



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:33 PM UTC

PDB ID : 6KOP / pdb_00006kop
Title : Mycobacterium tuberculosis initial transcription complex comprising sigma H
and 5'-OH RNA of 9 nt
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-08-12
Resolution : 3.30 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

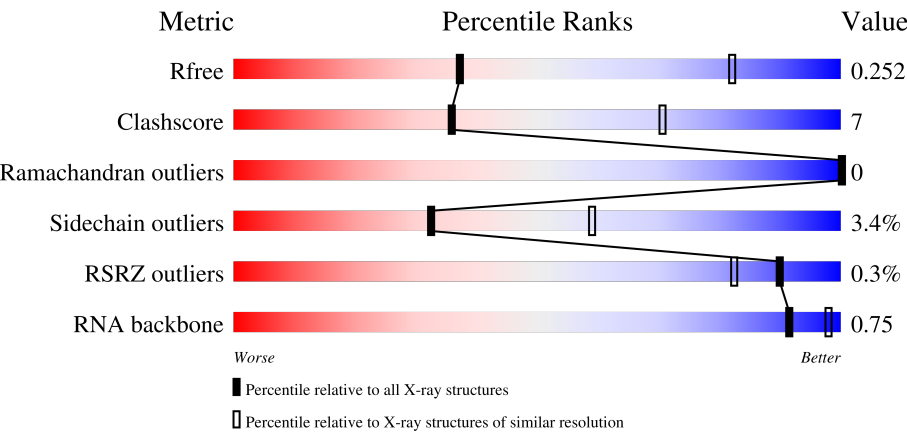
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



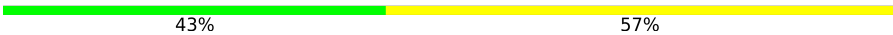
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	46%12%•41%
1	B	368	51%11%•38%
2	C	1174	79%18%••
3	D	1317	76%19%••

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Mol	Chain	Length	Quality of chain
4	E	110	 45% 22% 32%
5	F	218	 58% 15% 27%
6	G	23	 35% 65%
7	H	21	 43% 57%
8	I	9	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24560 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	218	Total	C	N	O	S	0	0	0
			1646	1038	281	325	2			
1	B	227	Total	C	N	O	S	0	0	0
			1606	1013	270	321	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
			8655	5413	1503	1701	38			

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	1263	Total	C	N	O	S	0	0	0
			9699	6086	1735	1837	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
			589	375	99	115			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	159	Total	C	N	O	S	0	0	0
			1252	788	220	240	4			

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*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
6	G	23	Total	C	N	O	P	0	0	0
			475	226	89	138	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(*CP*AP*CP*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	9	Total	C	N	O	P	0	0	0
			184	84	32	60	8			

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

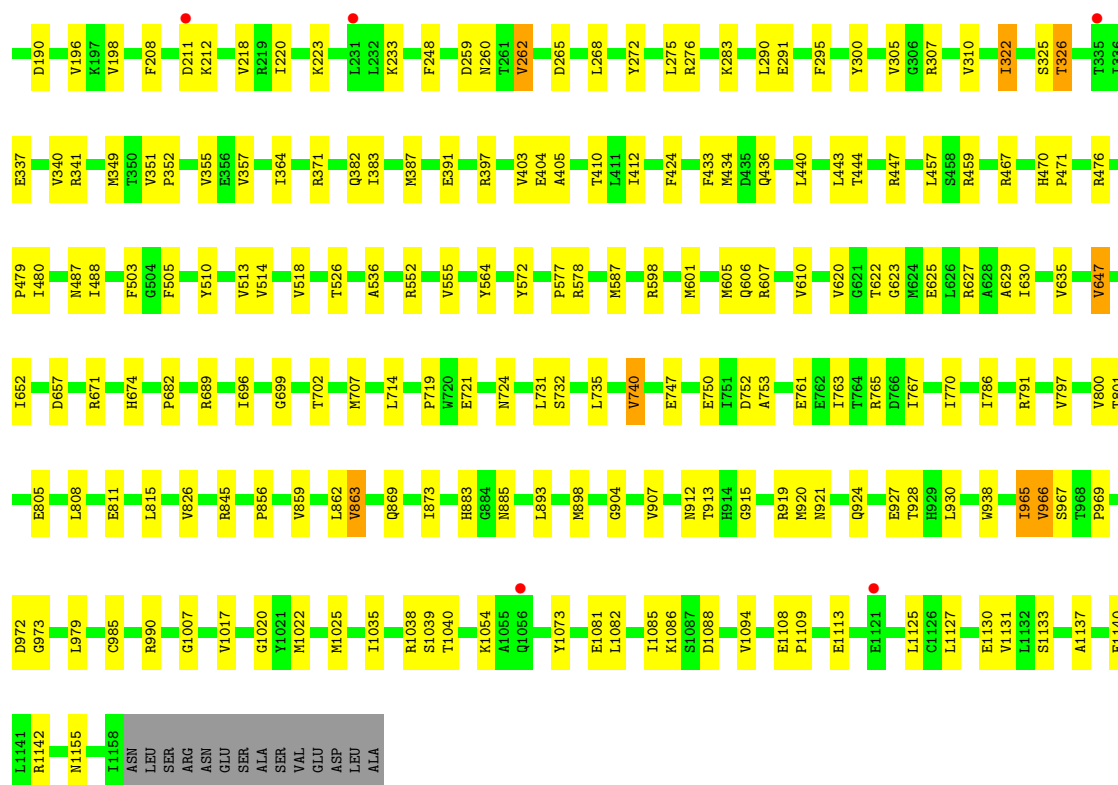
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		

