



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:30 PM UTC

PDB ID : 6JCX / pdb_00006jcx
Title : Mycobacterium tuberculosis transcription initiation complex with ECF sigma factor sigma H and 6nt RNA
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-01-30
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

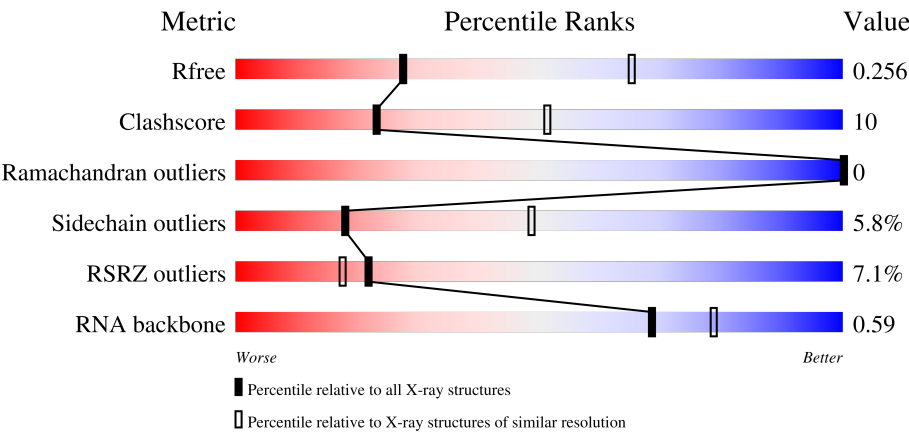
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	42%16%40% 10%
1	B	368	43%19%37% 10%
2	C	1174	70%26% 8%
3	D	1317	70%24% 4%

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	218	
6	H	20	
7	G	23	
8	I	6	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 25143 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	219	Total	C	N	O	S	0	0	0
			1654	1044	282	326	2			
1	B	232	Total	C	N	O	S	0	0	0
			1696	1073	287	334	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
			8731	5458	1528	1706	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY9
C	6	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
			9822	6153	1776	1852	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	71	Total	C	N	O	0	0	0
			566	362	95	109			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	186	Total	C	N	O	S	0	0	0
			1477	926	260	286	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*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	20	Total	C	N	O	P	0	0	0
			412	196	77	120	19			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*TP*GP*TP*GP*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
7	G	23	Total	C	N	O	P	0	0	0
			475	226	89	138	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	6	Total	C	N	O	P	0	0	0
			122	56	21	40	5			

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

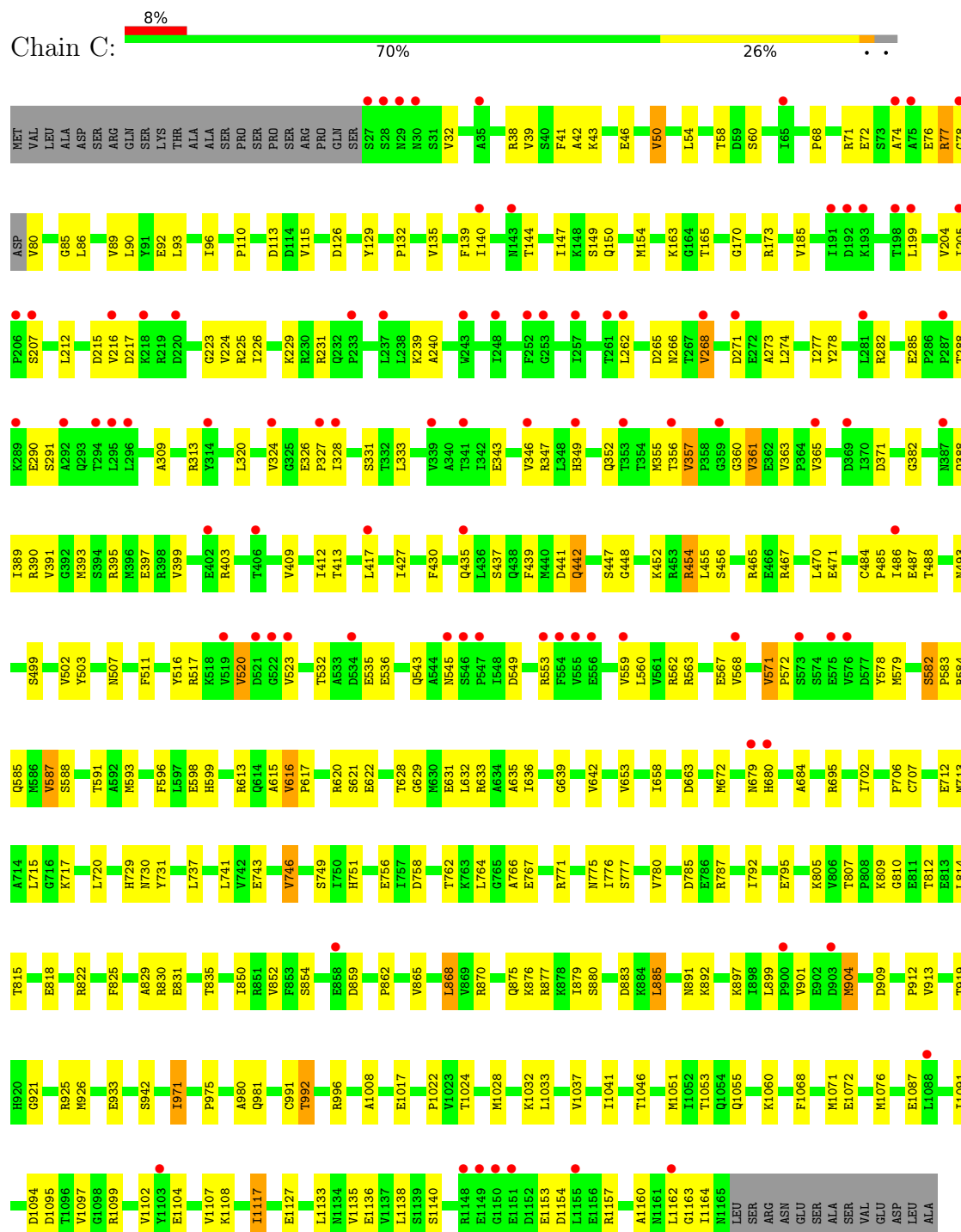
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

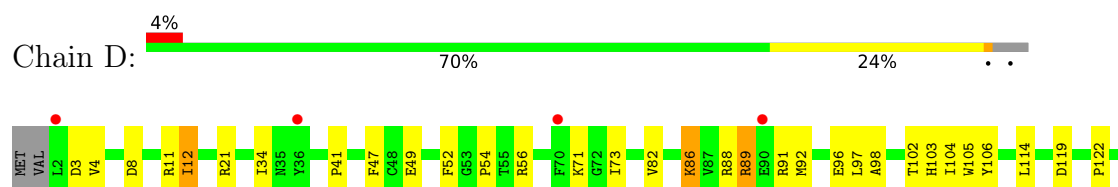
- Molecule 11 is water.

