



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:19 PM GMT

PDB ID : 4BXZ  
Title : RNA Polymerase II-Bye1 complex  
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.  
Deposited on : 2013-07-16  
Resolution : 4.80 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](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

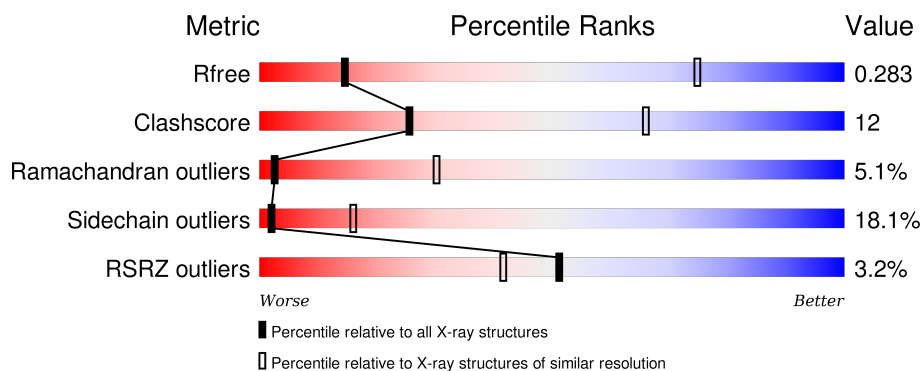
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 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))
$R_{free}$	91344	1117 (6.00-3.60)
Clashscore	102246	1017 (5.96-3.64)
Ramachandran outliers	100387	1156 (6.00-3.60)
Sidechain outliers	100360	1134 (6.00-3.60)
RSRZ outliers	91569	1120 (6.00-3.60)

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	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	155	<div><div></div><div>28%23%46%</div></div>
7	G	171	<div><div>4%</div><div>67%31%</div><div></div></div>
8	H	146	<div><div>6%</div><div>47%38%9%</div><div></div></div>
9	I	122	<div><div>11%</div><div>61%34%</div><div></div></div>
10	J	70	<div><div></div><div>47%37%6%7%</div><div></div></div>
11	K	120	<div><div>%</div><div>65%24%7%</div><div></div></div>
12	L	70	<div><div></div><div>37%20%7%34%</div><div></div></div>
13	X	594	<div><div>%</div><div>17%81%</div><div></div></div>

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31509 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 II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	X	113	Total	C	N	O	0	0	0
			564	338	113	113			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		

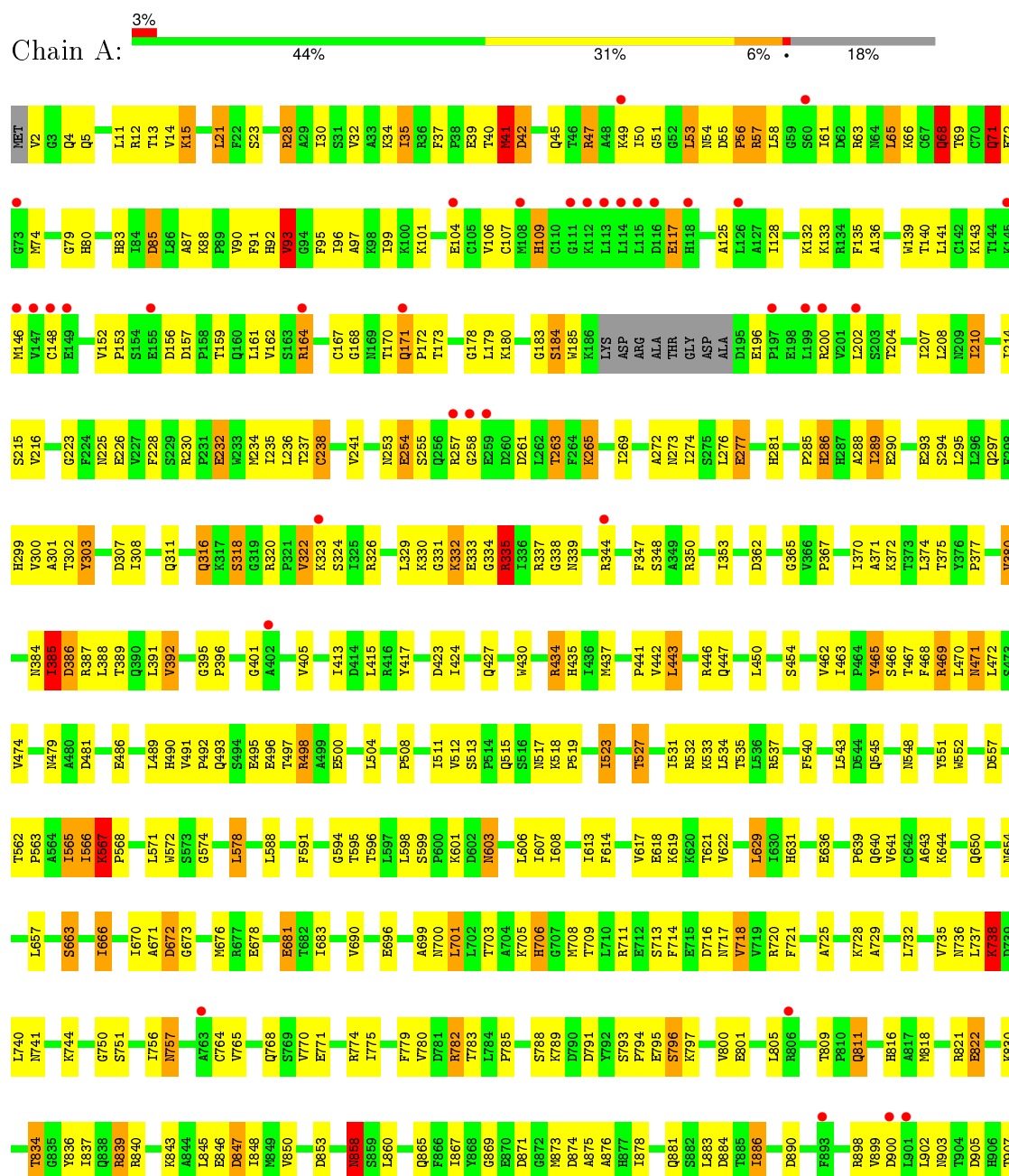
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

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.

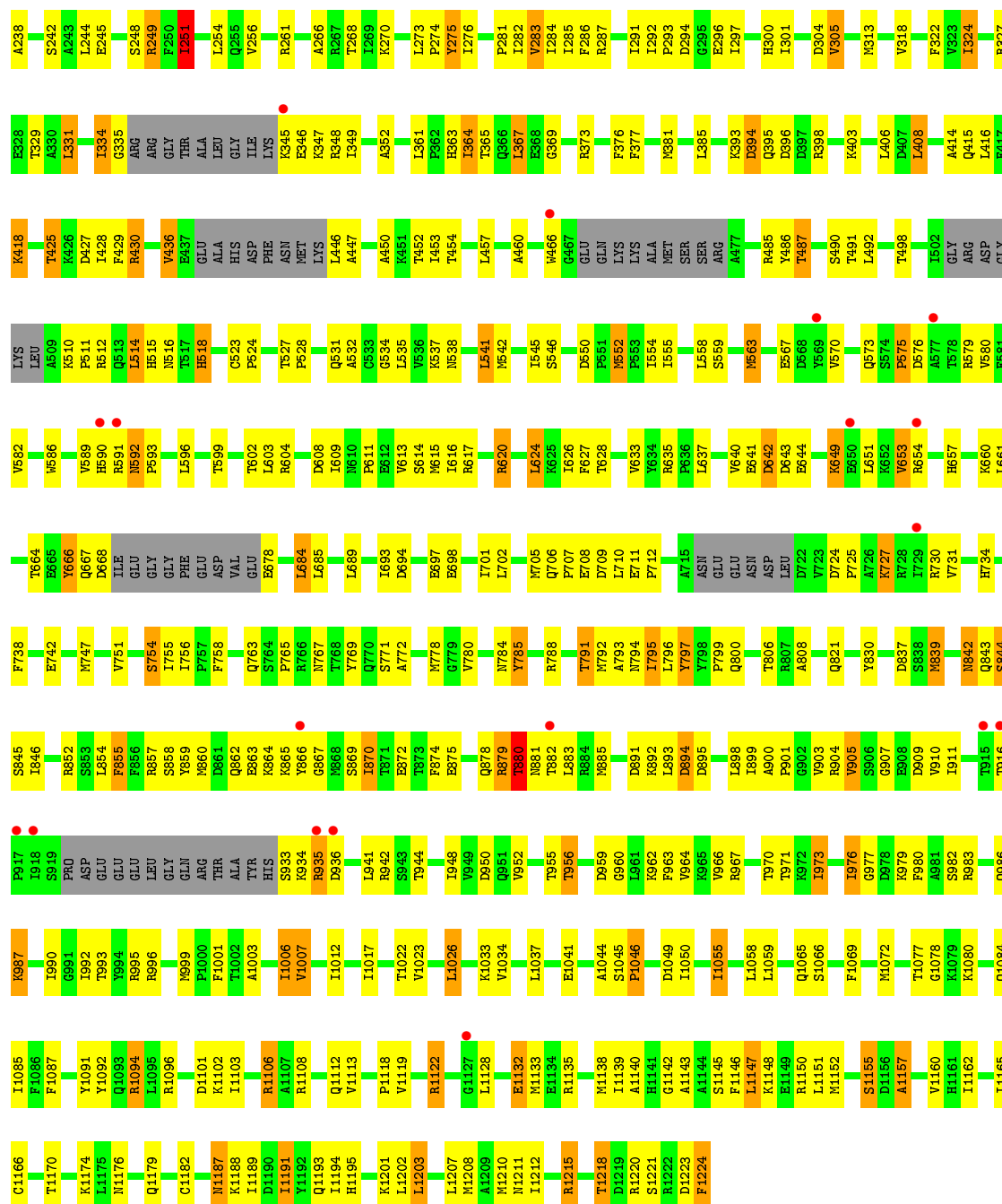
#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

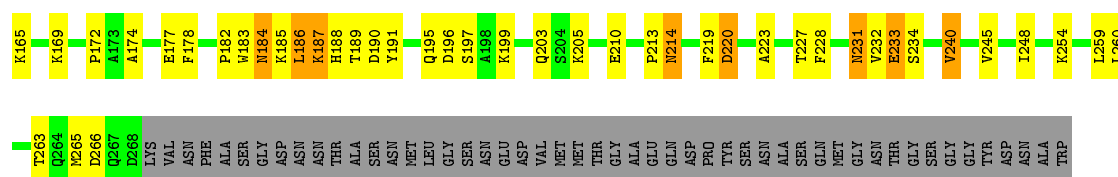




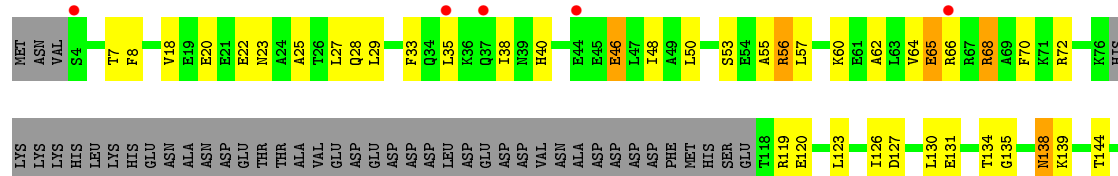
LEU	GLN	MET
LYS	HIS	SER
TYR	THR	ASP
GLU	THR	GLU
LEU	GLU	ALA
IIE	SER	ASN
ALA	ASP	SER
GLU	ASN	GLU
GLU	IIE	LVS
SER	SER	TYR
GLU	ARG	TYR
ASP	LVS	ASP
ASP	TYR	GLU
SER	GLU	ASP
GLU	I90	PRQ
GLY	S91	TYR
GLY	F92	GLY
K164	M101	PHE
G168	V102	D20
R169	N103	E21
L170		
P171	D106	I25
K177	G107	
	V108	V33
L181	L112	I34
D188	V113	S35
L189	P114	A36
	Q115	F37
L192	R118	F38
I204	L119	R39
I205	R120	E40
E206	N121	K41
G207	L122	V44
S208	T123	S45
E209	I124	Q46
K210	S125	
V211	S126	S50
	G127	F51
A214	L128	N52
Q215	F129	V55
E216	V130	D56
	D131	Y57
N221	V132	T58
I222	K133	L59
V223	K134	Q60
Q224	ARG	D61
V225	TYR	I62
F226	TYR	I63
K227	GLU	
K228	ALA	S67
A229	IIE	
	ASP	T70
S232	VAL	LEU
E236	GLY	GLU
H237	PHQ	GLN
	ARG	LEU
	GLU	ALA



