



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:15 AM GMT

PDB ID : 2WAQ  
Title : THE COMPLETE STRUCTURE OF THE ARCHAEAL 13-SUBUNIT DNA-DIRECTED RNA POLYMERASE  
Authors : Korkhin, Y.; Unligil, U.M.; Littlefield, O.; Nelson, P.J.; Stuart, D.I.; Sigler, P.B.; Bell, S.D.; Abrescia, N.G.A.  
Deposited on : 2009-02-11  
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

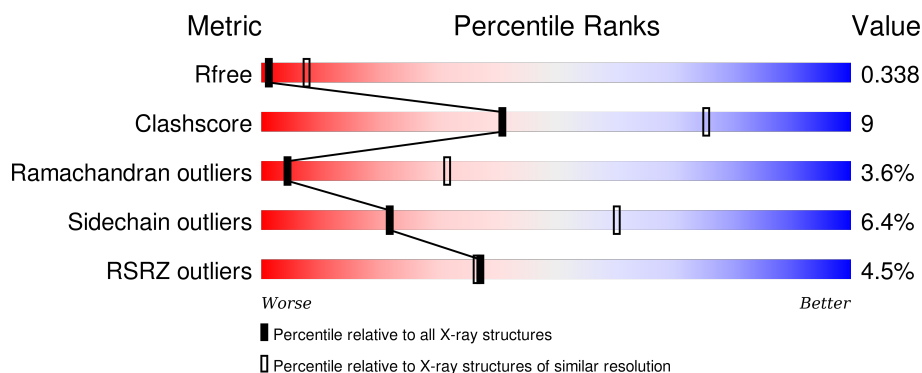
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	880	<div> <div>0%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• •</div> </div> </div>
2	B	1131	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• •</div> </div> </div>
3	C	395	<div> <div>8%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>• 7%</div> </div> </div>
4	D	265	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>• •</div> </div> </div>
5	E	180	<div> <div>19%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
6	F	113	
7	G	132	
8	H	84	
9	K	95	
10	L	92	
11	N	66	
12	P	48	
13	Q	104	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26471 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 RPO1N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6691	4256	1183	1226	26			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1090	Total	C	N	O	S	0	0	0
			8652	5484	1534	1605	29			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	367	Total	C	N	O	S	0	0	0
			2833	1797	481	547	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE RPO3 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	260	Total	C	N	O	S	0	0	0
			2071	1332	334	392	13			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1384	893	232	255	4			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	90	Total	C	N	O	S	0	0	0
			701	439	114	145	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	113	Total	C	N	O	S	0	0	0
			901	572	152	173	4			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O	S	0	0	0
			609	396	108	105				

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	91	Total	C	N	O	S	0	0	0
			707	454	114	137	2			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	45	Total	C	N	O	S	0	0	0
			387	243	68	75	1			

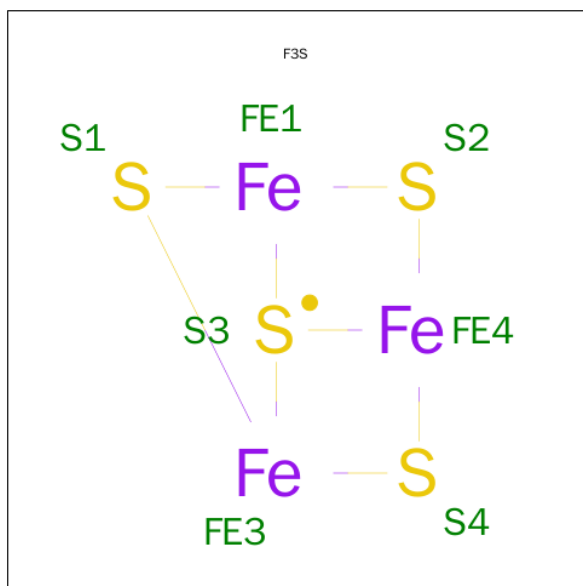
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	P	1	Total	Zn	0	0
			1	1		
14	B	3	Total	Zn	0	0
			3	3		
14	A	3	Total	Zn	0	0
			3	3		
14	C	1	Total	Zn	0	0
			1	1		
14	N	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

- Molecule 16 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).

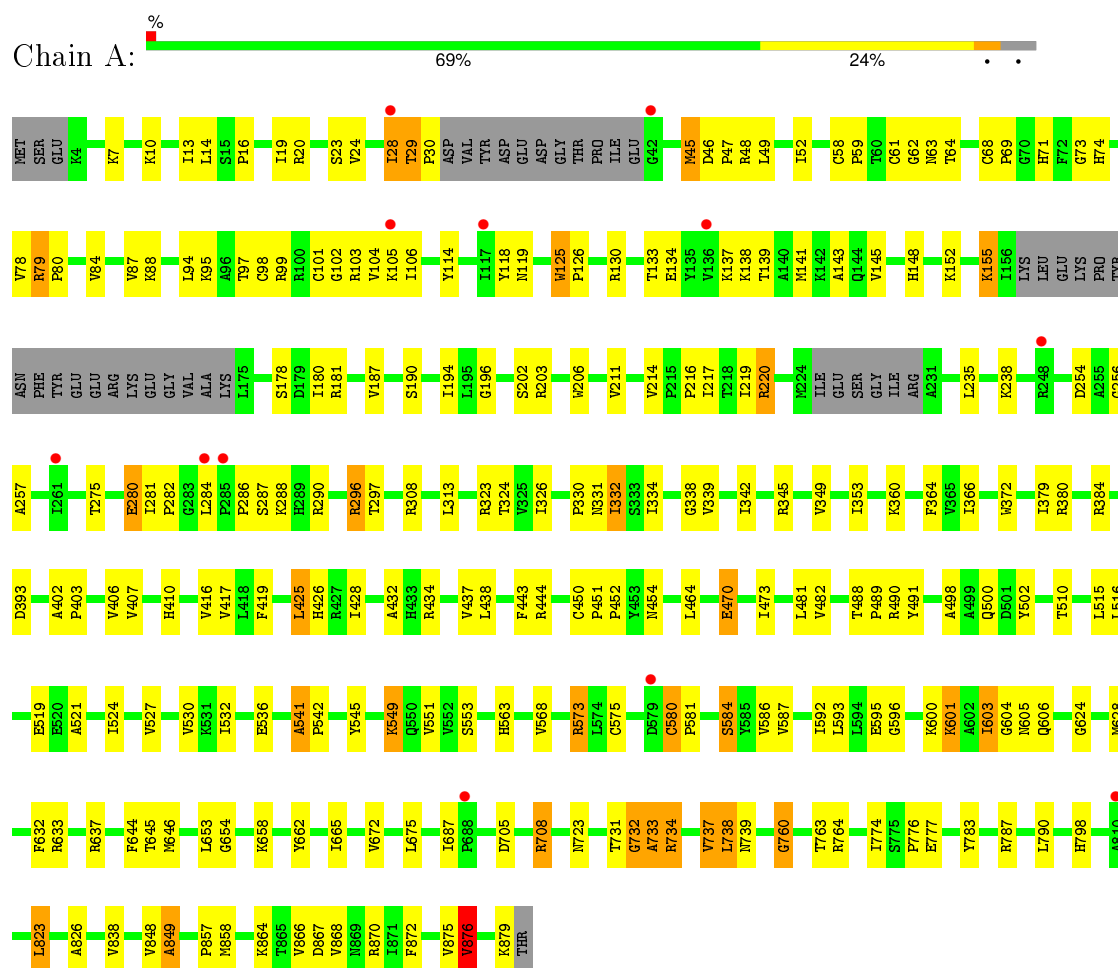


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	Fe	S	0	0
			7	3	4		

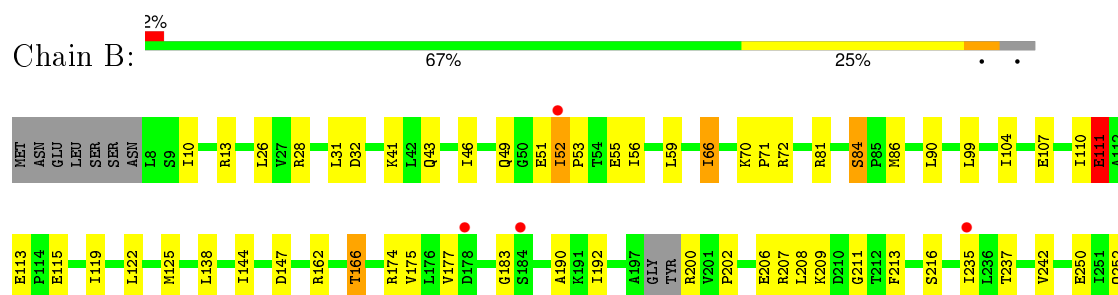
### 3 Residue-property plots [i](#)