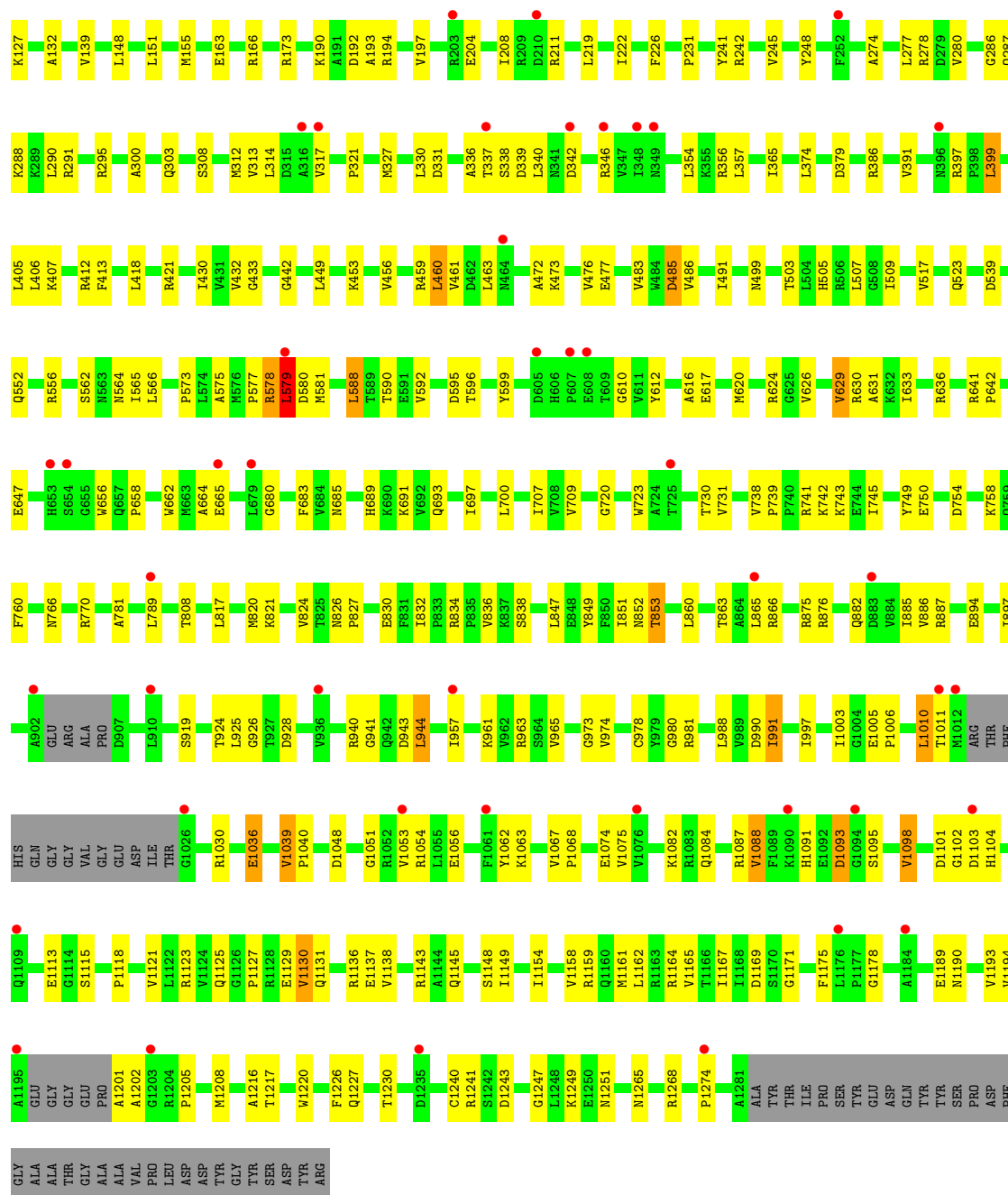
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	9	Total 9	O 9	0	0
11	B	9	Total 9	O 9	0	0
11	C	66	Total 66	O 66	0	0
11	D	71	Total 71	O 71	0	0
11	E	3	Total 3	O 3	0	0
11	F	11	Total 11	O 11	0	0
11	H	7	Total 7	O 7	0	0
11	G	4	Total 4	O 4	0	0
11	I	5	Total 5	O 5	0	0

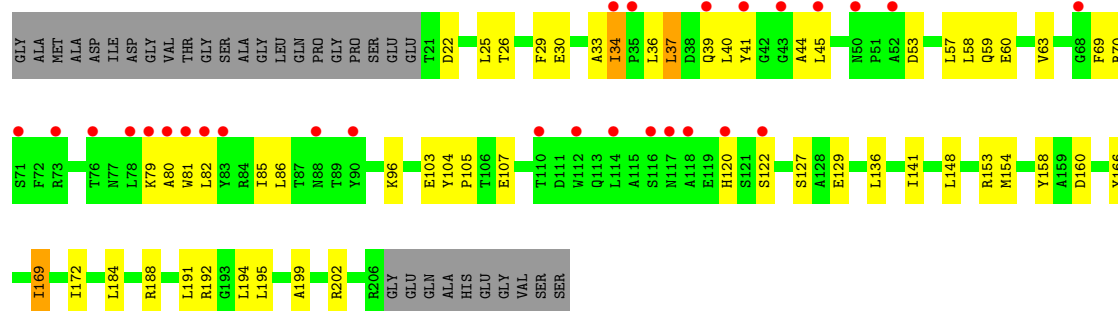
• Molecule 2: DNA-directed RNA polymerase subunit beta



• Molecule 3: DNA-directed RNA polymerase subunit beta'



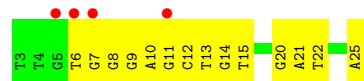




- Molecule 6: DNA (5'-D(*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*GP*T)-3')



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



- Molecule 8: RNA (5'-R(*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	125.14Å 161.00Å 128.85Å 90.00° 117.06° 90.00°	Depositor
Resolution (Å)	36.09 – 2.90 36.09 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (36.09-2.90) 97.6 (36.09-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.210 , 0.256 (Not available) , 0.256	Depositor DCC
R_{free} test set	2446 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25143	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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	0.22	0/1679	0.44	0/2285
1	B	0.17	0/1722	0.40	0/2351
2	C	0.22	0/8889	0.43	0/12067
3	D	0.22	0/9984	0.44	2/13500 (0.0%)
4	E	0.21	0/577	0.43	0/786
5	F	0.21	0/1506	0.41	0/2041
6	H	0.29	0/462	0.50	0/713
7	G	0.27	0/533	0.66	2/823 (0.2%)
8	I	0.24	0/135	0.52	0/208
All	All	0.22	0/25487	0.44	4/34774 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	8	DG	OP1-P-O3'	-8.63	82.12	108.00
7	G	8	DG	OP2-P-O3'	-8.32	83.03	108.00
3	D	578	ARG	CA-C-N	5.61	132.25	121.54
3	D	578	ARG	C-N-CA	5.61	132.25	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	579	LEU	Mainchain

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	1654	0	1687	38	0
1	B	1696	0	1683	41	0
2	C	8731	0	8564	205	0
3	D	9822	0	9862	209	0
4	E	566	0	567	11	0
5	F	1477	0	1422	39	0
6	H	412	0	227	11	0
7	G	475	0	261	18	0
8	I	122	0	66	4	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	A	9	0	0	0	0
11	B	9	0	0	1	0
11	C	66	0	0	4	0
11	D	71	0	0	2	0
11	E	3	0	0	0	0
11	F	11	0	0	0	0
11	G	4	0	0	0	0
11	H	7	0	0	0	0
11	I	5	0	0	0	0
All	All	25143	0	24339	507	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 10.