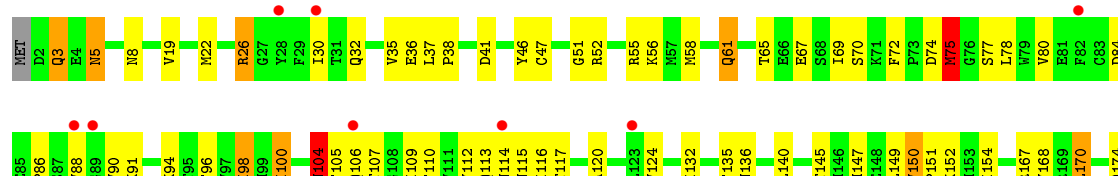




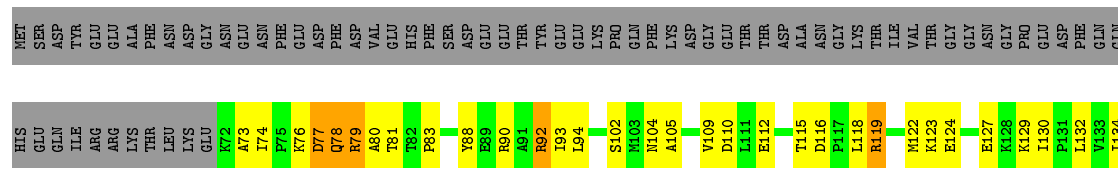
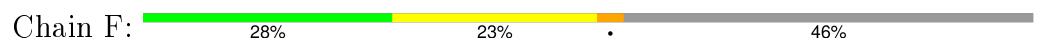
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

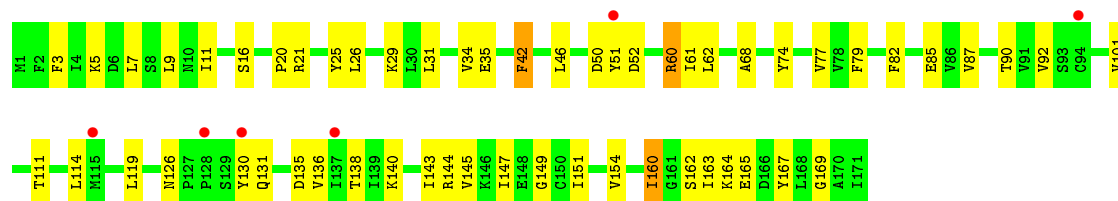


• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

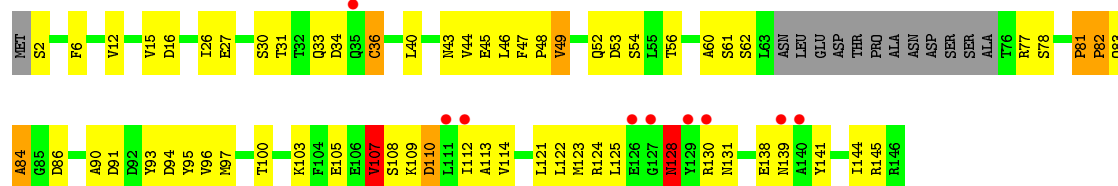


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

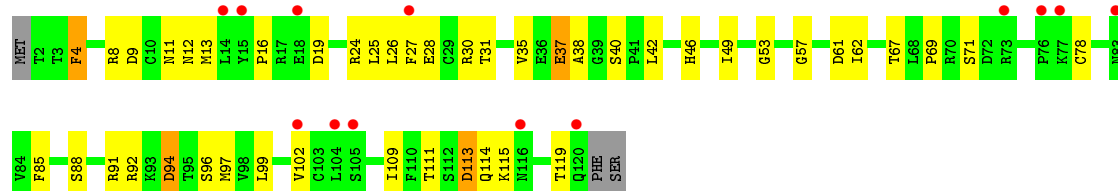




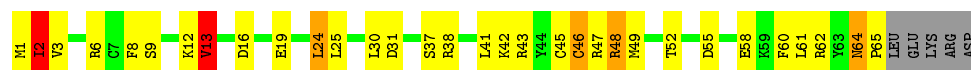
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3



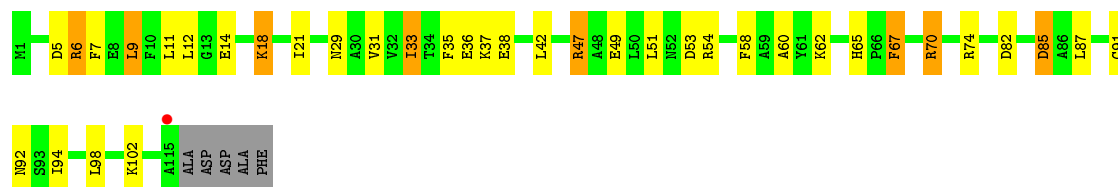
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



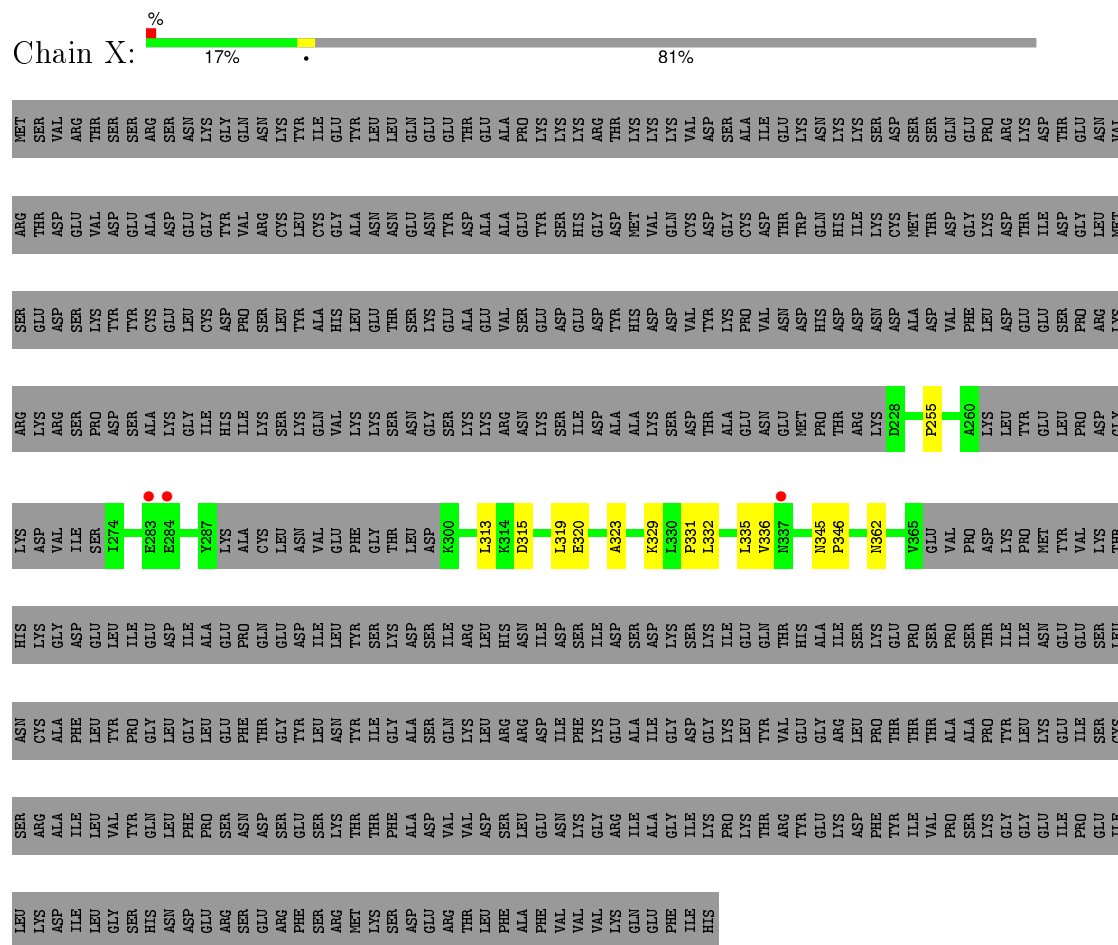
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



- Molecule 13: TRANSCRIPTION FACTOR BYE1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.55Å 392.09Å 279.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 4.80 49.63 – 4.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.63-4.80) 100.0 (49.63-4.80)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 4.86Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.191 , 0.253 0.218 , 0.283	Depositor DCC
$R_{free}$ test set	1169 reflections (1.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	151.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 289.9	EDS
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 59394 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	31509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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, 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	0.53	0/11339	0.82	2/15334 (0.0%)
2	B	0.52	0/8889	0.80	2/11987 (0.0%)
3	C	0.48	0/2133	0.77	0/2891
4	D	0.51	0/1365	0.82	0/1837
5	E	0.48	0/1788	0.77	0/2406
6	F	0.54	0/691	0.82	0/933
7	G	0.47	0/1368	0.78	0/1844
8	H	0.53	0/1086	0.85	2/1470 (0.1%)
9	I	0.48	0/989	0.79	0/1331
10	J	0.52	0/541	0.77	0/727
11	K	0.49	0/938	0.75	0/1267
12	L	0.54	0/365	0.94	0/485
13	X	0.62	0/561	0.88	3/780 (0.4%)
All	All	0.52	0/32053	0.81	9/43292 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	C-N-CA	6.43	137.77	121.70
13	X	255	PRO	N-CA-CB	6.15	110.67	103.30
13	X	346	PRO	N-CA-CB	5.66	110.09	103.30
13	X	331	PRO	N-CA-CB	5.54	109.94	103.30
1	A	858	ASN	C-N-CA	5.39	135.18	121.70
8	H	90	ALA	N-CA-C	-5.37	96.50	111.00
8	H	83	GLN	C-N-CA	5.36	135.09	121.70
2	B	784	ASN	C-N-CA	5.35	135.07	121.70
2	B	1187	ASN	C-N-CA	5.07	134.38	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11140	0	11218	359	0
2	B	8720	0	8745	225	0
3	C	2095	0	2051	71	0
4	D	1356	0	1319	31	0
5	E	1752	0	1776	46	0
6	F	679	0	701	21	0
7	G	1340	0	1357	26	0
8	H	1068	0	1040	29	0
9	I	971	0	930	25	0
10	J	532	0	543	16	0
11	K	920	0	929	27	0
12	L	363	0	386	12	0
13	X	564	0	239	4	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31509	0	31234	783	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 12.