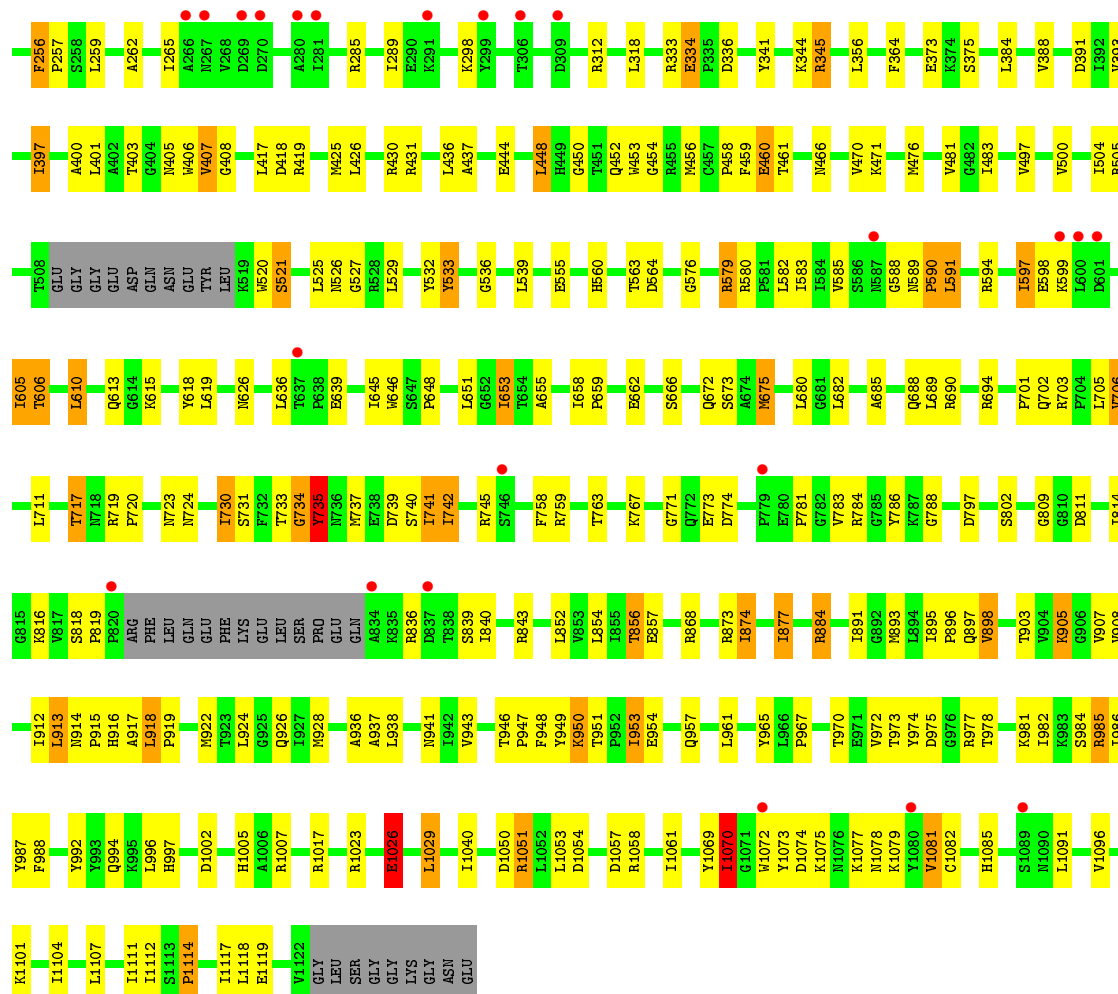
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 RPO1N SUBUNIT

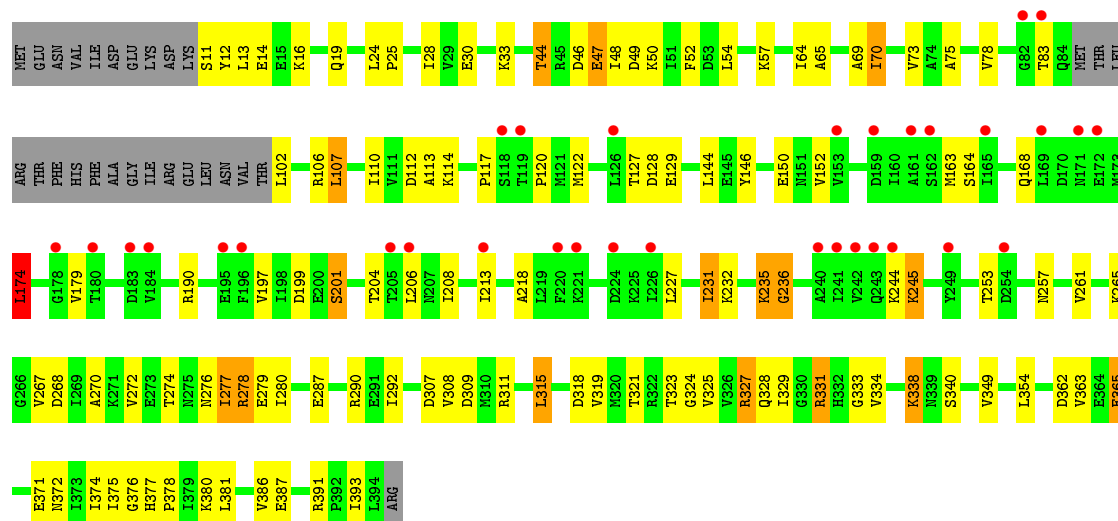


#### • Molecule 2: DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT



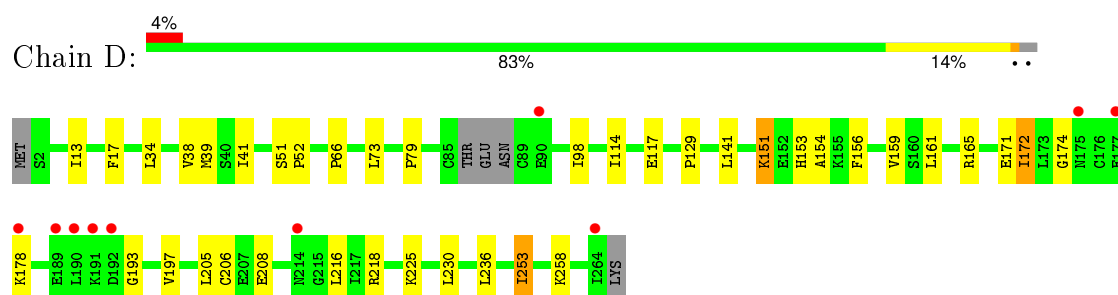


• Molecule 3: DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT

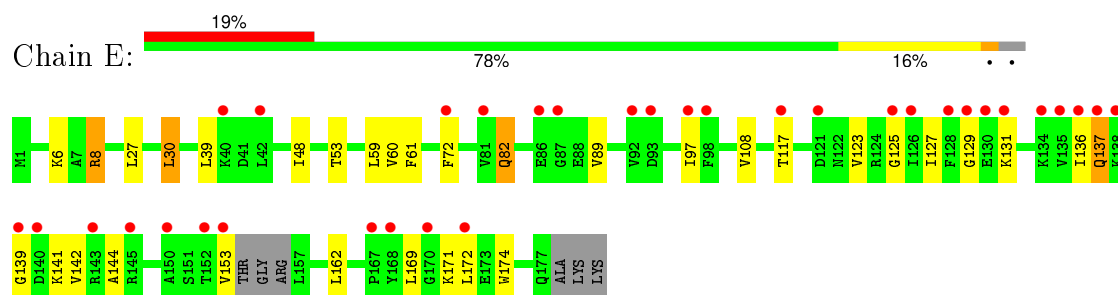


• Molecule 4: DNA-DIRECTED RNA POLYMERASE RPO3 SUBUNIT

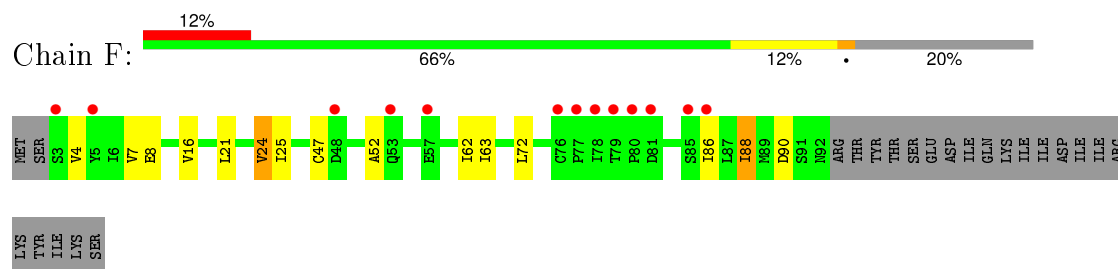




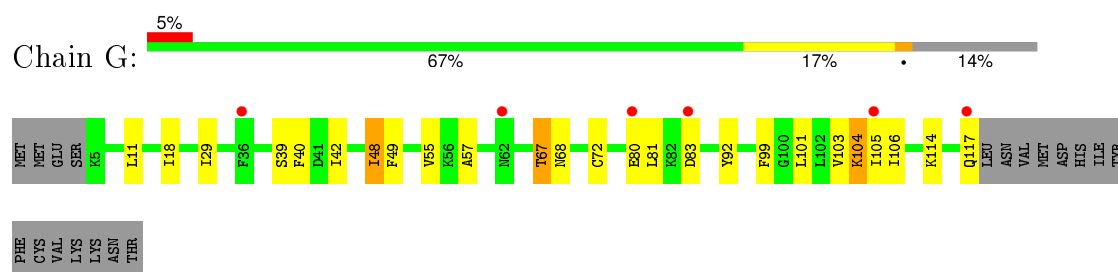
• Molecule 5: DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT



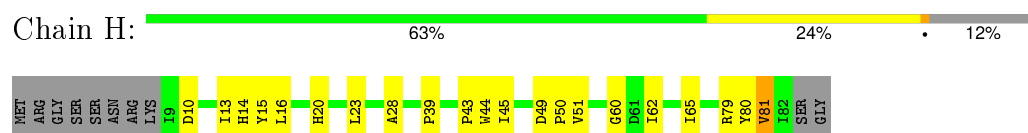
• Molecule 6: DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT



• Molecule 7: DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT



• Molecule 8: DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT

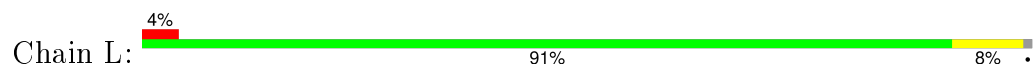


• Molecule 9: DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT

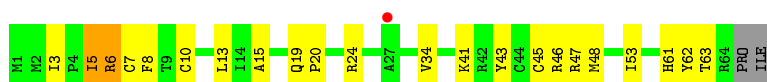




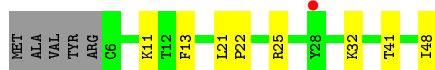
• Molecule 10: DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT



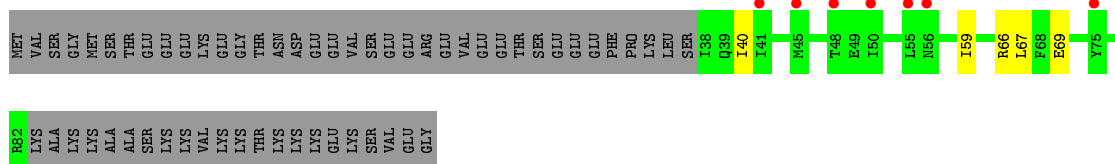
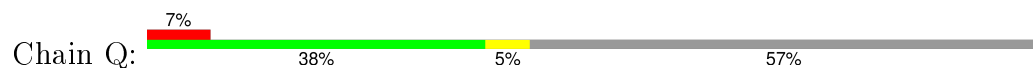
• Molecule 11: DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT



• Molecule 12: DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT



• Molecule 13: DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.50Å 212.62Å 129.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 3.35 42.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	77.0 (42.78-3.35) 72.5 (42.78-3.20)	Depositor EDS
$R_{merge}$	0.00	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.271 , 0.341 0.270 , 0.338	Depositor DCC
$R_{free}$ test set	3012 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63954 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	26471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, F3S, 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	0.33	0/6834	0.52	0/9247
2	B	0.32	0/8816	0.52	0/11926
3	C	0.34	0/2857	0.53	1/3847 (0.0%)
4	D	0.31	0/2106	0.50	0/2845
5	E	0.34	0/1405	0.47	0/1899
6	F	0.33	0/709	0.44	0/961
7	G	0.34	0/913	0.48	0/1224
8	H	0.34	0/623	0.52	0/845
9	K	0.33	0/667	0.51	0/903
10	L	0.29	0/717	0.47	0/968
11	N	0.33	0/524	0.45	0/706
12	P	0.37	0/354	0.51	0/475
13	Q	0.37	0/391	0.50	0/522
All	All	0.33	0/26916	0.51	1/36368 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	174	LEU	CA-CB-CG	5.09	127.01	115.30