All (507) 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)
2:C:485:PRO:HB2	3:D:853:THR:HG21	1.52	0.89
2:C:1051:MET:O	3:D:89:ARG:NH2	2.08	0.87
2:C:1053:THR:HG23	2:C:1055:GLN:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1024:THR:H	3:D:730:THR:HG21	1.43	0.84
3:D:505:HIS:HD2	3:D:1005:GLU:HG3	1.49	0.77
3:D:925:LEU:HG	3:D:944:LEU:HD21	1.67	0.77
4:E:59:ARG:HH22	4:E:79:GLY:HA3	1.49	0.77
3:D:1056:GLU:HB3	3:D:1063:LYS:HB3	1.66	0.76
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.69	0.74
4:E:37:PRO:HG2	4:E:42:LEU:HD11	1.70	0.74
3:D:578:ARG:H	3:D:581:MET:HE3	1.53	0.74
3:D:629:VAL:HG12	3:D:630:ARG:HG3	1.71	0.73
3:D:346:ARG:NH2	5:F:53:ASP:OD1	2.21	0.73
6:H:11:DT:H2'	6:H:12:DG:C8	2.24	0.72
2:C:78:GLY:O	2:C:80:VAL:N	2.23	0.72
2:C:50:VAL:O	2:C:633:ARG:NH2	2.22	0.71
3:D:190:LYS:HE2	3:D:192:ASP:HB3	1.73	0.71
6:H:17:DG:N2	8:I:5:C:O2	2.18	0.71
3:D:875:ARG:NH2	3:D:1226:PHE:O	2.24	0.70
2:C:92:GLU:OE1	2:C:390:ARG:NH2	2.25	0.70
2:C:1046:THR:HG21	5:F:129:GLU:H	1.56	0.70
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.74	0.70
4:E:31:PRO:HB2	4:E:35:THR:HG23	1.75	0.68
3:D:981:ARG:HA	3:D:988:LEU:HA	1.76	0.68
6:H:16:DC:H2'	6:H:17:DG:H5''	1.76	0.68
1:A:95:MET:HE3	1:A:112:PRO:HB3	1.74	0.68
4:E:46:VAL:HG21	4:E:52:LEU:HB2	1.76	0.68
2:C:395:ARG:NH1	7:G:10:DA:OP1	2.26	0.67
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	1.77	0.67
1:B:102:PRO:HA	1:B:128:LEU:O	1.95	0.67
1:A:144:ARG:NH2	1:B:27:GLU:OE1	2.25	0.67
2:C:1046:THR:HG22	5:F:127:SER:HB2	1.77	0.66
2:C:74:ALA:HA	2:C:77:ARG:HD2	1.76	0.66
3:D:1062:TYR:HE1	3:D:1082:LYS:HA	1.61	0.66
2:C:357:VAL:HG13	2:C:360:GLY:HA3	1.78	0.66
2:C:751:HIS:CD2	2:C:877:ARG:HG3	2.31	0.66
2:C:815:THR:HG23	2:C:818:GLU:H	1.61	0.66
3:D:1167:ILE:HD13	3:D:1175:PHE:HB3	1.78	0.65
3:D:876:ARG:NH1	3:D:1036:GLU:OE1	2.28	0.65
3:D:885:ILE:HG13	3:D:887:ARG:HD3	1.79	0.65
3:D:173:ARG:NE	3:D:204:GLU:OE1	2.27	0.65
2:C:631:GLU:OE1	2:C:631:GLU:N	2.26	0.65
2:C:593:MET:HE3	2:C:631:GLU:HG3	1.77	0.64
5:F:44:ALA:HB2	5:F:86:LEU:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:507:ASN:HD21	2:C:511:PHE:HB2	1.62	0.64
2:C:921:GLY:O	2:C:925:ARG:HG3	1.98	0.64
2:C:517:ARG:HD3	2:C:579:MET:HE2	1.79	0.64
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.80	0.64
3:D:97:LEU:HD22	3:D:374:LEU:HD21	1.79	0.64
3:D:973:GLY:O	3:D:1159:ARG:NH2	2.31	0.63
3:D:642:PRO:HG2	3:D:647:GLU:HB2	1.79	0.63
2:C:467:ARG:NH1	7:G:13:DT:O4'	2.32	0.63
2:C:582:SER:OG	2:C:583:PRO:O	2.16	0.63
3:D:163:GLU:HG2	3:D:166:ARG:HH21	1.62	0.63
5:F:141:ILE:HD13	5:F:195:LEU:HD11	1.82	0.62
2:C:239:LYS:HZ2	2:C:262:LEU:HD11	1.64	0.61
2:C:1136:GLU:OE1	3:D:11:ARG:NH2	2.34	0.61
3:D:47:PHE:O	3:D:88:ARG:NH2	2.33	0.61
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.82	0.60
1:A:87:SER:HB2	1:A:116:VAL:HG22	1.84	0.60
2:C:173:ARG:NH2	11:C:1202:HOH:O	2.34	0.60
3:D:562:SER:HA	3:D:565:ILE:HD11	1.83	0.60
2:C:822:ARG:NH2	2:C:829:ALA:O	2.34	0.60
7:G:13:DT:H1'	7:G:14:DG:H5''	1.83	0.60
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.82	0.60
1:B:220:GLY:HA2	1:B:223:ARG:HG2	1.82	0.60
2:C:901:VAL:HG22	2:C:912:PRO:HG2	1.83	0.60
1:B:110:ILE:HD11	1:B:118:VAL:HG21	1.84	0.60
2:C:1068:PHE:HZ	2:C:1076:MET:HE3	1.66	0.59
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.84	0.59
3:D:866:ARG:HD3	3:D:1010:LEU:O	2.02	0.59
2:C:388:GLN:HG2	2:C:430:PHE:HB2	1.84	0.59
1:B:97:LEU:HB2	1:B:110:ILE:HG22	1.85	0.59
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.68	0.59
2:C:313:ARG:HD3	2:C:331:SER:HA	1.85	0.59
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.85	0.59
2:C:536:GLU:OE2	2:C:562:ARG:NH2	2.35	0.59
2:C:741:LEU:HD22	2:C:746:VAL:HG21	1.85	0.58
2:C:1140:SER:HA	3:D:8:ASP:HB2	1.85	0.58
2:C:814:LEU:HD11	2:C:822:ARG:HH11	1.68	0.58
2:C:391:VAL:O	2:C:395:ARG:HG2	2.03	0.58
6:H:18:DA:H2'	6:H:19:DG:C8	2.38	0.58
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.38	0.58
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.86	0.58
3:D:1088:VAL:HA	3:D:1098:VAL:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:SER:O	1:A:199:LYS:NZ	2.29	0.58
2:C:96:ILE:HD13	2:C:397:GLU:HG3	1.86	0.58
2:C:756:GLU:OE1	2:C:870:ARG:NH1	2.37	0.58
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.84	0.58
3:D:539:ASP:OD1	8:I:7:A:O3'	2.20	0.58
2:C:805:LYS:NZ	2:C:835:THR:OG1	2.36	0.57
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.68	0.57
3:D:300:ALA:HA	3:D:303:GLN:HG2	1.86	0.57
5:F:160:ASP:OD1	5:F:188:ARG:NH1	2.33	0.57
3:D:505:HIS:CD2	3:D:1005:GLU:HG3	2.37	0.57
1:A:197:GLU:OE1	2:C:996:ARG:NH2	2.30	0.57
2:C:282:ARG:HD3	2:C:285:GLU:HG2	1.86	0.57
3:D:539:ASP:CG	8:I:7:A:O3'	2.48	0.57
2:C:560:LEU:HD11	2:C:568:VAL:HB	1.87	0.57
2:C:663:ASP:OD2	2:C:695:ARG:NH2	2.37	0.56
2:C:809:LYS:HA	5:F:122:SER:HB2	1.87	0.56
6:H:7:DT:H1'	6:H:8:DC:H5'	1.86	0.56
2:C:628:THR:HG23	2:C:975:PRO:HA	1.87	0.56
3:D:499:ASN:HB2	3:D:509:ILE:HG12	1.88	0.56
2:C:658:ILE:HD13	2:C:702:ILE:HG22	1.87	0.56
3:D:386:ARG:HH12	3:D:1230:THR:HG21	1.71	0.56
1:B:169:SER:HB3	3:D:620:MET:HE1	1.87	0.56
1:A:83:LEU:HG	1:A:123:MET:HE1	1.86	0.56
3:D:12:ILE:HD11	3:D:1220:TRP:CE3	2.41	0.56
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.87	0.56
3:D:92:MET:HG3	3:D:321:PRO:HD3	1.88	0.56
2:C:239:LYS:NZ	2:C:262:LEU:HD11	2.21	0.56
2:C:815:THR:HG22	2:C:818:GLU:HB2	1.87	0.56
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.87	0.56
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.87	0.56
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.87	0.56
1:B:9:LEU:HD13	1:B:23:ILE:HG12	1.87	0.55
2:C:587:VAL:HG13	2:C:591:THR:HB	1.87	0.55
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.89	0.55
2:C:140:ILE:HG12	2:C:147:ILE:HG12	1.88	0.55
2:C:792:ILE:HG13	2:C:850:ILE:HD12	1.88	0.55
3:D:1265:ASN:HA	3:D:1268:ARG:HG2	1.89	0.55
3:D:832:ILE:HG22	3:D:834:ARG:H	1.72	0.55
3:D:1136:ARG:HH21	3:D:1143:ARG:HH22	1.52	0.55
2:C:68:PRO:HA	2:C:71:ARG:HB3	1.89	0.55
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:GLU:OE1	4:E:99:HIS:NE2	2.30	0.55
6:H:3:DT:H2"	6:H:4:DG:C8	2.42	0.54
3:D:21:ARG:NE	3:D:96:GLU:OE2	2.32	0.54
3:D:1054:ARG:NH1	3:D:1056:GLU:OE1	2.40	0.54
5:F:39:GLN:OE1	5:F:79:LYS:NZ	2.34	0.54
2:C:454:ARG:HH11	2:C:499:SER:HB3	1.72	0.54
2:C:1041:ILE:O	2:C:1060:LYS:NZ	2.34	0.54
2:C:516:TYR:HB3	2:C:578:TYR:HB3	1.90	0.54
3:D:194:ARG:HA	3:D:197:VAL:HG22	1.90	0.54
1:A:213:LYS:HB2	1:B:223:ARG:HE	1.74	0.53
2:C:622:GLU:HB3	2:C:717:LYS:HD3	1.89	0.53
3:D:421:ARG:NH1	6:H:17:DG:OP1	2.40	0.53
6:H:5:DC:H2"	6:H:6:DA:C8	2.43	0.53
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.91	0.53
2:C:899:LEU:HB2	2:C:904:MET:CE	2.38	0.53
3:D:1087:ARG:NH1	3:D:1113:GLU:OE2	2.39	0.53
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.90	0.53
2:C:615:ALA:HB3	2:C:715:LEU:HD22	1.91	0.53
2:C:1068:PHE:CZ	2:C:1076:MET:HE3	2.44	0.53
3:D:453:LYS:NZ	5:F:129:GLU:OE2	2.42	0.53
2:C:729:HIS:CD2	2:C:897:LYS:HD2	2.43	0.53
2:C:741:LEU:HA	2:C:746:VAL:HG13	1.90	0.53
5:F:148:LEU:HD13	5:F:191:LEU:HD13	1.91	0.53
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.90	0.53
2:C:767:GLU:OE2	2:C:807:THR:OG1	2.25	0.53
3:D:963:ARG:NH1	3:D:978:CYS:SG	2.82	0.53
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.42	0.52
3:D:1091:HIS:HB3	3:D:1095:SER:O	2.10	0.52
1:A:146:TYR:CD2	2:C:743:GLU:HG2	2.44	0.52
2:C:880:SER:N	2:C:883:ASP:OD2	2.41	0.52
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.90	0.52
2:C:1117:ILE:HD13	3:D:3:ASP:HB2	1.90	0.52
1:B:75:GLU:HG2	3:D:636:ARG:NH2	2.25	0.52
3:D:1164:ARG:HD2	3:D:1208:MET:SD	2.50	0.52
3:D:683:PHE:HE1	3:D:685:ASN:HB2	1.75	0.52
1:A:72:ASP:OD1	1:A:72:ASP:N	2.42	0.52
1:A:62:GLU:OE2	2:C:876:LYS:NZ	2.31	0.52
2:C:135:VAL:HG21	2:C:154:MET:HE2	1.92	0.52
3:D:928:ASP:OD1	3:D:940:ARG:N	2.36	0.52
3:D:1158:VAL:HA	3:D:1161:MET:HE3	1.91	0.52
2:C:862:PRO:HG2	2:C:865:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLY:HA3	11:B:408:HOH:O	2.11	0.51
3:D:106:TYR:HB3	3:D:312:MET:HE3	1.92	0.51