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

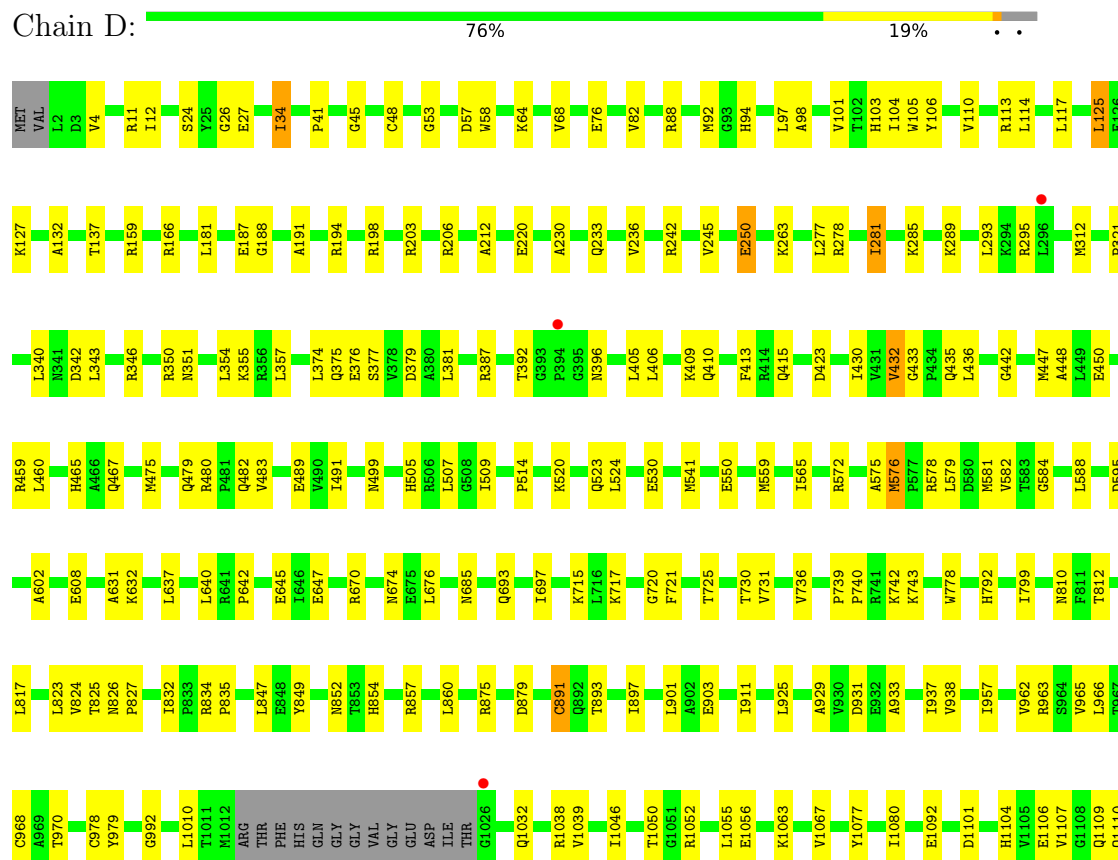
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total 1	Mg 1	0	0

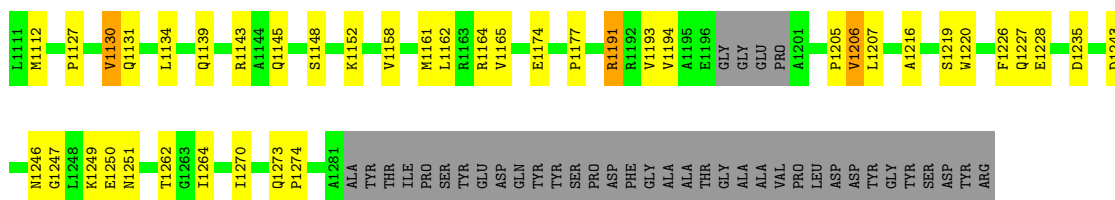
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total 1	O 1	0	0
11	C	7	Total 7	O 7	0	0
11	D	8	Total 8	O 8	0	0
11	H	1	Total 1	O 1	0	0



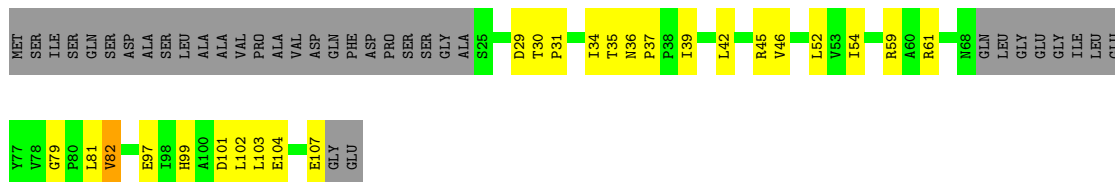
• Molecule 3: DNA-directed RNA polymerase subunit beta'





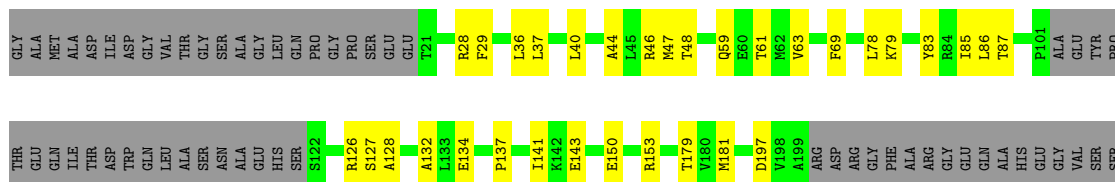
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 45% 22% 32%



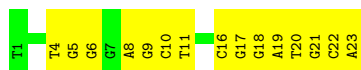
- Molecule 5: ECF RNA polymerase sigma factor SigH

Chain F: 58% 15% 27%



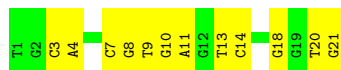
- Molecule 6: DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3')

