



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:14 PM BST

PDB ID : 6KOO
Title : Mycobacterium tuberculosis initial transcription complex comprising sigma H and 5'-OH RNA of 7 nt
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-08-12
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

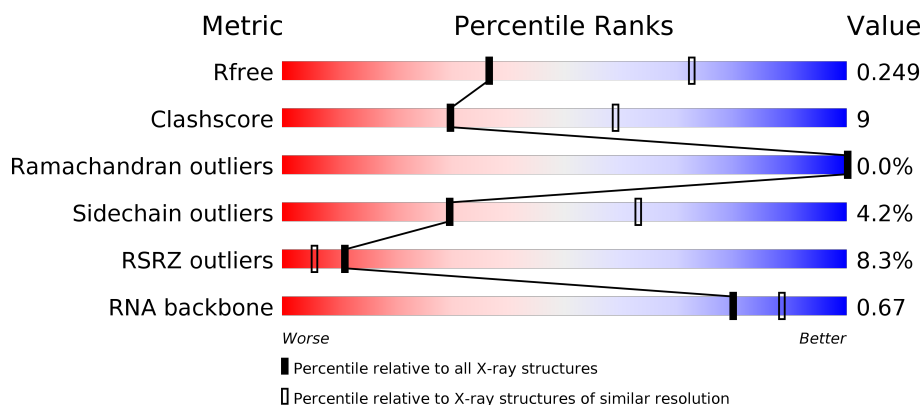
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

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

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24837 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
			1646	1035	285	324	2			
1	B	230	Total	C	N	O	S	0	0	0
			1670	1057	283	328	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

Continued on next page...

Continued from previous page...

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	1135	Total	C	N	O	S	0	0	0
			8673	5428	1519	1687	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
			9763	6118	1766	1838	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
			592	378	99	115			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	182	Total	C	N	O	S	0	0	0
			1432	896	251	280	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*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	20	Total	C	N	O	P	0	0	0
			412	196	77	120	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	P	0	0	0
			142	65	24	47	6			

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

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

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

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

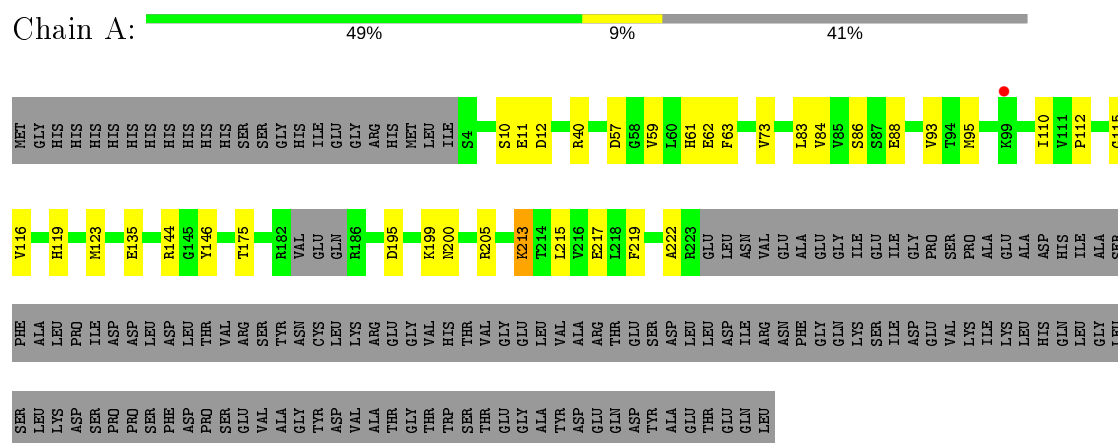
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	8	Total 8	O 8	0	0
11	D	12	Total 12	O 12	0	0
11	F	4	Total 4	O 4	0	0
11	H	3	Total 3	O 3	0	0
11	I	2	Total 2	O 2	0	0

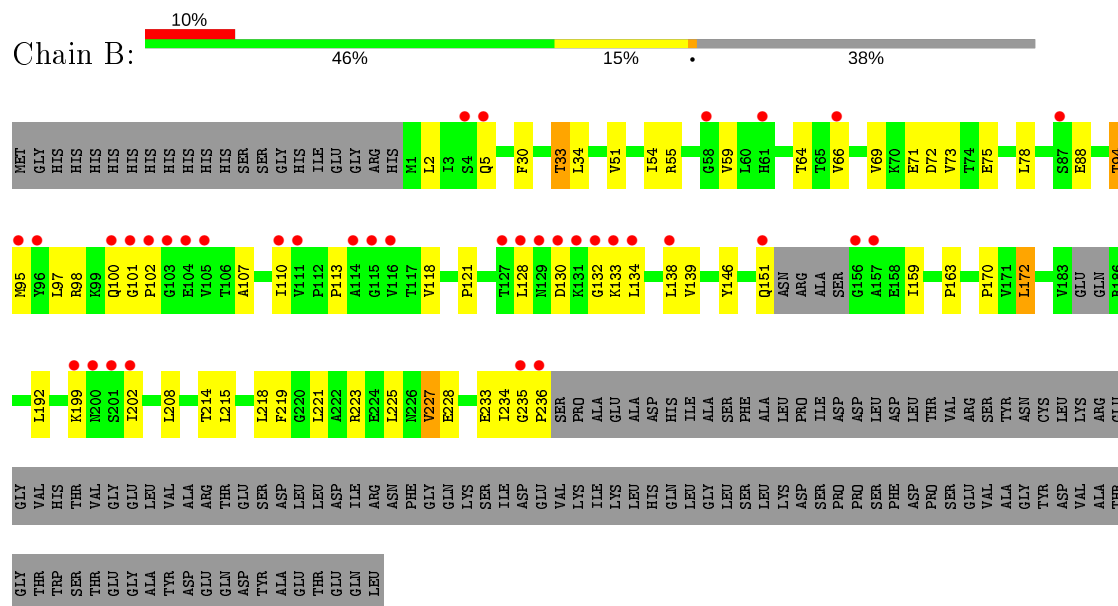
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit alpha