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	6691	0	6758	138	0
2	B	8652	0	8795	191	0
3	C	2833	0	2992	76	0
4	D	2071	0	2116	24	0
5	E	1384	0	1444	15	0
6	F	701	0	708	7	0
7	G	901	0	912	13	0
8	H	609	0	640	12	0
9	K	658	0	692	10	0
10	L	707	0	739	3	0
11	N	514	0	528	15	0
12	P	346	0	375	4	0
13	Q	387	0	388	2	0
14	A	3	0	0	0	0
14	B	3	0	0	0	0
14	C	1	0	0	0	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
15	A	1	0	0	0	0
16	D	7	0	0	0	0
All	All	26471	0	27087	460	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 (460) 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)
1:A:867:ASP:HA	1:A:870:ARG:HH22	1.14	1.12
2:B:110:ILE:HA	2:B:111:GLU:HB2	1.10	1.07
2:B:110:ILE:HA	2:B:111:GLU:CB	1.86	1.03
2:B:110:ILE:CA	2:B:111:GLU:HB2	1.96	0.95
2:B:953:ILE:HD13	2:B:953:ILE:H	1.35	0.92
3:C:64:ILE:HG22	3:C:65:ALA:H	1.37	0.89
2:B:1069:TYR:HA	2:B:1070:ILE:HB	1.56	0.84
3:C:244:LYS:HA	3:C:245:LYS:HB3	1.58	0.84
1:A:867:ASP:HA	1:A:870:ARG:NH2	1.94	0.82
8:H:45:ILE:O	8:H:81:VAL:HA	1.82	0.80
1:A:600:LYS:O	1:A:601:LYS:HB2	1.82	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ARG:NH1	2:B:992:TYR:HB3	2.00	0.76
1:A:63:ASN:HB2	1:A:68:CYS:HB2	1.66	0.75
1:A:342:ILE:HD13	1:A:345:ARG:HH12	1.50	0.75
2:B:905:LYS:H	2:B:905:LYS:HE2	1.51	0.75
2:B:1069:TYR:CA	2:B:1070:ILE:HB	2.16	0.74
1:A:875:VAL:HG12	1:A:876:VAL:H	1.52	0.74
1:A:553:SER:OG	1:A:592:ILE:HA	1.88	0.74
2:B:984:SER:O	2:B:985:ARG:HB2	1.86	0.73
3:C:163:MET:CB	3:C:164:SER:HA	2.17	0.73
1:A:524:ILE:HA	1:A:637:ARG:HG2	1.72	0.72
1:A:220:ARG:HG2	1:A:235:LEU:HD22	1.73	0.71
13:Q:66:ARG:HG2	13:Q:66:ARG:HH11	1.56	0.70
3:C:163:MET:HB2	3:C:164:SER:HA	1.72	0.70
2:B:256:PHE:HB2	2:B:257:PRO:HD3	1.74	0.69
1:A:235:LEU:HA	1:A:238:LYS:HE3	1.75	0.69
1:A:498:ALA:HB1	1:A:502:TYR:HB2	1.74	0.69
1:A:330:PRO:HG3	2:B:734:GLY:HA2	1.75	0.68
1:A:125:TRP:H	1:A:126:PRO:HD2	1.57	0.68
3:C:274:THR:HG22	3:C:276:ASN:H	1.57	0.68
2:B:1082:CYS:HB3	2:B:1091:LEU:HD21	1.74	0.67
3:C:338:LYS:HE2	3:C:338:LYS:H	1.59	0.67
3:C:117:PRO:HG2	3:C:120:PRO:HB3	1.77	0.67
2:B:954:GLU:HA	2:B:957:GLN:HB2	1.77	0.67
4:D:66:PRO:HG2	11:N:13:LEU:HD11	1.77	0.67
2:B:563:THR:HG22	2:B:564:ASP:H	1.58	0.67
3:C:70:ILE:HA	3:C:73:VAL:HG22	1.77	0.66
3:C:30:GLU:O	3:C:33:LYS:HG2	1.98	0.64
2:B:333:ARG:O	2:B:334:GLU:HB3	1.97	0.64
1:A:586:VAL:HA	1:A:596:GLY:HA3	1.79	0.64
2:B:742:ILE:HG23	2:B:912:ILE:HB	1.79	0.63
1:A:428:ILE:HG22	1:A:452:PRO:HB3	1.79	0.63
1:A:78:VAL:O	1:A:79:ARG:HB2	1.99	0.63
2:B:166:THR:HG23	2:B:431:ARG:O	1.99	0.63
1:A:603:ILE:HG21	1:A:632:PHE:HE1	1.63	0.63
1:A:49:LEU:HA	1:A:71:HIS:HB2	1.79	0.62
1:A:360:LYS:HE2	1:A:364:PHE:HE1	1.63	0.62
1:A:7:LYS:HB2	2:B:1119:GLU:HB2	1.82	0.62
1:A:28:ILE:HG22	1:A:30:PRO:HD2	1.81	0.61
4:D:98:ILE:HD11	4:D:114:ILE:HG12	1.83	0.61
2:B:119:ILE:HG22	2:B:393:VAL:HG21	1.82	0.61
9:K:78:ILE:HB	9:K:90:LEU:HD12	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:ILE:HD11	8:H:79:ARG:HG2	1.83	0.61
2:B:594:ARG:NH1	2:B:615:LYS:HB2	2.15	0.60
1:A:125:TRP:N	1:A:126:PRO:HD2	2.16	0.60
1:A:47:PRO:O	1:A:48:ARG:HB2	2.01	0.60
2:B:703:ARG:HD2	2:B:717:THR:HG22	1.82	0.60
2:B:207:ARG:HB2	2:B:216:SER:OG	2.00	0.60
2:B:162:ARG:HG2	2:B:401:LEU:O	2.02	0.60
5:E:6:LYS:HB2	6:F:8:GLU:HB2	1.84	0.60
1:A:603:ILE:HG21	1:A:632:PHE:CE1	2.37	0.59
3:C:244:LYS:HA	3:C:245:LYS:CB	2.27	0.59
2:B:733:THR:HG23	2:B:735:TYR:HB2	1.83	0.59
9:K:80:ARG:HB2	9:K:88:ILE:HB	1.83	0.59
2:B:682:LEU:HD23	2:B:719:ARG:HG2	1.84	0.59
2:B:974:TYR:CE2	2:B:981:LYS:HB3	2.37	0.59
2:B:364:PHE:HE1	2:B:388:VAL:HG13	1.66	0.59
2:B:730:ILE:HG12	2:B:986:ILE:HG21	1.85	0.59
2:B:953:ILE:CD1	2:B:953:ILE:H	2.10	0.58
8:H:43:PRO:HB2	8:H:79:ARG:HD3	1.85	0.58
1:A:338:GLY:O	1:A:443:PHE:HA	2.02	0.58
3:C:11:SER:HB2	3:C:14:GLU:HB2	1.83	0.58
1:A:20:ARG:HE	1:A:211:VAL:HG21	1.68	0.58
2:B:1104:ILE:HG23	2:B:1114:PRO:HG2	1.84	0.58
1:A:867:ASP:CA	1:A:870:ARG:HH22	2.02	0.58
4:D:34:LEU:HD22	4:D:151:LYS:HB2	1.84	0.58
1:A:130:ARG:HH11	1:A:196:GLY:HA2	1.68	0.58
3:C:277:ILE:HG22	3:C:278:ARG:H	1.69	0.57
1:A:573:ARG:HH11	1:A:573:ARG:CG	2.17	0.57
3:C:25:PRO:HA	3:C:28:ILE:HA	1.85	0.57
2:B:884:ARG:HB2	2:B:884:ARG:HH11	1.68	0.57
3:C:327:ARG:HB2	3:C:333:GLY:HA3	1.87	0.57
2:B:702:GLN:HB2	2:B:723:ASN:HA	1.87	0.57
3:C:152:VAL:HG23	3:C:174:LEU:HD12	1.85	0.57
2:B:460:GLU:HG2	2:B:673:SER:HB3	1.86	0.57
2:B:852:LEU:HB3	2:B:868:ARG:HG2	1.87	0.57
2:B:70:LYS:O	2:B:72:ARG:N	2.37	0.57
3:C:146:TYR:HD1	3:C:235:LYS:H	1.52	0.56
11:N:8:PHE:H	11:N:48:MET:HE3	1.71	0.56
1:A:600:LYS:HB2	1:A:732:GLY:HA3	1.86	0.56
2:B:898:VAL:HG21	4:D:34:LEU:HD21	1.87	0.56
1:A:134:GLU:HA	1:A:137:LYS:HD2	1.88	0.56
2:B:974:TYR:HA	2:B:981:LYS:HA	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:VAL:O	2:B:397:ILE:HB	2.06	0.56
3:C:150:GLU:HG3	3:C:227:LEU:HB3	1.88	0.56
2:B:1074:ASP:HB3	2:B:1075:LYS:HB3	1.87	0.56
2:B:605:ILE:HG12	2:B:606:THR:H	1.71	0.55
2:B:52:ILE:N	2:B:53:PRO:HD3	2.20	0.55
2:B:694:ARG:HA	2:B:758:PHE:O	2.06	0.55
1:A:510:THR:O	1:A:549:LYS:HD3	2.07	0.55
1:A:97:THR:HG22	1:A:99:ARG:H	1.72	0.55
2:B:701:PRO:HB2	2:B:720:PRO:HG2	1.89	0.55
7:G:72:CYS:HB3	7:G:114:LYS:HG2	1.89	0.55
3:C:47:GLU:HB3	3:C:50:LYS:HB2	1.89	0.55
7:G:80:GLU:HG3	7:G:81:LEU:H	1.71	0.55
1:A:864:LYS:O	1:A:864:LYS:HG3	2.06	0.55
3:C:290:ARG:HA	3:C:321:THR:HG21	1.88	0.55
2:B:742:ILE:CG2	2:B:912:ILE:HB	2.37	0.54
2:B:400:ALA:HA	2:B:403:THR:HG22	1.88	0.54
5:E:123:VAL:HG22	5:E:125:GLY:H	1.72	0.54
1:A:488:THR:HG22	1:A:490:ARG:H	1.71	0.54
3:C:64:ILE:HG22	3:C:65:ALA:N	2.16	0.54
5:E:60:VAL:HG22	5:E:61:PHE:H	1.72	0.54
5:E:89:VAL:HG13	5:E:139:GLY:HA2	1.90	0.54
3:C:331:ARG:H	3:C:331:ARG:HD3	1.73	0.54
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.88	0.54
4:D:171:GLU:HB2	4:D:218:ARG:HB3	1.90	0.54
1:A:16:PRO:HG2	1:A:181:ARG:HH22	1.72	0.54
3:C:102:LEU:HB2	3:C:106:ARG:HB2	1.88	0.54
1:A:125:TRP:H	1:A:126:PRO:CD	2.20	0.54
8:H:39:PRO:HG3	13:Q:67:LEU:HD11	1.89	0.54
1:A:490:ARG:HD2	1:A:491:TYR:HD1	1.73	0.54
1:A:777:GLU:HG3	1:A:783:TYR:HE2	1.72	0.53
1:A:330:PRO:HG3	2:B:734:GLY:CA	2.38	0.53
5:E:141:LYS:HB3	5:E:172:LEU:HD13	1.90	0.53
1:A:603:ILE:HG22	1:A:604:GLY:H	1.74	0.53
3:C:340:SER:HB3	3:C:371:GLU:HG2	1.90	0.53
6:F:72:LEU:HD11	6:F:86:ILE:HG12	1.91	0.53
2:B:972:VAL:HG21	4:D:205:LEU:HB3	1.91	0.53
4:D:174:GLY:HA3	4:D:216:LEU:HD22	1.89	0.53
2:B:10:ILE:HA	2:B:13:ARG:HG2	1.90	0.53
2:B:724:ASN:O	11:N:47:ARG:HD2	2.07	0.53
3:C:270:ALA:HA	8:H:14:HIS:HB3	1.91	0.53
9:K:26:ARG:HG2	9:K:27:LEU:H	1.73	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:372:ASN:HA	3:C:375:ILE:HG22	1.89	0.53
1:A:662:TYR:HA	1:A:665:ILE:HG12	1.91	0.53
5:E:82:GLN:HB3	6:F:88:ILE:HB	1.89	0.53
1:A:848:VAL:O	1:A:849:ALA:HB3	2.07	0.52
2:B:115:GLU:HG2	2:B:384:LEU:HD12	1.92	0.52
2:B:982:ILE:CD1	2:B:985:ARG:H	2.22	0.52
2:B:356:LEU:HA	2:B:407:VAL:HG21	1.91	0.52
3:C:127:THR:H	3:C:268:ASP:HB2	1.74	0.52
1:A:95:LYS:HD3	1:A:138:LYS:HG2	1.91	0.52
1:A:338:GLY:HA3	1:A:444:ARG:HG2	1.92	0.52
6:F:88:ILE:H	6:F:88:ILE:HD13	1.74	0.52
1:A:568:VAL:HG22	1:A:731:THR:HG22	1.91	0.52
3:C:144:LEU:HA	3:C:235:LYS:HG3	1.92	0.51
6:F:16:VAL:HB	6:F:52:ALA:HB3	1.92	0.51
9:K:82:LEU:HD12	9:K:86:LYS:HB3	1.91	0.51
1:A:98:CYS:O	1:A:99:ARG:HB2	2.11	0.51
1:A:879:LYS:NZ	3:C:44:THR:O	2.44	0.51
2:B:648:PRO:HB3	2:B:947:PRO:HG2	1.92	0.51
3:C:277:ILE:C	3:C:279:GLU:H	2.14	0.51
7:G:83:ASP:HB2	7:G:101:LEU:HG	1.92	0.51
2:B:560:HIS:HB3	2:B:626:ASN:HD21	1.75	0.51
2:B:1007:ARG:HH21	2:B:1026:GLU:C	2.13	0.51
2:B:406:TRP:CG	2:B:407:VAL:N	2.78	0.51
2:B:783:VAL:CG1	2:B:784:ARG:HB2	2.40	0.50
3:C:315:LEU:O	3:C:319:VAL:HG23	2.12	0.50
10:L:46:PRO:HD2	10:L:52:LYS:O	2.11	0.50
5:E:108:VAL:HB	5:E:162:LEU:HB2	1.94	0.50
2:B:192:ILE:HB	2:B:206:GLU:HB2	1.93	0.50
1:A:353:ILE:HD11	1:A:407:VAL:HG23	1.93	0.50
2:B:694:ARG:HE	2:B:759:ARG:HH21	1.60	0.50
9:K:50:LEU:HD13	9:K:75:PRO:HD3	1.94	0.50
1:A:654:GLY:HA2	1:A:658:LYS:HE3	1.93	0.50
2:B:483:ILE:HD11	2:B:555:GLU:HB2	1.94	0.50
1:A:870:ARG:HD2	3:C:57:LYS:HB3	1.93	0.50
2:B:31:LEU:HA	2:B:125:MET:HE1	1.93	0.49
2:B:1069:TYR:CB	2:B:1070:ILE:HB	2.42	0.49
2:B:1007:ARG:NH2	2:B:1026:GLU:O	2.42	0.49
2:B:59:LEU:HD23	2:B:107:GLU:HG2	1.94	0.49
1:A:281:ILE:N	1:A:282:PRO:CD	2.75	0.49
2:B:774:ASP:HB2	2:B:819:PRO:HD3	1.93	0.49
2:B:1069:TYR:HA	2:B:1070:ILE:CB	2.30	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:VAL:HG22	4:D:161:LEU:H	1.76	0.49
2:B:897:GLN:HG3	2:B:908:VAL:HG21	1.95	0.49
3:C:122:MET:HG2	3:C:274:THR:HG23	1.93	0.49
2:B:680:LEU:HD21	2:B:997:HIS:HB3	1.95	0.49
2:B:741:ILE:HG22	2:B:891:ILE:HA	1.94	0.49
2:B:591:LEU:HD23	2:B:615:LYS:HB3	1.93	0.49
2:B:520:TRP:O	2:B:521:SER:CB	2.60	0.49
3:C:274:THR:HB	3:C:280:ILE:HD11	1.95	0.49
2:B:961:LEU:HA	2:B:965:TYR:O	2.13	0.49
2:B:31:LEU:HA	2:B:125:MET:CE	2.43	0.48
2:B:448:LEU:HD11	2:B:458:PRO:HB3	1.94	0.48
2:B:1112:ILE:O	2:B:1114:PRO:HD3	2.12	0.48
1:A:541:ALA:HB2	7:G:72:CYS:HB2	1.95	0.48
2:B:734:GLY:HA3	2:B:735:TYR:CG	2.49	0.48
1:A:624:GLY:O	1:A:628:MET:HG2	2.13	0.48
7:G:11:LEU:HB2	7:G:57:ALA:HB3	1.95	0.48
7:G:29:ILE:O	7:G:39:SER:HA	2.14	0.48
11:N:8:PHE:CD1	11:N:48:MET:HE3	2.49	0.48
3:C:261:VAL:HG12	3:C:267:VAL:HG11	1.96	0.48
5:E:144:ALA:HA	5:E:169:LEU:HD23	1.94	0.48
4:D:73:LEU:HD11	4:D:236:LEU:HD21	1.95	0.48
2:B:55:GLU:HG3	2:B:373:GLU:HG3	1.96	0.48
3:C:112:ASP:HA	3:C:328:GLN:HG3	1.95	0.48
7:G:42:ILE:HG21	7:G:48:ILE:HG23	1.96	0.48
2:B:1051:ARG:HA	2:B:1051:ARG:NE	2.28	0.48
1:A:737:VAL:HG23	1:A:738:LEU:H	1.77	0.48
1:A:125:TRP:N	1:A:126:PRO:CD	2.77	0.47
1:A:402:ALA:HB1	1:A:403:PRO:HD2	1.95	0.47
7:G:55:VAL:HG23	7:G:117:GLN:HA	1.94	0.47
2:B:816:LYS:H	2:B:839:SER:HB3	1.79	0.47
4:D:253:ILE:HG13	10:L:73:ILE:HG23	1.95	0.47
5:E:171:LYS:HB2	5:E:174:TRP:HB2	1.96	0.47
4:D:153:HIS:HE2	12:P:48:ILE:HG23	1.79	0.47
2:B:856:THR:HG22	2:B:857:GLU:H	1.80	0.47
1:A:428:ILE:CG2	1:A:452:PRO:HB3	2.45	0.47
3:C:287:GLU:HG2	8:H:79:ARG:HH21	1.80	0.47
2:B:745:ARG:HD2	2:B:896:PRO:HG3	1.96	0.47
2:B:653:ILE:H	2:B:653:ILE:HD12	1.78	0.47
3:C:78:VAL:HG23	3:C:308:VAL:HG11	1.95	0.47
1:A:216:PRO:HD2	1:A:219:ILE:HD12	1.97	0.47
1:A:734:ARG:HH12	2:B:917:ALA:HA	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:PRO:HG3	2:B:884:ARG:NH2	2.30	0.47
1:A:488:THR:HG22	1:A:490:ARG:N	2.29	0.47
2:B:975:ASP:HB3	2:B:978:THR:HG22	1.97	0.47
1:A:432:ALA:O	1:A:482:VAL:HG23	2.15	0.47
2:B:200:ARG:HH12	2:B:298:LYS:HD2	1.80	0.47
2:B:742:ILE:HD11	2:B:895:ILE:HB	1.97	0.46
2:B:1074:ASP:HB3	2:B:1075:LYS:CA	2.45	0.46
1:A:541:ALA:HB3	1:A:542:PRO:HD3	1.96	0.46
2:B:175:VAL:HG22	2:B:192:ILE:HG12	1.97	0.46
4:D:66:PRO:HG3	11:N:6:ARG:HH21	1.81	0.46
1:A:28:ILE:HG22	1:A:29:THR:H	1.80	0.46
1:A:326:ILE:HG22	1:A:443:PHE:HB2	1.98	0.46
1:A:280:GLU:H	1:A:282:PRO:HD2	1.81	0.46
1:A:80:PRO:HD2	1:A:178:SER:HB3	1.97	0.46
7:G:40:PHE:HA	7:G:92:TYR:HD1	1.79	0.46
2:B:536:GLY:HA3	2:B:560:HIS:CE1	2.51	0.46
