0.41
2:C:351:VAL:O	2:C:353:GLY:N	2.53	0.41
2:C:719:PRO:HA	2:C:724:ASN:HD21	1.85	0.41
2:C:1125:LEU:HD13	3:D:105:TRP:CH2	2.56	0.41
3:D:1078:ASP:OD1	3:D:1078:ASP:N	2.53	0.41
3:D:86:LYS:HB3	3:D:86:LYS:HE2	1.95	0.41
2:C:598:ARG:CZ	2:C:919:ARG:HD3	2.51	0.41
7:H:13:DT:H2'	7:H:14:DC:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:470:HIS:CG	2:C:471:PRO:HD2	2.56	0.41
2:C:741:LEU:HB2	2:C:873:ILE:HB	2.02	0.41
3:D:34:ILE:HG22	3:D:41:PRO:HA	2.03	0.41
2:C:1083:LEU:HD22	3:D:420:LYS:HZ3	1.86	0.41
1:B:22:VAL:HG12	1:B:193:ILE:HG12	2.03	0.41
2:C:542:ILE:HA	2:C:547:ARG:O	2.20	0.41
3:D:917:GLU:HA	3:D:921:TYR:HB3	2.02	0.41
3:D:925:LEU:HD23	3:D:925:LEU:HA	1.74	0.41
2:C:1140:GLU:OE1	2:C:1142:ARG:HG2	2.20	0.41
3:D:860:LEU:O	3:D:863:THR:HG22	2.20	0.41
2:C:543:ASP:O	2:C:546:GLY:N	2.54	0.41
2:C:93:PHE:CZ	6:G:4:DT:C4'	3.03	0.41
3:D:901:LEU:HA	3:D:916:ILE:HG12	2.02	0.41
5:F:84:ARG:HD3	5:F:84:ARG:HA	1.86	0.41
2:C:592:GLU:HB3	2:C:971:PHE:CD1	2.56	0.41
3:D:1191:ARG:HG2	3:D:1191:ARG:H	1.53	0.41
3:D:670:ARG:HD3	3:D:685:ASN:HA	2.03	0.41
3:D:766:ASN:O	3:D:770:ARG:N	2.43	0.41
3:D:928:ASP:HB3	3:D:939:GLU:HA	2.03	0.41
1:B:182:ARG:CB	1:B:189:PHE:HB2	2.50	0.41
1:A:144:ARG:NH1	1:B:2:LEU:HB2	2.36	0.41
2:C:206:LEU:HD12	2:C:206:LEU:HA	1.92	0.41
2:C:251:ILE:H	2:C:251:ILE:HD12	1.86	0.41
3:D:343:LEU:HD13	3:D:381:LEU:HA	2.03	0.41
6:G:7:DG:N1	6:G:8:DA:N1	2.69	0.41
1:A:17:ASN:HB2	1:A:198:THR:O	2.22	0.40
1:A:202:ILE:HD11	1:A:207:ALA:HB2	2.03	0.40
1:B:226:ASN:O	1:B:227:VAL:CG1	2.69	0.40
2:C:328:THR:HB	2:C:330:GLU:OE2	2.21	0.40
2:C:66:GLU:HG2	2:C:66:GLU:H	1.61	0.40
3:D:342:ASP:O	3:D:346:ARG:HG3	2.21	0.40
2:C:548:PHE:HD2	2:C:567:SER:HB2	1.85	0.40
3:D:1053:VAL:HG12	3:D:1103:ASP:O	2.21	0.40
3:D:1080:ILE:HG21	3:D:1112:MET:HE2	2.04	0.40
3:D:879:ASP:OD2	3:D:1214:SER:HB3	2.21	0.40
3:D:481:PRO:HA	3:D:484:TRP:HD1	1.86	0.40
8:I:9:G:O6	8:I:10:A:N6	2.54	0.40
1:A:86:SER:O	1:A:116:VAL:HA	2.22	0.40
1:A:149:ALA:N	1:A:165:ASP:OD1	2.49	0.40
1:A:66:VAL:O	1:A:69:VAL:HG22	2.20	0.40
2:C:515:ASP:OD1	2:C:515:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:725:TYR:CE1	3:D:579:LEU:HD11	2.57	0.40