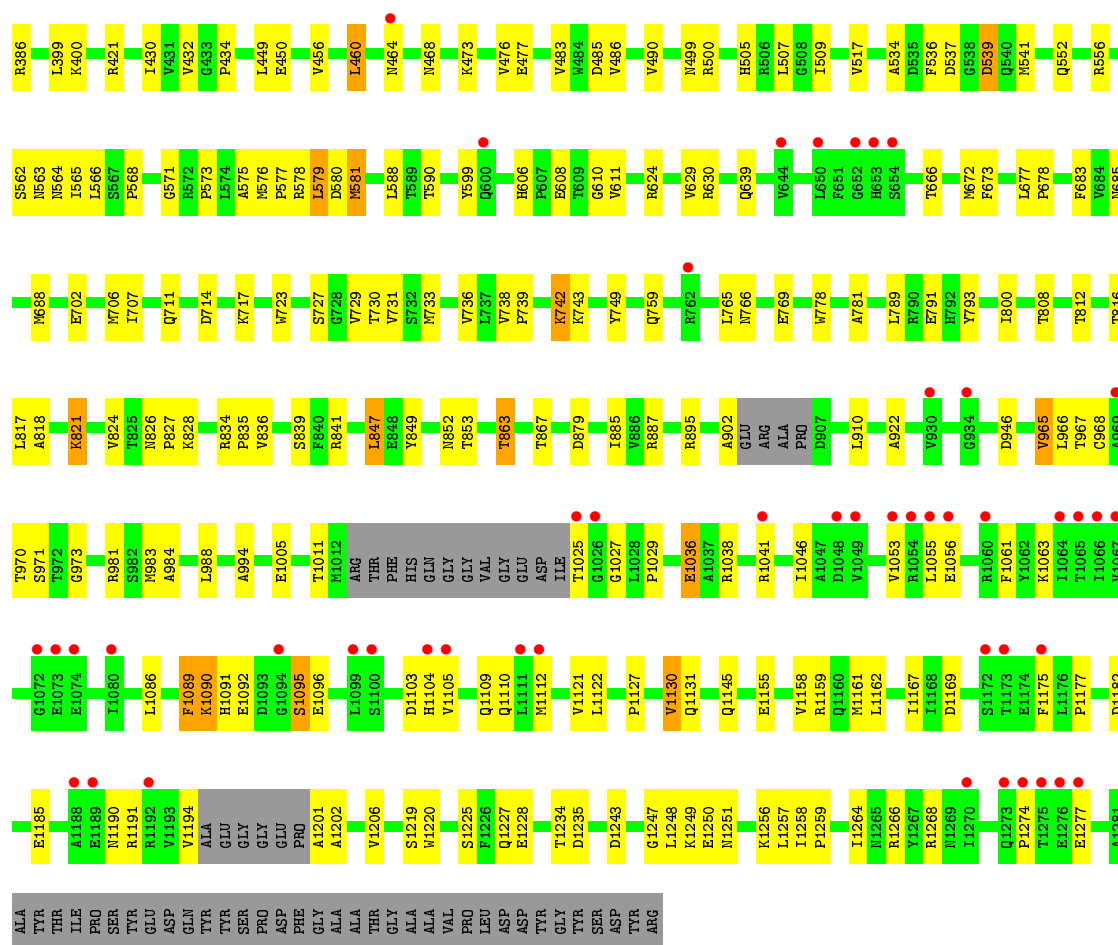


• Molecule 1: DNA-directed RNA polymerase subunit alpha

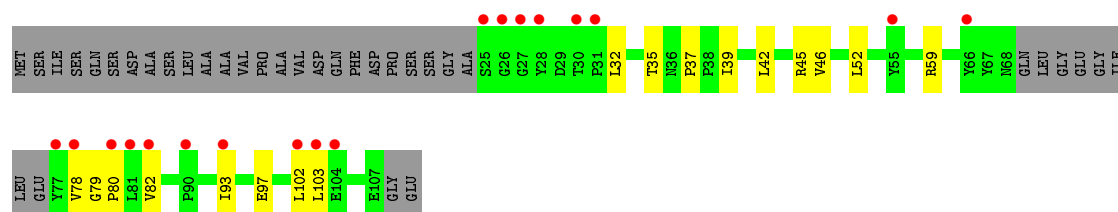


• Molecule 2: DNA-directed RNA polymerase subunit beta

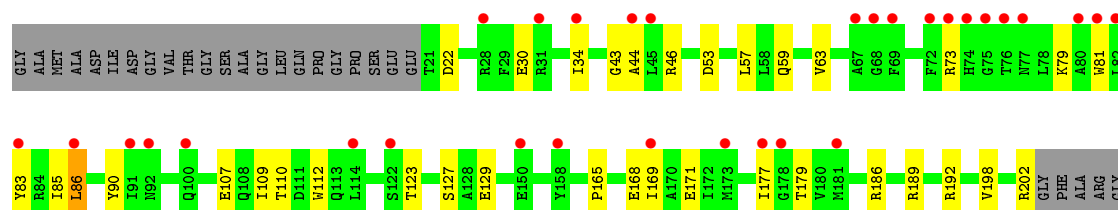




• Molecule 4: DNA-directed RNA polymerase subunit omega

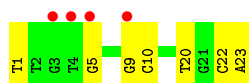


• Molecule 5: ECF RNA polymerase sigma factor SigH



GLU	GLN	ALA	HIS	GLU	GLY	VAL	SER
-----	-----	-----	-----	-----	-----	-----	-----

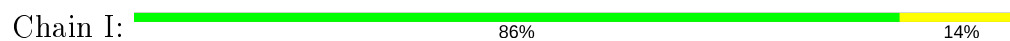
- Molecule 6: DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3')