1:A:286:PRO:HG2	1:A:288:LYS:HE3	1.96	0.46
1:A:848:VAL:O	1:A:849:ALA:CB	2.63	0.46
2:B:675:MET:HG3	2:B:996:LEU:HD21	1.97	0.46
1:A:380:ARG:HH11	1:A:384:ARG:HH21	1.63	0.46
4:D:154:ALA:C	4:D:156:PHE:H	2.19	0.46
2:B:877:ILE:HD12	2:B:877:ILE:H	1.81	0.46
1:A:600:LYS:O	1:A:601:LYS:CB	2.57	0.46
1:A:491:TYR:OH	1:A:606:GLN:HG2	2.16	0.46
7:G:48:ILE:HG22	7:G:49:PHE:H	1.81	0.46
2:B:459:PHE:O	2:B:461:THR:N	2.49	0.46
4:D:98:ILE:HD13	4:D:141:LEU:HD11	1.97	0.46
3:C:28:ILE:HD13	9:K:14:HIS:CE1	2.51	0.46
2:B:973:THR:HG21	2:B:988:PHE:CE1	2.50	0.46
1:A:296:ARG:HD2	1:A:296:ARG:H	1.80	0.46
1:A:323:ARG:HB2	2:B:1029:LEU:HD21	1.96	0.46
8:H:39:PRO:HB2	8:H:80:TYR:CD2	2.50	0.46
1:A:334:ILE:HD12	1:A:628:MET:HB3	1.98	0.46
3:C:168:GLN:HG2	3:C:204:THR:HG23	1.98	0.46
1:A:94:LEU:HD21	1:A:180:ILE:HG23	1.97	0.46
3:C:122:MET:HB2	3:C:253:THR:OG1	2.16	0.46
4:D:129:PRO:HD2	11:N:15:ALA:HB1	1.97	0.46
2:B:874:ILE:H	2:B:874:ILE:HD12	1.81	0.46
1:A:489:PRO:HA	1:A:858:MET:HB2	1.98	0.46
1:A:777:GLU:HG3	1:A:783:TYR:CE2	2.50	0.45
4:D:161:LEU:O	4:D:230:LEU:HA	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:61:VAL:H	9:K:64:ILE:HD12	1.81	0.45
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.47	0.45
2:B:532:TYR:O	2:B:533:TYR:HB3	2.17	0.45
3:C:70:ILE:H	3:C:70:ILE:HD13	1.82	0.45
2:B:1005:HIS:NE2	2:B:1023:ARG:HA	2.30	0.45
2:B:86:MET:O	2:B:90:LEU:HG	2.16	0.45
2:B:500:VAL:O	2:B:504:ILE:HG12	2.16	0.45
2:B:417:LEU:HD21	2:B:425:MET:HG3	1.98	0.45
1:A:530:VAL:HB	1:A:532:ILE:HG13	1.98	0.45
1:A:798:HIS:HE2	2:B:666:SER:H	1.64	0.45
1:A:519:GLU:HG2	10:L:33:ARG:HD2	1.99	0.45
4:D:38:VAL:HG12	4:D:39:MET:N	2.31	0.45
2:B:598:GLU:HB3	2:B:599:LYS:H	1.66	0.45
2:B:51:GLU:HB2	2:B:53:PRO:HD3	1.98	0.45
3:C:199:ASP:HB2	3:C:206:LEU:HB2	1.98	0.45
1:A:238:LYS:NZ	1:A:297:THR:HA	2.32	0.45
1:A:645:THR:OG1	1:A:646:MET:N	2.45	0.45
1:A:516:LEU:HD23	1:A:521:ALA:HA	1.99	0.45
3:C:28:ILE:H	3:C:28:ILE:HG13	1.57	0.45
3:C:340:SER:CB	3:C:371:GLU:HG2	2.47	0.45
1:A:275:THR:O	1:A:297:THR:HG21	2.17	0.44
2:B:1050:ASP:HA	2:B:1054:ASP:HB2	1.99	0.44
2:B:689:LEU:HD13	11:N:62:TYR:HB3	1.99	0.44
2:B:235:ILE:HA	2:B:312:ARG:HH21	1.83	0.44
1:A:331:ASN:O	1:A:332:ILE:HG12	2.17	0.44
6:F:21:LEU:O	6:F:24:VAL:HG12	2.17	0.44
2:B:341:TYR:CE1	2:B:452:GLN:HG2	2.52	0.44
1:A:190:SER:O	1:A:194:ILE:HG13	2.18	0.44
2:B:430:ARG:HH11	2:B:653:ILE:HG13	1.82	0.44
1:A:296:ARG:N	1:A:296:ARG:HD2	2.32	0.44
1:A:857:PRO:HB3	3:C:309:ASP:OD1	2.18	0.44
1:A:434:ARG:HD3	1:A:481:LEU:HD21	2.00	0.44
1:A:102:GLY:HA3	1:A:187:VAL:HG12	1.99	0.44
3:C:13:LEU:HD23	3:C:16:LYS:HD3	1.99	0.44
5:E:97:ILE:HB	5:E:108:VAL:HG13	1.98	0.44
1:A:644:PHE:HB3	2:B:731:SER:OG	2.18	0.44
2:B:110:ILE:CA	2:B:111:GLU:CB	2.71	0.44
3:C:13:LEU:HD13	3:C:48:ILE:HG12	1.99	0.44
2:B:970:THR:HA	2:B:987:TYR:HA	1.99	0.44
3:C:391:ARG:NH2	9:K:77:THR:OG1	2.51	0.44
12:P:25:ARG:HG2	12:P:32:LYS:HG2	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:786:TYR:CE2	2:B:788:GLY:HA2	2.53	0.44
1:A:527:VAL:HG12	1:A:633:ARG:HG2	1.99	0.44
2:B:937:ALA:O	11:N:46:ARG:HD2	2.18	0.44
2:B:742:ILE:HG12	2:B:893:MET:O	2.17	0.44
3:C:231:ILE:HG22	3:C:232:LYS:H	1.83	0.44
11:N:7:CYS:HB3	11:N:10:CYS:SG	2.58	0.44
2:B:597:ILE:HD13	2:B:597:ILE:H	1.82	0.44
2:B:985:ARG:HH12	4:D:208:GLU:HG2	1.83	0.44
2:B:583:ILE:HD12	2:B:591:LEU:HD21	1.99	0.44
1:A:573:ARG:NH1	1:A:573:ARG:HG3	2.33	0.44
1:A:733:ALA:O	1:A:734:ARG:C	2.56	0.44
2:B:737:MET:H	2:B:740:SER:HB3	1.82	0.44
2:B:242:VAL:HG22	2:B:256:PHE:HB3	2.00	0.43
2:B:936:ALA:HA	2:B:941:ASN:O	2.17	0.43
3:C:201:SER:HB2	3:C:204:THR:HB	2.00	0.43
1:A:450:CYS:HB2	1:A:451:PRO:HD3	2.00	0.43
1:A:672:VAL:HG11	1:A:776:PRO:HD3	2.00	0.43
2:B:46:ILE:HG13	2:B:66:ILE:HG12	2.00	0.43
2:B:582:LEU:HD12	2:B:619:LEU:HD12	2.00	0.43
4:D:159:VAL:HG21	4:D:230:LEU:HD22	1.99	0.43
1:A:23:SER:HB2	1:A:74:HIS:NE2	2.33	0.43
2:B:733:THR:HG23	2:B:734:GLY:N	2.34	0.43
8:H:62:ILE:HG22	8:H:80:TYR:HA	2.00	0.43
2:B:400:ALA:O	2:B:405:ASN:HA	2.17	0.43
3:C:268:ASP:O	3:C:272:VAL:HG23	2.19	0.43
1:A:425:LEU:HD23	3:C:83:THR:HG21	2.00	0.43
12:P:21:LEU:HD22	12:P:22:PRO:HA	2.01	0.43
3:C:197:VAL:HB	3:C:208:ILE:HB	2.00	0.43
1:A:823:LEU:HA	1:A:826:ALA:HB3	2.01	0.43
3:C:107:LEU:HA	3:C:110:ILE:HG22	2.00	0.43
2:B:594:ARG:HH12	2:B:615:LYS:HB2	1.82	0.43
2:B:961:LEU:HD12	2:B:967:PRO:HD3	2.01	0.43
2:B:873:ARG:HH22	2:B:1002:ASP:CG	2.22	0.43
2:B:209:LYS:C	2:B:211:GLY:H	2.22	0.43
2:B:594:ARG:HH11	2:B:610:LEU:HD23	1.84	0.43
12:P:21:LEU:HA	12:P:22:PRO:HA	1.87	0.43
5:E:30:LEU:HD22	5:E:72:PHE:CE1	2.54	0.43
3:C:127:THR:HB	3:C:128:ASP:H	1.66	0.43
1:A:10:LYS:HG2	3:C:363:VAL:HG13	2.01	0.43
2:B:345:ARG:HG3	2:B:576:GLY:HA3	2.01	0.43
1:A:372:TRP:O	1:A:410:HIS:ND1	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:VAL:HB	1:A:595:GLU:HB2	2.01	0.43
2:B:147:ASP:HB3	2:B:685:ALA:HB3	2.01	0.43
4:D:17:PHE:O	4:D:225:LYS:HA	2.19	0.43
2:B:454:GLY:HA3	2:B:580:ARG:HE	1.83	0.43
1:A:739:ASN:HB2	2:B:922:MET:SD	2.59	0.43
2:B:84:SER:HB2	2:B:144:ILE:HD12	2.01	0.43
3:C:127:THR:N	3:C:268:ASP:HB2	2.34	0.42
1:A:104:VAL:HG13	1:A:143:ALA:HB2	2.00	0.42
2:B:190:ALA:HB3	2:B:208:LEU:HD12	2.02	0.42
1:A:16:PRO:HA	1:A:19:ILE:HD12	2.00	0.42
2:B:406:TRP:O	2:B:408:GLY:N	2.52	0.42
2:B:816:LYS:N	2:B:839:SER:HB3	2.35	0.42
4:D:38:VAL:CG1	4:D:39:MET:N	2.82	0.42
2:B:262:ALA:HB1	2:B:265:ILE:HB	2.00	0.42
1:A:13:ILE:HD12	1:A:202:SER:HB2	2.01	0.42
3:C:50:LYS:O	3:C:54:LEU:HG	2.19	0.42
2:B:884:ARG:HH12	2:B:992:TYR:HB3	1.80	0.42
2:B:720:PRO:HG3	11:N:53:ILE:HD12	2.01	0.42
3:C:47:GLU:CB	3:C:50:LYS:HB2	2.50	0.42
3:C:179:VAL:HG11	3:C:232:LYS:HZ2	1.84	0.42
1:A:313:LEU:HD22	3:C:374:ILE:HG23	2.01	0.42
2:B:1061:ILE:HD13	2:B:1096:VAL:HB	2.00	0.42
5:E:129:GLY:H	5:E:137:GLN:HB3	1.85	0.42
1:A:575:CYS:SG	1:A:584:SER:HB3	2.60	0.42
2:B:430:ARG:HD3	2:B:653:ILE:CG1	2.50	0.42
2:B:174:ARG:HB3	2:B:527:GLY:HA3	2.01	0.42
1:A:760:GLY:HA2	2:B:450:GLY:HA3	2.02	0.42
2:B:1040:ILE:HG23	3:C:381:LEU:HD11	2.02	0.42
1:A:141:MET:HG3	1:A:148:HIS:HA	2.02	0.42
2:B:953:ILE:N	2:B:953:ILE:HD13	2.18	0.42
2:B:646:TRP:CD2	2:B:648:PRO:HD2	2.55	0.42
3:C:257:ASN:O	3:C:261:VAL:HG23	2.20	0.42
2:B:938:LEU:HD23	11:N:43:TYR:HB3	2.01	0.42
1:A:705:ASP:O	1:A:708:ARG:HG3	2.20	0.42
1:A:58:CYS:HA	1:A:59:PRO:HD3	1.91	0.42
2:B:41:LYS:O	2:B:43:GLN:N	2.52	0.42
2:B:651:LEU:HB3	2:B:655:ALA:HB3	2.01	0.42
7:G:18:ILE:HD12	7:G:29:ILE:HG12	2.02	0.42
2:B:918:LEU:H	2:B:919:PRO:HD2	1.85	0.42
2:B:430:ARG:HD3	2:B:653:ILE:HG12	2.02	0.42
1:A:450:CYS:O	1:A:454:ASN:N	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1107:LEU:HD21	3:C:354:LEU:HD13	2.01	0.42
2:B:783:VAL:HG13	2:B:784:ARG:HB2	2.02	0.41
2:B:1111:ILE:HG22	2:B:1111:ILE:O	2.20	0.41
2:B:705:LEU:O	2:B:706:VAL:HB	2.20	0.41
1:A:515:LEU:HB3	1:A:545:TYR:CD1	2.55	0.41
7:G:103:VAL:HG13	7:G:104:LYS:HG2	2.02	0.41
2:B:285:ARG:HD3	2:B:289:ILE:HD11	2.02	0.41
1:A:502:TYR:CD1	1:A:632:PHE:HB3	2.55	0.41
1:A:426:HIS:NE2	1:A:489:PRO:HD2	2.35	0.41
1:A:646:MET:HG2	2:B:918:LEU:HD13	2.01	0.41
2:B:589:ASN:HA	2:B:590:PRO:HD3	1.90	0.41
2:B:928:MET:HE3	2:B:953:ILE:HD12	2.02	0.41
2:B:914:ASN:HA	2:B:915:PRO:HD2	1.88	0.41
1:A:580:CYS:HA	1:A:581:PRO:HD3	1.88	0.41
8:H:44:TRP:O	8:H:79:ARG:HD2	2.20	0.41
2:B:99:LEU:HD11	2:B:122:LEU:HB2	2.02	0.41
5:E:8:ARG:HH12	6:F:7:VAL:HG11	1.85	0.41
2:B:1081:VAL:HG22	2:B:1085:HIS:HA	2.01	0.41
11:N:24:ARG:HD2	11:N:34:VAL:HG13	2.03	0.41
3:C:387:GLU:HG3	9:K:79:ARG:HB2	2.02	0.41
1:A:69:PRO:HG2	2:B:1101:LYS:HE3	2.02	0.41
9:K:74:LEU:HA	9:K:75:PRO:HD3	1.91	0.41
1:A:339:VAL:O	1:A:437:VAL:HA	2.20	0.41
3:C:377:HIS:HA	3:C:378:PRO:HD2	1.90	0.41
3:C:323:THR:O	3:C:325:VAL:N	2.53	0.41
4:D:172:ILE:HD11	4:D:197:VAL:HG23	2.03	0.41
1:A:866:VAL:O	1:A:870:ARG:NH1	2.35	0.41
2:B:974:TYR:CD2	2:B:981:LYS:HB3	2.56	0.41
1:A:379:ILE:HB	1:A:406:VAL:HB	2.03	0.41
1:A:416:VAL:HB	1:A:473:ILE:HG23	2.03	0.41
11:N:5:ILE:O	11:N:6:ARG:HB2	2.21	0.41
1:A:823:LEU:HD13	3:C:75:ALA:HB1	2.03	0.41
2:B:174:ARG:HH21	2:B:526:ASN:HA	1.86	0.41
1:A:52:ILE:HG23	1:A:217:ILE:HG23	2.02	0.41
2:B:818:SER:HB2	2:B:836:ARG:HB2	2.03	0.41
1:A:114:TYR:HA	1:A:118:TYR:HD2	1.85	0.41
2:B:497:VAL:HA	2:B:533:TYR:HB2	2.02	0.41
1:A:500:GLN:HB2	2:B:916:HIS:CD2	2.56	0.41
2:B:476:MET:HE1	2:B:645:ILE:HB	2.03	0.41
3:C:235:LYS:HB3	3:C:235:LYS:HE3	1.95	0.41
2:B:946:THR:HA	2:B:947:PRO:HD2	1.91	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ARG:HB2	1:A:206:TRP:CD2	2.56	0.41
2:B:1057:ASP:OD2	2:B:1057:ASP:N	2.54	0.41
1:A:73:GLY:O	1:A:214:VAL:N	2.53	0.41
2:B:658:ILE:HG12	2:B:672:GLN:HG2	2.01	0.41
8:H:20:HIS:CG	8:H:51:VAL:HG11	2.55	0.41
8:H:23:LEU:HB3	8:H:28:ALA:HB2	2.03	0.41
2:B:884:ARG:HB2	2:B:884:ARG:NH1	2.34	0.41
3:C:69:ALA:HB2	3:C:381:LEU:HD13	2.03	0.41
2:B:1053:LEU:HD13	3:C:376:GLY:HA3	2.03	0.41
2:B:1005:HIS:CE1	2:B:1007:ARG:CZ	3.04	0.40
2:B:86:MET:HE1	2:B:690:ARG:HD3	2.03	0.40
2:B:1077:LYS:HA	2:B:1078:ASN:HA	1.78	0.40
2:B:579:ARG:HD3	2:B:618:TYR:HB3	2.03	0.40
8:H:49:ASP:OD2	8:H:50:PRO:HD2	2.21	0.40
1:A:470:GLU:HG2	1:A:470:GLU:H	1.63	0.40
1:A:563:HIS:HB2	1:A:872:PHE:HE2	1.86	0.40
3:C:235:LYS:HB3	3:C:236:GLY:H	1.66	0.40
2:B:605:ILE:HG23	2:B:606:THR:N	2.36	0.40
2:B:1054:ASP:HA	2:B:1058:ARG:HD2	2.02	0.40
1:A:10:LYS:HG3	2:B:1117:ILE:HD11	2.03	0.40
4:D:41:ILE:HG12	4:D:41:ILE:H	1.72	0.40
1:A:235:LEU:HG	1:A:238:LYS:HE3	2.03	0.40
1:A:838:VAL:HG13	3:C:70:ILE:HD11	2.03	0.40
3:C:11:SER:O	3:C:13:LEU:N	2.54	0.40
2:B:720:PRO:HG3	11:N:53:ILE:CD1	2.51	0.40
1:A:14:LEU:HB3	2:B:1111:ILE:HG23	2.04	0.40
3:C:329:ILE:HA	3:C:334:VAL:HB	2.04	0.40
2:B:814:ILE:HB	2:B:840:ILE:HB	2.03	0.40
5:E:131:LYS:HD2	5:E:136:ILE:HD13	2.02	0.40
7:G:67:THR:HG22	7:G:68:ASN:H	1.86	0.40
2:B:81:ARG:HA	2:B:81:ARG:HD3	1.89	0.40
2:B:783:VAL:HG12	2:B:784:ARG:HB2	2.02	0.40
2:B:913:LEU:HD12	2:B:926:GLN:HE21	1.86	0.40
2:B:585:VAL:HG21	2:B:636:LEU:HD11	2.04	0.40
5:E:39:LEU:HA	5:E:153:VAL:HG23	2.04	0.40
1:A:29:THR:HB	1:A:30:PRO:HD3	2.03	0.40
2:B:84:SER:OG	2:B:144:ILE:HG23	2.21	0.40
11:N:19:GLN:N	11:N:20:PRO:HD2	2.37	0.40
3:C:265:LYS:HD2	3:C:265:LYS:H	1.86	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	833/880 (95%)	692 (83%)	112 (13%)	29 (4%)	4	32
2	B	1082/1131 (96%)	908 (84%)	127 (12%)	47 (4%)	3	26
3	C	363/395 (92%)	288 (79%)	61 (17%)	14 (4%)	4	29
4	D	256/265 (97%)	227 (89%)	25 (10%)	4 (2%)	12	49
5	E	170/180 (94%)	152 (89%)	16 (9%)	2 (1%)	16	56
6	F	88/113 (78%)	74 (84%)	11 (12%)	3 (3%)	5	33
7	G	111/132 (84%)	96 (86%)	13 (12%)	2 (2%)	11	47
8	H	72/84 (86%)	59 (82%)	8 (11%)	5 (7%)	1	12
9	K	80/95 (84%)	69 (86%)	7 (9%)	4 (5%)	3	21
10	L	89/92 (97%)	79 (89%)	8 (9%)	2 (2%)	8	43
11	N	62/66 (94%)	50 (81%)	10 (16%)	2 (3%)	5	34
12	P	41/48 (85%)	32 (78%)	7 (17%)	2 (5%)	3	22
13	Q	43/104 (41%)	36 (84%)	6 (14%)	1 (2%)	8	42
All	All	3290/3585 (92%)	2762 (84%)	411 (12%)	117 (4%)	4	31