All (783) 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)
3:C:83:SER:HA	3:C:95:CYS:HB2	1.36	1.05
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.38	1.04
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.46	0.97
1:A:821:ARG:HG2	2:B:514:LEU:H	1.31	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.53	0.89
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.53	0.89
1:A:51:GLY:HA2	1:A:56:PRO:HB3	1.53	0.89
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.53	0.89
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.54	0.89
4:D:183:LEU:HD23	7:G:144:ARG:HE	1.38	0.88
1:A:1121:GLU:HB3	1:A:1124:HIS:NE2	1.90	0.86
1:A:49:LYS:HD3	1:A:54:ASN:HB3	1.57	0.85
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.14	0.83
2:B:35:SER:HB3	2:B:39:ARG:HE	1.43	0.82
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.81
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.61	0.81
5:E:147:HIS:HD2	5:E:149:LEU:H	1.28	0.81
1:A:332:LYS:H	1:A:337:ARG:HB2	1.46	0.80
3:C:83:SER:HA	3:C:95:CYS:CB	2.12	0.80
2:B:866:TYR:CD2	2:B:870:ILE:HB	2.17	0.79
1:A:208:LEU:HD12	1:A:235:ILE:HB	1.64	0.79
1:A:329:LEU:HD22	2:B:1203:LEU:HD12	1.64	0.79
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.66	0.78
4:D:62:ALA:HB1	7:G:50:ASP:H	1.48	0.77
1:A:225:ASN:HD22	1:A:228:PHE:H	1.33	0.77
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.68	0.76
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.67	0.75
2:B:843:GLN:HB2	2:B:993:THR:HB	1.67	0.75
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.68	0.75
1:A:316:GLN:HB2	1:A:322:VAL:HG22	1.69	0.75
1:A:517:ASN:HD21	1:A:1362:TYR:HE2	1.33	0.75
2:B:702:LEU:HD13	9:I:67:THR:HA	1.67	0.74
2:B:346:GLU:H	2:B:349:ILE:HD12	1.53	0.74
1:A:567:LYS:HB3	8:H:96:VAL:H	1.52	0.73
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.71	0.73
1:A:1396:ALA:HA	1:A:1399:ARG:HH21	1.52	0.73
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.71	0.72
1:A:265:LYS:HD2	1:A:322:VAL:HG11	1.72	0.72
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.72	0.72
2:B:1001:PHE:CE2	3:C:178:PHE:HB3	2.25	0.72
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.55	0.72
9:I:85:PHE:HB2	9:I:99:LEU:HD22	1.72	0.72
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.72	0.72
8:H:105:GLU:HB3	8:H:113:ALA:HB3	1.70	0.72
12:L:55:ILE:HD12	12:L:56:LEU:H	1.55	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:HA	2:B:649:LYS:HA	1.73	0.71
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.73	0.71
11:K:38:GLU:HG3	11:K:42:LEU:HD22	1.71	0.70
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.72	0.70
2:B:624:LEU:HD22	2:B:626:ILE:HG13	1.72	0.70
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.73	0.70
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.73	0.70
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.31	0.70
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.74	0.70
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.74	0.70
3:C:177:GLU:HB3	3:C:231:ASN:HB3	1.72	0.69
1:A:1333:ILE:H	1:A:1333:ILE:HD13	1.57	0.69
1:A:1006:ILE:HD11	5:E:167:ARG:HB2	1.73	0.69
1:A:1279:ILE:HA	1:A:1310:GLY:HA3	1.75	0.69
3:C:11:ARG:HH12	3:C:205:LYS:HE3	1.58	0.69
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.57	0.69
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.74	0.69
1:A:1423:GLY:H	1:A:1426:GLU:HG3	1.57	0.68
2:B:558:LEU:HB3	2:B:563:MET:HG3	1.74	0.68
2:B:293:PRO:HB2	9:I:11:ASN:HD22	1.58	0.68
1:A:1002:GLY:HA3	1:A:1007:ILE:CG2	2.24	0.67
1:A:316:GLN:HB2	1:A:322:VAL:CG2	2.24	0.67
8:H:33:GLN:HB3	8:H:36:CYS:HB2	1.76	0.67
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.76	0.67
1:A:1228:TRP:HB3	1:A:1238:ILE:HG23	1.76	0.67
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.77	0.66
4:D:120:GLU:HA	4:D:123:LEU:HD12	1.78	0.66
1:A:1081:LEU:HD22	1:A:1096:SER:HB2	1.77	0.66
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.77	0.66
1:A:387:ARG:HH12	1:A:434:ARG:NH1	1.93	0.66
2:B:1160:VAL:HG11	2:B:1201:LYS:HG3	1.76	0.66
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.60	0.65
3:C:46:ILE:H	3:C:46:ILE:HD12	1.61	0.65
13:X:319:LEU:HA	13:X:345:ASN:HA	1.78	0.65
1:A:793:SER:HB2	1:A:796:SER:HB2	1.78	0.65
3:C:55:THR:HB	3:C:151:GLN:HA	1.78	0.65
1:A:565:ILE:HG13	8:H:97:MET:HG2	1.77	0.65
2:B:664:THR:HG1	2:B:678:GLU:N	1.95	0.65
4:D:68:ARG:HB2	4:D:72:ARG:HH21	1.62	0.65
2:B:797:TYR:HE1	2:B:971:THR:HG23	1.62	0.64
2:B:992:ILE:HG12	2:B:993:THR:N	2.12	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HD11	2:B:1103:ILE:HD11	1.79	0.64
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.80	0.64
1:A:830:LYS:O	1:A:834:THR:HB	1.97	0.64
1:A:709:THR:HG23	9:I:94:ASP:HA	1.80	0.64
1:A:28:ARG:HH12	1:A:85:ASP:HB3	1.63	0.63
2:B:866:TYR:HD2	2:B:870:ILE:HB	1.62	0.63
1:A:299:HIS:HA	1:A:302:THR:HB	1.80	0.63
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.64	0.63
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.78	0.63
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.24	0.63
1:A:1189:SER:HB3	1:A:1241:ARG:HB3	1.79	0.63
2:B:224:GLN:HE21	2:B:403:LYS:HD3	1.64	0.63
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.80	0.63
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.81	0.62
11:K:12:LEU:HA	11:K:37:LYS:HG3	1.81	0.62
1:A:788:SER:HB3	9:I:69:PRO:HG3	1.81	0.62
2:B:425:THR:HA	2:B:428:ILE:HD12	1.81	0.62
6:F:81:THR:HB	6:F:136:ARG:HH11	1.64	0.62
1:A:741:ASN:HD22	1:A:744:LYS:H	1.46	0.62
1:A:606:LEU:HG	1:A:613:ILE:HD13	1.80	0.62
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.81	0.62
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.81	0.62
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.82	0.62
1:A:2:VAL:HG23	2:B:1157:ALA:HB1	1.80	0.62
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.29	0.62
3:C:220:ASP:HB3	3:C:223:ALA:HB2	1.82	0.62
8:H:44:VAL:HG22	8:H:49:VAL:H	1.64	0.61
1:A:332:LYS:HE2	2:B:1132:GLU:HG3	1.81	0.61
3:C:83:SER:CA	3:C:95:CYS:HB2	2.20	0.61
2:B:1033:LYS:O	2:B:1037:LEU:HG	2.01	0.61
5:E:47:CYS:HB3	5:E:51:GLY:HA2	1.81	0.61
1:A:1260:LEU:HA	1:A:1263:ILE:HD12	1.82	0.61
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.83	0.61
10:J:42:LYS:HG3	10:J:43:ARG:H	1.65	0.61
9:I:4:PHE:HE2	9:I:13:MET:HG3	1.66	0.61
2:B:515:HIS:HB3	2:B:518:HIS:CE1	2.36	0.60
2:B:334:ILE:HG21	2:B:352:ALA:HB2	1.84	0.60
1:A:1386:ARG:HA	1:A:1390:ASN:HB2	1.82	0.60
1:A:12:ARG:HG2	1:A:13:THR:H	1.67	0.60
1:A:881:GLN:NE2	1:A:960:ILE:H	1.98	0.60
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.82	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ILE:HG13	1:A:925:LEU:HD13	1.83	0.60
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.84	0.60
2:B:992:ILE:HG12	2:B:993:THR:H	1.67	0.60
3:C:187:LYS:HB2	3:C:219:PHE:HE1	1.67	0.60
12:L:31:CYS:SG	12:L:55:ILE:HD11	2.42	0.59
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.85	0.59
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.84	0.59
5:E:3:GLN:HG2	5:E:5:ASN:HD22	1.68	0.59
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.85	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.83	0.59
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.85	0.58
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.83	0.58
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.86	0.58
1:A:774:ARG:HG3	1:A:797:LYS:HD3	1.85	0.58
2:B:114:PRO:HG3	2:B:181:LEU:HG	1.83	0.58
6:F:105:ALA:HA	7:G:16:SER:HA	1.86	0.58
2:B:778:MET:HB2	2:B:1094:ARG:HG2	1.86	0.58
1:A:672:ASP:HB3	1:A:736:ASN:HD21	1.69	0.58
2:B:512:ARG:HA	2:B:534:GLY:HA3	1.86	0.58
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.86	0.58
2:B:296:GLU:O	2:B:300:HIS:HD2	1.86	0.58
4:D:154:PHE:HA	4:D:219:THR:HB	1.85	0.58
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.86	0.58
5:E:147:HIS:NE2	5:E:149:LEU:HD12	2.19	0.58
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.16	0.58
2:B:281:PRO:HD2	2:B:284:ILE:HD13	1.86	0.57
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.40	0.57
1:A:1124:HIS:CD2	1:A:1130:GLN:HG2	2.39	0.57
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.86	0.57
1:A:1063:MET:HB2	2:B:1140:ALA:HA	1.86	0.57
1:A:1148:ILE:HG23	9:I:49:ILE:HB	1.87	0.57
8:H:47:PHE:CD2	8:H:95:TYR:HD2	2.23	0.57
2:B:780:VAL:HG13	2:B:795:ILE:HD11	1.87	0.57
2:B:603:LEU:HB3	2:B:609:ILE:H	1.70	0.57
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.85	0.57
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.05	0.57
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.87	0.57
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.86	0.57
1:A:265:LYS:HB3	1:A:303:TYR:HB2	1.87	0.56
2:B:38:PHE:C	2:B:40:GLU:H	2.09	0.56
2:B:843:GLN:HG3	11:K:6:ARG:HH21	1.69	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HB	1:A:929:LEU:HG	1.86	0.56
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.87	0.56
5:E:147:HIS:CD2	5:E:149:LEU:H	2.16	0.56
1:A:512:VAL:HG12	1:A:876:ALA:HB1	1.85	0.56
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.87	0.56
1:A:170:THR:HB	1:A:185:TRP:HD1	1.70	0.56
10:J:8:PHE:H	10:J:49:MET:HE3	1.69	0.56
3:C:98:VAL:HG22	3:C:158:VAL:HG13	1.86	0.56
11:K:58:PHE:CZ	11:K:60:ALA:HB3	2.40	0.56
1:A:101:LYS:HA	1:A:139:TRP:HE1	1.68	0.56
1:A:385:ILE:HG23	1:A:386:ASP:H	1.71	0.56
3:C:50:GLU:HB3	3:C:156:THR:HB	1.87	0.56
1:A:14:VAL:HB	1:A:1430:LEU:HD13	1.87	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.87	0.56
2:B:276:ILE:HG23	2:B:335:GLY:H	1.70	0.56
1:A:1102:LYS:O	1:A:1106:ASN:HB2	2.05	0.56
2:B:657:HIS:HA	2:B:660:LYS:HD2	1.88	0.56
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.88	0.55
1:A:91:PHE:HD1	1:A:99:ILE:HD13	1.69	0.55
1:A:1001:ARG:HB3	6:F:80:ALA:HA	1.86	0.55