- 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(*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	125.03Å 162.31Å 128.48Å 90.00° 117.03° 90.00°	Depositor
Resolution (Å)	31.38 – 2.80 48.67 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.9 (31.38-2.80) 97.1 (48.67-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.206 , 0.248 0.207 , 0.249	Depositor DCC
R_{free} test set	2398 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24837	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.32	0/1671	0.54	0/2273
1	B	0.32	0/1695	0.51	0/2314
2	C	0.35	0/8830	0.51	1/11988 (0.0%)
3	D	0.33	0/9923	0.50	0/13425
4	E	0.27	0/604	0.48	0/822
5	F	0.29	0/1460	0.43	0/1983
6	G	0.65	0/533	0.92	0/823
7	H	0.67	0/462	0.81	0/713
8	I	0.48	0/157	1.07	0/242
All	All	0.35	0/25335	0.53	1/34583 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	75	ASN	C-N-CD	5.77	140.51	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1646	0	1676	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1670	0	1651	43	0
2	C	8673	0	8508	177	0
3	D	9763	0	9772	195	0
4	E	592	0	587	11	0
5	F	1432	0	1359	22	0
6	G	475	0	261	6	0
7	H	412	0	227	22	0
8	I	142	0	78	1	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	C	8	0	0	0	0
11	D	12	0	0	0	0
11	F	4	0	0	0	0
11	H	3	0	0	0	0
11	I	2	0	0	0	0
All	All	24837	0	24119	458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (458) 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)
7:H:14:DC:H2'	7:H:15:DG:H5''	1.20	1.11
7:H:14:DC:C2'	7:H:15:DG:H5''	1.96	0.95
3:D:1090:LYS:HG3	3:D:1095:SER:O	1.75	0.87
3:D:1090:LYS:HG3	3:D:1095:SER:C	1.96	0.86
7:H:19:DG:C2'	7:H:20:DT:H5'	2.06	0.86
1:A:40:ARG:HE	1:B:33:THR:HG22	1.43	0.83
2:C:557:ARG:H	2:C:561:GLU:HB3	1.45	0.81
7:H:12:DG:H2''	7:H:13:DT:H5'	1.60	0.80
2:C:537:GLN:HG3	3:D:847:LEU:HD11	1.65	0.79
3:D:1090:LYS:CD	3:D:1091:HIS:H	1.96	0.79
4:E:59:ARG:HH22	4:E:79:GLY:HA3	1.47	0.79
2:C:1040:THR:HG22	5:F:127:SER:HB2	1.64	0.78
2:C:553:VAL:O	2:C:564:TYR:HA	1.83	0.78
7:H:16:DA:C2'	7:H:17:DG:H5'	2.15	0.77
3:D:1090:LYS:HD3	3:D:1091:HIS:H	1.50	0.76
3:D:92:MET:HG3	3:D:321:PRO:HD3	1.68	0.75
1:B:151:GLN:HG2	1:B:163:PRO:HG2	1.69	0.75
3:D:113:ARG:NH1	3:D:1235:ASP:OD1	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1090:LYS:CB	3:D:1096:GLU:HA	2.20	0.72
7:H:16:DA:H2''	7:H:17:DG:H5'	1.73	0.71
3:D:47:PHE:O	3:D:88:ARG:NH2	2.24	0.71
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.56	0.70
3:D:1089:PHE:HD1	3:D:1089:PHE:H	1.38	0.70
1:B:69:VAL:HG12	1:B:71:GLU:H	1.56	0.70
2:C:44:VAL:O	2:C:627:ARG:NH2	2.25	0.69
2:C:103:ASP:O	2:C:129:VAL:HA	1.93	0.69
2:C:56:GLU:OE1	2:C:63:ARG:HD3	1.93	0.69
1:B:30:PHE:HA	1:B:33:THR:HG23	1.73	0.69
7:H:19:DG:H2'	7:H:20:DT:H5'	1.74	0.69
2:C:144:GLN:HE22	2:C:409:GLN:HB2	1.57	0.68
2:C:745:HIS:HD2	2:C:871:ARG:HG3	1.57	0.68
2:C:1047:THR:HG23	2:C:1049:GLN:H	1.58	0.68
7:H:19:DG:H2''	7:H:20:DT:H5'	1.76	0.68
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.75	0.68
3:D:539:ASP:CG	8:I:10:A:O3'	2.33	0.68
2:C:803:LYS:O	3:D:56:ARG:NH2	2.28	0.67
2:C:913:THR:HG23	3:D:731:VAL:HG23	1.75	0.67
3:D:885:ILE:HG13	3:D:887:ARG:HD3	1.75	0.67
2:C:1062:PHE:HZ	2:C:1070:MET:HE2	1.59	0.66
1:B:64:THR:HA	1:B:73:VAL:HB	1.78	0.66
2:C:67:SER:O	2:C:71:ARG:HD3	1.96	0.66
4:E:46:VAL:HG21	4:E:52:LEU:HB2	1.77	0.66
2:C:542:ILE:HG23	2:C:547:ARG:H	1.59	0.66
1:B:97:LEU:HD13	1:B:110:ILE:HG22	1.79	0.65
3:D:365:ILE:HD12	5:F:34:ILE:HD13	1.77	0.65
1:A:83:LEU:HD13	1:A:123:MET:HE1	1.78	0.65
3:D:1247:GLY:HA3	3:D:1250:GLU:OE1	1.97	0.64
2:C:1040:THR:HG21	5:F:129:GLU:H	1.63	0.64
1:A:93:VAL:HG11	1:A:116:VAL:HG11	1.80	0.64
2:C:114:ASP:N	2:C:114:ASP:OD1	2.27	0.64
2:C:341:ARG:HD2	2:C:349:MET:HG3	1.78	0.64
3:D:1219:SER:CB	3:D:1250:GLU:OE2	2.45	0.64
2:C:1087:SER:HB3	3:D:421:ARG:O	1.98	0.63
7:H:3:DC:H2''	7:H:4:DA:N7	2.14	0.63
3:D:1090:LYS:HD3	3:D:1091:HIS:N	2.14	0.62
1:A:63:PHE:CD1	2:C:842:ILE:HD11	2.34	0.62
7:H:9:DT:H2'	7:H:10:DG:C8	2.34	0.62
5:F:186:ARG:HA	5:F:189:ARG:HD2	1.81	0.62
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:351:VAL:HG23	2:C:354:GLY:HA3	1.81	0.62
2:C:36:ALA:HB2	2:C:969:PRO:HG2	1.82	0.62
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.81	0.62
1:B:98:ARG:HA	1:B:134:LEU:O	1.99	0.61
2:C:1035:ILE:O	2:C:1054:LYS:NZ	2.30	0.61
2:C:1130:GLU:OE1	3:D:11:ARG:NH2	2.24	0.61
3:D:981:ARG:HA	3:D:988:LEU:HA	1.83	0.61
3:D:59:GLU:HG2	3:D:66:LYS:HG3	1.82	0.61
3:D:1011:THR:O	3:D:1145:GLN:NE2	2.32	0.60
3:D:1092:GLU:OE2	3:D:1104:HIS:ND1	2.34	0.60