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	734	ARG
1	A	737	VAL
2	B	28	ARG
2	B	111	GLU
2	B	460	GLU
2	B	521	SER
2	B	590	PRO
2	B	735	TYR
2	B	950	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1070	ILE
8	H	13	ILE
9	K	61	VAL
1	A	256	GLY
1	A	280	GLU
1	A	332	ILE
1	A	732	GLY
1	A	876	VAL
2	B	605	ILE
2	B	739	ASP
2	B	797	ASP
2	B	809	GLY
2	B	877	ILE
2	B	1072	TRP
3	C	12	TYR
3	C	245	LYS
3	C	324	GLY
3	C	365	GLU
3	C	393	ILE
4	D	117	GLU
4	D	206	CYS
1	A	45	MET
1	A	290	ARG
1	A	536	GLU
1	A	733	ALA
1	A	849	ALA
2	B	26	LEU
2	B	49	GLN
2	B	250	GLU
2	B	256	PHE
2	B	734	GLY
2	B	918	LEU
2	B	943	VAL
2	B	985	ARG
2	B	1026	GLU
2	B	1029	LEU
3	C	113	ALA
3	C	114	LYS
7	G	99	PHE
9	K	25	ASN
9	K	91	SER
11	N	41	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	P	13	PHE
1	A	46	ASP
1	A	79	ARG
1	A	155	LYS
1	A	287	SER
1	A	393	ASP
1	A	601	LYS
2	B	71	PRO
2	B	202	PRO
2	B	375	SER
2	B	407	VAL
2	B	606	THR
2	B	706	VAL
2	B	773	GLU
2	B	949	TYR
2	B	951	THR
3	C	201	SER
4	D	79	PRO
4	D	193	GLY
5	E	82	GLN
8	H	15	TYR
8	H	81	VAL
10	L	19	GLY
11	N	6	ARG
1	A	106	ILE
1	A	125	TRP
1	A	257	ALA
1	A	308	ARG
1	A	541	ALA
1	A	738	LEU
2	B	56	ILE
2	B	334	GLU
2	B	437	ALA
2	B	453	TRP
2	B	533	TYR
2	B	771	GLY
2	B	781	PRO
2	B	907	VAL
3	C	44	THR
3	C	218	ALA
3	C	349	VAL
9	K	14	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	L	10	SER
12	P	11	LYS
1	A	62	GLY
2	B	183	GLY
2	B	948	PHE
2	B	1073	TYR
3	C	190	ARG
3	C	235	LYS
3	C	236	GLY
5	E	127	ILE
6	F	47	CYS
7	G	105	ILE
8	H	10	ASP
8	H	60	GLY
1	A	145	VAL
1	A	29	THR
1	A	760	GLY
2	B	113	GLU
2	B	588	GLY
2	B	1114	PRO
13	Q	59	ILE
6	F	25	ILE
6	F	4	VAL