Chain G: 35% 65%



- 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: 43% 57%



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

Chain I: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.37Å 162.64Å 133.42Å 90.00° 117.95° 90.00°	Depositor
Resolution (Å)	49.25 – 3.30 49.25 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.25-3.30) 98.3 (49.25-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.217 , 0.255 0.218 , 0.252	Depositor DCC
R_{free} test set	2401 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	107.2	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24560	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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	0.11	0/1671	0.31	0/2274
1	B	0.12	0/1629	0.33	0/2233
2	C	0.12	0/8813	0.32	0/11978
3	D	0.11	0/9860	0.31	0/13357
4	E	0.12	0/601	0.35	0/818
5	F	0.11	0/1274	0.29	0/1724
6	G	0.19	0/533	0.45	0/823
7	H	0.19	0/487	0.40	0/752
8	I	0.14	0/204	0.26	0/315
All	All	0.12	0/25072	0.32	0/34274

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1646	0	1676	28	0
1	B	1606	0	1543	23	0
2	C	8655	0	8429	129	0
3	D	9699	0	9624	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	589	0	578	16	0
5	F	1252	0	1214	21	0
6	G	475	0	261	10	0
7	H	434	0	238	11	0
8	I	184	0	99	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	A	1	0	0	0	0
11	C	7	0	0	0	0
11	D	8	0	0	0	0
11	H	1	0	0	0	0
All	All	24560	0	23662	350	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 7.