3:D:97:LEU:HD22	3:D:374:LEU:HD21	1.83	0.60
5:F:110:THR:HG22	5:F:112:TRP:H	1.66	0.60
2:C:407:THR:HG23	2:C:409:GLN:H	1.66	0.60
7:H:12:DG:C2'	7:H:13:DT:H5'	2.30	0.60
1:B:228:GLU:HA	1:B:228:GLU:OE1	2.02	0.60
1:A:40:ARG:NE	1:B:33:THR:HG22	2.16	0.60
3:D:629:VAL:HG12	3:D:630:ARG:HG3	1.82	0.60
2:C:1098:GLU:HG2	2:C:1102:LYS:HE2	1.82	0.59
2:C:678:ALA:HA	2:C:700:PRO:HG3	1.83	0.59
1:A:213:LYS:HD2	1:B:223:ARG:HD2	1.83	0.59
2:C:848:SER:O	2:C:853:ASP:HB2	2.03	0.59
2:C:968:THR:HG23	2:C:974:ALA:H	1.68	0.59
3:D:1248:LEU:HD12	3:D:1249:LYS:N	2.18	0.58
2:C:536:ALA:HA	2:C:555:VAL:HG12	1.86	0.58
2:C:895:VAL:HG13	2:C:906:PRO:HG2	1.86	0.58
2:C:444:THR:OG1	2:C:607:ARG:HD2	2.03	0.58
1:A:57:ASP:HB2	1:A:135:GLU:HB3	1.86	0.57
7:H:19:DG:H2''	7:H:20:DT:C5'	2.33	0.57
2:C:337:GLU:OE2	2:C:341:ARG:NH2	2.36	0.57
3:D:847:LEU:H	3:D:847:LEU:HD12	1.68	0.57
2:C:926:LEU:HD22	3:D:733:MET:HE3	1.85	0.57
1:A:86:SER:OG	1:A:119:HIS:NE2	2.31	0.57
3:D:1055:LEU:HD11	3:D:1086:LEU:HD21	1.87	0.57
2:C:134:ILE:HG12	2:C:141:ILE:HG12	1.87	0.57
2:C:383:ILE:HG12	2:C:421:ILE:HD11	1.85	0.57
3:D:21:ARG:NE	3:D:96:GLU:OE2	2.29	0.57
3:D:1167:ILE:HG22	3:D:1177:PRO:HA	1.87	0.56
2:C:382:GLN:HG2	2:C:424:PHE:HB2	1.87	0.56
2:C:776:ALA:O	2:C:785:ARG:NH2	2.37	0.56
3:D:339:ASP:HB3	3:D:399:LEU:HB3	1.87	0.56
2:C:407:THR:HG22	2:C:410:THR:HG23	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLN:HA	1:B:233:GLU:HG3	1.87	0.56
2:C:856:PRO:HG2	2:C:859:VAL:HG21	1.87	0.56
2:C:32:ARG:HA	2:C:965:ILE:HG22	1.88	0.56
2:C:714:LEU:HD23	2:C:907:VAL:HA	1.87	0.56
4:E:37:PRO:HG2	4:E:42:LEU:HD11	1.88	0.56
3:D:1227:GLN:HG2	3:D:1228:GLU:HG3	1.87	0.56
2:C:1129:VAL:HG22	3:D:12:ILE:HG23	1.87	0.56
2:C:626:LEU:HB2	2:C:706:GLU:HG2	1.89	0.55
3:D:1182:ASP:HB3	3:D:1185:GLU:HG2	1.87	0.55
3:D:1219:SER:HB2	3:D:1250:GLU:OE2	2.06	0.55
2:C:581:VAL:HG13	2:C:585:THR:HB	1.87	0.55
2:C:735:LEU:HA	2:C:740:VAL:HG13	1.87	0.55
3:D:1089:PHE:N	3:D:1089:PHE:CD1	2.72	0.55
1:B:55:ARG:NH2	1:B:159:ILE:O	2.34	0.55
2:C:233:LYS:HZ3	2:C:262:VAL:HA	1.70	0.55
2:C:652:ILE:HD13	2:C:696:ILE:HG22	1.89	0.55
1:B:218:LEU:O	1:B:221:LEU:HB2	2.06	0.55
1:B:5:GLN:CB	1:B:234:ILE:H	2.20	0.55
3:D:86:LYS:O	3:D:89:ARG:HG2	2.06	0.55
2:C:133:PHE:CZ	2:C:406:ILE:HD11	2.42	0.55
2:C:593:HIS:HB3	2:C:922:ILE:HD12	1.89	0.55
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.72	0.55
3:D:879:ASP:OD1	3:D:1249:LYS:NZ	2.39	0.55
3:D:12:ILE:HD11	3:D:1220:TRP:CE3	2.42	0.55
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.89	0.55
2:C:541:PRO:HG2	2:C:550:GLU:HB2	1.90	0.54
7:H:3:DC:H2"	7:H:4:DA:C8	2.41	0.54
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.89	0.54
2:C:557:ARG:N	2:C:561:GLU:HB3	2.21	0.54
2:C:90:ILE:HD13	2:C:391:GLU:HG3	1.89	0.54
2:C:109:VAL:HG11	2:C:123:TYR:CE1	2.42	0.54
3:D:1190:ASN:HD21	3:D:1201:ALA:HB1	1.73	0.54
1:A:95:MET:HE2	1:A:112:PRO:HB3	1.89	0.54
3:D:1027:GLY:H	3:D:1029:PRO:HD2	1.73	0.53
1:B:54:ILE:HG22	1:B:138:LEU:HG	1.89	0.53
2:C:510:TYR:HB3	2:C:572:TYR:HB3	1.90	0.53
3:D:62:CYS:N	3:D:78:CYS:SG	2.81	0.53
1:B:34:LEU:HD12	1:B:192:LEU:HD22	1.90	0.53
2:C:1046:ILE:HD12	2:C:1046:ILE:H	1.74	0.53
1:B:59:VAL:HG11	1:B:66:VAL:HG22	1.91	0.53
5:F:110:THR:HG22	5:F:112:TRP:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:750:GLU:OE1	2:C:864:ARG:NH1	2.42	0.53
2:C:961:GLN:HG3	2:C:962:PRO:HD2	1.89	0.53
3:D:12:ILE:HD11	3:D:1220:TRP:CZ3	2.44	0.53
2:C:736:VAL:HG13	2:C:872:LYS:HD2	1.91	0.53
2:C:893:LEU:HB2	2:C:898:MET:HE1	1.90	0.53
2:C:97:MET:HB2	2:C:133:PHE:HE1	1.74	0.52
2:C:364:ILE:HD12	2:C:364:ILE:H	1.74	0.52
3:D:1090:LYS:HD2	3:D:1091:HIS:H	1.70	0.52
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.90	0.52
2:C:217:GLY:HA3	2:C:225:ARG:HD2	1.92	0.52
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.91	0.52
2:C:68:ALA:HA	2:C:71:ARG:HD3	1.92	0.52
5:F:30:GLU:HA	5:F:34:ILE:HD12	1.92	0.52
3:D:155:MET:HE1	3:D:219:LEU:HD22	1.91	0.52
3:D:116:TYR:O	3:D:295:ARG:NH1	2.43	0.51
1:A:217:GLU:HG2	1:B:233:GLU:OE1	2.10	0.51
2:C:842:ILE:HG12	2:C:868:ALA:HB2	1.92	0.51
4:E:80:PRO:HB3	4:E:93:ILE:HG21	1.91	0.51
2:C:181:PHE:CD2	2:C:196:VAL:HB	2.46	0.51
2:C:723:HIS:CD2	2:C:891:LYS:HD2	2.46	0.51
1:B:95:MET:HG2	1:B:113:PRO:HD2	1.91	0.51
2:C:481:GLU:OE2	2:C:607:ARG:NH2	2.41	0.51
2:C:786:ILE:HG13	2:C:844:ILE:HD12	1.92	0.51
7:H:2:DG:H2''	7:H:3:DC:O5'	2.11	0.51
3:D:1025:THR:HA	3:D:1041:ARG:HD2	1.93	0.51
3:D:1248:LEU:HA	3:D:1259:PRO:HD2	1.92	0.51
2:C:724:ASN:HB3	2:C:730:ILE:HG13	1.92	0.51
3:D:1090:LYS:HB2	3:D:1096:GLU:HA	1.91	0.51