### 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	729/766 (95%)	680 (93%)	49 (7%)	20	59
2	B	941/975 (96%)	866 (92%)	75 (8%)	15	50
3	C	315/341 (92%)	289 (92%)	26 (8%)	14	48
4	D	233/238 (98%)	226 (97%)	7 (3%)	48	80
5	E	154/158 (98%)	145 (94%)	9 (6%)	25	64
6	F	84/107 (78%)	79 (94%)	5 (6%)	24	62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	106/125 (85%)	102 (96%)	4 (4%)	40	75
8	H	67/75 (89%)	66 (98%)	1 (2%)	72	89
9	K	72/83 (87%)	70 (97%)	2 (3%)	51	82
10	L	79/80 (99%)	78 (99%)	1 (1%)	76	90
11	N	58/60 (97%)	53 (91%)	5 (9%)	13	46
12	P	39/43 (91%)	38 (97%)	1 (3%)	54	83
13	Q	43/96 (45%)	41 (95%)	2 (5%)	32	71
All	All	2920/3147 (93%)	2733 (94%)	187 (6%)	22	60

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	28	ILE
1	A	45	MET
1	A	61	CYS
1	A	64	THR
1	A	84	VAL
1	A	87	VAL
1	A	88	LYS
1	A	101	CYS
1	A	105	LYS
1	A	119	ASN
1	A	133	THR
1	A	139	THR
1	A	152	LYS
1	A	155	LYS
1	A	220	ARG
1	A	254	ASP
1	A	284	LEU
1	A	296	ARG
1	A	324	THR
1	A	349	VAL
1	A	366	ILE
1	A	417	VAL
1	A	419	PHE
1	A	425	LEU
1	A	438	LEU
1	A	464	LEU
1	A	470	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	549	LYS
1	A	551	VAL
1	A	573	ARG
1	A	580	CYS
1	A	584	SER
1	A	593	LEU
1	A	603	ILE
1	A	605	ASN
1	A	653	LEU
1	A	675	LEU
1	A	687	ILE
1	A	708	ARG
1	A	723	ASN
1	A	763	THR
1	A	764	ARG
1	A	774	ILE
1	A	787	ARG
1	A	790	LEU
1	A	823	LEU
1	A	868	VAL
1	A	876	VAL
2	B	32	ASP
2	B	52	ILE
2	B	66	ILE
2	B	84	SER
2	B	104	ILE
2	B	111	GLU
2	B	138	LEU
2	B	166	THR
2	B	177	VAL
2	B	213	PHE
2	B	237	THR
2	B	252	GLN
2	B	259	LEU
2	B	318	LEU
2	B	336	ASP
2	B	344	LYS
2	B	345	ARG
2	B	391	ASP
2	B	397	ILE
2	B	418	ASP
2	B	419	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	426	LEU
2	B	436	LEU
2	B	444	GLU
2	B	448	LEU
2	B	456	MET
2	B	466	ASN
2	B	470	VAL
2	B	471	LYS
2	B	481	VAL
2	B	505	ARG
2	B	525	LEU
2	B	529	LEU
2	B	539	LEU
2	B	579	ARG
2	B	591	LEU
2	B	597	ILE
2	B	610	LEU
2	B	613	GLN
2	B	639	GLU
2	B	653	ILE
2	B	662	GLU
2	B	675	MET
2	B	688	GLN
2	B	711	LEU
2	B	717	THR
2	B	730	ILE
2	B	735	TYR
2	B	741	ILE
2	B	742	ILE
2	B	763	THR
2	B	767	LYS
2	B	802	SER
2	B	811	ASP
2	B	843	ARG
2	B	854	LEU
2	B	856	THR
2	B	874	ILE
2	B	884	ARG
2	B	898	VAL
2	B	903	THR
2	B	905	LYS
2	B	913	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	924	LEU
2	B	950	LYS
2	B	953	ILE
2	B	977	ARG
2	B	994	GLN
2	B	1017	ARG
2	B	1026	GLU
2	B	1051	ARG
2	B	1070	ILE
2	B	1079	LYS
2	B	1081	VAL
2	B	1118	LEU
3	C	19	GLN
3	C	24	LEU
3	C	46	ASP
3	C	47	GLU
3	C	49	ASP
3	C	52	PHE
3	C	70	ILE
3	C	107	LEU
3	C	129	GLU
3	C	174	LEU
3	C	213	ILE
3	C	231	ILE
3	C	277	ILE
3	C	278	ARG
3	C	292	ILE
3	C	307	ASP
3	C	311	ARG
3	C	315	LEU
3	C	318	ASP
3	C	327	ARG
3	C	331	ARG
3	C	338	LYS
3	C	362	ASP
3	C	365	GLU
3	C	380	LYS
3	C	386	VAL
4	D	13	ILE
4	D	151	LYS
4	D	165	ARG
4	D	172	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	D	178	LYS
4	D	253	ILE
4	D	258	LYS
5	E	8	ARG
5	E	27	LEU
5	E	30	LEU
5	E	48	ILE
5	E	53	THR
5	E	59	LEU
5	E	117	THR
5	E	137	GLN
5	E	142	VAL
6	F	24	VAL
6	F	62	ILE
6	F	63	ILE
6	F	88	ILE
6	F	90	ASP
7	G	48	ILE
7	G	67	THR
7	G	104	LYS
7	G	106	ILE
8	H	16	LEU
9	K	52	ASP
9	K	74	LEU
10	L	24	LEU
11	N	3	ILE
11	N	5	ILE
11	N	45	CYS
11	N	61	HIS
11	N	63	THR
12	P	41	THR
13	Q	40	ILE
13	Q	69	GLU