2:B:115:GLN:HE21	2:B:119:LEU:HD21	1.70	0.55
1:A:881:GLN:HB2	1:A:956:LEU:HB2	1.88	0.55
1:A:348:SER:HB2	2:B:1128:LEU:HB2	1.88	0.55
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.89	0.55
1:A:185:TRP:CZ3	1:A:200:ARG:HB2	2.42	0.55
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.88	0.55
1:A:1138:ILE:HG13	1:A:1282:VAL:HG21	1.89	0.55
7:G:149:GLY:HA3	7:G:160:ILE:HD12	1.88	0.55
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.89	0.55
2:B:559:SER:HA	2:B:563:MET:HB2	1.89	0.55
1:A:387:ARG:HH12	1:A:434:ARG:HH11	1.55	0.55
3:C:12:GLU:HB2	3:C:19:ASP:HB2	1.88	0.55
2:B:879:ARG:O	2:B:934:LYS:HB2	2.06	0.55
3:C:102:GLN:HE21	3:C:154:LYS:HG3	1.71	0.55
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.56	0.55
7:G:114:LEU:HD12	7:G:162:SER:HB3	1.89	0.54
1:A:821:ARG:HG2	2:B:514:LEU:N	2.12	0.54
3:C:46:ILE:HD13	3:C:67:LEU:O	2.08	0.54
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.88	0.54
1:A:15:LYS:HA	1:A:15:LYS:HE3	1.88	0.54
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:CD2	2:B:516:ASN:H	2.26	0.54
1:A:330:LYS:O	1:A:334:GLY:HA3	2.06	0.54
5:E:168:TYR:HB3	5:E:170:LEU:HD12	1.89	0.54
1:A:335:ARG:HG2	2:B:1203:LEU:HB2	1.88	0.54
1:A:185:TRP:HZ3	1:A:200:ARG:HB2	1.73	0.54
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.90	0.54
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.38	0.54
12:L:40:LEU:HB3	12:L:44:ASP:HB3	1.89	0.54
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.90	0.53
1:A:153:PRO:HA	1:A:161:LEU:HA	1.89	0.53
7:G:163:ILE:HB	7:G:169:GLY:HA2	1.89	0.53
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.90	0.53
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.90	0.53
1:A:367:PRO:HA	1:A:463:ILE:O	2.09	0.53
2:B:52:ASN:HA	2:B:177:LYS:HG3	1.91	0.53
4:D:155:ARG:H	4:D:219:THR:HB	1.74	0.53
3:C:91:HIS:CE1	3:C:158:VAL:HG21	2.42	0.53
1:A:1115:SER:H	1:A:1330:ASN:HB3	1.74	0.53
1:A:765:VAL:HB	1:A:800:VAL:HB	1.90	0.53
2:B:453:ILE:HG22	2:B:457:LEU:HD11	1.91	0.53
4:D:66:ARG:HG3	7:G:51:TYR:HB2	1.89	0.53
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.91	0.53
3:C:187:LYS:HB2	3:C:219:PHE:CE1	2.43	0.53
1:A:1335:ILE:HG21	1:A:1347:ALA:HB2	1.91	0.53
1:A:183:GLY:O	1:A:184:SER:HB2	2.08	0.53
2:B:893:LEU:HG	2:B:899:ILE:HG13	1.91	0.53
2:B:283:VAL:HG23	2:B:284:ILE:HD12	1.91	0.53
1:A:1001:ARG:CD	6:F:83:PRO:HD3	2.38	0.53
1:A:1235:LYS:HD2	1:A:1237:ILE:HD11	1.89	0.53
2:B:654:ARG:H	2:B:657:HIS:HD2	1.56	0.52
7:G:60:ARG:NH2	7:G:62:LEU:HA	2.23	0.52
3:C:102:GLN:HG3	3:C:154:LYS:HG3	1.91	0.52
1:A:276:LEU:HD22	1:A:293:GLU:HA	1.90	0.52
2:B:881:ASN:HB2	2:B:933:SER:HB2	1.90	0.52
10:J:48:ARG:O	10:J:52:THR:HG22	2.09	0.52
1:A:15:LYS:HA	1:A:15:LYS:CE	2.39	0.52
2:B:614:SER:HB2	2:B:697:GLU:HB2	1.91	0.52
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.91	0.52
3:C:186:LEU:HD22	3:C:188:HIS:HE2	1.73	0.52
1:A:148:CYS:O	1:A:168:GLY:HA2	2.10	0.52
4:D:168:LYS:HE3	4:D:174:PRO:HA	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ILE:HA	2:B:208:SER:O	2.10	0.52
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.91	0.52
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.45	0.52
1:A:1009:ASN:HD22	1:A:1012:ARG:HH11	1.57	0.52
1:A:913:LEU:HD22	1:A:1032:LEU:HD13	1.91	0.52
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.91	0.52
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.92	0.52
2:B:283:VAL:HG11	2:B:318:VAL:HA	1.92	0.52
10:J:24:LEU:HD21	10:J:38:ARG:HD2	1.90	0.52
3:C:165:LYS:HE2	11:K:9:LEU:HD22	1.91	0.52
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.90	0.52
2:B:1142:GLY:HA3	6:F:88:TYR:HE1	1.75	0.52
3:C:100:THR:HG22	3:C:119:VAL:HB	1.92	0.52
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.92	0.52
2:B:944:THR:HB	2:B:1122:ARG:NH2	2.25	0.52
1:A:332:LYS:N	1:A:337:ARG:HB2	2.20	0.51
2:B:979:LYS:HE2	2:B:987:LYS:HB2	1.91	0.51
1:A:738:LYS:H	1:A:738:LYS:HE2	1.76	0.51
1:A:873:MET:HG3	1:A:1056:SER:HB3	1.92	0.51
9:I:4:PHE:CE2	9:I:13:MET:HG3	2.44	0.51
2:B:125:SER:HA	2:B:171:PRO:HA	1.93	0.51
2:B:532:ALA:HA	2:B:535:LEU:HD12	1.91	0.51
1:A:845:LEU:HA	1:A:848:ILE:HD12	1.93	0.51
1:A:1347:ALA:O	1:A:1351:GLU:HB2	2.11	0.51
5:E:135:PHE:HE1	5:E:186:LEU:HB3	1.75	0.51
7:G:25:TYR:CE2	7:G:29:LYS:HD3	2.46	0.51
1:A:939:ASP:OD2	1:A:1023:ARG:HD2	2.11	0.51
1:A:230:ARG:HB3	1:A:232:GLU:HG2	1.92	0.51
1:A:690:VAL:HG22	1:A:718:VAL:HG22	1.92	0.51
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.92	0.51
1:A:1119:TYR:HA	1:A:1305:VAL:HG22	1.93	0.51
1:A:708:MET:SD	1:A:713:SER:HA	2.50	0.51
1:A:11:LEU:HD13	2:B:1193:GLN:HE21	1.74	0.51
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.46	0.51
2:B:1001:PHE:HB3	2:B:1007:VAL:HG23	1.93	0.51
1:A:333:GLU:HA	1:A:338:GLY:HA3	1.92	0.51
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.92	0.51
3:C:16:ASP:HA	3:C:234:SER:HB3	1.92	0.51
1:A:973:ILE:HG12	1:A:1037:LEU:HA	1.92	0.51
1:A:1063:MET:HG3	2:B:1139:ILE:HG22	1.92	0.51
1:A:1004:ASN:HD21	1:A:1007:ILE:HG13	1.74	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG22	2:B:808:ALA:H	1.76	0.51
1:A:898:ARG:HD3	1:A:933:TYR:CG	2.46	0.51
1:A:867:ILE:HD11	1:A:1010:ALA:HB1	1.91	0.51
1:A:1120:LEU:HD22	1:A:1304:TRP:HB2	1.92	0.51
1:A:1150:SER:H	9:I:46:HIS:HB3	1.75	0.51
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.92	0.51
2:B:361:LEU:HG	2:B:363:HIS:CE1	2.46	0.51
5:E:151:PRO:HG3	5:E:200:ARG:HG3	1.93	0.51
1:A:92:HIS:HE2	1:A:1410:PHE:HE2	1.59	0.51
2:B:651:LEU:HD21	2:B:707:PRO:HB3	1.92	0.51
1:A:395:GLY:O	1:A:401:GLY:HA3	2.11	0.51
1:A:171:GLN:HG3	1:A:172:PRO:HD2	1.93	0.51
8:H:114:VAL:HG22	8:H:125:LEU:HB3	1.92	0.51
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	1.93	0.50
1:A:523:ILE:HG23	1:A:527:THR:HB	1.93	0.50
1:A:1189:SER:CB	1:A:1242:VAL:H	2.25	0.50
3:C:50:GLU:HG2	12:L:64:LEU:HD12	1.93	0.50
2:B:950:ASP:HB3	2:B:967:ARG:HB3	1.92	0.50
1:A:162:VAL:HG12	1:A:164:ARG:H	1.77	0.50
2:B:487:THR:HG23	2:B:490:SER:HB3	1.94	0.50
1:A:706:HIS:HB2	13:X:362:ASN:O	2.10	0.50
1:A:471:ASN:O	1:A:474:VAL:HG12	2.11	0.50
2:B:620:ARG:HD2	9:I:62:ILE:HD11	1.93	0.50
1:A:1134:ILE:HG22	1:A:1138:ILE:HD13	1.94	0.50
2:B:554:ILE:HG21	2:B:626:ILE:HG21	1.93	0.50
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.30	0.50
1:A:512:VAL:HG13	1:A:631:HIS:CE1	2.47	0.50
3:C:142:VAL:H	10:J:16:ASP:HB3	1.76	0.50
3:C:145:CYS:HA	10:J:2:ILE:HD12	1.94	0.50
1:A:65:LEU:HB3	1:A:71:GLN:CB	2.42	0.50
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.93	0.50
5:E:202:SER:HB3	5:E:205:SER:OG	2.12	0.50
3:C:98:VAL:H	3:C:122:SER:HB3	1.76	0.50
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.94	0.50
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.94	0.50
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.94	0.50
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.93	0.50
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.93	0.50
1:A:353:ILE:HA	1:A:468:PHE:O	2.12	0.50
1:A:1006:ILE:CD1	5:E:167:ARG:HB2	2.42	0.50
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.38	0.49
1:A:79:GLY:H	2:B:1201:LYS:HZ1	1.60	0.49
1:A:922:ASP:HB3	1:A:925:LEU:HB2	1.94	0.49
1:A:986:ILE:HG12	1:A:1031:VAL:HG11	1.94	0.49
1:A:1412:ALA:HA	1:A:1417:GLU:HB2	1.94	0.49
2:B:641:GLU:C	2:B:643:ASP:H	2.15	0.49
2:B:893:LEU:HD23	2:B:898:LEU:HA	1.94	0.49
1:A:294:SER:HA	1:A:297:GLN:HB3	1.94	0.49
2:B:545:ILE:HG13	2:B:633:VAL:HG13	1.95	0.49
2:B:36:ALA:HA	2:B:39:ARG:HB2	1.94	0.49
1:A:690:VAL:HG11	1:A:794:PRO:HD3	1.95	0.49
2:B:791:THR:HA	2:B:858:SER:H	1.78	0.49
2:B:115:GLN:O	2:B:119:LEU:HG	2.12	0.49
1:A:1135:ARG:HG3	1:A:1136:SER:H	1.77	0.49
9:I:19:ASP:HB3	9:I:24:ARG:HG3	1.95	0.49
7:G:92:VAL:HG12	7:G:140:LYS:NZ	2.26	0.49
6:F:112:GLU:HB2	6:F:123:LYS:HE2	1.95	0.49
6:F:77:ASP:O	6:F:78:GLN:HB2	2.12	0.49
2:B:284:ILE:HG13	2:B:324:ILE:HG21	1.95	0.49
1:A:1332:PHE:HA	1:A:1335:ILE:HG13	1.95	0.49
1:A:1008:GLN:HB3	1:A:1012:ARG:NH2	2.28	0.49
3:C:169:LYS:HZ2	12:L:69:ALA:HB3	1.77	0.49
1:A:619:LYS:HD2	1:A:750:GLY:HA3	1.95	0.49
1:A:757:ASN:HD22	1:A:757:ASN:H	1.59	0.49
1:A:867:ILE:HD12	5:E:208:TYR:HD1	1.78	0.49
1:A:1422:ARG:HH12	2:B:1224:PHE:HB2	1.76	0.49
1:A:51:GLY:CA	1:A:56:PRO:HB3	2.34	0.49
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.94	0.49
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.94	0.49
5:E:56:LYS:HD2	5:E:84:ASP:HB2	1.95	0.49
9:I:27:PHE:CE2	9:I:38:ALA:HA	2.48	0.49
1:A:1100:ARG:HE	1:A:1104:ILE:HD11	1.77	0.49
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.95	0.48
1:A:1404:GLU:O	1:A:1408:ILE:HD12	2.13	0.48
1:A:347:PHE:HB3	1:A:491:VAL:HB	1.95	0.48
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.95	0.48
1:A:55:ASP:C	1:A:57:ARG:H	2.17	0.48
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.95	0.48
8:H:81:PRO:CB	8:H:82:PRO:HD3	2.40	0.48
1:A:1386:ARG:HG3	1:A:1387:HIS:CE1	2.48	0.48
11:K:58:PHE:HE2	11:K:74:ARG:HB3	1.78	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:HD11	1:A:1038:THR:HG23	1.95	0.48
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.96	0.48
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.94	0.48
1:A:107:CYS:HA	1:A:171:GLN:OE1	2.14	0.48
2:B:613:VAL:HG13	2:B:627:PHE:O	2.14	0.48
1:A:725:ALA:HA	1:A:728:LYS:HG2	1.94	0.48
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.94	0.48
7:G:61:ILE:HG13	7:G:68:ALA:HB2	1.96	0.48
2:B:885:MET:HA	2:B:936:ASP:HB3	1.95	0.48
1:A:551:TYR:HB2	11:K:58:PHE:HZ	1.79	0.48
1:A:699:ALA:HB1	9:I:114:GLN:HB2	1.95	0.48
12:L:53:HIS:HB3	12:L:55:ILE:HG12	1.95	0.48
1:A:1002:GLY:HA3	1:A:1007:ILE:HG22	1.95	0.48
2:B:795:ILE:HG22	2:B:854:LEU:HB2	1.95	0.48
8:H:56:THR:O	8:H:144:ILE:HA	2.14	0.48
2:B:797:TYR:HB2	2:B:852:ARG:O	2.13	0.48
1:A:537:ARG:HH12	8:H:122:LEU:HG	1.79	0.48