2:C:955:ASP:OD1	2:C:955:ASP:N	2.43	0.50
3:D:1225:SER:OG	3:D:1249:LYS:HE3	2.10	0.50
3:D:226:PHE:CE1	3:D:248:TYR:HB3	2.46	0.50
3:D:430:ILE:HD11	3:D:539:ASP:HB2	1.94	0.50
3:D:702:GLU:HG3	3:D:946:ASP:HB2	1.93	0.50
2:C:80:LEU:HD21	2:C:383:ILE:HD13	1.94	0.50
3:D:1056:GLU:HB2	3:D:1063:LYS:HB3	1.93	0.50
3:D:1219:SER:OG	3:D:1250:GLU:OE2	2.30	0.50
2:C:186:ASP:N	2:C:191:LYS:O	2.43	0.50
3:D:331:ASP:OD1	3:D:331:ASP:N	2.44	0.50
3:D:184:LEU:HD11	3:D:197:VAL:HG21	1.94	0.49
3:D:666:THR:HG21	3:D:683:PHE:CE1	2.47	0.49
2:C:626:LEU:HA	2:C:706:GLU:HA	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:32:LEU:O	4:E:35:THR:HG22	2.12	0.49
2:C:305:VAL:HG12	2:C:503:PHE:HB3	1.92	0.49
3:D:67:ARG:HH12	3:D:69:ARG:HH21	1.59	0.49
3:D:565:ILE:H	3:D:706:MET:HE1	1.76	0.49
2:C:252:MET:HA	2:C:255:THR:HG22	1.94	0.49
2:C:898:MET:HG2	2:C:907:VAL:O	2.12	0.49
2:C:1133:SER:OG	2:C:1134:SER:N	2.45	0.49
2:C:511:ARG:HD3	2:C:573:MET:HE2	1.95	0.49
2:C:893:LEU:HB2	2:C:898:MET:CE	2.43	0.49
3:D:973:GLY:O	3:D:1159:ARG:NH2	2.45	0.49
3:D:562:SER:HA	3:D:565:ILE:HD11	1.94	0.49
4:E:82:VAL:HG22	4:E:102:LEU:HD22	1.93	0.49
2:C:157:LYS:HD2	2:C:633:GLY:HA3	1.95	0.49
7:H:18:DG:H2'	7:H:19:DG:H5''	1.95	0.49
6:G:9:DG:H2'	6:G:10:DC:O4'	2.13	0.49
1:B:94:THR:O	1:B:113:PRO:HG3	2.11	0.49
3:D:173:ARG:NE	3:D:204:GLU:OE2	2.41	0.49
3:D:499:ASN:HB2	3:D:509:ILE:HG12	1.95	0.49
5:F:43:GLY:HA2	5:F:46:ARG:HD3	1.95	0.49
2:C:107:ASP:HB3	2:C:126:PRO:HD2	1.94	0.48
1:A:84:VAL:HG13	1:A:119:HIS:HB2	1.96	0.48
1:B:146:TYR:O	3:D:624:ARG:NE	2.46	0.48
2:C:803:LYS:HG2	2:C:807:GLU:HB2	1.95	0.48
2:C:1146:ASP:OD1	3:D:71:LYS:NZ	2.40	0.48
3:D:1053:VAL:HG12	3:D:1103:ASP:O	2.13	0.48
2:C:922:ILE:HG12	3:D:817:LEU:HD11	1.95	0.48
3:D:812:THR:O	3:D:816:THR:HG23	2.14	0.48
3:D:922:ALA:HA	3:D:981:ARG:HD3	1.95	0.48
2:C:1089:ASP:OD2	2:C:1110:GLY:N	2.46	0.48
2:C:1148:ASP:N	2:C:1148:ASP:OD1	2.47	0.48
3:D:1257:LEU:HD12	3:D:1268:ARG:HE	1.78	0.48
3:D:966:LEU:HD22	3:D:1131:GLN:HB3	1.96	0.48
2:C:135:ASN:O	2:C:139:GLY:N	2.47	0.48
2:C:219:ARG:HG3	2:C:223:LYS:O	2.14	0.48
2:C:874:SER:N	2:C:877:ASP:OD2	2.47	0.47
1:B:102:PRO:HA	1:B:128:LEU:O	2.13	0.47
3:D:78:CYS:HB3	3:D:80:VAL:HG23	1.95	0.47
3:D:67:ARG:NH1	3:D:69:ARG:HH21	2.12	0.47
3:D:337:THR:HG22	3:D:341:ASN:HD22	1.80	0.47
3:D:563:ASN:ND2	4:E:39:ILE:HD12	2.29	0.47
3:D:759:GLN:HG2	3:D:765:LEU:HG	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:793:TYR:HB3	3:D:800:ILE:HG13	1.97	0.47
2:C:576:SER:OG	2:C:577:PRO:O	2.30	0.47
2:C:786:ILE:HD12	2:C:786:ILE:H	1.79	0.47
3:D:1248:LEU:C	3:D:1248:LEU:HD12	2.34	0.47
3:D:885:ILE:HG22	3:D:994:ALA:HA	1.97	0.47
1:B:100:GLN:HA	1:B:133:LYS:HA	1.95	0.47
2:C:1039:SER:HB3	3:D:450:GLU:O	2.15	0.47
2:C:778:LEU:HD12	2:C:784:VAL:HA	1.96	0.47
1:B:102:PRO:HD3	1:B:130:ASP:HA	1.96	0.47
1:B:172:LEU:HD13	1:B:199:LYS:HG3	1.97	0.47
2:C:899:PRO:HB3	2:C:1013:PHE:HE2	1.80	0.47
2:C:593:HIS:HB3	2:C:922:ILE:CD1	2.45	0.47
2:C:888:VAL:HG22	3:D:536:PHE:O	2.14	0.47
7:H:16:DA:N6	7:H:17:DG:O6	2.48	0.47
2:C:71:ARG:HH11	2:C:71:ARG:HG2	1.79	0.47
1:A:219:PHE:CE1	1:B:215:LEU:HD13	2.50	0.46
3:D:1131:GLN:HG3	3:D:1162:LEU:HD12	1.97	0.46
3:D:1264:ILE:HG22	3:D:1266:ARG:H	1.80	0.46
3:D:460:LEU:HD21	3:D:483:VAL:HG12	1.97	0.46
3:D:568:PRO:HB3	3:D:984:ALA:HB2	1.97	0.46
3:D:577:PRO:HB3	3:D:581:MET:HB3	1.97	0.46
3:D:588:LEU:HD13	3:D:723:TRP:CE2	2.51	0.46
3:D:902:ALA:HB1	3:D:910:LEU:HB2	1.97	0.46
2:C:196:VAL:HG13	2:C:208:PHE:HB2	1.97	0.46
2:C:198:VAL:HB	2:C:206:LEU:HB3	1.96	0.46
3:D:400:LYS:HG3	5:F:107:GLU:HG3	1.97	0.46
3:D:863:THR:O	3:D:867:THR:HG22	2.16	0.46
2:C:302:LEU:O	2:C:325:SER:HB2	2.16	0.46
2:C:577:PRO:O	2:C:578:ARG:HG2	2.15	0.46
2:C:647:VAL:HG21	2:C:684:VAL:HG23	1.98	0.46
5:F:198:VAL:O	5:F:202:ARG:N	2.44	0.46
2:C:337:GLU:HA	2:C:340:VAL:HG22	1.98	0.46
2:C:86:GLU:OE1	2:C:384:ARG:NH2	2.49	0.46
3:D:1090:LYS:CD	3:D:1091:HIS:N	2.72	0.46
3:D:468:ASN:N	3:D:468:ASN:OD1	2.48	0.46
2:C:205:TRP:CH2	6:G:10:DC:H2'	2.51	0.46
1:B:72:ASP:OD1	1:B:73:VAL:N	2.48	0.46
3:D:1167:ILE:HD13	3:D:1175:PHE:HB3	1.98	0.46
3:D:73:ILE:O	3:D:82:VAL:HG12	2.16	0.46
5:F:44:ALA:HB2	5:F:86:LEU:HD11	1.98	0.46
2:C:577:PRO:C	2:C:579:GLN:H	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:571:GLY:HA2	3:D:983:MET:O	2.16	0.46
2:C:435:ASP:HA	2:C:674:HIS:NE2	2.31	0.46
3:D:1110:GLN:NE2	3:D:1112:MET:O	2.36	0.46
3:D:346:ARG:NH2	5:F:53:ASP:OD1	2.40	0.46
1:B:110:ILE:HD11	1:B:118:VAL:HG21	1.98	0.45
1:B:51:VAL:HA	1:B:139:VAL:O	2.16	0.45
2:C:144:GLN:NE2	2:C:409:GLN:HB2	2.28	0.45
