



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:12 PM UTC

PDB ID : 6KOQ / pdb_00006koq
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 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

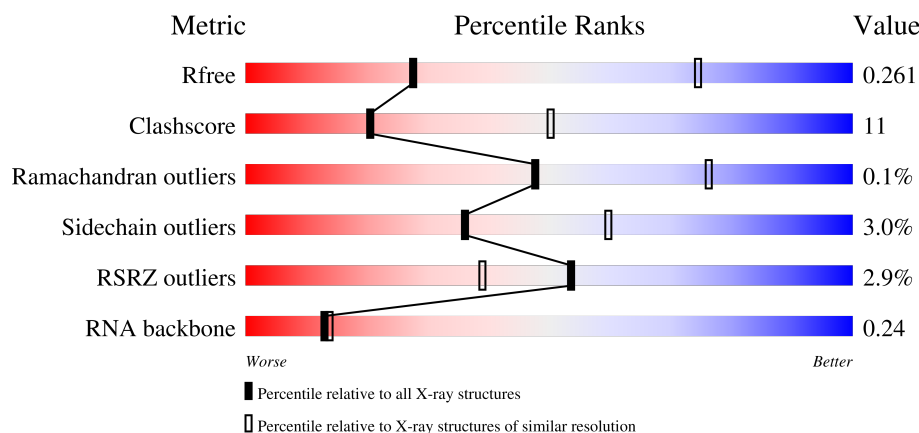
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	
2	C	1174	
3	D	1317	

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Mol	Chain	Length	Quality of chain
4	E	110	2%58%10%32%
5	F	218	4%44%22%32%
6	G	23	9%30%70%
7	H	21	24%76%
8	I	10	30%40%30%

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 (CCD ID: ZN) (formula: Zn).

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

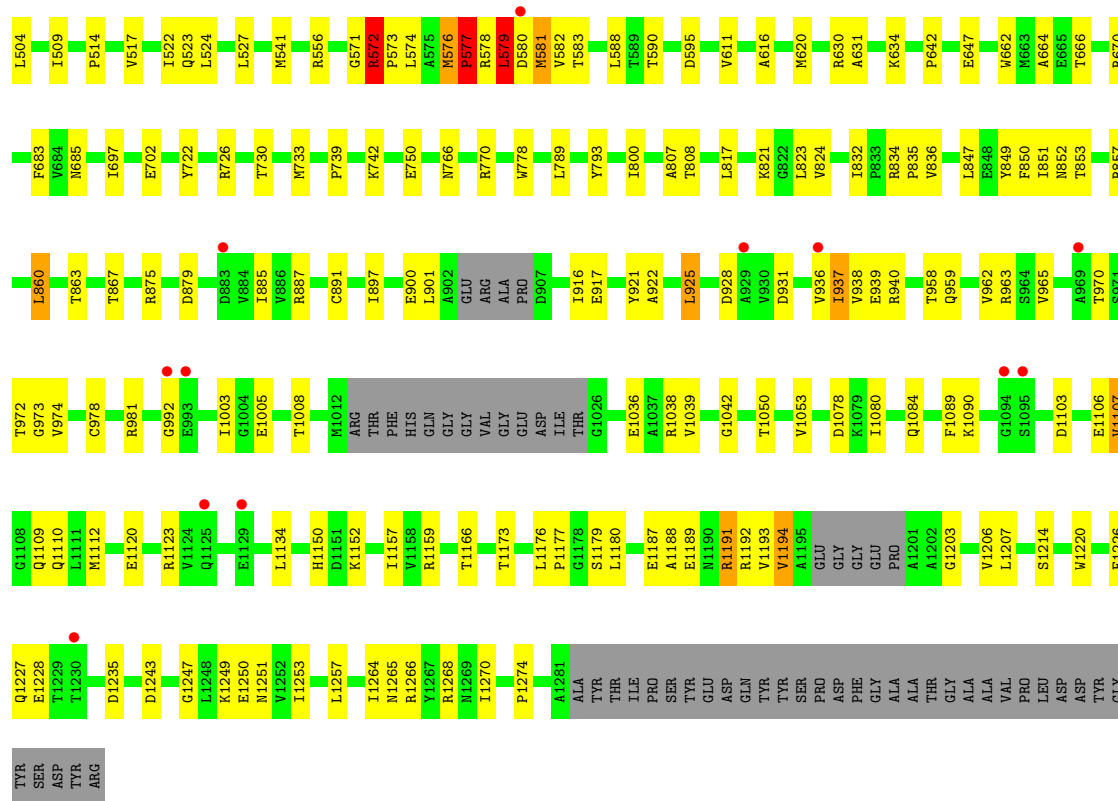
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