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.96	0.48
2:B:604:ARG:HG2	2:B:611:PRO:HA	1.95	0.48
2:B:862:GLN:HB2	2:B:864:LYS:HE3	1.95	0.48
3:C:174:ALA:HB3	3:C:233:GLU:HB3	1.96	0.48
1:A:973:ILE:HD11	1:A:1038:THR:H	1.79	0.47
3:C:125:MET:HB2	3:C:127:ARG:HE	1.79	0.47
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.13	0.47
2:B:901:PRO:HD3	2:B:952:VAL:HB	1.96	0.47
2:B:121:ASN:HB2	2:B:963:PHE:CE2	2.48	0.47
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.94	0.47
2:B:249:ARG:O	2:B:251:ILE:HG13	2.15	0.47
8:H:112:ILE:HD12	8:H:128:ASN:HA	1.95	0.47
5:E:145:THR:HG21	5:E:187:TYR:CG	2.49	0.47
8:H:100:THR:HA	8:H:138:GLU:HA	1.96	0.47
8:H:12:VAL:HB	8:H:52:GLN:H	1.79	0.47
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.95	0.47
1:A:903:ASN:HD22	1:A:905:ASP:H	1.61	0.47
2:B:168:GLY:H	2:B:450:ALA:HB1	1.78	0.47
1:A:1386:ARG:HD3	1:A:1403:GLU:HB3	1.96	0.47
5:E:72:PHE:HB3	5:E:75:MET:HB2	1.96	0.47
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.97	0.47
1:A:1111:MET:HE2	1:A:1333:ILE:HD11	1.96	0.47
3:C:11:ARG:HD3	3:C:21:ILE:HD11	1.96	0.47
1:A:1386:ARG:HG3	1:A:1387:HIS:NE2	2.30	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:THR:HB	2:B:537:LYS:O	2.14	0.47
6:F:116:ASP:HB3	6:F:119:ARG:HB2	1.96	0.47
1:A:117:GLU:H	1:A:117:GLU:CD	2.18	0.47
4:D:29:LEU:HB3	7:G:82:PHE:CZ	2.49	0.47
11:K:18:LYS:HD3	11:K:38:GLU:HG2	1.96	0.47
5:E:80:VAL:HG22	5:E:109:ILE:HB	1.97	0.47
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.96	0.47
1:A:152:VAL:HG22	1:A:153:PRO:HD2	1.97	0.47
1:A:907:THR:OG1	1:A:920:LEU:HG	2.14	0.47
1:A:1035:TYR:HB3	1:A:1037:LEU:HG	1.97	0.47
13:X:313:LEU:C	13:X:315:ASP:H	2.17	0.47
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.97	0.47
1:A:1009:ASN:HA	1:A:1012:ARG:HD2	1.97	0.47
1:A:511:ILE:HD11	1:A:643:ALA:HB2	1.96	0.47
5:E:26:ARG:HH22	5:E:107:THR:HG21	1.79	0.47
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.47
1:A:1333:ILE:CD1	1:A:1333:ILE:H	2.21	0.46
2:B:880:THR:HB	2:B:934:LYS:HD2	1.96	0.46
5:E:77:SER:O	5:E:105:PHE:HB3	2.16	0.46
2:B:297:ILE:O	2:B:301:ILE:HD12	2.15	0.46
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.80	0.46
1:A:903:ASN:ND2	1:A:905:ASP:H	2.13	0.46
2:B:956:THR:HG23	2:B:960:GLY:HA2	1.96	0.46
1:A:255:SER:H	2:B:935:ARG:HH21	1.61	0.46
3:C:185:LYS:HD3	3:C:213:PRO:HA	1.96	0.46
1:A:1197:LEU:O	1:A:1236:LEU:HD13	2.15	0.46
1:A:497:THR:HG23	2:B:1146:PHE:CD1	2.49	0.46
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.55	0.46
3:C:68:GLY:HA3	12:L:69:ALA:HB1	1.97	0.46
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.30	0.46
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.80	0.46
2:B:1162:ILE:HG12	2:B:1194:ILE:HG12	1.96	0.46
1:A:671:ALA:HB3	1:A:676:MET:HG2	1.97	0.46
2:B:304:ASP:CG	2:B:305:VAL:H	2.18	0.46
4:D:62:ALA:HA	4:D:65:GLU:HB2	1.98	0.46
1:A:809:THR:HB	2:B:730:ARG:HG2	1.97	0.46
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.98	0.46
9:I:102:VAL:HG13	9:I:109:ILE:HG13	1.97	0.46
2:B:615:MET:HG2	2:B:626:ILE:HG12	1.96	0.46
1:A:28:ARG:HG3	1:A:238:CYS:SG	2.55	0.46
10:J:42:LYS:HG3	10:J:43:ARG:N	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:H	1:A:297:GLN:HE22	1.63	0.46
1:A:172:PRO:HB2	1:A:183:GLY:HA2	1.97	0.46
1:A:537:ARG:HG2	8:H:121:LEU:HD23	1.98	0.46
4:D:57:LEU:HD23	4:D:60:LYS:HD3	1.97	0.46
2:B:882:THR:HG1	2:B:933:SER:N	2.14	0.46
2:B:698:GLU:HA	2:B:701:ILE:HG12	1.98	0.46
2:B:1023:VAL:HG13	2:B:1026:LEU:HD12	1.97	0.46
2:B:899:ILE:O	2:B:952:VAL:HG21	2.15	0.46
1:A:285:PRO:HD2	1:A:289:ILE:HD12	1.97	0.46
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.51	0.46
9:I:111:THR:HB	9:I:113:ASP:HB2	1.98	0.46
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.98	0.46
1:A:125:ALA:HA	1:A:128:ILE:HD12	1.98	0.46
1:A:941:LYS:HA	1:A:944:ARG:HB2	1.98	0.46
1:A:540:PHE:HB3	1:A:571:LEU:HG	1.98	0.46
3:C:183:TRP:HB2	3:C:185:LYS:HE2	1.97	0.46
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.98	0.46
5:E:196:VAL:HG23	5:E:212:ARG:HB2	1.98	0.46
1:A:179:LEU:HD22	1:A:297:GLN:HG3	1.98	0.46
2:B:1142:GLY:HA3	6:F:88:TYR:CE1	2.51	0.46
1:A:1343:ALA:HB2	5:E:150:VAL:HG13	1.97	0.46
11:K:65:HIS:HD2	11:K:67:PHE:H	1.63	0.46
1:A:1000:LEU:HB3	1:A:1007:ILE:HG23	1.98	0.46
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.96	0.46
3:C:146:LYS:CB	10:J:61:LEU:HD11	2.46	0.46
2:B:944:THR:HB	2:B:1122:ARG:HH21	1.81	0.46
4:D:190:GLU:HG3	7:G:167:TYR:CG	2.51	0.46
2:B:221:ASN:OD1	2:B:242:SER:HA	2.15	0.46
4:D:29:LEU:HB2	4:D:33:PHE:O	2.15	0.45
2:B:590:HIS:HD2	2:B:592:ASN:H	1.64	0.45
2:B:523:CYS:HA	2:B:524:PRO:HD3	1.80	0.45
1:A:1433:MET:HE1	6:F:92:ARG:HD2	1.98	0.45
2:B:1187:ASN:HB3	2:B:1191:ILE:HD11	1.98	0.45
1:A:68:GLN:HE22	1:A:80:HIS:HB2	1.80	0.45
7:G:60:ARG:HH21	7:G:62:LEU:HG	1.78	0.45
3:C:184:ASN:HB2	3:C:191:TYR:OH	2.17	0.45
10:J:41:LEU:HD13	10:J:47:ARG:HA	1.97	0.45
1:A:35:ILE:HB	1:A:83:HIS:O	2.16	0.45
1:A:551:TYR:CE2	11:K:62:LYS:HG2	2.52	0.45
5:E:55:ARG:HA	5:E:58:MET:HB3	1.99	0.45
3:C:263:THR:HA	3:C:266:ASP:HB2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:HIS:HB2	3:C:96:SER:OG	2.16	0.45
7:G:34:VAL:HG11	7:G:74:TYR:CE2	2.52	0.45
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.98	0.45
1:A:1158:PRO:HB3	1:A:1188:GLN:HB2	1.98	0.45
1:A:1220:PHE:HZ	1:A:1267:MET:HG2	1.81	0.45
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	1.98	0.45
2:B:1055:ILE:HA	2:B:1058:LEU:HD12	1.99	0.45
2:B:364:ILE:HD11	2:B:377:PHE:CD2	2.51	0.45
11:K:49:GLU:HB2	11:K:94:ILE:HD11	1.97	0.45
9:I:109:ILE:HD12	9:I:109:ILE:H	1.82	0.45
4:D:7:THR:HA	7:G:7:LEU:HD23	1.98	0.45
2:B:1208:MET:C	2:B:1210:MET:H	2.19	0.45
1:A:41:MET:HA	1:A:49:LYS:HG2	1.99	0.45
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.99	0.45
1:A:956:LEU:HD11	1:A:1017:LEU:HD23	1.99	0.45
3:C:104:PHE:CE1	3:C:150:GLY:HA2	2.52	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.45
1:A:90:VAL:HG11	1:A:300:VAL:HB	1.98	0.45
1:A:830:LYS:HD3	1:A:1098:VAL:HG21	1.99	0.45
1:A:1376:THR:HG22	5:E:212:ARG:HH22	1.82	0.45
1:A:563:PRO:HG2	1:A:566:ILE:HG23	1.98	0.45
4:D:33:PHE:CZ	7:G:42:PHE:HA	2.51	0.45
2:B:541:LEU:HD11	2:B:754:SER:HB2	1.99	0.45
2:B:542:MET:HB2	2:B:747:MET:HB3	1.99	0.45
1:A:986:ILE:HG21	1:A:1028:THR:HA	1.99	0.44
1:A:143:LYS:O	1:A:146:MET:HG3	2.17	0.44
11:K:82:ASP:HB3	11:K:85:ASP:HB2	1.99	0.44
1:A:135:PHE:HD2	1:A:223:GLY:H	1.65	0.44
1:A:780:VAL:O	1:A:782:ARG:HD3	2.18	0.44
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.99	0.44
2:B:867:GLY:C	2:B:869:SER:H	2.21	0.44
1:A:65:LEU:HB3	1:A:71:GLN:HB2	1.99	0.44
2:B:90:ILE:HA	2:B:133:LYS:O	2.18	0.44
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.98	0.44
1:A:959:ASN:OD1	1:A:961:ARG:HB3	2.17	0.44
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.98	0.44
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.18	0.44
3:C:254:LYS:HB3	11:K:42:LEU:HD11	2.00	0.44
5:E:197:LYS:HG3	5:E:211:TYR:CE1	2.52	0.44
1:A:850:VAL:CG2	1:A:1064:VAL:HG21	2.48	0.44
1:A:1289:ARG:HD3	1:A:1290:LYS:H	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:LEU:HA	4:D:201:LYS:HB2	1.98	0.44
1:A:272:ALA:HB2	1:A:295:LEU:HD23	1.99	0.44
2:B:971:THR:HG22	2:B:973:ILE:HD13	2.00	0.44
1:A:12:ARG:HB3	2:B:1218:THR:HG22	2.00	0.44
11:K:7:PHE:C	11:K:9:LEU:H	2.21	0.44
1:A:55:ASP:HA	1:A:58:LEU:H	1.81	0.44
1:A:512:VAL:HG13	1:A:631:HIS:HE1	1.81	0.44
5:E:98:ILE:HG13	5:E:98:ILE:H	1.62	0.44
8:H:82:PRO:C	8:H:84:ALA:H	2.21	0.44
2:B:270:LYS:HA	2:B:281:PRO:HA	1.99	0.44
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.53	0.44
2:B:620:ARG:HG3	9:I:57:GLY:O	2.18	0.44
2:B:274:PRO:O	2:B:275:TYR:HB2	2.17	0.44
1:A:1111:MET:HE3	1:A:1331:SER:HA	1.99	0.44
1:A:1081:LEU:HD11	1:A:1358:SER:O	2.18	0.44
1:A:1340:GLY:H	5:E:183:PRO:HD2	1.83	0.44
3:C:97:VAL:O	3:C:159:ALA:HB3	2.18	0.44
1:A:768:GLN:HG2	1:A:816:HIS:HA	2.00	0.44
1:A:663:SER:CB	2:B:1085:ILE:HA	2.48	0.43
8:H:40:LEU:HD13	8:H:123:MET:HG3	2.00	0.43
2:B:573:GLN:O	2:B:575:PRO:HD3	2.18	0.43
1:A:405:VAL:HG12	1:A:413:ILE:HD12	2.00	0.43
2:B:844:SER:HB2	2:B:995:ARG:HA	1.99	0.43
2:B:839:MET:O	2:B:990:ILE:HA	2.17	0.43
11:K:38:GLU:OE1	11:K:42:LEU:HD13	2.17	0.43
1:A:709:THR:HG22	1:A:711:ARG:H	1.83	0.43
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.19	0.43
2:B:1166:CYS:HA	2:B:1215:ARG:HD3	2.00	0.43
1:A:277:GLU:HG2	1:A:281:HIS:CD2	2.54	0.43
1:A:594:GLY:HA3	1:A:601:LYS:HD3	2.00	0.43
2:B:900:ALA:HA	12:L:58:LYS:HD3	2.01	0.43
1:A:512:VAL:HA	1:A:519:PRO:HA	2.00	0.43
1:A:207:ILE:HA	1:A:210:ILE:HD12	2.01	0.43
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.53	0.43
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.18	0.43
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.00	0.43
1:A:467:THR:HG21	2:B:977:GLY:HA3	2.01	0.43
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.45	0.43
10:J:42:LYS:HE3	10:J:43:ARG:HD3	1.98	0.43
5:E:100:ILE:O	5:E:104:ASN:HA	2.19	0.43
3:C:163:ILE:CD1	3:C:165:LYS:HB2	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:724:ASP:HB3	2:B:727:LYS:HB2	2.00	0.43
6:F:118:LEU:O	6:F:122:MET:HG3	2.18	0.43
1:A:1015:VAL:HG11	1:A:1053:PHE:CZ	2.54	0.43
1:A:95:PHE:HB3	1:A:234:MET:SD	2.58	0.43
2:B:515:HIS:HB3	2:B:518:HIS:ND1	2.34	0.43
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.48	0.43
1:A:899:VAL:HG22	1:A:1029:ARG:HD2	2.01	0.43
1:A:527:THR:HG21	1:A:650:GLN:HG2	2.00	0.43
1:A:706:HIS:CD2	1:A:1135:ARG:HH22	2.35	0.43
2:B:666:TYR:C	2:B:668:ASP:H	2.22	0.43
8:H:62:SER:HA	8:H:141:TYR:HE2	1.83	0.43
1:A:588:LEU:HD22	1:A:629:LEU:HD23	2.00	0.43
3:C:169:LYS:HE2	12:L:70:ARG:HG3	2.00	0.43
2:B:864:LYS:HB2	2:B:872:GLU:OE1	2.18	0.43
5:E:26:ARG:NH2	5:E:107:THR:HG21	2.33	0.43
2:B:414:ALA:O	2:B:418:LYS:HB2	2.18	0.43