2:C:352:GLN:O	2:C:365:VAL:HB	2.10	0.51
2:C:395:ARG:HH22	7:G:10:DA:H5"	1.75	0.51
5:F:79:LYS:HE3	7:G:7:DG:C8	2.46	0.51
3:D:943:ASP:OD1	3:D:981:ARG:HD2	2.11	0.51
2:C:93:LEU:HD22	2:C:393:MET:HE3	1.92	0.51
1:B:124:HIS:CE1	1:B:127:THR:HG23	2.46	0.51
3:D:1167:ILE:O	3:D:1178:GLY:N	2.41	0.51
2:C:442:GLN:H	2:C:680:HIS:HD2	1.59	0.51
3:D:1158:VAL:HG22	3:D:1161:MET:HE3	1.92	0.51
1:B:98:ARG:HA	1:B:134:LEU:O	2.10	0.51
3:D:1006:PRO:HG3	3:D:1149:ILE:HD11	1.93	0.51
1:B:146:TYR:O	3:D:624:ARG:NE	2.44	0.50
2:C:46:GLU:OE1	2:C:503:TYR:OH	2.28	0.50
3:D:356:ARG:NH2	5:F:60:GLU:OE1	2.43	0.50
2:C:326:GLU:N	2:C:327:PRO:HD3	2.27	0.50
3:D:1190:ASN:HD21	3:D:1201:ALA:HB1	1.77	0.50
1:B:218:LEU:O	1:B:221:LEU:HB2	2.12	0.50
3:D:599:TYR:HB2	3:D:610:GLY:HA3	1.94	0.50
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.93	0.50
4:E:32:LEU:O	4:E:35:THR:HG22	2.12	0.50
2:C:737:LEU:HD22	2:C:741:LEU:HD12	1.94	0.50
3:D:190:LYS:HD3	3:D:193:ALA:HB2	1.94	0.50
3:D:1053:VAL:HG12	3:D:1103:ASP:O	2.12	0.50
1:A:175:THR:HG22	1:A:195:ASP:HB3	1.93	0.49
2:C:632:LEU:HB2	2:C:712:GLU:HG2	1.93	0.49
2:C:854:SER:O	2:C:859:ASP:HB2	2.12	0.49
3:D:242:ARG:HA	3:D:245:VAL:HG22	1.93	0.49
2:C:470:LEU:H	2:C:470:LEU:HD12	1.77	0.49
2:C:758:ASP:OD1	5:F:120:HIS:NE2	2.45	0.49
3:D:365:ILE:HD12	5:F:34:ILE:HD13	1.93	0.49
2:C:41:PHE:CG	2:C:980:ALA:HB2	2.48	0.49
2:C:1104:GLU:HG2	2:C:1108:LYS:HE2	1.93	0.49
3:D:1011:THR:O	3:D:1145:GLN:NE2	2.46	0.49
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.94	0.49
3:D:689:HIS:CE1	3:D:691:LYS:HE2	2.47	0.49
3:D:847:LEU:O	3:D:851:ILE:HG12	2.12	0.49
3:D:1030:ARG:NH2	3:D:1137:GLU:OE1	2.40	0.49
2:C:60:SER:HG	2:C:382:GLY:H	1.53	0.49
3:D:86:LYS:O	3:D:89:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:926:GLY:O	3:D:940:ARG:NH2	2.40	0.49
2:C:113:ASP:HB3	2:C:132:PRO:HD2	1.94	0.49
7:G:9:DG:H2''	7:G:10:DA:C8	2.48	0.49
2:C:38:ARG:HA	2:C:971:ILE:HG22	1.93	0.49
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.93	0.49
2:C:412:ILE:HD12	2:C:417:LEU:HD21	1.95	0.49
2:C:583:PRO:O	2:C:584:ARG:HG2	2.12	0.49
2:C:810:GLY:H	3:D:56:ARG:NH2	2.10	0.49
3:D:219:LEU:HA	3:D:222:ILE:HD12	1.95	0.49
2:C:207:SER:OG	2:C:309:ALA:N	2.46	0.49
3:D:73:ILE:O	3:D:82:VAL:HG12	2.13	0.49
3:D:552:GLN:O	3:D:556:ARG:HG3	2.13	0.49
3:D:1003:ILE:O	11:D:2101:HOH:O	2.20	0.49
2:C:532:THR:HG22	2:C:535:GLU:HG3	1.95	0.48
7:G:11:DG:H2''	7:G:12:DC:H5''	1.94	0.48
2:C:762:THR:HG22	2:C:764:LEU:H	1.79	0.48
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.96	0.48
2:C:265:ASP:OD1	2:C:266:ASN:N	2.46	0.48
2:C:583:PRO:C	2:C:585:GLN:H	2.20	0.48
3:D:579:LEU:HD23	3:D:808:THR:HB	1.95	0.48
3:D:1226:PHE:CD2	3:D:1227:GLN:HG2	2.48	0.48
3:D:1274:PRO:HB3	4:E:81:LEU:HD11	1.94	0.48
2:C:139:PHE:CZ	2:C:412:ILE:HD11	2.49	0.48
3:D:754:ASP:O	3:D:758:LYS:HG2	2.12	0.48
2:C:1135:VAL:HG13	3:D:12:ILE:HG23	1.95	0.48
3:D:114:LEU:HG	3:D:312:MET:HE2	1.96	0.48
3:D:208:ILE:HG23	3:D:211:ARG:HH22	1.78	0.48
1:A:3:ILE:HG13	1:A:4:SER:H	1.78	0.48
3:D:750:GLU:OE1	3:D:834:ARG:NH2	2.47	0.48
5:F:22:ASP:O	5:F:26:THR:HG23	2.14	0.48
2:C:320:LEU:C	2:C:363:VAL:HG11	2.39	0.48
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.96	0.48
3:D:459:ARG:NH2	4:E:87:GLN:OE1	2.47	0.48
2:C:441:ASP:HA	2:C:680:HIS:NE2	2.29	0.48
3:D:876:ARG:HG2	3:D:1226:PHE:HZ	1.78	0.48
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.96	0.48
2:C:467:ARG:HA	7:G:15:DT:H5'	1.95	0.47
3:D:449:LEU:HD11	3:D:476:VAL:HG13	1.96	0.47
1:A:149:ALA:HB1	1:A:163:PRO:HB2	1.95	0.47
2:C:199:LEU:HG	2:C:216:VAL:HG23	1.96	0.47
2:C:815:THR:CG2	2:C:818:GLU:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:173:ARG:NH1	2:C:437:SER:O	2.47	0.47
2:C:642:VAL:HG21	2:C:672:MET:HE1	1.96	0.47
7:G:13:DT:H2''	7:G:14:DG:OP2	2.15	0.47
2:C:749:SER:OG	2:C:751:HIS:NE2	2.46	0.47
2:C:1076:MET:HE1	3:D:509:ILE:HG21	1.96	0.47
3:D:566:LEU:HA	3:D:573:PRO:HA	1.95	0.47
1:A:86:SER:HG	1:A:119:HIS:HE2	1.60	0.47
2:C:616:VAL:HG13	2:C:1032:LYS:O	2.14	0.47
2:C:549:ASP:OD1	2:C:553:ARG:N	2.27	0.47
2:C:892:LYS:NZ	8:I:7:A:OP1	2.35	0.47
3:D:155:MET:HE1	3:D:219:LEU:HD22	1.95	0.47
3:D:683:PHE:CE1	3:D:685:ASN:HB2	2.50	0.47
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.96	0.47
3:D:612:TYR:HD2	3:D:617:GLU:HG2	1.79	0.47
3:D:1062:TYR:CE1	3:D:1082:LYS:HA	2.45	0.47
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.47	0.47
3:D:847:LEU:HD12	3:D:847:LEU:H	1.80	0.47
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.96	0.47
3:D:287:GLN:HA	3:D:290:LEU:HD12	1.96	0.47
2:C:448:GLY:O	2:C:452:LYS:HG3	2.14	0.46
2:C:598:GLU:OE1	2:C:598:GLU:N	2.27	0.46
3:D:633:ILE:O	3:D:665:GLU:HA	2.15	0.46
2:C:165:THR:HB	2:C:173:ARG:O	2.15	0.46
2:C:273:ALA:O	2:C:277:ILE:HG12	2.16	0.46
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.96	0.46
3:D:127:LYS:HA	3:D:132:ALA:HB3	1.96	0.46
3:D:596:THR:HG22	3:D:626:VAL:O	2.15	0.46
3:D:760:PHE:CG	3:D:770:ARG:HD3	2.50	0.46
2:C:216:VAL:HG21	2:C:349:HIS:NE2	2.30	0.46
2:C:1154:ASP:OD2	2:C:1157:ARG:NH2	2.48	0.46
3:D:280:VAL:HG13	3:D:288:LYS:HE3	1.98	0.46
2:C:1160:ALA:HA	2:C:1164:ILE:HB	1.97	0.46
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.98	0.46
3:D:1101:ASP:OD1	3:D:1102:GLY:N	2.48	0.46
3:D:1136:ARG:HD2	3:D:1136:ARG:HA	1.71	0.46
2:C:1072:GLU:OE2	3:D:503:THR:OG1	2.28	0.46
3:D:460:LEU:HD12	3:D:486:VAL:HG21	1.98	0.46
6:H:15:DT:H2'	6:H:16:DC:C6	2.51	0.46
2:C:628:THR:HG22	2:C:629:GLY:H	1.81	0.46
2:C:632:LEU:HA	2:C:712:GLU:HA	1.97	0.46
2:C:926:MET:HE1	3:D:817:LEU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:981:GLN:NE2	11:C:1201:HOH:O	2.30	0.46
3:D:689:HIS:O	3:D:693:GLN:HG3	2.16	0.46
1:B:128:LEU:HD21	1:B:134:LEU:HB2	1.98	0.46
2:C:60:SER:OG	2:C:382:GLY:N	2.36	0.46
2:C:879:ILE:HD12	2:C:1032:LYS:HE3	1.98	0.46
3:D:461:VAL:HG23	3:D:472:ALA:HB2	1.97	0.46
1:A:95:MET:HE2	1:A:110:ILE:CG2	2.45	0.46
2:C:229:LYS:HD3	2:C:229:LYS:HA	1.75	0.45
2:C:766:ALA:O	2:C:830:ARG:NH1	2.49	0.45
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.98	0.45
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.97	0.45
3:D:581:MET:HA	3:D:720:GLY:HA3	1.97	0.45
5:F:41:TYR:HB2	5:F:58:LEU:HD22	1.97	0.45
6:H:4:DG:H2''	6:H:5:DC:O5'	2.15	0.45
3:D:1136:ARG:NH2	3:D:1143:ARG:HH22	2.14	0.45
2:C:225:ARG:HG3	2:C:229:LYS:O	2.17	0.45
2:C:731:TYR:HB3	3:D:432:VAL:HG21	1.98	0.45
3:D:924:THR:HG22	3:D:941:GLY:HA2	1.98	0.45
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.97	0.45
2:C:239:LYS:HZ3	2:C:268:VAL:HA	1.80	0.45
2:C:1127:GLU:OE1	3:D:412:ARG:HG3	2.16	0.45
2:C:343:GLU:HA	2:C:346:VAL:HG22	1.98	0.45
2:C:347:ARG:HD2	2:C:355:MET:HG3	1.99	0.45
2:C:520:VAL:O	2:C:523:VAL:HG12	2.17	0.45
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.52	0.45
3:D:1131:GLN:HG3	3:D:1162:LEU:HD12	1.99	0.45
2:C:1104:GLU:HG3	5:F:136:LEU:HD21	1.99	0.45
3:D:741:ARG:O	3:D:745:ILE:HG13	2.16	0.45
3:D:92:MET:HB2	3:D:92:MET:HE3	1.63	0.45
3:D:826:ASN:OD1	3:D:827:PRO:HD2	2.17	0.45
3:D:1093:ASP:OD2	3:D:1104:HIS:ND1	2.44	0.45
5:F:154:MET:HG3	5:F:158:TYR:CE2	2.51	0.45
5:F:166:TYR:HA	5:F:169:ILE:HG22	1.99	0.45
2:C:771:ARG:O	2:C:771:ARG:HG2	2.17	0.45
2:C:288:THR:HB	2:C:291:SER:OG	2.17	0.45
2:C:751:HIS:HD2	2:C:877:ARG:HG3	1.81	0.45
2:C:775:ASN:HA	5:F:202:ARG:HB3	1.99	0.45
2:C:1133:LEU:HD11	3:D:105:TRP:CZ3	2.52	0.45
3:D:342:ASP:O	3:D:346:ARG:HG3	2.16	0.45
3:D:980:GLY:O	3:D:988:LEU:HD12	2.17	0.45
7:G:20:DG:H2''	7:G:21:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:ILE:HG12	2:C:427:ILE:HD11	1.97	0.44
2:C:596:PHE:HB3	2:C:599:HIS:CD2	2.52	0.44
3:D:226:PHE:CE1	3:D:248:TYR:HB3	2.52	0.44
3:D:616:ALA:O	3:D:620:MET:HG3	2.17	0.44
3:D:641:ARG:HD3	3:D:680:GLY:O	2.17	0.44
5:F:29:PHE:HB2	5:F:69:PHE:CE2	2.51	0.44
1:A:213:LYS:HZ3	1:B:223:ARG:HH21	1.65	0.44
1:B:100:GLN:HA	1:B:133:LYS:HA	1.99	0.44
1:B:107:ALA:HB3	1:B:121:PRO:HA	2.00	0.44
3:D:287:GLN:N	3:D:287:GLN:OE1	2.51	0.44
3:D:592:VAL:HB	3:D:595:ASP:HB2	1.99	0.44
3:D:894:GLU:O	3:D:961:LYS:NZ	2.45	0.44
3:D:1171:GLY:H	3:D:1201:ALA:N	2.15	0.44