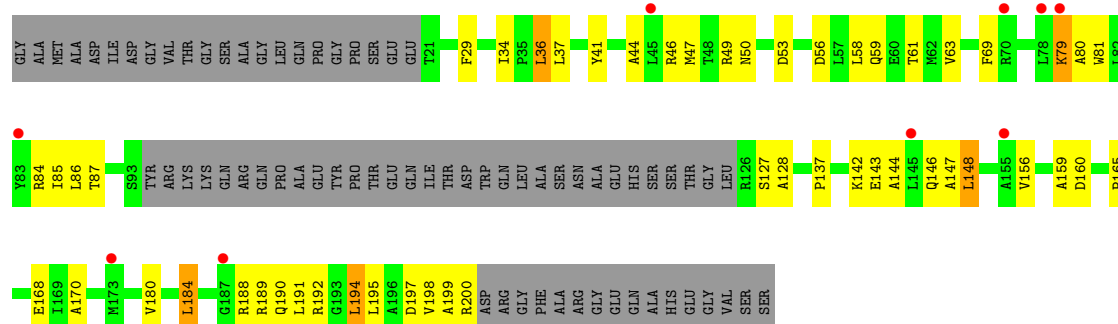
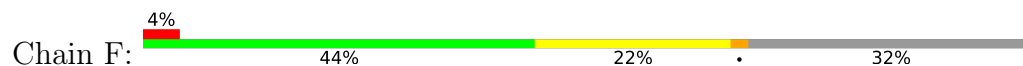




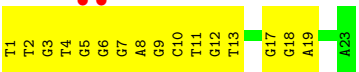
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: ECF RNA polymerase sigma factor SigH



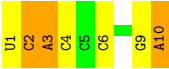
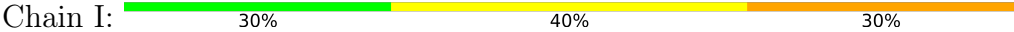
- Molecule 6: DNA (5'-D(*TP*TP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3')



● 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')



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



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 36.51 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (36.51-3.35) 97.1 (36.51-3.35)	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 0.222 , 0.261	Depositor DCC
R_{free} test set	2395 reflections (3.71%)	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)	0.31 , 73.5	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: MG, ZN

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	0.14	0/1657	0.35	0/2256
1	B	0.37	0/1663	0.48	1/2275 (0.0%)
2	C	0.21	0/8815	0.40	2/11982 (0.0%)
3	D	0.28	2/9880 (0.0%)	0.41	5/13377 (0.0%)
4	E	0.13	0/598	0.35	0/815
5	F	0.22	0/1155	0.44	0/1568
6	G	0.22	0/497	0.44	0/765
7	H	0.19	0/487	0.37	0/752
8	I	0.22	0/226	0.43	0/349
All	All	0.25	2/24978 (0.0%)	0.41	8/34139 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	577	PRO	C-O	-5.10	1.17	1.23
3	D	574	LEU	CA-C	-5.03	1.46	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	579	LEU	N-CA-C	10.52	122.50	111.14
3	D	574	LEU	N-CA-C	-9.00	95.91	109.86
1	B	229	ALA	N-CA-C	6.33	119.53	110.10
2	C	558	LYS	N-CA-C	-6.10	104.63	111.28
2	C	73	ASP	N-CA-C	-5.97	98.14	108.52
3	D	1189	GLU	N-CA-C	-5.84	104.92	111.28
3	D	576	MET	N-CA-C	-5.81	100.06	109.82
3	D	572	ARG	N-CA-C	-5.63	100.75	109.87