3:D:666:THR:HG22	3:D:685:ASN:OD1	2.15	0.45
3:D:507:LEU:HD11	3:D:564:ASN:HB3	1.98	0.45
3:D:500:ARG:HD2	3:D:534:ALA:HB2	1.98	0.45
7:H:16:DA:C6	7:H:17:DG:C6	3.04	0.45
1:B:235:GLY:HA2	1:B:236:PRO:HD3	1.83	0.45
2:C:390:MET:HG3	2:C:413:ASN:O	2.17	0.45
2:C:611:PRO:HD2	2:C:676:THR:HB	1.99	0.45
3:D:579:LEU:HD23	3:D:808:THR:HB	1.98	0.45
7:H:19:DG:H5"	7:H:19:DG:H8	1.82	0.45
3:D:1127:PRO:HA	3:D:1130:VAL:HG23	1.97	0.45
2:C:346:GLN:O	2:C:359:VAL:HB	2.16	0.45
3:D:1248:LEU:HB2	3:D:1258:ILE:HB	1.99	0.45
3:D:67:ARG:HG3	3:D:69:ARG:H	1.80	0.45
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.39	0.45
3:D:599:TYR:CE1	3:D:608:GLU:HB2	2.52	0.45
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.52	0.45
2:C:226:GLN:HG3	2:C:274:LYS:HD3	1.99	0.45
2:C:317:HIS:HB3	2:C:321:PRO:HG2	1.98	0.45
2:C:318:VAL:HG21	2:C:355:VAL:HG21	1.98	0.45
2:C:168:VAL:HG23	2:C:434:MET:HB2	1.99	0.45
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.52	0.45
3:D:566:LEU:HA	3:D:573:PRO:HA	1.98	0.45
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.99	0.45
3:D:749:TYR:CG	3:D:781:ALA:HB2	2.52	0.45
4:E:59:ARG:NH2	4:E:79:GLY:HA3	2.22	0.45
3:D:766:ASN:HB3	3:D:769:GLU:HG3	1.99	0.45
1:A:215:LEU:HD13	1:B:219:PHE:CE1	2.52	0.44
3:D:105:TRP:HB3	3:D:1234:THR:HG22	1.98	0.44
3:D:369:ASN:OD1	3:D:372:ARG:NH2	2.50	0.44
2:C:543:ASP:OD1	2:C:543:ASP:N	2.49	0.44
3:D:707:ILE:O	3:D:711:GLN:HG3	2.17	0.44
3:D:727:SER:OG	3:D:729:VAL:HG22	2.18	0.44
2:C:621:GLY:O	2:C:967:SER:HA	2.18	0.44
3:D:565:ILE:HG23	3:D:575:ALA:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1274:PRO:HA	4:E:103:LEU:HA	1.99	0.44
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.99	0.44
2:C:246:PHE:HB3	2:C:252:MET:HG3	1.98	0.44
3:D:155:MET:HE2	3:D:219:LEU:HB3	1.97	0.44
1:A:205:ARG:HG3	1:B:225:LEU:HD13	2.00	0.44
2:C:1017:VAL:HA	3:D:730:THR:HG21	2.00	0.44
5:F:168:GLU:O	5:F:171:GLU:HG2	2.18	0.44
2:C:1081:GLU:HG3	2:C:1085:ILE:HD11	1.99	0.44
2:C:526:THR:HG22	2:C:529:GLU:OE2	2.16	0.44
3:D:1105:VAL:HG13	3:D:1109:GLN:HB3	2.00	0.44
3:D:677:LEU:HB3	3:D:678:PRO:HD2	1.99	0.44
2:C:715:VAL:HG23	2:C:909:ILE:HG23	1.99	0.44
3:D:278:ARG:O	3:D:281:ILE:HG13	2.17	0.44
3:D:57:ASP:HB3	3:D:58:TRP:CD1	2.53	0.44
7:H:13:DT:H2'	7:H:14:DC:C6	2.53	0.44
1:B:170:PRO:HB2	1:B:202:ILE:HD11	2.00	0.44
2:C:200:PRO:HG3	2:C:300:TYR:CE2	2.53	0.44
2:C:950:ALA:O	2:C:954:PRO:HD2	2.18	0.44
3:D:159:ARG:HH12	3:D:220:GLU:HB2	1.83	0.44
1:A:144:ARG:NH1	1:B:2:LEU:O	2.50	0.43
2:C:351:VAL:H	2:C:354:GLY:HA3	1.83	0.43
3:D:460:LEU:HD12	3:D:486:VAL:HG21	2.00	0.43
5:F:81:TRP:NE1	6:G:1:DT:H2'	2.32	0.43
1:A:11:GLU:HG2	1:A:12:ASP:N	2.34	0.43
2:C:211:ASP:OD1	2:C:211:ASP:N	2.51	0.43
3:D:895:ARG:HB2	3:D:967:THR:HB	2.00	0.43
1:A:112:PRO:HB2	1:A:116:VAL:HG22	1.99	0.43
1:A:110:ILE:O	1:A:112:PRO:HD3	2.18	0.43
1:A:146:TYR:CD2	2:C:737:GLU:HG2	2.54	0.43
2:C:120:ASP:HA	2:C:164:GLY:HA3	1.99	0.43
2:C:196:VAL:CG1	2:C:208:PHE:HB2	2.48	0.43
3:D:500:ARG:HB2	3:D:541:MET:HG2	2.01	0.43
3:D:61:TYR:HB3	3:D:78:CYS:SG	2.58	0.43
4:E:97:GLU:HB3	4:E:103:LEU:HD22	2.00	0.43
5:F:177:ILE:H	5:F:177:ILE:HD12	1.82	0.43
5:F:59:GLN:O	5:F:63:VAL:HG23	2.18	0.43
5:F:79:LYS:HE2	6:G:5:DG:C8	2.53	0.43
1:B:107:ALA:HB3	1:B:121:PRO:HA	2.01	0.43
2:C:542:ILE:HG22	2:C:543:ASP:O	2.19	0.43
2:C:886:LYS:HE3	3:D:537:ASP:HB2	2.01	0.43
2:C:36:ALA:HA	2:C:972:ASP:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:588:LEU:HD11	3:D:672:MET:HE3	2.00	0.43
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.99	0.43
2:C:1098:GLU:OE2	2:C:1151:ARG:NH2	2.52	0.43
3:D:1251:ASN:OD1	3:D:1256:LYS:HD2	2.18	0.43
2:C:481:GLU:OE2	2:C:607:ARG:HD3	2.18	0.43
3:D:325:ARG:HD2	3:D:341:ASN:OD1	2.18	0.43
3:D:968:CYS:SG	3:D:970:THR:HG23	2.59	0.43
2:C:1111:ILE:HD13	3:D:3:ASP:HB2	2.00	0.43
2:C:288:THR:O	2:C:291:GLU:HG2	2.18	0.43
2:C:606:GLN:HG2	2:C:1025:MET:CE	2.49	0.43
2:C:732:SER:HA	2:C:898:MET:CE	2.49	0.43
2:C:32:ARG:CZ	2:C:965:ILE:HG23	2.49	0.43
3:D:581:MET:HG2	3:D:717:LYS:HA	2.00	0.43
2:C:435:ASP:HA	2:C:674:HIS:CD2	2.53	0.43
3:D:473:LYS:O	3:D:477:GLU:HG3	2.19	0.43
1:A:62:GLU:OE2	2:C:870:LYS:NZ	2.39	0.43
2:C:97:MET:HB2	2:C:133:PHE:CE1	2.51	0.43
2:C:303:ALA:HB3	2:C:305:VAL:HG22	2.00	0.43
2:C:88:SER:HB2	2:C:100:SER:HA	2.01	0.42
2:C:237:TRP:CZ2	2:C:333:VAL:HG21	2.53	0.42
2:C:509:PRO:HB2	2:C:575:VAL:HG11	2.01	0.42
3:D:98:ALA:HB3	3:D:354:LEU:HD23	2.01	0.42
3:D:849:TYR:O	3:D:853:THR:HG23	2.19	0.42
7:H:15:DG:H8	7:H:15:DG:C5'	2.32	0.42
1:A:61:HIS:HE1	1:A:63:PHE:O	2.03	0.42
2:C:314:LEU:O	2:C:357:VAL:HG21	2.19	0.42