2:C:54:LEU:O	2:C:58:THR:HG23	2.18	0.44
2:C:435:GLN:NE2	11:C:1205:HOH:O	2.48	0.44
2:C:792:ILE:HD12	2:C:792:ILE:H	1.82	0.44
3:D:507:LEU:HD11	3:D:564:ASN:HB3	2.00	0.44
3:D:826:ASN:HB2	3:D:830:GLU:O	2.17	0.44
7:G:14:DG:H4'	7:G:15:DT:OP1	2.16	0.44
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.32	0.44
1:A:93:VAL:HG11	1:A:116:VAL:HG21	2.00	0.44
1:B:182:ARG:CB	1:B:189:PHE:HB2	2.47	0.44
3:D:1048:ASP:OD2	3:D:1123:ARG:NH2	2.40	0.44
3:D:1051:GLY:HA3	3:D:1067:VAL:O	2.18	0.44
2:C:85:GLY:O	2:C:89:VAL:HG23	2.18	0.44
3:D:339:ASP:CG	3:D:397:ARG:HH22	2.26	0.44
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.47	0.44
1:A:78:LEU:HD23	2:C:620:ARG:NH1	2.32	0.44
2:C:737:LEU:HD11	2:C:885:LEU:HD21	2.00	0.44
3:D:97:LEU:HD11	3:D:317:VAL:HG23	2.00	0.44
3:D:274:ALA:O	3:D:278:ARG:HG3	2.17	0.44
3:D:656:TRP:CH2	3:D:658:PRO:HA	2.53	0.44
7:G:6:DT:H2''	7:G:7:DG:O5'	2.17	0.44
2:C:215:ASP:OD1	2:C:215:ASP:N	2.50	0.44
1:B:146:TYR:CE2	3:D:617:GLU:HG3	2.52	0.43
2:C:313:ARG:HB2	2:C:331:SER:HB2	1.99	0.43
2:C:1163:GLY:O	5:F:153:ARG:HD2	2.18	0.43
3:D:391:VAL:HG12	3:D:399:LEU:HD22	2.00	0.43
3:D:122:PRO:HG2	7:G:22:DT:H3'	2.01	0.43
3:D:204:GLU:O	3:D:208:ILE:HG13	2.17	0.43
3:D:886:VAL:HB	3:D:991:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.84	0.43
3:D:965:VAL:HG13	3:D:974:VAL:HG11	2.00	0.43
3:D:1217:THR:O	3:D:1241:ARG:NH2	2.52	0.43
3:D:155:MET:CE	3:D:219:LEU:HB3	2.48	0.43
3:D:473:LYS:O	3:D:477:GLU:HG3	2.18	0.43
4:E:88:GLU:OE2	4:E:96:ARG:NH1	2.51	0.43
1:A:95:MET:HE2	1:A:110:ILE:HG21	2.01	0.43
3:D:430:ILE:HD11	3:D:539:ASP:HB2	2.00	0.43
3:D:432:VAL:HG13	3:D:433:GLY:H	1.83	0.43
3:D:588:LEU:HG	3:D:723:TRP:CD1	2.53	0.43
3:D:990:ASP:CG	4:E:48:SER:HB2	2.44	0.43
3:D:397:ARG:HH21	5:F:107:GLU:HG2	1.82	0.43
5:F:81:TRP:O	5:F:85:ILE:HG13	2.19	0.43
3:D:693:GLN:O	3:D:697:ILE:HG13	2.18	0.43
1:A:66:VAL:O	1:A:69:VAL:HG22	2.18	0.43
2:C:240:ALA:HA	2:C:274:LEU:HG	2.01	0.43
2:C:399:VAL:O	2:C:403:ARG:HG2	2.19	0.43
2:C:730:ASN:OD1	2:C:730:ASN:N	2.48	0.43
1:B:176:TYR:HB3	1:B:194:LEU:HD23	2.01	0.43
3:D:330:LEU:HD11	3:D:336:ALA:HB2	2.00	0.43
5:F:59:GLN:O	5:F:63:VAL:HG23	2.19	0.43
1:A:46:ILE:HD12	1:A:210:SER:OG	2.19	0.43
1:A:152:ASN:HA	1:A:157:ALA:HB3	2.01	0.43
1:B:84:VAL:HG12	1:B:120:ASN:CG	2.44	0.43
2:C:371:ASP:OD1	7:G:14:DG:N2	2.51	0.42
2:C:442:GLN:HG3	2:C:679:ASN:HB2	2.00	0.42
2:C:891:ASN:HD21	2:C:1028:MET:CE	2.32	0.42
2:C:1138:LEU:HD11	3:D:11:ARG:NH1	2.33	0.42
7:G:10:DA:H2''	7:G:11:DG:H5''	2.01	0.42
1:B:7:PRO:HB3	1:B:25:PRO:O	2.19	0.42
1:B:69:VAL:HG22	1:B:128:LEU:HD23	2.01	0.42
2:C:163:LYS:HD2	2:C:639:GLY:HA3	2.02	0.42
2:C:389:ILE:O	2:C:393:MET:HG2	2.18	0.42
11:C:1238:HOH:O	3:D:418:LEU:HD13	2.20	0.42
3:D:1162:LEU:HD23	3:D:1162:LEU:HA	1.92	0.42
3:D:1189:GLU:O	3:D:1193:VAL:HG23	2.19	0.42
1:A:146:TYR:CG	2:C:743:GLU:HG2	2.54	0.42
5:F:104:TYR:HA	5:F:105:PRO:HD3	1.87	0.42
1:A:173:LYS:HD3	2:C:909:ASP:O	2.20	0.42
2:C:899:LEU:HD12	2:C:904:MET:HE2	2.01	0.42
3:D:327:MET:HE3	5:F:103:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:577:PRO:HB3	3:D:581:MET:HB2	2.02	0.42
1:A:61:HIS:HE1	1:A:63:PHE:O	2.02	0.42
1:B:28:PRO:HB3	1:B:188:ASP:O	2.20	0.42
2:C:439:PHE:CE2	2:C:679:ASN:HB3	2.55	0.42
2:C:1095:ASP:O	2:C:1099:ARG:HG3	2.19	0.42
3:D:1125:GLN:NE2	3:D:1129:GLU:HG2	2.35	0.42
1:A:205:ARG:HG2	1:B:225:LEU:HD22	2.02	0.42
1:B:101:GLY:N	1:B:132:GLY:O	2.53	0.42
2:C:324:VAL:HG11	2:C:361:VAL:HG21	2.02	0.42
3:D:151:LEU:HD22	3:D:248:TYR:HE1	1.85	0.42
3:D:749:TYR:CG	3:D:781:ALA:HB2	2.55	0.42
5:F:44:ALA:HB1	5:F:57:LEU:HD23	2.02	0.42
5:F:79:LYS:HE3	7:G:7:DG:H8	1.84	0.42
1:B:94:THR:O	1:B:113:PRO:HG3	2.20	0.42
3:D:119:ASP:HB2	3:D:295:ARG:NH2	2.35	0.42
3:D:241:TYR:O	3:D:245:VAL:HG13	2.20	0.42
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.89	0.42
5:F:82:LEU:HD23	5:F:85:ILE:HD12	2.01	0.42
3:D:460:LEU:HD21	3:D:483:VAL:HG12	2.02	0.42
5:F:25:LEU:HD12	5:F:70:ARG:NH1	2.35	0.42
5:F:40:LEU:HD11	5:F:82:LEU:HB3	2.02	0.42
2:C:825:PHE:CE2	5:F:192:ARG:HG3	2.55	0.42
2:C:617:PRO:HA	2:C:707:CYS:SG	2.60	0.41
3:D:71:LYS:HB3	3:D:71:LYS:HE3	1.80	0.41
5:F:26:THR:O	5:F:30:GLU:HG3	2.20	0.41
1:B:186:ARG:O	1:B:187:THR:HG22	2.20	0.41
3:D:405:LEU:HD23	3:D:405:LEU:HA	1.94	0.41
2:C:713:MET:HE3	2:C:713:MET:HB3	1.87	0.41
2:C:1017:GLU:H	2:C:1017:GLU:HG2	1.66	0.41
3:D:641:ARG:HG3	3:D:642:PRO:HD2	2.02	0.41
2:C:32:VAL:HG11	2:C:632:LEU:HD11	2.01	0.41
2:C:72:GLU:O	2:C:76:GLU:N	2.50	0.41
2:C:86:LEU:HD21	2:C:389:ILE:HD13	2.02	0.41
2:C:502:VAL:HG23	2:C:587:VAL:O	2.20	0.41
1:A:213:LYS:NZ	1:B:223:ARG:HH21	2.19	0.41
7:G:25:DA:OP2	7:G:25:DA:H3'	2.20	0.41
1:A:11:GLU:OE1	1:A:205:ARG:HD3	2.19	0.41
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.87	0.41
2:C:223:GLY:HA3	2:C:231:ARG:HE	1.86	0.41
1:A:57:ASP:HB2	1:A:135:GLU:HB3	2.03	0.41
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLU:HG2	3:D:485:ASP:OD2	2.21	0.41
2:C:212:LEU:HD22	2:C:333:LEU:HD21	2.02	0.41
3:D:12:ILE:HD11	3:D:1220:TRP:CZ3	2.55	0.41
3:D:700:LEU:HB3	3:D:709:VAL:HG22	2.02	0.41
5:F:34:ILE:HA	5:F:37:LEU:HD23	2.03	0.41
6:H:17:DG:H5"	6:H:17:DG:H8	1.86	0.41
1:A:182:ARG:HA	1:A:188:ASP:CG	2.45	0.41
1:B:172:LEU:HD13	1:B:199:LYS:HG3	2.02	0.41
2:C:185:VAL:HG22	2:C:204:VAL:HG22	2.01	0.41
3:D:52:PHE:O	3:D:91:ARG:HD2	2.21	0.41
3:D:413:PHE:HB2	11:D:2104:HOH:O	2.20	0.41
3:D:887:ARG:HA	3:D:887:ARG:HD2	1.95	0.41
1:B:24:GLU:HB2	1:B:191:LYS:HG3	2.03	0.41
1:B:112:PRO:HA	1:B:113:PRO:HD2	1.92	0.41
2:C:507:ASN:ND2	2:C:511:PHE:HB2	2.32	0.41
2:C:771:ARG:NH1	2:C:785:ASP:O	2.49	0.41
2:C:776:ILE:HG23	2:C:780:VAL:HB	2.02	0.41
3:D:49:GLU:HG2	3:D:54:PRO:HA	2.01	0.41
3:D:287:GLN:O	3:D:291:ARG:HG2	2.20	0.41
5:F:33:ALA:O	5:F:36:LEU:HB2	2.21	0.41
5:F:80:ALA:HA	7:G:7:DG:O6	2.20	0.41
1:A:46:ILE:HD11	1:A:211:ALA:HB2	2.03	0.41
1:A:199:LYS:O	1:A:200:ASN:HB2	2.21	0.41
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.88	0.41
2:C:90:LEU:HD12	2:C:110:PRO:HG3	2.03	0.41
2:C:223:GLY:HA3	2:C:231:ARG:HH21	1.85	0.41
3:D:12:ILE:HD11	3:D:1220:TRP:CD2	2.56	0.41
3:D:277:LEU:HD21	3:D:295:ARG:NH1	2.36	0.41
1:A:151:GLN:HB3	2:C:795:GLU:OE2	2.22	0.40
2:C:454:ARG:O	2:C:455:LEU:HD23	2.20	0.40
2:C:149:SER:OG	2:C:150:GLN:N	2.54	0.40
2:C:465:ARG:NH2	2:C:493:ASN:OD1	2.54	0.40
2:C:563:ARG:N	2:C:567:GLU:O	2.53	0.40
2:C:891:ASN:HD21	2:C:1028:MET:HE1	1.85	0.40
2:C:899:LEU:HB2	2:C:904:MET:HE1	2.03	0.40
2:C:942:SER:OG	2:C:992:THR:HG23	2.20	0.40
3:D:925:LEU:HD23	3:D:925:LEU:HA	1.92	0.40
3:D:1127:PRO:HA	3:D:1130:VAL:HG23	2.03	0.40
1:B:10:SER:HB3	1:B:22:VAL:HG23	2.03	0.40
2:C:217:ASP:OD2	2:C:231:ARG:NH1	2.54	0.40
2:C:278:TYR:CZ	2:C:282:ARG:HD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:484:CYS:CB	2:C:588:SER:HB3	2.51	0.40
3:D:286:GLY:O	3:D:290:LEU:HG	2.21	0.40
3:D:1138:VAL:HG12	3:D:1154:ILE:HD13	2.02	0.40
1:B:30:PHE:HA	1:B:33:THR:HB	2.03	0.40
2:C:262:LEU:HA	2:C:265:ASP:HB2	2.02	0.40
2:C:271:ASP:N	2:C:271:ASP:OD1	2.52	0.40
2:C:825:PHE:CZ	5:F:199:ALA:HB2	2.56	0.40
2:C:1008:ALA:O	2:C:1022:PRO:HA	2.21	0.40
3:D:821:LYS:HB3	3:D:836:VAL:HB	2.03	0.40
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.37	0.40
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.49	0.40
3:D:766:ASN:O	3:D:770:ARG:N	2.46	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	215/368 (58%)	210 (98%)	5 (2%)	0	100	100
1	B	228/368 (62%)	213 (93%)	15 (7%)	0	100	100
2	C	1134/1174 (97%)	1084 (96%)	50 (4%)	0	100	100
3	D	1250/1317 (95%)	1205 (96%)	45 (4%)	0	100	100
4	E	67/110 (61%)	62 (92%)	5 (8%)	0	100	100
5	F	184/218 (84%)	180 (98%)	4 (2%)	0	100	100
All	All	3078/3555 (87%)	2954 (96%)	124 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	186/315 (59%)	171 (92%)	15 (8%)	11	33
1	B	181/315 (58%)	164 (91%)	17 (9%)	8	26
2	C	940/995 (94%)	885 (94%)	55 (6%)	18	48
3	D	1040/1096 (95%)	987 (95%)	53 (5%)	21	53
4	E	62/90 (69%)	61 (98%)	1 (2%)	55	83
5	F	149/175 (85%)	141 (95%)	8 (5%)	20	51
All	All	2558/2986 (86%)	2409 (94%)	149 (6%)	18	49