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	24	0
1	B	1637	0	1607	33	0
2	C	8656	0	8438	202	0
3	D	9719	0	9680	223	0
4	E	586	0	576	8	0
5	F	1137	0	1088	56	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	536	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 (536) 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
3:D:527:LEU:CD2	3:D:581:MET:HE1	1.65	1.25
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:2:DT:H2''	6:G:3:DG:OP2	1.49	1.06
3:D:527:LEU:HD23	3:D:581:MET:HE1	1.37	1.05
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
2:C:70:GLU:N	2:C:70:GLU:OE1	1.95	1.00
3:D:527:LEU:HD23	3:D:581:MET:CE	1.92	0.99
3:D:527:LEU:HD21	3:D:581:MET:HE1	1.43	0.98
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
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
3:D:577:PRO:HA	3:D:581:MET:HE3	1.60	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:1193:VAL:C	3:D:1194:VAL:HG23	2.15	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:572:ARG:HH11	3:D:572:ARG:HG2	1.56	0.70
3:D:1188:ALA:CA	3:D:1191:ARG:HD2	2.18	0.70
2:C:1038:ARG:NH2	3:D:423:ASP:OD1	2.22	0.69
3:D:293:LEU:HD21	3:D:1177:PRO:HG2	1.74	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
2:C:1145:GLU:HB3	3:D:84:ARG:HH11	1.57	0.68
3:D:834:ARG:HD3	3:D:835:PRO:HD2	1.75	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
2:C:732:SER:HA	2:C:898:MET:HE3	1.75	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
3:D:1188:ALA:C	3:D:1191:ARG:HG2	2.21	0.66
2:C:62:PRO:O	2:C:66:GLU:HG2	1.96	0.65
2:C:605:MET:HE1	2:C:886:LYS:HD3	1.79	0.65
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.79	0.65
2:C:554:LEU:HD12	2:C:563:GLU:O	1.96	0.65
2:C:1131:VAL:HG21	2:C:1141:LEU:HD13	1.79	0.65
2:C:922:ILE:HD12	3:D:817:LEU:HD21	1.78	0.65
3:D:576:MET:HG2	3:D:697:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H8	6:G:7:DG:OP2	1.80	0.63
3:D:1188:ALA:C	3:D:1191:ARG:CG	2.72	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
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
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
2:C:129:VAL:HG21	2:C:148:MET:HE2	1.83	0.60
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:83:LEU:HA	1:A:123:MET:HE1	1.84	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:HG12	5:F:198:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1146:ASP:OD1	3:D:71:LYS:NZ	2.36	0.58
3:D:1270:ILE:HG12	4:E:107:GLU:HA	1.86	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:172:GLN:OE1	2:C:373:ARG:NH2	2.37	0.57
2:C:305:VAL:HG22	2:C:503:PHE:HD1	1.69	0.57
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:461:ARG:NH1	6:G:11:DT:O4'	2.37	0.56
2:C:725:TYR:HE1	3:D:579:LEU:CD1	2.18	0.56
2:C:605:MET:HE1	2:C:886:LYS:HB3	1.86	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
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
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:69:ALA:HB3	2:C:70:GLU:OE1	2.07	0.55
2:C:1081:GLU:HG3	2:C:1085:ILE:HD11	1.87	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
3:D:1188:ALA:O	3:D:1191:ARG:HG2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:142:LYS:O	5:F:146:GLN:HG3	2.07	0.55
2:C:709:LEU:HB2	2:C:1025:MET:HE2	1.87	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:A:40:ARG:NH2	2:C:1007:GLY:O	2.40	0.54
1:B:129:ASN:OD1	1:B:130:ASP:N	2.38	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
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:320:GLU:N	2:C:321:PRO:HD3	2.24	0.52
2:C:1111:ILE:HD13	3:D:3:ASP:HB2	1.90	0.52
3:D:386:ARG:NH2	7:H:9:DT:OP1	2.42	0.52
3:D:582:VAL:O	3:D:583:THR:C	2.51	0.52
5:F:44:ALA:HB2	5:F:86:LEU:HD11	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:480:ILE:HD11	3:D:849:TYR:HE1	1.75	0.52
2:C:510:TYR:HB3	2:C:572:TYR:HB3	1.92	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:HH11	3:D:572:ARG:CG	2.22	0.51
8:I:4:C:H2'	8:I:4:C:O2	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
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: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:832:ILE:HD12	3:D:851:ILE:HG23	1.93	0.50