2:C:644:ILE:HG22	2:C:686:ALA:HA	2.00	0.42
2:C:735:LEU:HD22	2:C:740:VAL:HG21	2.00	0.42
3:D:327:MET:HG3	3:D:337:THR:HG23	2.01	0.42
1:A:11:GLU:OE2	1:A:205:ARG:HD3	2.19	0.42
3:D:281:ILE:O	3:D:289:LYS:NZ	2.45	0.42
2:C:541:PRO:HD2	2:C:550:GLU:OE2	2.19	0.42
2:C:786:ILE:HG13	2:C:844:ILE:CD1	2.49	0.42
1:B:78:LEU:HD21	3:D:611:VAL:HG23	2.01	0.42
3:D:449:LEU:HD11	3:D:476:VAL:HG13	2.01	0.42
3:D:1122:LEU:HA	3:D:1130:VAL:CG2	2.49	0.42
1:B:66:VAL:HG23	1:B:73:VAL:HG22	2.02	0.42
2:C:496:VAL:HG23	2:C:581:VAL:O	2.19	0.42
2:C:761:GLU:OE2	2:C:801:THR:OG1	2.32	0.42
3:D:357:LEU:CD2	5:F:63:VAL:HG22	2.49	0.42
3:D:23:TRP:HB3	3:D:92:MET:HE3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:GLY:HA3	2:C:225:ARG:CG	2.50	0.42
3:D:238:GLU:O	3:D:242:ARG:HG2	2.20	0.42
1:A:40:ARG:HG2	2:C:896:GLU:HB2	2.02	0.42
2:C:795:ILE:HD12	2:C:795:ILE:H	1.84	0.42
2:C:873:ILE:HA	2:C:873:ILE:HD12	1.96	0.42
3:D:1046:ILE:HG22	3:D:1110:GLN:HA	2.01	0.42
3:D:30:LYS:HE3	3:D:32:GLU:OE1	2.20	0.42
3:D:552:GLN:O	3:D:556:ARG:HG3	2.20	0.42
5:F:81:TRP:O	5:F:85:ILE:HG13	2.20	0.42
2:C:1122:LEU:HD13	2:C:1129:VAL:HG21	2.02	0.41
2:C:48:LEU:CD2	2:C:446:LYS:HD2	2.50	0.41
2:C:779:ASP:OD1	2:C:781:ARG:HG3	2.20	0.41
3:D:505:HIS:CD2	3:D:1005:GLU:HG3	2.55	0.41
3:D:432:VAL:HG13	3:D:434:PRO:HD3	2.01	0.41
1:A:199:LYS:O	1:A:200:ASN:HB2	2.18	0.41
3:D:1036:GLU:HB3	3:D:1038:ARG:HG3	2.02	0.41
3:D:1277:GLU:H	3:D:1277:GLU:CD	2.22	0.41
3:D:263:LYS:HD3	3:D:263:LYS:HA	1.94	0.41
3:D:66:LYS:HE3	3:D:66:LYS:HB2	1.75	0.41
5:F:57:LEU:HD11	5:F:90:TYR:HB2	2.02	0.41
3:D:131:PHE:HB2	3:D:372:ARG:NH1	2.35	0.41
3:D:155:MET:CE	3:D:219:LEU:HB3	2.50	0.41
3:D:320:ILE:HG21	3:D:340:LEU:HD23	2.03	0.41
3:D:673:PHE:CE2	3:D:688:MET:HG3	2.56	0.41
3:D:1122:LEU:HD13	3:D:1130:VAL:HG21	2.02	0.41
3:D:12:ILE:HG21	3:D:12:ILE:HD13	1.85	0.41
5:F:165:PRO:O	5:F:169:ILE:HG13	2.20	0.41
1:B:128:LEU:HD21	1:B:134:LEU:HG	2.02	0.41
2:C:898:MET:HE3	2:C:898:MET:HB2	1.90	0.41
3:D:97:LEU:HD11	3:D:317:VAL:HG23	2.02	0.41
3:D:52:PHE:CD1	3:D:322:PRO:HD3	2.55	0.41
3:D:122:PRO:HG2	6:G:20:DT:H3'	2.01	0.41
2:C:154:MET:HA	2:C:159:THR:O	2.21	0.41
2:C:807:GLU:OE1	3:D:56:ARG:NH2	2.54	0.41
3:D:1227:GLN:HG3	7:H:10:DG:H5'	2.03	0.41
7:H:19:DG:C2'	7:H:20:DT:C5'	2.85	0.41
1:B:101:GLY:N	1:B:132:GLY:O	2.52	0.41
1:B:227:VAL:O	1:B:228:GLU:CG	2.69	0.41
1:B:30:PHE:O	1:B:34:LEU:HG	2.19	0.41
2:C:245:ARG:NH2	2:C:351:VAL:HG12	2.35	0.41
2:C:80:LEU:HA	2:C:80:LEU:HD23	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1121:VAL:HG22	3:D:1130:VAL:HG13	2.02	0.41
3:D:736:VAL:HG12	3:D:818:ALA:HB2	2.03	0.41
3:D:817:LEU:O	3:D:839:SER:HB2	2.20	0.41
2:C:941:ASP:C	2:C:943:ALA:H	2.24	0.41
3:D:965:VAL:HG22	3:D:1155:GLU:HB3	2.03	0.41
6:G:22:DC:H2"	6:G:23:DA:N7	2.35	0.41
3:D:1122:LEU:HA	3:D:1130:VAL:HG22	2.03	0.41
1:A:62:GLU:O	1:A:73:VAL:HB	2.20	0.41
2:C:265:ASP:HB2	2:C:283:LYS:HG3	2.03	0.41
3:D:1090:LYS:HB3	3:D:1096:GLU:HA	2.02	0.41
3:D:64:LYS:HE3	3:D:65:TYR:OH	2.21	0.41
1:A:88:GLU:HG2	1:A:115:GLY:O	2.21	0.40
3:D:71:LYS:HB2	3:D:71:LYS:HE3	1.71	0.40
3:D:826:ASN:HB3	3:D:828:LYS:H	1.86	0.40
2:C:1125:LEU:HD13	3:D:105:TRP:CZ2	2.56	0.40
2:C:767:ILE:HG21	2:C:770:ILE:HD12	2.03	0.40
2:C:936:SER:OG	2:C:986:THR:HG23	2.21	0.40
1:B:170:PRO:HA	1:B:199:LYS:HE3	2.04	0.40
2:C:1005:PHE:HA	2:C:1012:PRO:HA	2.03	0.40
2:C:443:LEU:O	2:C:447:ARG:HG3	2.22	0.40
2:C:720:TRP:HE1	2:C:899:PRO:HD3	1.86	0.40
2:C:753:ALA:HB2	2:C:763:ILE:HG13	2.02	0.40
3:D:1158:VAL:HA	3:D:1161:MET:HE2	2.03	0.40
1:A:175:THR:HG22	1:A:195:ASP:HB3	2.04	0.40
3:D:573:PRO:O	3:D:576:MET:HE2	2.21	0.40
3:D:736:VAL:O	3:D:841:ARG:NE	2.52	0.40
3:D:826:ASN:OD1	3:D:827:PRO:HD2	2.21	0.40
2:C:261:THR:HB	2:C:266:GLU:OE1	2.21	0.40
2:C:580:MET:HG3	2:C:581:VAL:HG23	2.03	0.40
3:D:821:LYS:HB3	3:D:836:VAL:HB	2.04	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%)	208 (98%)	5 (2%)	0	100	100
1	B	224/368 (61%)	211 (94%)	13 (6%)	0	100	100
2	C	1131/1174 (96%)	1082 (96%)	48 (4%)	1 (0%)	51	81
3	D	1250/1317 (95%)	1211 (97%)	39 (3%)	0	100	100
4	E	71/110 (64%)	68 (96%)	3 (4%)	0	100	100
5	F	180/218 (83%)	177 (98%)	3 (2%)	0	100	100
All	All	3069/3555 (86%)	2957 (96%)	111 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	185/315 (59%)	182 (98%)	3 (2%)	62	88
1	B	177/315 (56%)	170 (96%)	7 (4%)	31	65
2	C	929/995 (93%)	888 (96%)	41 (4%)	28	61
3	D	1026/1096 (94%)	981 (96%)	45 (4%)	28	61
4	E	64/90 (71%)	63 (98%)	1 (2%)	62	88
5	F	143/175 (82%)	135 (94%)	8 (6%)	21	51
All	All	2524/2986 (84%)	2419 (96%)	105 (4%)	30	63