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	10	SER
1	A	51	VAL
1	A	53	SER
1	A	85	VAL
1	A	88	GLU
1	A	93	VAL
1	A	100	GLN
1	A	111	VAL
1	A	133	LYS
1	A	159	ILE
1	A	178	VAL
1	A	208	LEU
1	A	213	LYS
1	A	218	LEU
1	B	11	GLU
1	B	16	ASP
1	B	27	GLU
1	B	34	LEU
1	B	45	SER
1	B	59	VAL
1	B	62	GLU

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Mol	Chain	Res	Type
1	B	64	THR
1	B	65	THR
1	B	74	THR
1	B	111	VAL
1	B	116	VAL
1	B	171	VAL
1	B	172	LEU
1	B	175	THR
1	B	196	VAL
1	B	202	ILE
2	C	39	VAL
2	C	43	LYS
2	C	50	VAL
2	C	77	ARG
2	C	144	THR
2	C	205	ILE
2	C	224	VAL
2	C	226	ILE
2	C	268	VAL
2	C	290	GLU
2	C	328	ILE
2	C	356	THR
2	C	357	VAL
2	C	361	VAL
2	C	409	VAL
2	C	442	GLN
2	C	447	SER
2	C	454	ARG
2	C	456	SER
2	C	471	GLU
2	C	488	THR
2	C	520	VAL
2	C	543	GLN
2	C	545	ASN
2	C	559	VAL
2	C	571	VAL
2	C	582	SER
2	C	587	VAL
2	C	616	VAL
2	C	621	SER
2	C	636	ILE
2	C	653	VAL