2:C:93:PHE:CE2	6:G:4:DT:H4'	2.57	0.40
3:D:1193:VAL:CG1	3:D:1194:VAL:N	2.83	0.40
3:D:435:GLN:H	3:D:435:GLN:HG2	1.73	0.40
3:D:666:THR:HG21	3:D:683:PHE:CE1	2.56	0.40
3:D:353:ARG:HH12	5:F:56:ASP:HA	1.86	0.40
1:A:40:ARG:NE	1:B:33:THR:HG22	2.36	0.40
2:C:342:LEU:HD13	2:C:359:VAL:HG12	2.03	0.40
3:D:339:ASP:OD2	3:D:397:ARG:NH2	2.55	0.40
1:B:24:GLU:HA	1:B:25:PRO:HA	1.81	0.40
6:G:1:DT:H2''	6:G:2:DT:OP2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/368 (58%)	209 (98%)	4 (2%)	0	100	100
1	B	224/368 (61%)	212 (95%)	12 (5%)	0	100	100
2	C	1136/1174 (97%)	1096 (96%)	39 (3%)	1 (0%)	51	82
3	D	1250/1317 (95%)	1223 (98%)	25 (2%)	2 (0%)	47	78
4	E	71/110 (64%)	68 (96%)	3 (4%)	0	100	100
5	F	144/218 (66%)	140 (97%)	4 (3%)	0	100	100
All	All	3038/3555 (86%)	2948 (97%)	87 (3%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1194	VAL

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Mol	Chain	Res	Type
3	D	573	PRO
2	C	76	PRO

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	183/315 (58%)	181 (99%)	2 (1%)	73	86
1	B	171/315 (54%)	169 (99%)	2 (1%)	71	85
2	C	923/995 (93%)	908 (98%)	15 (2%)	62	81
3	D	1016/1096 (93%)	1004 (99%)	12 (1%)	71	85
4	E	63/90 (70%)	62 (98%)	1 (2%)	62	81
5	F	112/175 (64%)	105 (94%)	7 (6%)	18	49
All	All	2468/2986 (83%)	2429 (98%)	39 (2%)	62	81

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	188	ASP
1	B	88	GLU
1	B	225	LEU
2	C	66	GLU
2	C	70	GLU
2	C	215	THR
2	C	293	LEU
2	C	316	LEU
2	C	324	SER
2	C	326	THR
2	C	517	VAL
2	C	557	ARG
2	C	578	ARG
2	C	620	VAL
2	C	635	VAL

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Mol	Chain	Res	Type
2	C	958	LEU
2	C	983	LEU
2	C	1135	ASP
3	D	314	LEU
3	D	330	LEU
3	D	577	PRO
3	D	579	LEU
3	D	581	MET
3	D	925	LEU
3	D	958	THR
3	D	972	THR
3	D	1070	ASP
3	D	1107	VAL
3	D	1191	ARG
3	D	1192	ARG
4	E	55	TYR
5	F	36	LEU
5	F	79	LYS
5	F	143	GLU
5	F	148	LEU
5	F	184	LEU
5	F	194	LEU
5	F	195	LEU

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
8	I	9/10 (90%)	4 (44%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	2	C
8	I	3	A
8	I	6	C
8	I	10	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	217/368 (58%)	-0.08	4 (1%) 68 71	63, 81, 120, 150	0