2:B:118:ARG:HA	2:B:207:GLY:HA2	2.01	0.43
6:F:132:LEU:O	6:F:148:VAL:HG13	2.18	0.43
1:A:1189:SER:HB3	1:A:1242:VAL:H	1.82	0.43
1:A:333:GLU:H	1:A:338:GLY:HA3	1.84	0.43
11:K:18:LYS:HG2	11:K:36:GLU:O	2.18	0.43
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.01	0.43
3:C:220:ASP:HB3	3:C:223:ALA:CB	2.48	0.43
1:A:88:LYS:HB2	1:A:276:LEU:HD21	2.00	0.43
1:A:392:VAL:HA	1:A:415:LEU:HD21	2.01	0.43
2:B:486:TYR:CD1	2:B:1096:ARG:HD2	2.54	0.43
6:F:76:LYS:O	6:F:79:ARG:HD3	2.18	0.43
5:E:90:VAL:HA	5:E:120:ALA:HB2	2.00	0.43
2:B:905:VAL:HB	2:B:941:LEU:HD22	2.01	0.43
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.00	0.43
1:A:531:ILE:HG13	1:A:578:LEU:HD11	2.00	0.43
4:D:144:THR:HG22	4:D:148:LEU:HD12	1.99	0.43
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.34	0.43
2:B:637:LEU:HD23	2:B:742:GLU:HA	2.00	0.43
4:D:185:CYS:SG	4:D:190:GLU:HG2	2.59	0.43
2:B:118:ARG:HH11	2:B:788:ARG:NH1	2.17	0.43
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.19	0.43
1:A:696:GLU:HA	1:A:701:LEU:HD12	2.01	0.43
1:A:1170:ILE:O	1:A:1174:PHE:HB2	2.18	0.43
1:A:839:ARG:HH22	1:A:843:LYS:HZ1	1.67	0.43
2:B:879:ARG:HB3	2:B:883:LEU:HG	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:ARG:HG3	7:G:51:TYR:CB	2.48	0.42
4:D:33:PHE:HZ	7:G:42:PHE:HA	1.82	0.42
2:B:590:HIS:HD2	2:B:592:ASN:N	2.17	0.42
1:A:1342:GLU:HG3	5:E:198:ILE:HD13	2.01	0.42
2:B:427:ASP:HA	2:B:430:ARG:HB2	2.01	0.42
8:H:15:VAL:HA	8:H:26:ILE:HG13	2.01	0.42
1:A:371:ALA:O	1:A:435:HIS:HB3	2.19	0.42
2:B:765:PRO:O	2:B:769:TYR:HD1	2.02	0.42
4:D:25:ALA:C	4:D:27:LEU:H	2.23	0.42
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.00	0.42
1:A:909:ASP:C	1:A:911:SER:H	2.22	0.42
1:A:924:LYS:HA	1:A:927:VAL:HB	2.02	0.42
2:B:893:LEU:HD11	2:B:910:VAL:HB	2.01	0.42
4:D:120:GLU:O	4:D:123:LEU:HB2	2.18	0.42
1:A:1355:VAL:HA	1:A:1358:SER:OG	2.18	0.42
2:B:842:ASN:HD22	2:B:845:SER:N	2.18	0.42
6:F:127:GLU:HB3	6:F:129:LYS:HE3	2.00	0.42
1:A:1386:ARG:HA	1:A:1390:ASN:CB	2.49	0.42
1:A:232:GLU:HG2	1:A:232:GLU:H	1.70	0.42
3:C:182:PRO:HD2	3:C:210:GLU:CD	2.40	0.42
3:C:17:ASN:HA	3:C:232:VAL:O	2.20	0.42
7:G:101:VAL:HG21	7:G:145:VAL:HG11	2.01	0.42
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.53	0.42
4:D:66:ARG:HG2	4:D:70:PHE:CE2	2.54	0.42
1:A:1163:ILE:HD13	1:A:1194:ARG:HD2	2.01	0.42
9:I:26:LEU:HB3	9:I:35:VAL:CG1	2.49	0.42
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.02	0.42
3:C:245:VAL:HG13	11:K:102:LYS:HD3	2.00	0.42
3:C:248:ILE:HG23	11:K:98:LEU:HD22	2.01	0.42
1:A:869:GLY:C	1:A:871:ASP:H	2.23	0.42
1:A:140:THR:HA	1:A:143:LYS:NZ	2.34	0.42
1:A:588:LEU:HD23	1:A:607:ILE:HD12	2.00	0.42
2:B:322:PHE:HZ	9:I:30:ARG:HB2	1.84	0.42
2:B:797:TYR:CD1	2:B:852:ARG:HB3	2.54	0.42
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.01	0.42
2:B:534:GLY:O	2:B:537:LYS:HE2	2.19	0.42
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.34	0.42
11:K:35:PHE:O	11:K:70:ARG:HA	2.20	0.42
1:A:678:GLU:O	1:A:681:GLU:HB3	2.20	0.42
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	2.35	0.42
9:I:40:SER:C	9:I:42:LEU:H	2.22	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:O	1:A:101:LYS:HG2	2.18	0.42
7:G:9:LEU:HD23	7:G:11:ILE:HD11	2.01	0.42
5:E:22:MET:O	5:E:26:ARG:HB2	2.20	0.42
1:A:377:PRO:HD3	1:A:493:GLN:CD	2.40	0.42
7:G:130:TYR:O	7:G:136:VAL:HA	2.20	0.42
1:A:567:LYS:HD2	1:A:568:PRO:HD3	2.01	0.42
1:A:867:ILE:HG12	1:A:1000:LEU:HD11	2.02	0.42
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.67	0.42
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.34	0.42
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	2.02	0.42
1:A:770:VAL:HG13	1:A:822:GLU:HG3	2.02	0.42
2:B:756:ILE:HG21	2:B:767:ASN:OD1	2.20	0.42
1:A:1387:HIS:HA	1:A:1391:ARG:HG2	2.00	0.42
1:A:548:ASN:HA	11:K:60:ALA:HB1	2.02	0.42
2:B:364:ILE:HG21	2:B:373:ARG:HB3	2.01	0.42
2:B:394:ASP:HB2	9:I:91:ARG:HD2	2.01	0.42
8:H:43:ASN:OD1	8:H:45:GLU:HB3	2.20	0.42
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.35	0.42
1:A:789:LYS:HG3	9:I:67:THR:HB	2.01	0.41
1:A:847:ASP:HA	1:A:1424:VAL:HG23	2.02	0.41
1:A:1423:GLY:N	1:A:1426:GLU:HG3	2.30	0.41
1:A:672:ASP:HB2	3:C:195:GLN:HE22	1.84	0.41
1:A:1289:ARG:HB2	1:A:1303:GLU:HG2	2.02	0.41
11:K:70:ARG:HE	11:K:70:ARG:HB3	1.67	0.41
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.71	0.41
3:C:60:ASP:HB3	12:L:67:PHE:CE2	2.55	0.41
2:B:552:MET:HA	2:B:555:ILE:HB	2.02	0.41
2:B:123:THR:HG23	2:B:205:ILE:HA	2.02	0.41
13:X:320:GLU:HA	13:X:323:ALA:HB3	2.02	0.41
1:A:782:ARG:HB3	1:A:789:LYS:HA	2.01	0.41
5:E:35:VAL:C	5:E:37:LEU:H	2.24	0.41
2:B:327:ARG:HG2	2:B:331:LEU:HD13	2.01	0.41
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.56	0.41
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.18	0.41
2:B:580:VAL:O	2:B:586:TRP:HD1	2.04	0.41
2:B:1003:ALA:O	3:C:177:GLU:HA	2.21	0.41
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.61	0.41
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.68	0.41
1:A:101:LYS:HA	1:A:139:TRP:NE1	2.34	0.41
1:A:92:HIS:NE2	1:A:1410:PHE:HE2	2.17	0.41
1:A:886:ILE:HG23	1:A:944:ARG:HG3	2.02	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:LEU:H	1:A:952:ALA:HB1	1.85	0.41
1:A:683:ILE:HD13	1:A:801:GLU:HG3	2.02	0.41
6:F:74:ILE:HG13	6:F:142:SER:HB2	2.01	0.41
2:B:705:MET:H	2:B:710:LEU:HD12	1.85	0.41
1:A:641:VAL:O	1:A:644:LYS:HB3	2.20	0.41
2:B:286:PHE:CD2	2:B:297:ILE:HG23	2.55	0.41
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.20	0.41
1:A:843:LYS:HZ3	1:A:1401:SER:HB2	1.85	0.41
1:A:273:ASN:HD22	1:A:274:ILE:HD12	1.84	0.41
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.41
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.01	0.41
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.55	0.41
2:B:1078:GLY:HA3	3:C:27:LEU:HD11	2.02	0.41
2:B:210:LYS:HD2	2:B:210:LYS:HA	1.84	0.41
2:B:580:VAL:HG13	2:B:624:LEU:HB3	2.01	0.41
5:E:154:ILE:O	5:E:196:VAL:HA	2.20	0.41
7:G:31:LEU:O	7:G:35:GLU:HB3	2.21	0.41
4:D:130:LEU:O	4:D:134:THR:HB	2.20	0.41
1:A:42:ASP:CG	1:A:47:ARG:HA	2.41	0.41
1:A:500:GLU:CD	1:A:1438:THR:HG21	2.41	0.41
1:A:571:LEU:HD22	8:H:46:LEU:HD11	2.02	0.41
1:A:344:ARG:HA	2:B:1128:LEU:O	2.20	0.41
1:A:65:LEU:HB3	1:A:71:GLN:HB3	2.02	0.41
1:A:374:LEU:HB3	1:A:491:VAL:HG21	2.03	0.41
3:C:104:PHE:HE1	3:C:150:GLY:HA2	1.85	0.41
8:H:2:SER:HA	8:H:62:SER:HB3	2.02	0.41
2:B:653:VAL:HG13	2:B:689:LEU:HB3	2.02	0.41
1:A:608:ILE:H	1:A:613:ILE:CD1	2.32	0.41
1:A:1190:PRO:HG2	1:A:1191:TRP:CD1	2.55	0.41
3:C:149:LYS:HB3	3:C:150:GLY:H	1.58	0.41
1:A:717:ASN:O	1:A:720:ARG:HB2	2.21	0.41
2:B:345:LYS:C	2:B:347:LYS:H	2.24	0.41
2:B:1006:ILE:H	2:B:1006:ILE:HG13	1.62	0.41
8:H:105:GLU:HG2	8:H:107:VAL:HG13	2.03	0.41
10:J:41:LEU:HD22	10:J:46:CYS:HB2	2.03	0.41
1:A:21:LEU:HD12	1:A:1414:ALA:HA	2.02	0.41
9:I:16:PRO:HB3	9:I:25:LEU:HD11	2.02	0.41
1:A:874:ASP:HA	1:A:1058:VAL:HG13	2.03	0.41
2:B:579:ARG:HA	2:B:589:VAL:HG12	2.02	0.41
1:A:465:TYR:HB3	2:B:976:ILE:CG2	2.37	0.41
1:A:91:PHE:CE1	1:A:99:ILE:HG21	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:VAL:O	1:A:1035:TYR:HB2	2.20	0.41
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.85	0.41
1:A:1431:GLY:HA3	2:B:1152:MET:HG3	2.02	0.41
1:A:928:LEU:HA	1:A:931:GLU:OE2	2.21	0.41
2:B:793:ALA:O	2:B:855:PHE:HA	2.20	0.41
1:A:531:ILE:HD11	1:A:578:LEU:HD21	2.03	0.40
1:A:840:ARG:HH12	1:A:1102:LYS:HG3	1.87	0.40
1:A:1095:THR:HB	1:A:1100:ARG:HB2	2.02	0.40
4:D:8:PHE:H	7:G:5:LYS:HE3	1.85	0.40
1:A:596:THR:C	1:A:598:LEU:H	2.25	0.40
1:A:811:GLN:HG3	1:A:811:GLN:H	1.52	0.40
6:F:130:ILE:HG22	6:F:132:LEU:H	1.85	0.40
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	2.02	0.40
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	2.02	0.40
5:E:176:PRO:HD2	5:E:211:TYR:O	2.21	0.40
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	2.03	0.40
1:A:1191:TRP:HB3	1:A:1260:LEU:HD22	2.02	0.40
1:A:737:LEU:HA	1:A:738:LYS:HE2	2.04	0.40
2:B:486:TYR:CE1	2:B:1096:ARG:HD2	2.57	0.40
5:E:88:VAL:HB	5:E:116:ILE:HG12	2.02	0.40
2:B:188:ASP:O	2:B:192:LEU:HB2	2.21	0.40
1:A:133:LYS:HA	1:A:136:ALA:HB3	2.03	0.40
1:A:567:LYS:HE3	8:H:46:LEU:HD12	2.02	0.40
1:A:865:GLN:HA	5:E:208:TYR:OH	2.21	0.40
2:B:92:PHE:HZ	2:B:428:ILE:HD13	1.86	0.40
1:A:913:LEU:HD12	1:A:915:SER:OG	2.22	0.40
5:E:136:ASN:O	5:E:140:LEU:HD12	2.21	0.40
4:D:35:LEU:O	4:D:46:GLU:HA	2.19	0.40
1:A:1413:GLY:HA3	2:B:1212:ILE:HG12	2.03	0.40
11:K:38:GLU:HG3	11:K:42:LEU:CD2	2.47	0.40
1:A:700:ASN:O	9:I:115:LYS:HD2	2.21	0.40
3:C:72:LEU:HA	3:C:132:PRO:HA	2.03	0.40
1:A:53:LEU:HD22	1:A:263:THR:HG22	2.04	0.40
6:F:90:ARG:HG2	6:F:94:LEU:CD1	2.52	0.40
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.36	0.40
1:A:1194:ARG:HG3	1:A:1237:ILE:HG23	2.03	0.40
6:F:79:ARG:HG2	6:F:146:TRP:CZ2	2.56	0.40
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.04	0.40
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.02	0.40
5:E:112:TYR:CD2	5:E:115:ASN:HA	2.57	0.40
1:A:365:GLY:HA3	1:A:469:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1111 (79%)	218 (16%)	77 (6%)	2	29
2	B	1075/1224 (88%)	861 (80%)	155 (14%)	59 (6%)	2	29
3	C	264/318 (83%)	208 (79%)	47 (18%)	9 (3%)	5	41
4	D	173/221 (78%)	144 (83%)	18 (10%)	11 (6%)	2	25
5	E	212/215 (99%)	176 (83%)	30 (14%)	6 (3%)	6	45
6	F	82/155 (53%)	69 (84%)	11 (13%)	2 (2%)	7	48
7	G	169/171 (99%)	143 (85%)	22 (13%)	4 (2%)	7	48
8	H	129/146 (88%)	96 (74%)	17 (13%)	16 (12%)	0	8
9	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	7	46
10	J	63/70 (90%)	46 (73%)	14 (22%)	3 (5%)	3	32
11	K	113/120 (94%)	94 (83%)	18 (16%)	1 (1%)	21	67
12	L	44/70 (63%)	25 (57%)	13 (30%)	6 (14%)	0	7
13	X	107/594 (18%)	83 (78%)	20 (19%)	4 (4%)	4	39
All	All	3954/5159 (77%)	3152 (80%)	601 (15%)	201 (5%)	2	30