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Mol	Chain	Res	Type
2	C	746	VAL
2	C	777	SER
2	C	787	ARG
2	C	812	THR
2	C	831	GLU
2	C	852	VAL
2	C	868	LEU
2	C	875	GLN
2	C	885	LEU
2	C	904	MET
2	C	933	GLU
2	C	971	ILE
2	C	991	CYS
2	C	992	THR
2	C	1033	LEU
2	C	1037	VAL
2	C	1071	MET
2	C	1094	ASP
2	C	1097	VAL
2	C	1107	VAL
2	C	1117	ILE
2	C	1153	GLU
2	C	1162	LEU
3	D	4	VAL
3	D	12	ILE
3	D	86	LYS
3	D	89	ARG
3	D	148	LEU
3	D	308	SER
3	D	314	LEU
3	D	331	ASP
3	D	337	THR
3	D	338	SER
3	D	340	LEU
3	D	399	LEU
3	D	406	LEU
3	D	407	LYS
3	D	456	VAL
3	D	460	LEU
3	D	463	LEU
3	D	485	ASP
3	D	491	ILE

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Mol	Chain	Res	Type
3	D	517	VAL
3	D	579	LEU
3	D	580	ASP
3	D	588	LEU
3	D	590	THR
3	D	629	VAL
3	D	707	ILE
3	D	738	VAL
3	D	743	LYS
3	D	820	MET
3	D	838	SER
3	D	853	THR
3	D	860	LEU
3	D	863	THR
3	D	865	LEU
3	D	897	ILE
3	D	919	SER
3	D	944	LEU
3	D	957	ILE
3	D	991	ILE
3	D	1010	LEU
3	D	1036	GLU
3	D	1039	VAL
3	D	1075	VAL
3	D	1084	GLN
3	D	1088	VAL
3	D	1093	ASP
3	D	1098	VAL
3	D	1115	SER
3	D	1130	VAL
3	D	1148	SER
3	D	1194	VAL
3	D	1240	CYS
3	D	1249	LYS
4	E	82	VAL
5	F	34	ILE
5	F	37	LEU
5	F	45	LEU
5	F	96	LYS
5	F	169	ILE
5	F	172	ILE
5	F	184	LEU

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Mol	Chain	Res	Type
5	F	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	232	GLN
2	C	415	GLN
2	C	545	ASN
3	D	766	ASN
3	D	767	HIS
3	D	882	GLN
3	D	1084	GLN
3	D	1109	GLN
3	D	1125	GLN
3	D	1160	GLN
3	D	1190	ASN
4	E	64	ASN
4	E	68	ASN
4	E	105	HIS
5	F	117	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