3:D:1134:LEU:HD11	3:D:1207:LEU:HD21	1.92	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:776:ALA:O	2:C:785:ARG:NH2	2.45	0.50
2:C:899:PRO:HB3	2:C:1013:PHE:HE2	1.76	0.50
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.47	0.50
3:D:327:MET:HG3	3:D:337:THR:HG22	1.93	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
2:C:606:GLN:HG2	2:C:1025:MET:HE1	1.93	0.50
3:D:328:VAL:HG11	8:I:1:U:H3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:74:VAL:HG13	2:C:75:ASN:N	2.27	0.49
2:C:557:ARG:C	2:C:560:GLY:H	2.20	0.49
3:D:527:LEU:CD2	3:D:581:MET:HE3	2.38	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: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
2:C:1130:GLU:OE1	3:D:11:ARG:NH2	2.40	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
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:198:VAL:HB	2:C:206:LEU:HB3	1.95	0.48
2:C:1040:THR:HG21	5:F:128:ALA:HB3	1.95	0.48
2:C:1140:GLU:OE1	2:C:1141:LEU:N	2.46	0.48
3:D:556:ARG:HD3	4:E:91:LEU:HD22	1.95	0.48
2:C:803:LYS:HG2	2:C:805:GLU:H	1.77	0.48
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.95	0.48
3:D:1089:PHE:O	3:D:1109:GLN:NE2	2.45	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
3:D:1080:ILE:HG21	3:D:1112:MET:HE2	1.95	0.48
2:C:652:ILE:HD13	2:C:696:ILE:HG22	1.96	0.48
2:C:1088:ASP:HB3	2:C:1112:PRO:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:717:ILE:O	3:D:730:THR:HG23	2.14	0.48
3:D:219:LEU:HA	3:D:222:ILE:HD12	1.96	0.48
3:D:1264:ILE:HG22	3:D:1266:ARG:H	1.78	0.48
5:F:59:GLN:O	5:F:63:VAL:HG23	2.12	0.48
3:D:230:ALA:N	3:D:233:GLN:OE1	2.45	0.48
3:D:1193:VAL:HG12	3:D:1194:VAL:N	2.29	0.48
2:C:93:PHE:CG	6:G:5:DG:OP1	2.67	0.47
2:C:508:THR:HG22	2:C:579:GLN:HE21	1.78	0.47
2:C:756:THR:N	2:C:759:GLY:O	2.45	0.47
2:C:1005:PHE:HA	2:C:1012:PRO:HA	1.97	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
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
2:C:233:LYS:HZ2	2:C:262:VAL:HA	1.80	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
2:C:1083:LEU:HB3	3:D:420:LYS:HZ1	1.80	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:238:THR:O	2:C:242:ILE:HG12	2.15	0.47
2:C:1039:SER:HB3	3:D:450:GLU:O	2.14	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:707:MET:HE3	2:C:707:MET:HB3	1.82	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:N	3:D:931:ASP:OD1	2.47	0.46
5:F:148:LEU:HD11	5:F:190:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:PHE:HA	1:B:33:THR:OG1	2.15	0.46
1:B:49:ALA:HA	1:B:142:ARG:HA	1.97	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
3:D:576:MET:HE2	3:D:576:MET:HB3	1.71	0.46
2:C:534:VAL:CG2	2:C:555:VAL:HG21	2.45	0.46
2:C:1090:THR:HG22	2:C:1093:ARG:HH21	1.80	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:45:GLY:H	3:D:48:CYS:HB2	1.81	0.46
3:D:100:PRO:HG3	3:D:315:ASP:OD1	2.16	0.46
6:G:9:DG:H2''	6:G:10:DC:C6	2.51	0.46
2:C:93:PHE:CD2	6:G:4:DT:H4'	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
2:C:803:LYS:HE3	2:C:827:ARG:HB3	1.96	0.46
3:D:114:LEU:HG	3:D:312:MET:HE2	1.97	0.46
3:D:1227:GLN:HG3	7:H:10:DG:H5''	1.96	0.46
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:HD13	5:F:36:LEU:HA	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:850:PHE:O	3:D:853:THR:OG1	2.32	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:873:ILE:HD12	2:C:873:ILE:HA	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:80:LEU:O	2:C:84:LEU:HG	2.17	0.45
2:C:1001:LYS:HA	2:C:1018:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:501:ASN:HB3	2:C:505:PHE:H	1.82	0.44
2:C:813:ARG:HD2	3:D:67:ARG:HH12	1.83	0.44
2:C:1047:THR:HG23	2:C:1049:GLN:H	1.83	0.44
3:D:461:VAL:HG21	3:D:469:ILE:HD12	2.00	0.44
5:F:191:LEU:CG	5:F:195:LEU:HD21	2.48	0.44
2:C:87:LEU:HD11	2:C:391:GLU:HB2	2.00	0.44
2:C:652:ILE:HD11	2:C:682:PRO:HB3	2.00	0.44
3:D:1193:VAL:C	3:D:1194:VAL:CG2	2.86	0.44
2:C:93:PHE:CE2	6:G:4:DT:H5'	2.50	0.44
2:C:393:VAL:HG11	2:C:413:ASN:HB3	2.00	0.44
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
3:D:1090:LYS:HA	3:D:1109:GLN:HE22	1.82	0.44
7:H:1:DT:H4'	7:H:2:DG:H5'	1.99	0.44
2:C:235:LEU:HD23	2:C:235:LEU:HA	1.83	0.44