All (350) 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:122:THR:HG22	2:C:163:ASN:H	1.40	0.85
2:C:652:ILE:HD11	2:C:682:PRO:HB3	1.63	0.81
3:D:925:LEU:HA	3:D:962:VAL:HA	1.66	0.76
3:D:1050:THR:HG23	3:D:1107:VAL:HG23	1.67	0.76
4:E:31:PRO:HB2	4:E:36:ASN:HB3	1.67	0.75
2:C:1155:ASN:HB2	5:F:137:PRO:HB3	1.69	0.75
3:D:968:CYS:SG	3:D:978:CYS:HB3	2.28	0.74
3:D:92:MET:HG2	3:D:321:PRO:HD3	1.69	0.73
3:D:392:THR:HB	3:D:396:ASN:HA	1.72	0.71
3:D:891:CYS:SG	3:D:970:THR:OG1	2.49	0.71
2:C:721:GLU:H	3:D:725:THR:HG22	1.56	0.71
3:D:460:LEU:HD11	3:D:483:VAL:HG12	1.72	0.71
1:B:24:GLU:HB3	1:B:191:LYS:HG3	1.73	0.70
2:C:151:PHE:HE1	2:C:383:ILE:HD11	1.57	0.70
3:D:530:GLU:OE1	3:D:578:ARG:NH1	2.25	0.70
1:A:40:ARG:NH2	2:C:1007:GLY:O	2.26	0.69
2:C:1040:THR:HG22	5:F:127:SER:HB2	1.76	0.68
2:C:883:HIS:NE2	2:C:927:GLU:OE1	2.24	0.68
2:C:536:ALA:HA	2:C:555:VAL:HG12	1.77	0.67
2:C:732:SER:HA	2:C:898:MET:HE3	1.77	0.67
3:D:879:ASP:OD2	3:D:1249:LYS:NZ	2.28	0.66
3:D:293:LEU:HD21	3:D:1177:PRO:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1080:ILE:HG12	3:D:1112:MET:HE1	1.77	0.65
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.62	0.64
3:D:642:PRO:HG2	3:D:647:GLU:HB2	1.79	0.64
2:C:341:ARG:HH11	2:C:349:MET:HG2	1.61	0.64
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.79	0.64
2:C:1017:VAL:HA	3:D:730:THR:HG21	1.79	0.64
2:C:921:ASN:OD1	2:C:924:GLN:NE2	2.32	0.63
4:E:42:LEU:HB3	4:E:52:LEU:HD11	1.81	0.63
3:D:285:LYS:HA	3:D:289:LYS:HD2	1.78	0.63
1:B:179:ASP:HB2	1:B:191:LYS:HE2	1.81	0.63
2:C:1130:GLU:OE1	3:D:11:ARG:NH2	2.31	0.63
2:C:1133:SER:HB3	2:C:1137:ALA:HB3	1.81	0.62
2:C:587:MET:HE3	2:C:625:GLU:HG3	1.80	0.62
3:D:550:GLU:OE2	4:E:61:ARG:NH1	2.33	0.62
3:D:1274:PRO:HB3	4:E:81:LEU:HD11	1.81	0.61
2:C:627:ARG:HA	2:C:630:ILE:HG12	1.83	0.61
3:D:181:LEU:HD21	3:D:198:ARG:HB2	1.82	0.61
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.83	0.61
2:C:972:ASP:OD1	2:C:973:GLY:N	2.30	0.61
6:G:4:DT:OP2	6:G:4:DT:H3'	2.00	0.61
2:C:606:GLN:HG2	2:C:1025:MET:HE1	1.83	0.60
2:C:1038:ARG:NH2	3:D:423:ASP:OD1	2.25	0.60
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.83	0.60
1:A:83:LEU:HA	1:A:123:MET:HE1	1.83	0.60
6:G:20:DT:H2''	6:G:21:DG:C8	2.37	0.60
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.84	0.60
3:D:965:VAL:HG22	3:D:979:TYR:HA	1.83	0.60
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.83	0.59
2:C:272:TYR:OH	2:C:276:ARG:NH1	2.36	0.59
1:A:176:TYR:HB3	1:A:194:LEU:HD23	1.85	0.59
1:A:181:THR:O	1:A:188:ASP:HA	2.02	0.59
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.29	0.59
2:C:436:GLN:H	2:C:674:HIS:CD2	2.21	0.59
3:D:963:ARG:NH1	3:D:978:CYS:SG	2.76	0.59
2:C:752:ASP:HB3	2:C:862:LEU:HD23	1.84	0.58
3:D:430:ILE:HD13	3:D:541:MET:HG3	1.86	0.58
3:D:505:HIS:CE1	3:D:507:LEU:HB2	2.39	0.58
3:D:530:GLU:HB2	3:D:578:ARG:HD2	1.86	0.58
1:A:98:ARG:HG3	1:A:135:GLU:HG3	1.86	0.58
2:C:699:GLY:N	2:C:702:THR:OG1	2.36	0.58
3:D:281:ILE:HD11	3:D:293:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:671:ARG:HE	2:C:747:GLU:HA	1.68	0.57
3:D:376:GLU:HG2	3:D:387:ARG:HH12	1.70	0.57
2:C:647:VAL:HG12	2:C:652:ILE:HG12	1.86	0.56
2:C:1140:GLU:OE1	2:C:1142:ARG:NH2	2.39	0.56
3:D:740:PRO:HD3	3:D:792:HIS:CD2	2.40	0.56
2:C:791:ARG:NH2	3:D:479:GLN:OE1	2.37	0.56
2:C:815:LEU:HD11	5:F:141:ILE:HD12	1.87	0.56
2:C:265:ASP:HA	2:C:268:LEU:HD12	1.88	0.56
3:D:581:MET:HE2	3:D:717:LYS:HG3	1.87	0.56
3:D:1227:GLN:HG2	3:D:1228:GLU:HG3	1.86	0.56
2:C:118:ASP:OD2	2:C:845:ARG:NH1	2.39	0.55
2:C:397:ARG:NH1	2:C:410:THR:O	2.40	0.55
2:C:577:PRO:O	2:C:578:ARG:HG2	2.06	0.55
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.39	0.55
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.89	0.55
2:C:915:GLY:O	2:C:919:ARG:HG2	2.06	0.55
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.87	0.55
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.87	0.55
2:C:33:VAL:HG23	2:C:966:VAL:HG13	1.89	0.55
3:D:1050:THR:HG22	3:D:1106:GLU:HA	1.87	0.55
2:C:179:VAL:HG22	2:C:198:VAL:HG22	1.89	0.55
3:D:1262:THR:HB	4:E:54:ILE:HD11	1.87	0.55
2:C:129:VAL:HG21	2:C:148:MET:HE2	1.88	0.55
2:C:1081:GLU:HG3	2:C:1085:ILE:HD11	1.89	0.54
3:D:459:ARG:NE	3:D:489:GLU:OE2	2.39	0.54
3:D:1032:GLN:HG2	3:D:1038:ARG:HH12	1.72	0.54
1:A:56:ILE:HG12	1:A:136:VAL:HG22	1.90	0.54
3:D:64:LYS:NZ	3:D:76:GLU:OE2	2.36	0.54
2:C:114:ASP:OD1	2:C:114:ASP:N	2.41	0.54
2:C:179:VAL:HG23	2:C:310:VAL:HG12	1.90	0.54
1:A:37:SER:HG	1:B:37:SER:HG	1.56	0.54
4:E:37:PRO:HG2	4:E:42:LEU:HD11	1.89	0.54
1:B:186:ARG:O	1:B:187:THR:HG22	2.07	0.54
6:G:8:DA:H2''	6:G:9:DG:C8	2.43	0.54
2:C:480:ILE:HD11	3:D:849:TYR:HE1	1.72	0.53
3:D:721:PHE:O	3:D:725:THR:HG23	2.08	0.53
2:C:657:ASP:OD2	2:C:689:ARG:NH2	2.41	0.53
3:D:676:LEU:HD22	3:D:715:LYS:HB3	1.91	0.53
1:B:174:VAL:HG22	1:B:196:VAL:HG23	1.91	0.52
1:B:6:ARG:O	1:B:25:PRO:HD2	2.09	0.52
2:C:721:GLU:H	3:D:725:THR:CG2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:ILE:HG23	3:D:514:PRO:HG2	1.91	0.52
1:A:95:MET:HG2	1:A:113:PRO:HD2	1.91	0.52
2:C:248:PHE:HZ	2:C:341:ARG:HE	1.56	0.52
1:B:22:VAL:HG12	1:B:193:ILE:HG12	1.92	0.52
1:B:215:LEU:HD23	1:B:218:LEU:HD12	1.91	0.52
2:C:622:THR:HG23	2:C:969:PRO:HA	1.91	0.52
1:A:48:GLY:O	1:A:142:ARG:HG3	2.10	0.52
1:A:95:MET:HE3	1:A:112:PRO:HB3	1.91	0.52
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.91	0.52
2:C:622:THR:HG22	2:C:623:GLY:H	1.75	0.52
2:C:382:GLN:HG2	2:C:424:PHE:HB2	1.91	0.52
3:D:101:VAL:HA	3:D:375:GLN:HE22	1.75	0.52
2:C:719:PRO:HA	2:C:724:ASN:HD21	1.75	0.51
2:C:1035:ILE:O	2:C:1054:LYS:NZ	2.38	0.51
2:C:1127:LEU:HD13	3:D:12:ILE:HD11	1.92	0.51