1	B	228/368 (61%)	0.42	18 (7%) 12 14	86, 124, 151, 168	0
2	C	1138/1174 (96%)	0.24	73 (6%) 19 21	47, 86, 169, 207	0
3	D	1258/1317 (95%)	0.21	50 (3%) 38 40	48, 97, 146, 197	0
4	E	75/110 (68%)	0.62	10 (13%) 3 4	99, 124, 149, 176	0
5	F	148/218 (67%)	1.04	27 (18%) 1 1	90, 146, 168, 198	0
6	G	23/23 (100%)	2.29	11 (47%) 0 0	101, 152, 199, 204	2 (8%)
7	H	21/21 (100%)	1.04	5 (23%) 0 0	59, 85, 160, 170	0
8	I	10/10 (100%)	0.08	0 100 100	53, 70, 118, 142	0
All	All	3118/3609 (86%)	0.29	198 (6%) 19 21	47, 99, 159, 207	2 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	G	5	DG	8.7
3	D	908	GLY	7.3
3	D	336	ALA	5.8
3	D	334	ARG	5.7
4	E	25	SER	5.6
6	G	23	DA	5.5
6	G	3	DG	5.5
2	C	281	PRO	5.4
3	D	333	GLY	5.3
2	C	568	SER	5.1
1	B	4	SER	5.0
3	D	332	GLY	4.9
2	C	263	GLY	4.9
2	C	282	THR	4.7
3	D	907	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
6	G	6	DG	4.7
5	F	193	GLY	4.7
2	C	141	ILE	4.6
6	G	4	DT	4.6
3	D	653	HIS	4.6
3	D	933	ALA	4.5
3	D	1093	ASP	4.5
2	C	133	PHE	4.5
5	F	173	MET	4.5
2	C	286	ALA	4.4
2	C	285	SER	4.3
1	B	235	GLY	4.3
1	B	12	ASP	4.2
7	H	1	DT	4.1
5	F	70	ARG	4.1
2	C	279	GLU	4.1
3	D	654	SER	4.0
3	D	337	THR	4.0
2	C	138	THR	3.9
2	C	569	GLU	3.9
2	C	134	ILE	3.9
2	C	1158	ILE	3.9
2	C	321	PRO	3.9
5	F	68	GLY	3.9
2	C	290	LEU	3.8
2	C	515	ASP	3.8
1	B	133	LYS	3.8
3	D	1190	ASN	3.8
5	F	145	LEU	3.7
5	F	187	GLY	3.7
5	F	74	HIS	3.7
6	G	1	DT	3.6
3	D	1095	SER	3.6
1	B	117	THR	3.6
3	D	1094	GLY	3.5
2	C	352	PRO	3.5
2	C	354	GLY	3.5
1	B	184	GLU	3.5
2	C	323	THR	3.5
2	C	280	PRO	3.4
2	C	514	VAL	3.4
2	C	262	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	278	GLY	3.4
2	C	22	SER	3.4
5	F	78	LEU	3.3
5	F	155	ALA	3.3
2	C	137	ASN	3.3
5	F	69	PHE	3.3
3	D	331	ASP	3.3
3	D	335	PHE	3.3
2	C	820	GLY	3.3
2	C	283	LYS	3.3
3	D	1203	GLY	3.2
2	C	224	ARG	3.2
2	C	140	GLU	3.2
2	C	545	ASP	3.2
2	C	1145	GLU	3.2
2	C	231	LEU	3.2
5	F	46	ARG	3.2
4	E	55	TYR	3.2
2	C	1154	ALA	3.1
3	D	59	GLU	3.1
1	B	101	GLY	3.1
2	C	1155	ASN	3.1
3	D	1189	GLU	3.1
3	D	1272	VAL	3.1
2	C	1144	GLY	3.1
1	B	13	VAL	3.1
7	H	4	DA	3.0
2	C	567	SER	3.0
3	D	251	TYR	3.0
2	C	824	ARG	3.0
4	E	26	GLY	3.0
2	C	265	ASP	3.0