7:H:19:DG:H2''	7:H:20:DT:H5'	1.99	0.44
1:A:95:MET:HE3	1:A:112:PRO:HB3	2.00	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:P	6:G:3:DG:C3'	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
2:C:407:THR:HG23	2:C:410:THR:H	1.83	0.43
2:C:70:GLU:N	2:C:70:GLU:CD	2.73	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
3:D:666:THR:HG22	3:D:685:ASN:CG	2.44	0.43
5:F:198:VAL:O	5:F:199:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:725:TYR:CE1	3:D:579:LEU:CD1	3.00	0.43
3:D:524:LEU:HD13	3:D:541:MET:HE1	1.99	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:HB2	3:D:71:LYS:HE3	1.80	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
2:C:93:PHE:CZ	6:G:4:DT:C5'	3.02	0.42
2:C:592:GLU:H	2:C:592:GLU:CD	2.24	0.42
3:D:437:LYS:HA	3:D:437:LYS:HD3	1.75	0.42
3:D:1176:LEU:O	3:D:1179:SER:OG	2.34	0.42
2:C:542:ILE:HG22	2:C:543:ASP:O	2.19	0.42
2:C:1132:LEU:HD21	3:D:11:ARG:NH1	2.34	0.42
3:D:465:HIS:CD2	3:D:482:GLN:HB3	2.55	0.42
2:C:93:PHE:CZ	6:G:4:DT:H5'	2.54	0.42
2:C:347:THR:O	2:C:358:PRO:HA	2.18	0.42
2:C:918:ARG:NH1	3:D:808:THR:OG1	2.53	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
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
3:D:453:LYS:HZ1	3:D:473:LYS:HG3	1.84	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
3:D:571:GLY:C	3:D:572:ARG:O	2.56	0.42
5:F:47:MET:HE1	5:F:87:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:430:ILE:HG21	3:D:541:MET:HE2	2.01	0.41
3:D:925:LEU:HD12	3:D:938:VAL:HG12	2.02	0.41
3:D:1042:GLY:O	3:D:1084:GLN:NE2	2.53	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
2:C:1155:ASN:HB3	5:F:137:PRO:HB3	2.01	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
7:H:13:DT:H2'	7:H:14:DC:H6	1.86	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:1011:GLU:H	2:C:1011:GLU:HG2	1.62	0.41
2:C:1125:LEU:HD13	3:D:105:TRP:CH2	2.56	0.41
3:D:86:LYS:HE2	3:D:86:LYS:HB3	1.95	0.41
3:D:1078:ASP:OD1	3:D:1078:ASP:N	2.53	0.41
2:C:221:ASP:OD1	2:C:221:ASP:N	2.52	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
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
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:HA	3:D:925:LEU:HD23	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:93:PHE:CZ	6:G:4:DT:C4'	3.03	0.41
2:C:246:PHE:CD2	2:C:252:MET:HE2	2.55	0.41
2:C:543:ASP:O	2:C:546:GLY:N	2.54	0.41
2:C:592:GLU:HB3	2:C:971:PHE:CD1	2.56	0.41
3:D:447:MET:HE2	3:D:447:MET:HB3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:901:LEU:HA	3:D:916:ILE:HG12	2.02	0.41
3:D:928:ASP:HB3	3:D:939:GLU:HA	2.03	0.41
3:D:1191:ARG:HG2	3:D:1191:ARG:H	1.53	0.41
5:F:84:ARG:HD3	5:F:84:ARG:HA	1.86	0.41
1:A:144:ARG:NH1	1:B:2:LEU:HB2	2.36	0.41
1:B:182:ARG:CB	1:B:189:PHE:HB2	2.50	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:66:GLU:HG2	2:C:66:GLU:H	1.61	0.40
2:C:261:THR:HB	2:C:266:GLU:CD	2.46	0.40
2:C:328:THR:HB	2:C:330:GLU:OE2	2.21	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:481:PRO:HA	3:D:484:TRP:HD1	1.86	0.40
3:D:879:ASP:OD2	3:D:1214:SER:HB3	2.21	0.40
3:D:1053:VAL:HG12	3:D:1103:ASP:O	2.21	0.40
8:I:9:G:O6	8:I:10:A:N6	2.54	0.40
1:A:66:VAL:O	1:A:69:VAL:HG22	2.20	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:B:226:ASN:C	1:B:227:VAL:HG12	2.46	0.40
2:C:93:PHE:CE2	6:G:4:DT:H4'	2.57	0.40
2:C:515:ASP:OD1	2:C:515:ASP:N	2.54	0.40
2:C:725:TYR:CE1	3:D:579:LEU:HD11	2.57	0.40
3:D:353:ARG:HH12	5:F:56:ASP:HA	1.86	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:1193:VAL:CG1	3:D:1194:VAL:N	2.83	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	48	76
3	D	1250/1317 (95%)	1223 (98%)	25 (2%)	2 (0%)	43	70
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%)	48	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1194	VAL
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%)	179 (98%)	4 (2%)	45	63
1	B	171/315 (54%)	162 (95%)	9 (5%)	20	48
2	C	923/995 (93%)	896 (97%)	27 (3%)	37	60
3	D	1016/1096 (93%)	989 (97%)	27 (3%)	39	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	63/90 (70%)	62 (98%)	1 (2%)	55	67
5	F	112/175 (64%)	106 (95%)	6 (5%)	20	47
All	All	2468/2986 (83%)	2394 (97%)	74 (3%)	36	60