5:F:78:LEU:HD23	5:F:78:LEU:H	1.75	0.51
5:F:150:GLU:HG2	5:F:153:ARG:HH12	1.76	0.51
5:F:47:MET:HE1	5:F:87:THR:HG22	1.91	0.51
3:D:448:ALA:HB1	3:D:491:ILE:HD11	1.93	0.51
3:D:1250:GLU:OE1	3:D:1250:GLU:N	2.41	0.51
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.92	0.51
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.45	0.51
2:C:735:LEU:HD22	2:C:740:VAL:HG21	1.92	0.51
4:E:29:ASP:OD1	4:E:30:THR:N	2.37	0.51
1:B:171:VAL:HA	1:B:198:THR:HA	1.93	0.51
2:C:856:PRO:HG2	2:C:859:VAL:HG21	1.93	0.50
3:D:1162:LEU:HD21	3:D:1207:LEU:HD12	1.92	0.50
5:F:46:ARG:HD3	6:G:6:DG:H5"	1.92	0.50
3:D:1270:ILE:HG12	4:E:107:GLU:HA	1.93	0.50
3:D:823:LEU:HD23	3:D:835:PRO:HB3	1.93	0.50
7:H:9:DT:H2'	7:H:10:DG:C8	2.47	0.50
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.93	0.50
2:C:223:LYS:HG3	2:C:275:LEU:HD23	1.93	0.50
2:C:440:LEU:HB2	2:C:707:MET:HE2	1.94	0.50
2:C:885:ASN:HD21	2:C:1022:MET:HE1	1.77	0.50
3:D:1134:LEU:HD11	3:D:1207:LEU:HD11	1.92	0.50
2:C:291:GLU:HA	2:C:295:PHE:HD2	1.76	0.49
1:A:12:ASP:OD1	1:A:13:VAL:N	2.45	0.49
3:D:576:MET:HB2	3:D:697:ILE:HD12	1.94	0.49
3:D:810:ASN:OD1	3:D:812:THR:OG1	2.21	0.49
3:D:1227:GLN:HG3	7:H:10:DG:H5"	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:159:ARG:HH12	3:D:220:GLU:HB2	1.78	0.49
1:A:171:VAL:HA	1:A:198:THR:HA	1.94	0.49
2:C:805:GLU:HA	2:C:808:LEU:HD13	1.95	0.49
3:D:929:ALA:HB1	3:D:957:ILE:HD13	1.94	0.49
3:D:480:ARG:NH1	3:D:482:GLN:OE1	2.46	0.49
2:C:436:GLN:H	2:C:674:HIS:HD2	1.60	0.49
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.46	0.49
2:C:259:ASP:OD1	2:C:260:ASN:N	2.45	0.49
2:C:32:ARG:HA	2:C:965:ILE:HG22	1.94	0.48
2:C:731:LEU:HD13	2:C:735:LEU:HD12	1.95	0.48
2:C:797:VAL:HG11	2:C:863:VAL:HG11	1.93	0.48
2:C:1082:LEU:HA	2:C:1086:LYS:HD2	1.95	0.48
3:D:278:ARG:O	3:D:281:ILE:HG22	2.13	0.48
3:D:114:LEU:HG	3:D:312:MET:HE2	1.95	0.48
4:E:59:ARG:HH22	4:E:79:GLY:HA3	1.78	0.48
7:H:20:DT:H2''	7:H:21:DG:H8	1.79	0.48
3:D:45:GLY:H	3:D:48:CYS:HB2	1.78	0.48
3:D:1046:ILE:HG22	3:D:1110:GLN:HA	1.96	0.47
3:D:832:ILE:HG22	3:D:834:ARG:H	1.79	0.47
1:A:97:LEU:HD22	1:A:110:ILE:HG12	1.95	0.47
2:C:196:VAL:HG13	2:C:208:PHE:HB2	1.97	0.47
3:D:410:GLN:HA	3:D:415:GLN:HB2	1.96	0.47
7:H:7:DC:H2''	7:H:8:DG:C8	2.49	0.47
1:A:144:ARG:NH1	1:B:2:LEU:HB2	2.30	0.47
2:C:37:LYS:NZ	2:C:973:GLY:O	2.31	0.47
3:D:53:GLY:O	3:D:88:ARG:NH1	2.46	0.47
3:D:351:ASN:HD21	3:D:355:LYS:HE3	1.78	0.47
3:D:1055:LEU:HD13	3:D:1101:ASP:HA	1.96	0.47
3:D:1174:GLU:OE2	3:D:1174:GLU:N	2.47	0.47
3:D:1273:GLN:O	4:E:104:GLU:HG2	2.14	0.47
2:C:307:ARG:HD3	2:C:325:SER:HA	1.97	0.47
7:H:13:DT:H2'	7:H:14:DC:C6	2.50	0.47
2:C:800:VAL:HB	2:C:826:VAL:HB	1.95	0.47
6:G:22:DC:H2''	6:G:23:DA:C8	2.49	0.47
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.80	0.47
3:D:475:MET:HG3	3:D:480:ARG:HD3	1.97	0.47
5:F:79:LYS:HE3	6:G:5:DG:N7	2.29	0.47
3:D:670:ARG:HD3	3:D:685:ASN:HA	1.97	0.47
4:E:31:PRO:HB3	4:E:35:THR:HG23	1.96	0.47
5:F:61:THR:HG23	5:F:85:ILE:HG22	1.97	0.47
1:A:64:THR:OG1	1:A:65:THR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:230:ALA:N	3:D:233:GLN:OE1	2.48	0.47
7:H:3:DC:H2''	7:H:4:DA:C8	2.50	0.47
1:A:34:LEU:HD11	1:B:218:LEU:HD13	1.97	0.47
1:B:17:ASN:OD1	1:B:17:ASN:N	2.48	0.47
3:D:342:ASP:O	3:D:346:ARG:HG3	2.14	0.47
3:D:1274:PRO:HA	4:E:103:LEU:HA	1.97	0.46
3:D:103:HIS:ND1	3:D:105:TRP:HB2	2.30	0.46
3:D:847:LEU:HD12	3:D:847:LEU:H	1.81	0.46
3:D:891:CYS:HB3	3:D:893:THR:HG22	1.97	0.46
2:C:479:PRO:O	3:D:857:ARG:NH2	2.45	0.46
2:C:1040:THR:HG21	5:F:128:ALA:HB3	1.97	0.46
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.97	0.46
3:D:1106:GLU:HB2	3:D:1109:GLN:HG3	1.96	0.46
1:B:9:LEU:HD13	1:B:23:ILE:HG12	1.97	0.46
3:D:827:PRO:HD3	3:D:854:HIS:CE1	2.51	0.46
1:A:9:LEU:HD22	1:B:222:ALA:HA	1.97	0.46
3:D:637:LEU:HD13	3:D:640:LEU:HD12	1.97	0.46
2:C:930:LEU:HB2	2:C:979:LEU:HD21	1.97	0.46
3:D:602:ALA:HB2	3:D:608:GLU:HG3	1.97	0.46
2:C:32:ARG:CZ	2:C:965:ILE:HG23	2.46	0.46
3:D:875:ARG:NH2	3:D:1226:PHE:O	2.41	0.46
1:B:223:ARG:HE	1:B:223:ARG:HB2	1.47	0.45
2:C:337:GLU:HA	2:C:340:VAL:HG22	1.98	0.45
2:C:873:ILE:HD12	2:C:873:ILE:HA	1.84	0.45
2:C:1039:SER:HB3	3:D:450:GLU:O	2.17	0.45
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.98	0.45
2:C:598:ARG:HG3	2:C:921:ASN:HD22	1.81	0.45
1:B:83:LEU:HB2	1:B:123:MET:HE1	1.99	0.45
2:C:233:LYS:HZ2	2:C:262:VAL:HA	1.81	0.45
2:C:364:ILE:HD12	2:C:364:ILE:H	1.82	0.45
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.52	0.45
2:C:433:PHE:CE2	7:H:18:DG:H4'	2.51	0.45
3:D:432:VAL:HG13	3:D:433:GLY:H	1.82	0.45
2:C:459:ARG:NH2	2:C:487:ASN:OD1	2.50	0.45
2:C:1094:VAL:HG23	5:F:132:ALA:HB2	1.99	0.45
3:D:572:ARG:NH2	3:D:1148:SER:OG	2.50	0.45
3:D:1139:GLN:HG3	3:D:1143:ARG:HD2	1.98	0.45
2:C:265:ASP:OD1	2:C:265:ASP:N	2.50	0.45
3:D:250:GLU:CD	3:D:250:GLU:H	2.25	0.45
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.99	0.44
3:D:24:SER:OG	3:D:26:GLY:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:351:VAL:HG22	2:C:352:PRO:HD2	1.98	0.44
2:C:786:ILE:HD12	2:C:786:ILE:H	1.82	0.44
3:D:340:LEU:HD21	3:D:405:LEU:HD11	1.99	0.44
4:E:45:ARG:NE	4:E:101:ASP:OD1	2.50	0.44
2:C:443:LEU:O	2:C:447:ARG:HG3	2.18	0.44
3:D:1010:LEU:HA	3:D:1145:GLN:HG3	2.00	0.44
6:G:18:DG:H2''	6:G:19:DA:N7	2.32	0.44
1:B:202:ILE:HD13	1:B:207:ALA:HB2	1.99	0.44
3:D:465:HIS:CD2	3:D:482:GLN:HB3	2.53	0.44
3:D:826:ASN:CG	3:D:827:PRO:HD2	2.42	0.44
3:D:1158:VAL:HA	3:D:1161:MET:HE2	2.00	0.44
4:E:81:LEU:HB3	4:E:102:LEU:HD23	2.00	0.44
2:C:457:LEU:HD23	2:C:457:LEU:H	1.83	0.44
3:D:203:ARG:HD2	3:D:206:ARG:HD2	2.00	0.44