3	D	5	ASN	3.0
3	D	330	LEU	3.0
1	B	236	PRO	3.0
5	F	154	MET	3.0
7	H	2	DG	2.9
1	A	4	SER	2.9
3	D	1175	PHE	2.9
2	C	405	ALA	2.9
4	E	81	LEU	2.9
4	E	103	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
6	G	9	DG	2.8
5	F	45	LEU	2.8
1	B	6	ARG	2.8
4	E	28	TYR	2.8
4	E	78	VAL	2.8
2	C	229	THR	2.8
2	C	277	PRO	2.8
2	C	238	THR	2.8
1	B	140	VAL	2.8
3	D	188	GLY	2.7
3	D	38	THR	2.7
5	F	184	LEU	2.7
4	E	30	THR	2.7
2	C	320	GLU	2.7
3	D	1092	GLU	2.7
2	C	324	SER	2.7
2	C	347	THR	2.7
2	C	517	VAL	2.7
7	H	3	DC	2.7
5	F	194	LEU	2.7
2	C	406	ILE	2.6
6	G	2	DT	2.6
3	D	82	VAL	2.6
4	E	27	GLY	2.6
2	C	288	THR	2.6
2	C	818	ILE	2.6
2	C	246	PHE	2.6
3	D	1188	ALA	2.6
2	C	242	ILE	2.6
1	B	132	GLY	2.6
5	F	77	ASN	2.6
2	C	825	GLU	2.5
1	B	5	GLN	2.5
3	D	45	GLY	2.5
5	F	29	PHE	2.5
1	B	16	ASP	2.5
2	C	71	ARG	2.5
3	D	39	LEU	2.5
5	F	65	ALA	2.5
5	F	153	ARG	2.4
2	C	234	ALA	2.4
5	F	76	THR	2.4

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Mol	Chain	Res	Type	RSRZ
5	F	198	VAL	2.4
2	C	271	ILE	2.4
3	D	192	ASP	2.4
1	A	189	PHE	2.4
3	D	80	VAL	2.4
3	D	958	THR	2.4
2	C	819	PHE	2.4
2	C	267	ALA	2.4
2	C	1153	ALA	2.4
1	B	185	GLN	2.4
2	C	823	ALA	2.4
2	C	98	SER	2.4
1	B	14	LEU	2.4
6	G	8	DA	2.4
1	B	116	VAL	2.4
2	C	1152	ALA	2.4
2	C	1157	GLY	2.3
2	C	142	LYS	2.3
5	F	166	TYR	2.3
5	F	174	ASP	2.3
5	F	73	ARG	2.3
3	D	931	ASP	2.3
2	C	544	ALA	2.3
7	H	21	DG	2.3
3	D	1202	ALA	2.3
3	D	81	GLU	2.3
3	D	1187	GLU	2.3
3	D	91	ARG	2.2
3	D	957	ILE	2.2
2	C	546	GLY	2.2
3	D	1280	ALA	2.2
2	C	139	GLY	2.2
3	D	1275	THR	2.2
3	D	194	ARG	2.2
3	D	189	ALA	2.2
5	F	71	SER	2.2
3	D	41	PRO	2.2
3	D	909	THR	2.2
2	C	760	ALA	2.1
2	C	73	ASP	2.1
6	G	11	DT	2.1
2	C	74	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	E	80	PRO	2.1
6	G	7	DG	2.1
2	C	623	GLY	2.1
3	D	1060	ARG	2.1
1	A	187	THR	2.1
2	C	355	VAL	2.1
3	D	305	SER	2.1
2	C	1067	CYS	2.0
1	A	221	LEU	2.0
1	B	102	PRO	2.0
5	F	160	ASP	2.0
5	F	25	LEU	2.0
2	C	31	ASN	2.0
3	D	1050	THR	2.0
3	D	934	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	MG	D	2003	1/1	0.90	0.10	68,68,68,68	0
9	ZN	D	2002	1/1	0.92	0.04	129,129,129,129	0
9	ZN	D	2001	1/1	0.98	0.08	109,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.