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	51	VAL
1	A	111	VAL
1	A	141	GLU
1	B	84	VAL
1	B	88	GLU
1	B	111	VAL
1	B	136	VAL
1	B	150	VAL
1	B	191	LYS
1	B	199	LYS
1	B	202	ILE
1	B	225	LEU
2	C	66	GLU
2	C	70	GLU
2	C	196	VAL
2	C	215	THR
2	C	218	VAL
2	C	262	VAL
2	C	293	LEU
2	C	316	LEU
2	C	324	SER
2	C	326	THR
2	C	364	ILE
2	C	441	SER
2	C	517	VAL
2	C	557	ARG
2	C	565	VAL
2	C	578	ARG
2	C	610	VAL
2	C	620	VAL
2	C	635	VAL
2	C	643	VAL
2	C	654	VAL

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Mol	Chain	Res	Type
2	C	717	ILE
2	C	731	LEU
2	C	958	LEU
2	C	976	GLU
2	C	983	LEU
2	C	1148	ASP
3	D	4	VAL
3	D	34	ILE
3	D	110	VAL
3	D	135	VAL
3	D	187	GLU
3	D	236	VAL
3	D	243	GLU
3	D	314	LEU
3	D	330	LEU
3	D	517	VAL
3	D	572	ARG
3	D	577	PRO
3	D	579	LEU
3	D	581	MET
3	D	588	LEU
3	D	733	MET
3	D	860	LEU
3	D	897	ILE
3	D	925	LEU
3	D	936	VAL
3	D	937	ILE
3	D	958	THR
3	D	972	THR
3	D	1039	VAL
3	D	1107	VAL
3	D	1191	ARG
3	D	1192	ARG
4	E	39	ILE
5	F	36	LEU
5	F	79	LYS
5	F	143	GLU
5	F	148	LEU
5	F	184	LEU
5	F	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	733	ASN
2	C	883	HIS
2	C	885	ASN
3	D	262	GLN
3	D	287	GLN
3	D	303	GLN
3	D	748	HIS
3	D	766	ASN
3	D	771	ASN
3	D	935	ASN
3	D	1160	GLN
3	D	1269	ASN
4	E	68	ASN
4	E	105	HIS
5	F	77	ASN
5	F	88	ASN