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

Mol	Chain	Res	Type
1	A	565	GLN
2	B	442	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	F3S	D	1001	4	0,9,9	0.00	-	0,15,15	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	F3S	D	1001	4	-	0/0/24/24	0/0/3/3

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	841/880 (95%)	-0.05	12 (1%) 78 79	40, 69, 119, 184	0
2	B	1090/1131 (96%)	0.08	27 (2%) 61 60	43, 71, 136, 201	0
3	C	367/395 (92%)	0.46	33 (8%) 12 12	48, 81, 151, 202	0
4	D	260/265 (98%)	0.26	10 (3%) 44 44	66, 93, 131, 200	0
5	E	174/180 (96%)	0.96	34 (19%) 1 2	58, 144, 188, 210	0
6	F	90/113 (79%)	0.83	13 (14%) 3 3	95, 175, 222, 230	0
7	G	113/132 (85%)	0.37	6 (5%) 30 30	66, 105, 147, 156	0
8	H	74/84 (88%)	0.02	0 100 100	60, 84, 103, 108	0
9	K	82/95 (86%)	0.01	2 (2%) 62 62	50, 67, 90, 99	0
10	L	91/92 (98%)	0.17	4 (4%) 38 37	51, 90, 121, 140	0
11	N	64/66 (96%)	0.00	1 (1%) 74 75	60, 71, 113, 140	0
12	P	43/48 (89%)	0.17	1 (2%) 64 64	72, 93, 135, 146	0
13	Q	45/104 (43%)	1.00	7 (15%) 3 3	83, 121, 150, 169	0
All	All	3334/3585 (92%)	0.19	150 (4%) 37 36	40, 81, 156, 230	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	153	VAL	5.8
5	E	135	VAL	5.7
2	B	267	ASN	5.3
5	E	87	GLY	5.0
6	F	81	ASP	4.9
5	E	125	GLY	4.8
5	E	140	ASP	4.3
5	E	167	PRO	4.2
5	E	92	VAL	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	159	ASP	3.8
5	E	130	GLU	3.8
5	E	86	GLU	3.7
4	D	190	LEU	3.6
1	A	28	ILE	3.6
6	F	78	ILE	3.6
3	C	244	LYS	3.6
2	B	600	LEU	3.6
3	C	184	VAL	3.5
6	F	77	PRO	3.5
3	C	242	VAL	3.4
5	E	172	LEU	3.3
2	B	291	LYS	3.3
4	D	191	LYS	3.3
6	F	85	SER	3.3
3	C	161	ALA	3.3
2	B	309	ASP	3.2
4	D	177	GLU	3.2
5	E	93	ASP	3.2
2	B	266	ALA	3.2
3	C	162	SER	3.1
2	B	299	TYR	3.1
3	C	249	TYR	3.0
5	E	98	PHE	3.0
13	Q	75	TYR	3.0
6	F	76	CYS	3.0
3	C	241	ILE	3.0
2	B	269	ASP	3.0
3	C	254	ASP	3.0
3	C	180	THR	3.0
6	F	57	GLU	3.0
5	E	136	ILE	2.9
2	B	280	ALA	2.9
5	E	129	GLY	2.9
5	E	143	ARG	2.9
3	C	118	SER	2.9
2	B	306	THR	2.9
3	C	183	ASP	2.9
3	C	82	GLY	2.8
5	E	168	TYR	2.8
7	G	105	ILE	2.8
9	K	51	ILE	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
13	Q	48	THR	2.8
7	G	62	ASN	2.8
13	Q	50	ILE	2.8
2	B	601	ASP	2.8
2	B	599	LYS	2.7
5	E	134	LYS	2.7
1	A	285	PRO	2.7
3	C	221	LYS	2.7
2	B	1072	TRP	2.7
2	B	270	ASP	2.7
3	C	196	PHE	2.7
1	A	248	ARG	2.7
3	C	226	ILE	2.7
5	E	137	GLN	2.6
3	C	126	LEU	2.6
10	L	89	GLY	2.6
3	C	165	ILE	2.6
1	A	117	ILE	2.6
6	F	80	PRO	2.6
2	B	1089	SER	2.6
2	B	1080	TYR	2.6
2	B	837	ASP	2.5
10	L	83	TYR	2.5
4	D	264	ILE	2.5
1	A	284	LEU	2.5
7	G	36	PHE	2.5
5	E	81	VAL	2.5
2	B	820	PRO	2.5
5	E	145	ARG	2.5
6	F	5	TYR	2.5
3	C	119	THR	2.4
2	B	52	ILE	2.4
7	G	117	GLN	2.4
2	B	281	ILE	2.4
3	C	206	LEU	2.4
6	F	3	SER	2.4
6	F	79	THR	2.4
1	A	579	ASP	2.4
9	K	58	SER	2.4
5	E	117	THR	2.4
7	G	83	ASP	2.4
6	F	53	GLN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	195	GLU	2.4
5	E	97	ILE	2.4
2	B	834	ALA	2.3
4	D	178	LYS	2.3
1	A	810	ALA	2.3
5	E	139	GLY	2.3
2	B	587	ASN	2.3
3	C	224	ASP	2.3
3	C	169	LEU	2.3
5	E	150	ALA	2.3
5	E	40	LYS	2.3
4	D	189	GLU	2.3
5	E	152	THR	2.3
4	D	175	ASN	2.3
4	D	90	GLU	2.3
12	P	28	TYR	2.3
3	C	220	PHE	2.3
13	Q	56	ASN	2.3
3	C	171	ASN	2.2
3	C	205	THR	2.2
3	C	178	GLY	2.2
1	A	136	VAL	2.2
1	A	105	LYS	2.2
4	D	214	ASN	2.2
2	B	235	ILE	2.2
1	A	42	GLY	2.2
1	A	261	ILE	2.2
2	B	178	ASP	2.2
5	E	131	LYS	2.1
2	B	637	THR	2.1
11	N	27	ALA	2.1
5	E	138	LYS	2.1
1	A	688	PRO	2.1
2	B	746	SER	2.1
6	F	48	ASP	2.1
5	E	121	ASP	2.1
3	C	243	GLN	2.1
5	E	42	LEU	2.1
5	E	72	PHE	2.1
5	E	128	PHE	2.1
13	Q	55	LEU	2.1
3	C	240	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	G	80	GLU	2.1
3	C	213	ILE	2.1
13	Q	41	ILE	2.1
3	C	172	GLU	2.1
5	E	170	GLY	2.1
4	D	192	ASP	2.1
13	Q	45	MET	2.1
5	E	126	ILE	2.0
2	B	779	PRO	2.0
3	C	153	VAL	2.0
10	L	1	MET	2.0
2	B	184	SER	2.0
3	C	83	THR	2.0
6	F	86	ILE	2.0
10	L	12	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	ZN	B	1400	1/1	0.98	0.21	-0.39	62,62,62,62	0
16	F3S	D	1001	7/7	0.98	0.16	-1.01	67,67,67,67	0
14	ZN	P	50	1/1	0.97	0.08	-1.16	71,71,71,71	0
14	ZN	B	1300	1/1	0.99	0.06	-1.70	62,62,62,62	0
14	ZN	A	1300	1/1	1.00	0.04	-1.86	58,58,58,58	0
14	ZN	N	100	1/1	0.97	0.14	-2.03	63,63,63,63	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
14	ZN	A	1350	1/1	0.97	0.07	-2.44	58,58,58,58	0
14	ZN	C	1000	1/1	0.98	0.05	-	58,58,58,58	0
14	ZN	B	1500	1/1	0.99	0.08	-	62,62,62,62	0
15	MG	A	1400	1/1	0.92	0.36	-	58,58,58,58	0
14	ZN	A	1360	1/1	0.98	0.20	-	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.