All (201) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	47	ARG
1	A	57	ARG
1	A	65	LEU
1	A	71	GLN
1	A	93	VAL
1	A	164	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	323	LYS
1	A	331	GLY
1	A	332	LYS
1	A	335	ARG
1	A	385	ILE
1	A	424	ILE
1	A	462	VAL
1	A	466	SER
1	A	543	LEU
1	A	567	LYS
1	A	751	SER
1	A	775	ILE
1	A	875	ALA
1	A	1097	GLY
1	A	1223	ASP
1	A	1281	ARG
2	B	67	SER
2	B	108	VAL
2	B	177	LYS
2	B	229	ALA
2	B	249	ARG
2	B	266	ALA
2	B	364	ILE
2	B	367	LEU
2	B	731	VAL
2	B	734	HIS
2	B	785	TYR
2	B	880	THR
2	B	962	LYS
2	B	1041	GLU
2	B	1132	GLU
2	B	1157	ALA
2	B	1165	ILE
2	B	1188	LYS
3	C	40	GLU
3	C	197	SER
3	C	240	VAL
4	D	18	VAL
5	E	104	ASN
5	E	174	GLN
6	F	78	GLN
7	G	20	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	84	ALA
8	H	128	ASN
10	J	2	ILE
12	L	55	ILE
13	X	332	LEU
13	X	335	LEU
13	X	336	VAL
1	A	41	MET
1	A	42	ASP
1	A	66	LYS
1	A	68	GLN
1	A	167	CYS
1	A	184	SER
1	A	286	HIS
1	A	318	SER
1	A	673	GLY
1	A	846	GLU
1	A	923	LEU
1	A	1206	ASP
1	A	1314	SER
1	A	1388	GLY
1	A	1403	GLU
1	A	1437	GLY
2	B	45	SER
2	B	55	VAL
2	B	245	GLU
2	B	251	ILE
2	B	275	TYR
2	B	369	GLY
2	B	447	ALA
2	B	667	GLN
2	B	711	GLU
2	B	712	PRO
2	B	751	VAL
2	B	772	ALA
2	B	1046	PRO
2	B	1113	VAL
2	B	1223	ASP
3	C	142	VAL
4	D	53	SER
4	D	56	ARG
4	D	119	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	135	GLY
4	D	184	ALA
5	E	36	GLU
7	G	154	VAL
8	H	6	PHE
8	H	81	PRO
8	H	82	PRO
8	H	94	ASP
8	H	108	SER
8	H	131	ASN
8	H	139	ASN
10	J	13	VAL
11	K	6	ARG
12	L	33	GLU
12	L	45	ALA
1	A	40	THR
1	A	322	VAL
1	A	396	PRO
1	A	639	PRO
1	A	738	LYS
1	A	858	ASN
1	A	981	LEU
1	A	1122	PRO
1	A	1236	LEU
1	A	1416	ALA
1	A	1421	CYS
2	B	40	GLU
2	B	305	VAL
2	B	511	PRO
2	B	608	ASP
2	B	649	LYS
2	B	725	PRO
2	B	907	GLY
2	B	982	SER
2	B	1066	SER
2	B	1102	LYS
2	B	1215	ARG
3	C	90	ASP
4	D	40	HIS
4	D	55	ALA
4	D	138	ASN
5	E	3	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	75	MET
8	H	78	SER
8	H	110	ASP
9	I	61	ASP
9	I	88	SER
12	L	50	ASP
1	A	5	GLN
1	A	63	ARG
1	A	196	GLU
1	A	465	TYR
1	A	1396	ALA
1	A	1440	ALA
2	B	41	LYS
2	B	106	ASP
2	B	214	ALA
2	B	575	PRO
2	B	642	ASP
2	B	1119	VAL
3	C	214	ASN
4	D	22	GLU
6	F	73	ALA
8	H	60	ALA
8	H	77	ARG
13	X	329	LYS
1	A	4	GLN
1	A	45	GLN
1	A	109	HIS
1	A	117	GLU
1	A	253	ASN
1	A	958	VAL
1	A	1107	VAL
1	A	1255	GLU
2	B	1189	ILE
3	C	149	LYS
4	D	20	GLU
5	E	185	ALA
7	G	52	ASP
8	H	109	LYS
12	L	39	SER
12	L	56	LEU
1	A	254	GLU
1	A	380	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	479	ASN
1	A	1256	GLU
1	A	1424	VAL
1	A	1454	MET
2	B	514	LEU
2	B	593	PRO
2	B	894	ASP
2	B	1108	ARG
2	B	1143	ALA
2	B	1155	SER
7	G	147	ILE
8	H	103	LYS
9	I	53	GLY
10	J	64	ASN
1	A	916	GLY
1	A	178	GLY
1	A	599	SER
2	B	168	GLY
2	B	436	VAL
3	C	5	GLY
8	H	107	VAL
1	A	910	PRO
1	A	1189	SER
1	A	1327	ILE
3	C	141	GLY
1	A	258	GLY