3:D:992:GLY:HA2	3:D:1264:ILE:HD12	1.99	0.44
3:D:1056:GLU:HB2	3:D:1063:LYS:HB3	2.00	0.44
2:C:434:MET:HG2	2:C:436:GLN:HG3	1.99	0.44
2:C:322:ILE:H	2:C:322:ILE:HG13	1.58	0.43
2:C:467:ARG:HD3	2:C:488:ILE:O	2.18	0.43
2:C:552:ARG:HB3	2:C:564:TYR:HD2	1.83	0.43
3:D:406:LEU:HD23	3:D:413:PHE:HE1	1.83	0.43
3:D:499:ASN:HB2	3:D:509:ILE:HG12	2.00	0.43
3:D:1191:ARG:HA	3:D:1194:VAL:HG12	2.00	0.43
7:H:10:DG:H2'	7:H:11:DA:C8	2.52	0.43
1:B:120:ASN:ND2	1:B:123:MET:SD	2.91	0.43
2:C:913:THR:HG23	3:D:731:VAL:HG23	2.00	0.43
5:F:59:GLN:O	5:F:63:VAL:HG23	2.18	0.43
3:D:435:GLN:CD	3:D:435:GLN:H	2.26	0.43
3:D:937:ILE:HG13	3:D:957:ILE:HD11	2.00	0.43
3:D:1219:SER:OG	3:D:1243:ASP:OD2	2.31	0.43
2:C:300:TYR:HD1	2:C:326:THR:HG22	1.84	0.43
5:F:36:LEU:O	5:F:40:LEU:HG	2.18	0.43
2:C:146:VAL:HG21	2:C:412:ILE:HD12	2.01	0.43
2:C:513:VAL:HG22	2:C:518:VAL:HG22	1.99	0.43
3:D:1127:PRO:HA	3:D:1130:VAL:HG23	2.00	0.43
4:E:37:PRO:HG3	4:E:99:HIS:HB2	2.00	0.43
4:E:82:VAL:HG23	4:E:97:GLU:HG2	2.01	0.43
6:G:16:DC:H2''	6:G:17:DG:C8	2.53	0.43
2:C:211:ASP:OD1	2:C:212:LYS:N	2.49	0.43
2:C:1035:ILE:HG21	3:D:520:LYS:HD3	2.00	0.43
2:C:371:ARG:HB3	2:C:505:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:912:ASN:OD1	2:C:913:THR:N	2.52	0.43
1:B:170:PRO:HB2	1:B:202:ILE:HD11	2.01	0.43
2:C:32:ARG:HG2	2:C:967:SER:HB3	2.01	0.43
2:C:58:LEU:HD21	2:C:151:PHE:HZ	1.84	0.43
2:C:383:ILE:O	2:C:387:MET:HG2	2.18	0.43
3:D:1165:VAL:HA	3:D:1206:VAL:HG23	2.00	0.42
7:H:20:DT:H2"	7:H:21:DG:C8	2.54	0.42
2:C:920:MET:HE1	3:D:817:LEU:HA	2.01	0.42
3:D:376:GLU:HG2	3:D:387:ARG:NH1	2.34	0.42
3:D:966:LEU:HD13	3:D:1131:GLN:HB3	2.01	0.42
1:A:62:GLU:HG2	1:A:162:ILE:HG23	2.01	0.42
2:C:1035:ILE:HD11	3:D:447:MET:HG3	2.00	0.42
2:C:1125:LEU:HD13	3:D:105:TRP:CH2	2.54	0.42
3:D:736:VAL:HG22	3:D:799:ILE:HD11	2.01	0.42
1:B:226:ASN:OD1	1:B:227:VAL:N	2.52	0.42
2:C:761:GLU:HG2	2:C:801:THR:HA	2.01	0.42
3:D:277:LEU:HD21	3:D:295:ARG:HE	1.84	0.42
1:A:175:THR:HB	2:C:904:GLY:HA3	2.02	0.42
3:D:27:GLU:HB2	3:D:94:HIS:CE1	2.54	0.42
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.54	0.42
2:C:444:THR:OG1	2:C:607:ARG:HD2	2.20	0.42
2:C:1088:ASP:HB3	2:C:1113:GLU:H	1.85	0.42
3:D:191:ALA:HA	3:D:194:ARG:HD3	2.00	0.42
3:D:1092:GLU:HB2	3:D:1104:HIS:HB3	2.02	0.42
5:F:61:THR:HG21	5:F:86:LEU:HB3	2.00	0.42
7:H:7:DC:H2"	7:H:8:DG:H8	1.84	0.42
1:A:66:VAL:O	1:A:69:VAL:HG22	2.20	0.42
2:C:90:ILE:HD13	2:C:391:GLU:HG3	2.02	0.42
2:C:476:ARG:HH11	2:C:526:THR:C	2.27	0.42
3:D:281:ILE:HD12	3:D:289:LYS:HG3	2.01	0.42
3:D:584:GLY:HA3	3:D:720:GLY:O	2.19	0.42
2:C:601:MET:HB3	2:C:605:MET:HE3	2.01	0.42
3:D:579:LEU:O	3:D:582:VAL:HB	2.19	0.42
3:D:931:ASP:C	3:D:933:ALA:H	2.28	0.42
2:C:305:VAL:HG22	2:C:503:PHE:HD1	1.85	0.42
2:C:403:VAL:C	2:C:405:ALA:H	2.27	0.42
3:D:350:ARG:HH11	3:D:377:SER:HB3	1.85	0.42
3:D:524:LEU:HD13	3:D:541:MET:HE1	2.01	0.42
3:D:903:GLU:O	3:D:911:ILE:HG13	2.20	0.42
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	2.01	0.42
1:B:49:ALA:HA	1:B:142:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1073:TYR:CD2	3:D:559:MET:HG2	2.55	0.42
3:D:97:LEU:HD22	3:D:374:LEU:HD21	2.02	0.42
5:F:29:PHE:HB2	5:F:69:PHE:CE2	2.55	0.42
2:C:433:PHE:HE2	7:H:18:DG:H4'	1.85	0.41
2:C:135:ASN:HB3	2:C:140:GLU:HG2	2.02	0.41
2:C:629:ALA:HB2	2:C:707:MET:HG2	2.02	0.41
2:C:470:HIS:CG	2:C:471:PRO:HD2	2.55	0.41
2:C:765:ARG:O	2:C:767:ILE:HG12	2.19	0.41
3:D:963:ARG:HB3	3:D:978:CYS:HA	2.02	0.41
1:A:57:ASP:OD1	1:A:57:ASP:N	2.54	0.41
2:C:84:LEU:HD12	2:C:104:PRO:HG3	2.01	0.41
3:D:281:ILE:HD12	3:D:281:ILE:HA	1.74	0.41
2:C:750:GLU:HG3	2:C:862:LEU:HD21	2.01	0.41
3:D:1046:ILE:O	3:D:1077:TYR:OH	2.31	0.41
6:G:17:DG:H2''	6:G:18:DG:C8	2.55	0.41
2:C:753:ALA:HB2	2:C:763:ILE:HG13	2.02	0.41
1:A:3:ILE:HD12	1:A:3:ILE:HA	1.91	0.41
2:C:928:THR:HG22	2:C:1020:GLY:HA3	2.02	0.41
2:C:938:TRP:HB2	2:C:985:CYS:HB2	2.02	0.41
3:D:242:ARG:HA	3:D:245:VAL:HG22	2.03	0.41
5:F:44:ALA:O	5:F:48:THR:OG1	2.25	0.41
5:F:126:ARG:NH2	5:F:134:GLU:OE2	2.51	0.41
2:C:510:TYR:HB3	2:C:572:TYR:HB3	2.02	0.41
3:D:979:TYR:CZ	3:D:1152:LYS:HD3	2.56	0.41
1:A:7:PRO:HG2	1:B:221:LEU:HD11	2.02	0.41
1:A:112:PRO:HB2	1:A:116:VAL:HG23	2.02	0.41
3:D:187:GLU:CD	3:D:188:GLY:H	2.29	0.41
3:D:1112:MET:HE3	3:D:1112:MET:HB2	1.95	0.41
1:A:197:GLU:OE1	2:C:990:ARG:NH2	2.38	0.41
3:D:137:THR:HB	3:D:263:LYS:HG2	2.02	0.41
5:F:47:MET:HE2	5:F:47:MET:HB3	1.94	0.41
5:F:126:ARG:HH22	5:F:134:GLU:CD	2.28	0.41
2:C:714:LEU:HD23	2:C:907:VAL:HA	2.03	0.40
6:G:10:DC:H2''	6:G:11:DT:H5'	2.04	0.40
2:C:1108:GLU:HA	2:C:1109:PRO:HD3	1.96	0.40
3:D:166:ARG:HD3	3:D:212:ALA:HB3	2.03	0.40
2:C:283:LYS:HE3	2:C:283:LYS:HB3	1.90	0.40
2:C:893:LEU:HB2	2:C:898:MET:CE	2.51	0.40
3:D:127:LYS:HA	3:D:132:ALA:HB3	2.03	0.40
5:F:197:ASP:OD1	5:F:197:ASP:N	2.53	0.40
3:D:1052:ARG:HG3	3:D:1067:VAL:HB	2.03	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	214/368 (58%)	210 (98%)	4 (2%)	0	100	100
1	B	223/368 (61%)	215 (96%)	8 (4%)	0	100	100
2	C	1136/1174 (97%)	1095 (96%)	41 (4%)	0	100	100
3	D	1257/1317 (95%)	1226 (98%)	31 (2%)	0	100	100
4	E	71/110 (64%)	70 (99%)	1 (1%)	0	100	100
5	F	155/218 (71%)	150 (97%)	5 (3%)	0	100	100
All	All	3056/3555 (86%)	2966 (97%)	90 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	185/315 (59%)	178 (96%)	7 (4%)	29	57
1	B	165/315 (52%)	157 (95%)	8 (5%)	23	52
2	C	925/995 (93%)	900 (97%)	25 (3%)	39	63
3	D	1007/1096 (92%)	974 (97%)	33 (3%)	33	59
4	E	63/90 (70%)	59 (94%)	4 (6%)	16	44
5	F	125/175 (71%)	119 (95%)	6 (5%)	23	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2470/2986 (83%)	2387 (97%)	83 (3%)	32 59