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.01	0 100 100	63, 81, 120, 150	0
1	B	228/368 (61%)	0.53	10 (4%) 39 28	86, 124, 151, 168	0
2	C	1138/1174 (96%)	0.26	35 (3%) 51 38	47, 86, 169, 207	0
3	D	1258/1317 (95%)	0.31	33 (2%) 57 42	48, 97, 146, 197	0
4	E	75/110 (68%)	0.38	2 (2%) 56 41	99, 124, 149, 176	0
5	F	148/218 (67%)	0.71	9 (6%) 27 20	90, 146, 168, 198	0
6	G	23/23 (100%)	0.79	2 (8%) 16 14	101, 132, 199, 204	2 (8%)
7	H	21/21 (100%)	0.27	0 100 100	59, 85, 160, 170	0
8	I	10/10 (100%)	0.07	0 100 100	53, 70, 118, 142	0
All	All	3118/3609 (86%)	0.31	91 (2%) 53 39	47, 99, 159, 207	2 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	246	PHE	5.2
3	D	1095	SER	4.3
6	G	6	DG	4.1
5	F	173	MET	3.6
2	C	231	LEU	3.6
2	C	567	SER	3.4
3	D	883	ASP	3.4
2	C	1156	LEU	3.4
6	G	5	DG	3.4
1	B	183	VAL	3.4
1	B	201	SER	3.1
5	F	70	ARG	3.0
3	D	580	ASP	3.0
3	D	334	ARG	3.0
3	D	337	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	252	MET	2.9
2	C	230	VAL	2.9
2	C	212	LYS	2.8
2	C	141	ILE	2.8
2	C	263	GLY	2.8
3	D	992	GLY	2.8
5	F	83	TYR	2.8
5	F	78	LEU	2.8
4	E	55	TYR	2.8
2	C	187	LYS	2.7
2	C	289	LEU	2.7
3	D	303	GLN	2.7
2	C	138	THR	2.6
2	C	229	THR	2.6
2	C	134	ILE	2.6
2	C	133	PHE	2.6
3	D	1125	GLN	2.6
3	D	331	ASP	2.6
3	D	1129	GLU	2.6
3	D	5	ASN	2.5
3	D	82	VAL	2.5
5	F	155	ALA	2.5
3	D	59	GLU	2.5
1	B	4	SER	2.5
3	D	929	ALA	2.4
2	C	1114	SER	2.4
2	C	190	ASP	2.4
4	E	30	THR	2.4
2	C	515	ASP	2.4
5	F	187	GLY	2.4
5	F	145	LEU	2.4
3	D	1094	GLY	2.3
3	D	969	ALA	2.3
2	C	209	ASP	2.3
3	D	124	ASP	2.3
2	C	285	SER	2.3
2	C	569	GLU	2.3
3	D	7	PHE	2.3
2	C	71	ARG	2.3
2	C	189	THR	2.3
2	C	333	VAL	2.3
1	B	117	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	248	TYR	2.2
3	D	68	VAL	2.2
3	D	81	GLU	2.2
2	C	352	PRO	2.2
3	D	332	GLY	2.2
5	F	45	LEU	2.2
3	D	1230	THR	2.2
3	D	251	TYR	2.2
2	C	232	LEU	2.2
2	C	186	ASP	2.2
1	B	30	PHE	2.2
2	C	22	SER	2.2
2	C	193	LEU	2.2
3	D	336	ALA	2.2
2	C	514	VAL	2.1
3	D	80	VAL	2.1
3	D	936	VAL	2.1
1	B	90	ASP	2.1
2	C	220	ILE	2.1
5	F	79	LYS	2.1
2	C	1075	ALA	2.1
1	B	184	GLU	2.1
3	D	79	GLY	2.1
3	D	993	GLU	2.1
1	B	138	LEU	2.1
3	D	39	LEU	2.1
3	D	91	ARG	2.1
1	B	43	LEU	2.0
2	C	226	GLN	2.0
2	C	1142	ARG	2.0
1	B	12	ASP	2.0
2	C	294	PHE	2.0
3	D	333	GLY	2.0
3	D	454	PRO	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MG	D	2003	1/1	0.95	0.06	68,68,68,68	0
9	ZN	D	2002	1/1	0.98	0.06	129,129,129,129	0
9	ZN	D	2001	1/1	0.99	0.03	109,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.