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	59	VAL
1	A	213	LYS
1	B	33	THR
1	B	75	GLU
1	B	88	GLU
1	B	94	THR
1	B	172	LEU
1	B	214	THR
1	B	227	VAL
2	C	24	ASN
2	C	71	ARG
2	C	87	LEU
2	C	114	ASP
2	C	199	ILE
2	C	209	ASP
2	C	211	ASP
2	C	238	THR
2	C	284	GLU
2	C	343	HIS
2	C	347	THR
2	C	350	THR
2	C	351	VAL
2	C	372	LEU
2	C	441	SER
2	C	444	THR
2	C	458	SER
2	C	482	THR
2	C	548	PHE
2	C	562	VAL
2	C	565	VAL
2	C	576	SER
2	C	615	SER
2	C	635	VAL
2	C	648	SER
2	C	756	THR
2	C	766	ASP
2	C	770	ILE
2	C	778	LEU
2	C	781	ARG
2	C	824	ARG
2	C	825	GLU
2	C	842	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	846	VAL
2	C	1027	LEU
2	C	1031	VAL
2	C	1032	ASP
2	C	1088	ASP
2	C	1134	SER
2	C	1145	GLU
2	C	1147	GLU
3	D	12	ILE
3	D	148	LEU
3	D	150	THR
3	D	165	GLN
3	D	177	LEU
3	D	192	ASP
3	D	287	GLN
3	D	308	SER
3	D	331	ASP
3	D	337	THR
3	D	386	ARG
3	D	456	VAL
3	D	460	LEU
3	D	464	ASN
3	D	485	ASP
3	D	490	VAL
3	D	517	VAL
3	D	539	ASP
3	D	578	ARG
3	D	579	LEU
3	D	580	ASP
3	D	581	MET
3	D	590	THR
3	D	606	HIS
3	D	639	GLN
3	D	714	ASP
3	D	738	VAL
3	D	742	LYS
3	D	743	LYS
3	D	791	GLU
3	D	821	LYS
3	D	834	ARG
3	D	847	LEU
3	D	863	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	965	VAL
3	D	971	SER
3	D	1036	GLU
3	D	1061	PHE
3	D	1089	PHE
3	D	1090	LYS
3	D	1095	SER
3	D	1130	VAL
3	D	1191	ARG
3	D	1194	VAL
3	D	1206	VAL
4	E	45	ARG
5	F	22	ASP
5	F	73	ARG
5	F	83	TYR
5	F	86	LEU
5	F	109	ILE
5	F	123	THR
5	F	179	THR
5	F	192	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	144	GLN
3	D	854	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	6/7 (85%)	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/368 (58%)	0.03	1 (0%) 91 88	53, 75, 108, 128	0
1	B	230/368 (62%)	0.76	37 (16%) 1 1	75, 112, 147, 156	0
2	C	1135/1174 (96%)	0.42	93 (8%) 11 6	47, 75, 147, 169	0
3	D	1258/1317 (95%)	0.26	76 (6%) 21 14	48, 79, 122, 153	0
4	E	75/110 (68%)	1.03	18 (24%) 0 0	73, 99, 138, 175	0
5	F	182/218 (83%)	1.02	31 (17%) 1 1	52, 103, 132, 147	12 (6%)
6	G	23/23 (100%)	0.68	4 (17%) 1 1	87, 118, 154, 161	3 (13%)
7	H	20/21 (95%)	0.27	2 (10%) 7 4	54, 78, 136, 137	0
8	I	7/7 (100%)	-0.32	0 100 100	53, 54, 81, 87	0
All	All	3147/3606 (87%)	0.40	262 (8%) 11 6	47, 81, 139, 175	15 (0%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	GLY	11.8
1	B	236	PRO	9.8
2	C	262	VAL	8.7
3	D	65	TYR	7.4
5	F	76	THR	7.4
5	F	73	ARG	7.3
5	F	68	GLY	7.3
3	D	189	ALA	7.0
2	C	406	ILE	6.7
2	C	553	VAL	6.7
2	C	246	PHE	6.6
2	C	568	SER	6.6
2	C	214	ASP	6.4
3	D	654	SER	6.1
2	C	544	ALA	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	321	PRO	5.9
1	B	61	HIS	5.9
3	D	197	VAL	5.8
2	C	139	GLY	5.7
3	D	1055	LEU	5.7
2	C	567	SER	5.6
2	C	323	THR	5.6
2	C	22	SER	5.6
1	B	235	GLY	5.4
1	B	128	LEU	5.4
3	D	190	LYS	5.4
5	F	72	PHE	5.4
4	E	27	GLY	5.3
2	C	93	PHE	5.3
2	C	255	THR	5.3
6	G	3	DG	5.3
4	E	25	SER	5.2
4	E	82	VAL	5.2
4	E	30	THR	5.0
2	C	569	GLU	5.0
2	C	545	ASP	5.0
1	B	58	GLY	4.9
4	E	81	LEU	4.8
2	C	247	GLY	4.7
3	D	184	LEU	4.7
5	F	82	LEU	4.7
5	F	83	TYR	4.7
1	B	103	GLY	4.7
2	C	324	SER	4.7
2	C	251	ILE	4.7
4	E	28	TYR	4.6
2	C	253	ARG	4.6
2	C	243	VAL	4.6
2	C	347	THR	4.6
3	D	1025	THR	4.6
1	B	102	PRO	4.5
1	B	133	LYS	4.5
3	D	305	SER	4.5
2	C	245	ARG	4.5
5	F	177	ILE	4.4
2	C	138	THR	4.3
5	F	67	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	263	GLY	4.3
3	D	59	GLU	4.2
3	D	181	LEU	4.2
1	B	87	SER	4.1
1	B	157	ALA	4.1
2	C	229	THR	4.1
3	D	188	GLY	4.0
4	E	80	PRO	4.0
3	D	1066	ILE	3.9
2	C	239	SER	3.9
5	F	173	MET	3.9
2	C	231	LEU	3.8
4	E	103	LEU	3.8
3	D	1056	GLU	3.8
1	B	151	GLN	3.8
3	D	1188	ALA	3.8
3	D	1054	ARG	3.7
3	D	1192	ARG	3.7
4	E	78	VAL	3.7
5	F	81	TRP	3.7
3	D	1053	VAL	3.6
1	B	201	SER	3.6
5	F	45	LEU	3.6
3	D	1173	THR	3.6
3	D	1049	VAL	3.6
5	F	169	ILE	3.6
2	C	546	GLY	3.5
4	E	93	ILE	3.5
2	C	348	THR	3.5
2	C	137	ASN	3.5
3	D	187	GLU	3.5
2	C	286	ALA	3.4
2	C	133	PHE	3.4
2	C	340	VAL	3.4
2	C	351	VAL	3.4
2	C	68	ALA	3.4
2	C	237	TRP	3.4
4	E	31	PRO	3.3
3	D	1099	LEU	3.3
2	C	346	GLN	3.3
4	E	102	LEU	3.3
3	D	653	HIS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	G	5	DG	3.2
2	C	252	MET	3.2
6	G	4	DT	3.2
3	D	186	ALA	3.2
2	C	519	SER	3.2
2	C	1145	GLU	3.2
5	F	74	HIS	3.1
3	D	201	GLY	3.1
2	C	242	ILE	3.1
2	C	250	GLU	3.1
2	C	282	THR	3.1
2	C	249	SER	3.1
3	D	762	ARG	3.1
1	B	130	ASP	3.1
1	B	105	VAL	3.1
2	C	548	PHE	3.1
3	D	1189	GLU	3.0
3	D	205	MET	3.0
3	D	1175	PHE	3.0
3	D	1277	GLU	3.0
2	C	520	ASP	3.0
2	C	256	LEU	3.0
2	C	283	LYS	3.0
3	D	1094	GLY	3.0
3	D	61	TYR	3.0
3	D	1274	PRO	3.0
2	C	90	ILE	3.0
2	C	141	ILE	3.0
1	B	96	TYR	2.9
3	D	60	CYS	2.9
4	E	77	TYR	2.9
3	D	1060	ARG	2.9
3	D	70	PHE	2.9
2	C	140	GLU	2.9
2	C	248	PHE	2.9
3	D	80	VAL	2.8
5	F	114	LEU	2.8
2	C	352	PRO	2.8
2	C	1144	GLY	2.8
2	C	69	ALA	2.8
1	B	5	GLN	2.8
5	F	77	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	131	LYS	2.8
3	D	243	GLU	2.8
1	B	101	GLY	2.8
5	F	69	PHE	2.7
2	C	67	SER	2.7
2	C	359	VAL	2.7
2	C	135	ASN	2.7
2	C	411	LEU	2.7
2	C	278	GLY	2.7
1	B	100	GLN	2.7
2	C	353	GLY	2.7
3	D	73	ILE	2.7
1	B	134	LEU	2.7
3	D	1074	GLU	2.7
3	D	930	VAL	2.7
5	F	28	ARG	2.7
3	D	1105	VAL	2.7
2	C	131	ALA	2.7
3	D	1067	VAL	2.6
2	C	222	ARG	2.6
1	B	115	GLY	2.6
2	C	354	GLY	2.6
3	D	652	GLY	2.6
2	C	325	SER	2.6
3	D	1041	ARG	2.6
1	B	104	GLU	2.6
3	D	1064	ILE	2.6
5	F	91	ILE	2.6
1	B	95	MET	2.6
2	C	257	GLU	2.6
2	C	254	SER	2.6
2	C	215	THR	2.5
3	D	216	LEU	2.5
3	D	1104	HIS	2.5
5	F	31	ARG	2.5
4	E	66	TYR	2.5
3	D	600	GLN	2.5
2	C	143	SER	2.5
1	B	116	VAL	2.5
5	F	158	TYR	2.5
1	B	111	VAL	2.5
3	D	969	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	319	GLY	2.5
2	C	396	GLU	2.5
1	B	138	LEU	2.5
3	D	177	LEU	2.5
4	E	104	GLU	2.5
3	D	934	GLY	2.5
3	D	1065	THR	2.4
3	D	1276	GLU	2.4
1	B	199	LYS	2.4
2	C	517	VAL	2.4
5	F	75	GLY	2.4
5	F	178	GLY	2.4
2	C	274	LYS	2.4
2	C	236	GLY	2.4
4	E	55	TYR	2.4
3	D	644	VAL	2.4
1	A	99	LYS	2.4
3	D	72	GLY	2.4
3	D	1073	GLU	2.4
1	B	129	ASN	2.4
3	D	1270	ILE	2.4
1	B	132	GLY	2.4
2	C	238	THR	2.4
3	D	1112	MET	2.4
3	D	1172	SER	2.4
3	D	650	LEU	2.4
3	D	146	ASN	2.3
5	F	122	SER	2.3
3	D	1080	ILE	2.3
4	E	26	GLY	2.3
2	C	132	GLU	2.3
3	D	194	ARG	2.3
2	C	551	PRO	2.3
5	F	92	ASN	2.3
2	C	623	GLY	2.3
3	D	155	MET	2.3
3	D	1100	SER	2.3
5	F	86	LEU	2.3
3	D	180	ASP	2.2
2	C	258	LYS	2.2
5	F	80	ALA	2.2
1	B	4	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	1111	LEU	2.2
2	C	213	ARG	2.2
7	H	5	DT	2.2
3	D	1275	THR	2.2
2	C	656	HIS	2.2
2	C	513	VAL	2.2
1	B	200	ASN	2.2
2	C	265	ASP	2.2
1	B	114	ALA	2.2
5	F	44	ALA	2.2
3	D	1273	GLN	2.2
2	C	281	PRO	2.2
2	C	261	THR	2.1
5	F	34	ILE	2.1
2	C	134	ILE	2.1
5	F	100	GLN	2.1
5	F	181	MET	2.1
2	C	94	SER	2.1
2	C	684	VAL	2.1
7	H	1	DT	2.1
1	B	202	ILE	2.1
3	D	464	ASN	2.1
3	D	246	ASP	2.1
6	G	9	DG	2.1
5	F	150	GLU	2.1
3	D	219	LEU	2.1
1	B	127	THR	2.1
3	D	1072	GLY	2.1
1	B	66	VAL	2.1
1	B	110	ILE	2.0
4	E	90	PRO	2.0
2	C	401	GLN	2.0
3	D	1048	ASP	2.0
2	C	514	VAL	2.0
2	C	280	PRO	2.0
2	C	652	ILE	2.0
3	D	1026	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	ZN	D	2002	1/1	0.94	0.08	105,105,105,105	0
10	MG	D	2003	1/1	0.94	0.25	54,54,54,54	0
9	ZN	D	2001	1/1	0.99	0.12	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.