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	62	GLU
1	A	84	VAL
1	A	111	VAL
1	A	134	LEU
1	A	150	VAL
1	A	171	VAL
1	B	54	ILE
1	B	66	VAL
1	B	84	VAL
1	B	111	VAL
1	B	183	VAL
1	B	202	ILE
1	B	223	ARG
1	B	225	LEU
2	C	74	VAL
2	C	190	ASP
2	C	218	VAL
2	C	220	ILE
2	C	262	VAL
2	C	290	LEU
2	C	322	ILE
2	C	326	THR
2	C	355	VAL
2	C	357	VAL
2	C	404	GLU
2	C	514	VAL
2	C	610	VAL
2	C	620	VAL
2	C	635	VAL
2	C	647	VAL
2	C	696	ILE
2	C	740	VAL
2	C	770	ILE
2	C	811	GLU
2	C	863	VAL
2	C	869	GLN

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Mol	Chain	Res	Type
2	C	965	ILE
2	C	966	VAL
2	C	1131	VAL
3	D	4	VAL
3	D	34	ILE
3	D	68	VAL
3	D	82	VAL
3	D	110	VAL
3	D	117	LEU
3	D	125	LEU
3	D	236	VAL
3	D	250	GLU
3	D	281	ILE
3	D	409	LYS
3	D	432	VAL
3	D	436	LEU
3	D	467	GLN
3	D	576	MET
3	D	588	LEU
3	D	632	LYS
3	D	645	GLU
3	D	674	ASN
3	D	693	GLN
3	D	743	LYS
3	D	825	THR
3	D	860	LEU
3	D	891	CYS
3	D	897	ILE
3	D	901	LEU
3	D	938	VAL
3	D	1039	VAL
3	D	1130	VAL
3	D	1191	ARG
3	D	1193	VAL
3	D	1206	VAL
3	D	1246	ASN
4	E	34	ILE
4	E	39	ILE
4	E	46	VAL
4	E	82	VAL
5	F	28	ARG
5	F	37	LEU