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	219/368 (59%)	0.32	5 (2%) 61 52	46, 62, 95, 132	0
1	B	232/368 (63%)	1.14	36 (15%) 5 4	64, 100, 128, 144	0
2	C	1138/1174 (96%)	0.51	89 (7%) 19 16	36, 64, 143, 173	0
3	D	1258/1317 (95%)	0.43	48 (3%) 44 36	39, 67, 111, 144	0
4	E	71/110 (64%)	0.90	12 (16%) 4 3	65, 84, 112, 120	0
5	F	186/218 (85%)	1.19	28 (15%) 5 4	24, 92, 131, 141	12 (6%)
6	H	20/20 (100%)	0.15	1 (5%) 34 27	47, 70, 137, 142	0
7	G	23/23 (100%)	1.03	4 (17%) 4 3	80, 102, 159, 169	3 (13%)
8	I	6/6 (100%)	-0.42	0 100 100	47, 52, 64, 69	0
All	All	3153/3604 (87%)	0.56	223 (7%) 22 17	24, 70, 129, 173	15 (0%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	114	LEU	6.7
5	F	68	GLY	5.8
2	C	75	ALA	5.0
1	B	60	LEU	5.0
2	C	1151	GLU	4.8
2	C	252	PHE	4.6
1	B	188	ASP	4.6
2	C	143	ASN	4.2
3	D	316	ALA	4.1
5	F	117	ASN	4.1
2	C	559	VAL	4.0
4	E	30	THR	4.0
1	B	187	THR	4.0
5	F	79	LYS	3.8
1	B	61	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
4	E	31	PRO	3.8
1	B	138	LEU	3.8
7	G	5	DG	3.8
1	A	3	ILE	3.8
2	C	271	ASP	3.8
1	B	236	PRO	3.8
2	C	402	GLU	3.7
1	B	96	TYR	3.6
2	C	369	ASP	3.6
2	C	268	VAL	3.6
5	F	71	SER	3.6
4	E	34	ILE	3.6
2	C	220	ASP	3.6
1	B	147	VAL	3.5
5	F	45	LEU	3.5
3	D	605	ASP	3.5
2	C	522	GLY	3.4
3	D	865	LEU	3.4
2	C	253	GLY	3.4
2	C	575	GLU	3.4
1	B	57	ASP	3.3
2	C	192	ASP	3.3
5	F	83	TYR	3.3
5	F	112	TRP	3.3
1	B	157	ALA	3.3
2	C	554	PHE	3.3
2	C	328	ILE	3.2
3	D	464	ASN	3.2
2	C	206	PRO	3.2
3	D	654	SER	3.1
5	F	116	SER	3.1
2	C	233	PRO	3.1
2	C	74	ALA	3.0
3	D	1053	VAL	3.0
5	F	118	ALA	3.0
2	C	296	LEU	2.9
2	C	237	LEU	2.9
2	C	568	VAL	2.9
5	F	78	LEU	2.9
3	D	579	LEU	2.9
5	F	76	THR	2.9
3	D	1235	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	789	LEU	2.8
7	G	7	DG	2.8
2	C	1150	GLY	2.8
2	C	287	PRO	2.8
2	C	547	PRO	2.8
4	E	77	TYR	2.8
5	F	120	HIS	2.8
3	D	349	ASN	2.8
3	D	1274	PRO	2.8
2	C	1148	ARG	2.8
2	C	314	TYR	2.8
1	B	162	ILE	2.8
2	C	243	TRP	2.7
1	A	2	LEU	2.7
7	G	6	DT	2.7
2	C	521	ASP	2.7
3	D	346	ARG	2.7
2	C	295	LEU	2.7
4	E	36	ASN	2.7
2	C	346	VAL	2.7
2	C	1162	LEU	2.7
4	E	94	ALA	2.7
5	F	50	ASN	2.7
1	B	111	VAL	2.7
2	C	216	VAL	2.7
5	F	81	TRP	2.7
1	B	90	ASP	2.7
2	C	519	VAL	2.7
3	D	348	ILE	2.6
2	C	198	THR	2.6
2	C	294	THR	2.6
1	B	80	LEU	2.6
1	B	93	VAL	2.6
5	F	82	LEU	2.6
1	B	229	ALA	2.6
2	C	27	SER	2.6
1	B	168	TYR	2.6
3	D	607	PRO	2.6
2	C	324	VAL	2.6
1	B	159	ILE	2.6
3	D	1026	GLY	2.6
3	D	1094	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	903	ASP	2.6
2	C	573	SER	2.6
2	C	900	PRO	2.6
2	C	262	LEU	2.6
2	C	261	THR	2.6
2	C	556	GLU	2.6
3	D	210	ASP	2.6
3	D	1061	PHE	2.5
2	C	28	SER	2.5
4	E	32	LEU	2.5
1	B	58	GLY	2.5
2	C	191	ILE	2.5
5	F	52	ALA	2.5
2	C	30	ASN	2.5
2	C	218	LYS	2.5
2	C	523	VAL	2.5
1	B	129	ASN	2.5
2	C	359	GLY	2.4
2	C	193	LYS	2.4
4	E	84	PRO	2.4
3	D	1184	ALA	2.4
3	D	1203	GLY	2.4
1	B	63	PHE	2.4
1	A	222	ALA	2.4
6	H	22	DT	2.4
2	C	140	ILE	2.4
3	D	1195	ALA	2.4
1	B	151	GLN	2.4
2	C	680	HIS	2.4
5	F	122	SER	2.3
1	B	74	THR	2.3
2	C	353	THR	2.3
2	C	339	VAL	2.3
3	D	203	ARG	2.3
3	D	910	LEU	2.3
5	F	43	GLY	2.3
7	G	11	DG	2.3
2	C	387	ASN	2.3
3	D	2	LEU	2.3
2	C	349	HIS	2.3
3	D	36	TYR	2.3
1	B	59	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	1109	GLN	2.3
2	C	406	THR	2.3
5	F	35	PRO	2.3
2	C	417	LEU	2.2
2	C	248	ILE	2.2
1	B	118	VAL	2.2
2	C	207	SER	2.2
2	C	327	PRO	2.2
3	D	725	THR	2.2
2	C	365	VAL	2.2
3	D	936	VAL	2.2
3	D	1076	VAL	2.2
3	D	252	PHE	2.2
5	F	80	ALA	2.2
1	B	56	ILE	2.2
2	C	205	ILE	2.2
3	D	1103	ASP	2.2
1	B	84	VAL	2.2
3	D	317	VAL	2.2
4	E	92	SER	2.2
2	C	199	LEU	2.2
2	C	1088	LEU	2.2
3	D	396	ASN	2.2
2	C	257	ILE	2.2
1	B	175	THR	2.2
3	D	1011	THR	2.2
1	B	160	GLY	2.2
3	D	1012	MET	2.2
5	F	73	ARG	2.2
2	C	679	ASN	2.2
2	C	534	ASP	2.2
5	F	41	TYR	2.2
3	D	1176	LEU	2.2
2	C	555	VAL	2.1
3	D	70	PHE	2.1
2	C	35	ALA	2.1
2	C	486	ILE	2.1
2	C	545	ASN	2.1
2	C	576	VAL	2.1
1	A	221	LEU	2.1
3	D	665	GLU	2.1
3	D	653	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	78	GLY	2.1
4	E	86	LEU	2.1
3	D	337	THR	2.1
1	B	23	ILE	2.1
3	D	902	ALA	2.1
1	B	233	GLU	2.1
2	C	1103	TYR	2.1
2	C	1149	GLU	2.1
3	D	1090	LYS	2.1
5	F	88	ASN	2.1
1	B	2	LEU	2.1
1	A	145	GLY	2.1
2	C	341	THR	2.1
2	C	356	THR	2.1
3	D	342	ASP	2.1
3	D	883	ASP	2.1
5	F	110	THR	2.1
2	C	292	ALA	2.1
4	E	39	ILE	2.1
4	E	55	TYR	2.1
2	C	281	LEU	2.0
3	D	679	LEU	2.0
2	C	553	ARG	2.0
2	C	65	ILE	2.0
2	C	858	GLU	2.0
2	C	435	GLN	2.0
2	C	546	SER	2.0
5	F	39	GLN	2.0
1	B	92	PRO	2.0
2	C	1155	LEU	2.0
1	B	182	ARG	2.0
2	C	29	ASN	2.0
3	D	957	ILE	2.0
5	F	34	ILE	2.0
1	B	184	GLU	2.0
2	C	289	LYS	2.0
3	D	90	GLU	2.0
3	D	608	GLU	2.0
5	F	90	TYR	2.0
1	B	150	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MG	D	2003	1/1	0.89	0.17	46,46,46,46	0
9	ZN	D	2002	1/1	0.99	0.02	91,91,91,91	0
9	ZN	D	2001	1/1	0.99	0.02	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.