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Mol	Chain	Res	Type
5	F	83	TYR
5	F	143	GLU
5	F	179	THR
5	F	181	MET

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

Mol	Chain	Res	Type
1	A	200	ASN
1	B	124	HIS
2	C	194	HIS
2	C	409	GLN
2	C	656	HIS
2	C	835	HIS
2	C	961	GLN
2	C	1049	GLN
2	C	1155	ASN
3	D	499	ASN
3	D	505	HIS
3	D	563	ASN
3	D	767	HIS
3	D	854	HIS
3	D	1133	HIS
4	E	68	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	8/9 (88%)	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 [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	218/368 (59%)	-0.44	0	100	100	75, 107, 150, 192	0
1	B	227/368 (61%)	-0.26	1 (0%)	88	79	116, 158, 181, 191	0
2	C	1138/1174 (96%)	-0.31	5 (0%)	88	79	68, 103, 172, 200	0
3	D	1263/1317 (95%)	-0.35	3 (0%)	91	86	74, 115, 182, 215	0
4	E	75/110 (68%)	-0.21	0	100	100	120, 143, 166, 172	0
5	F	159/218 (72%)	-0.24	0	100	100	101, 151, 174, 197	2 (1%)
6	G	23/23 (100%)	-0.40	0	100	100	112, 135, 180, 190	3 (13%)
7	H	21/21 (100%)	-0.75	0	100	100	76, 91, 167, 177	0
8	I	9/9 (100%)	-0.91	0	100	100	71, 79, 130, 133	0
All	All	3133/3608 (86%)	-0.33	9 (0%)	90	82	68, 117, 176, 215	5 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	231	LEU	2.7
2	C	1121	GLU	2.6
3	D	296	LEU	2.5
3	D	394	PRO	2.3
2	C	335	THR	2.3
1	B	164	VAL	2.2
2	C	211	ASP	2.1
3	D	1026	GLY	2.0
2	C	1056	GLN	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	0.95	0.07	81,81,81,81	0
9	ZN	D	2002	1/1	0.97	0.04	150,150,150,150	0
9	ZN	D	2001	1/1	0.99	0.02	117,117,117,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.