### 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	1239/1520 (82%)	998 (80%)	241 (20%)	2	13
2	B	952/1061 (90%)	773 (81%)	179 (19%)	2	14
3	C	234/274 (85%)	197 (84%)	37 (16%)	3	22
4	D	140/200 (70%)	115 (82%)	25 (18%)	2	16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	164 (84%)	32 (16%)	3	21
6	F	74/137 (54%)	62 (84%)	12 (16%)	3	21
7	G	152/152 (100%)	130 (86%)	22 (14%)	4	26
8	H	117/128 (91%)	101 (86%)	16 (14%)	4	28
9	I	113/116 (97%)	98 (87%)	15 (13%)	5	29
10	J	60/65 (92%)	45 (75%)	15 (25%)	1	6
11	K	99/102 (97%)	82 (83%)	17 (17%)	2	18
12	L	40/57 (70%)	31 (78%)	9 (22%)	1	9
All	All	3416/4009 (85%)	2796 (82%)	620 (18%)	2	16

All (620) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	21	LEU
1	A	23	SER
1	A	28	ARG
1	A	30	ILE
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	39	GLU
1	A	41	MET
1	A	50	ILE
1	A	53	LEU
1	A	61	ILE
1	A	68	GLN
1	A	69	THR
1	A	71	GLN
1	A	72	GLU
1	A	74	MET
1	A	85	ASP
1	A	93	VAL
1	A	96	ILE
1	A	104	GLU
1	A	109	HIS
1	A	132	LYS
1	A	141	LEU
1	A	156	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	157	ASP
1	A	159	THR
1	A	171	GLN
1	A	173	THR
1	A	180	LYS
1	A	204	THR
1	A	210	ILE
1	A	215	SER
1	A	216	VAL
1	A	226	GLU
1	A	232	GLU
1	A	236	LEU
1	A	237	THR
1	A	238	CYS
1	A	254	GLU
1	A	257	ARG
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	277	GLU
1	A	286	HIS
1	A	289	ILE
1	A	290	GLU
1	A	303	TYR
1	A	307	ASP
1	A	308	ILE
1	A	311	GLN
1	A	316	GLN
1	A	318	SER
1	A	320	ARG
1	A	324	SER
1	A	335	ARG
1	A	372	LYS
1	A	384	ASN
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
1	A	392	VAL
1	A	417	TYR
1	A	423	ASP
1	A	434	ARG
1	A	437	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	442	VAL
1	A	443	LEU
1	A	446	ARG
1	A	447	GLN
1	A	450	LEU
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	471	ASN
1	A	472	LEU
1	A	481	ASP
1	A	486	GLU
1	A	489	LEU
1	A	495	GLU
1	A	496	GLU
1	A	498	ARG
1	A	504	LEU
1	A	513	SER
1	A	515	GLN
1	A	518	LYS
1	A	523	ILE
1	A	527	THR
1	A	532	ARG
1	A	533	LYS
1	A	545	GLN
1	A	552	TRP
1	A	557	ASP
1	A	562	THR
1	A	565	ILE
1	A	566	ILE
1	A	567	LYS
1	A	578	LEU
1	A	591	PHE
1	A	603	ASN
1	A	618	GLU
1	A	621	THR
1	A	629	LEU
1	A	636	GLU
1	A	640	GLN
1	A	654	ASN
1	A	657	LEU
1	A	663	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	681	GLU
1	A	701	LEU
1	A	703	THR
1	A	705	LYS
1	A	706	HIS
1	A	714	PHE
1	A	716	ASP
1	A	718	VAL
1	A	721	PHE
1	A	735	VAL
1	A	738	LYS
1	A	756	ILE
1	A	757	ASN
1	A	764	CYS
1	A	771	GLU
1	A	782	ARG
1	A	783	THR
1	A	791	ASP
1	A	795	GLU
1	A	796	SER
1	A	805	LEU
1	A	811	GLN
1	A	818	MET
1	A	822	GLU
1	A	834	THR
1	A	837	ILE
1	A	839	ARG
1	A	847	ASP
1	A	853	ASP
1	A	858	ASN
1	A	860	LEU
1	A	884	ASP
1	A	886	ILE
1	A	890	ASP
1	A	909	ASP
1	A	913	LEU
1	A	915	SER
1	A	917	SER
1	A	919	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	920	LEU
1	A	926	GLN
1	A	928	LEU
1	A	929	LEU
1	A	937	VAL
1	A	942	PHE
1	A	947	PHE
1	A	948	VAL
1	A	964	ILE
1	A	968	GLN
1	A	972	HIS
1	A	973	ILE
1	A	974	ASP
1	A	976	THR
1	A	982	THR
1	A	988	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1017	LEU
1	A	1019	CYS
1	A	1037	LEU
1	A	1048	ASN
1	A	1050	GLU
1	A	1052	GLN
1	A	1058	VAL
1	A	1067	LEU
1	A	1094	VAL
1	A	1095	THR
1	A	1098	VAL
1	A	1100	ARG
1	A	1110	ASN
1	A	1113	THR
1	A	1135	ARG
1	A	1142	THR
1	A	1155	ASP
1	A	1159	ARG
1	A	1174	PHE
1	A	1175	SER
1	A	1195	LEU
1	A	1204	ASP
1	A	1207	LEU
1	A	1215	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1226	VAL
1	A	1227	ILE
1	A	1233	ASP
1	A	1234	GLU
1	A	1238	ILE
1	A	1240	CYS
1	A	1242	VAL
1	A	1256	GLU
1	A	1259	MET
1	A	1264	GLU
1	A	1266	THR
1	A	1277	GLU
1	A	1280	GLU
1	A	1285	MET
1	A	1287	TYR
1	A	1289	ARG
1	A	1293	SER
1	A	1295	THR
1	A	1298	TYR
1	A	1299	VAL
1	A	1303	GLU
1	A	1315	GLU
1	A	1322	ILE
1	A	1331	SER
1	A	1333	ILE
1	A	1335	ILE
1	A	1341	ILE
1	A	1345	ARG
1	A	1356	ILE
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1373	ASP
1	A	1382	THR
1	A	1391	ARG
1	A	1392	SER
1	A	1393	ASN
1	A	1400	CYS
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1443	VAL
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
2	B	20	ASP
2	B	21	GLU
2	B	25	ILE
2	B	33	VAL
2	B	44	VAL
2	B	46	GLN
2	B	50	SER
2	B	56	ASP
2	B	58	THR
2	B	59	LEU
2	B	61	ASP
2	B	63	ILE
2	B	101	MET
2	B	102	VAL
2	B	103	ASN
2	B	108	VAL
2	B	119	LEU
2	B	126	SER
2	B	128	LEU
2	B	131	ASP
2	B	177	LYS
2	B	189	LEU
2	B	192	LEU
2	B	211	VAL
2	B	223	VAL
2	B	232	SER
2	B	244	LEU
2	B	248	SER
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG
2	B	268	THR
2	B	273	LEU
2	B	283	VAL
2	B	294	ASP
2	B	313	MET
2	B	324	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	329	THR
2	B	331	LEU
2	B	334	ILE
2	B	348	ARG
2	B	365	THR
2	B	367	LEU
2	B	376	PHE
2	B	381	MET
2	B	393	LYS
2	B	394	ASP
2	B	395	GLN
2	B	396	ASP
2	B	398	ARG
2	B	408	LEU
2	B	415	GLN
2	B	418	LYS
2	B	425	THR
2	B	429	PHE
2	B	430	ARG
2	B	436	VAL
2	B	446	LEU
2	B	452	THR
2	B	466	TRP
2	B	485	ARG
2	B	487	THR
2	B	491	THR
2	B	492	LEU
2	B	510	LYS
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	541	LEU
2	B	546	SER
2	B	550	ASP
2	B	552	MET
2	B	563	MET
2	B	567	GLU
2	B	576	ASP
2	B	582	VAL
2	B	591	ARG
2	B	592	ASN
2	B	596	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	599	THR
2	B	602	THR
2	B	616	ILE
2	B	617	ARG
2	B	620	ARG
2	B	624	LEU
2	B	628	THR
2	B	635	ARG
2	B	644	GLU
2	B	653	VAL
2	B	666	TYR
2	B	684	LEU
2	B	694	ASP
2	B	708	GLU
2	B	727	LYS
2	B	738	PHE
2	B	754	SER
2	B	755	ILE
2	B	771	SER
2	B	785	TYR
2	B	791	THR
2	B	792	MET
2	B	795	ILE
2	B	797	TYR
2	B	830	TYR
2	B	837	ASP
2	B	839	MET
2	B	842	ASN
2	B	844	SER
2	B	855	PHE
2	B	857	ARG
2	B	860	MET
2	B	863	GLU
2	B	865	LYS
2	B	870	ILE
2	B	874	PHE
2	B	875	GLU
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	891	ASP
2	B	892	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	894	ASP
2	B	895	ASP
2	B	903	VAL
2	B	905	VAL
2	B	909	ASP
2	B	916	THR
2	B	935	ARG
2	B	942	ARG
2	B	956	THR
2	B	959	ASP
2	B	970	THR
2	B	973	ILE
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	996	ARG
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1012	ILE
2	B	1017	ILE
2	B	1022	THR
2	B	1026	LEU
2	B	1034	VAL
2	B	1045	SER
2	B	1049	ASP
2	B	1050	ILE
2	B	1055	ILE
2	B	1059	LEU
2	B	1072	MET
2	B	1077	THR
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1094	ARG
2	B	1101	ASP
2	B	1106	ARG
2	B	1112	GLN
2	B	1122	ARG
2	B	1133	MET
2	B	1145	SER
2	B	1147	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1148	LYS
2	B	1151	LEU
2	B	1155	SER
2	B	1170	THR
2	B	1176	ASN
2	B	1182	CYS
2	B	1191	ILE
2	B	1195	HIS
2	B	1202	LEU
2	B	1203	LEU
2	B	1207	LEU
2	B	1211	ASN
2	B	1218	THR
2	B	1220	ARG
2	B	1221	SER
2	B	1224	PHE
3	C	16	ASP
3	C	19	ASP
3	C	25	VAL
3	C	26	ASP
3	C	34	ARG
3	C	35	ARG
3	C	36	VAL
3	C	38	ILE
3	C	49	VAL
3	C	52	GLU
3	C	55	THR
3	C	62	PHE
3	C	66	ARG
3	C	80	LEU
3	C	87	PHE
3	C	104	PHE
3	C	106	GLU
3	C	120	ILE
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	136	ASP
3	C	155	LEU
3	C	184	ASN
3	C	186	LEU
3	C	187	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	189	THR
3	C	190	ASP
3	C	203	GLN
3	C	214	ASN
3	C	220	ASP
3	C	227	THR
3	C	231	ASN
3	C	233	GLU
3	C	240	VAL
3	C	260	LEU
3	C	265	MET
4	D	28	GLN
4	D	38	ILE
4	D	46	GLU
4	D	48	ILE
4	D	50	LEU
4	D	64	VAL
4	D	65	GLU
4	D	68	ARG
4	D	126	ILE
4	D	127	ASP
4	D	131	GLU
4	D	138	ASN
4	D	139	LYS
4	D	147	TYR
4	D	153	ARG
4	D	156	ASP
4	D	157	GLN
4	D	158	GLU
4	D	180	LEU
4	D	185	CYS
4	D	189	ASP
4	D	197	SER
4	D	206	GLU
4	D	208	GLU
4	D	216	ASN
5	E	5	ASN
5	E	8	ASN
5	E	26	ARG
5	E	30	ILE
5	E	32	GLN
5	E	46	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	52	ARG
5	E	61	GLN
5	E	65	THR
5	E	67	GLU
5	E	69	ILE
5	E	70	SER
5	E	74	ASP
5	E	75	MET
5	E	91	LYS
5	E	94	LYS
5	E	96	PHE
5	E	98	ILE
5	E	100	ILE
5	E	104	ASN
5	E	106	GLN
5	E	110	PHE
5	E	114	ASN
5	E	117	THR
5	E	150	VAL
5	E	152	LYS
5	E	170	LEU
5	E	179	GLN
5	E	182	ASP
5	E	184	VAL
5	E	196	VAL
5	E	208	TYR
6	F	77	ASP
6	F	79	ARG
6	F	92	ARG
6	F	102	SER
6	F	104	ASN
6	F	110	ASP
6	F	115	THR
6	F	119	ARG
6	F	135	ARG
6	F	138	LEU
6	F	140	ASP
6	F	153	VAL
7	G	3	PHE
7	G	21	ARG
7	G	26	LEU
7	G	42	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	G	46	LEU
7	G	60	ARG
7	G	77	VAL
7	G	79	PHE
7	G	85	GLU
7	G	87	VAL
7	G	90	THR
7	G	111	THR
7	G	119	LEU
7	G	126	ASN
7	G	131	GLN
7	G	135	ASP
7	G	138	THR
7	G	143	ILE
7	G	151	ILE
7	G	160	ILE
7	G	164	LYS
7	G	165	GLU
8	H	16	ASP
8	H	27	GLU
8	H	31	THR
8	H	34	ASP
8	H	36	CYS
8	H	49	VAL
8	H	53	ASP
8	H	54	SER
8	H	61	SER
8	H	86	ASP
8	H	91	ASP
8	H	107	VAL
8	H	110	ASP
8	H	124	ARG
8	H	128	ASN
8	H	130	ARG
9	I	4	PHE
9	I	8	ARG
9	I	9	ASP
9	I	12	ASN
9	I	28	GLU
9	I	31	THR
9	I	37	GLU
9	I	71	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	I	78	CYS
9	I	92	ARG
9	I	94	ASP
9	I	96	SER
9	I	97	MET
9	I	113	ASP
9	I	119	THR
10	J	2	ILE
10	J	3	VAL
10	J	9	SER
10	J	12	LYS
10	J	13	VAL
10	J	19	GLU
10	J	24	LEU
10	J	25	LEU
10	J	30	LEU
10	J	31	ASP
10	J	37	SER
10	J	46	CYS
10	J	48	ARG
10	J	55	ASP
10	J	62	ARG
11	K	5	ASP
11	K	9	LEU
11	K	11	LEU
11	K	14	GLU
11	K	18	LYS
11	K	21	ILE
11	K	29	ASN
11	K	31	VAL
11	K	33	ILE
11	K	47	ARG
11	K	51	LEU
11	K	53	ASP
11	K	54	ARG
11	K	67	PHE
11	K	70	ARG
11	K	85	ASP
11	K	92	ASN
12	L	30	ILE
12	L	38	LEU
12	L	50	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	L	55	ILE
12	L	57	LEU
12	L	58	LYS
12	L	61	THR
12	L	64	LEU
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	209	ASN
1	A	225	ASN
1	A	273	ASN
1	A	281	HIS
1	A	297	GLN
1	A	299	HIS
1	A	358	ASN
1	A	390	GLN
1	A	394	ASN
1	A	399	HIS
1	A	435	HIS
1	A	517	ASN
1	A	548	ASN
1	A	587	HIS
1	A	626	ASN
1	A	654	ASN
1	A	741	ASN
1	A	757	ASN
1	A	767	GLN
1	A	877	HIS
1	A	881	GLN
1	A	903	ASN
1	A	1009	ASN
1	A	1078	GLN
1	A	1188	GLN
1	A	1232	ASN
1	A	1354	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	110	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	115	GLN
2	B	121	ASN
2	B	206	ASN
2	B	215	GLN
2	B	224	GLN
2	B	300	HIS
2	B	415	GLN
2	B	449	ASN
2	B	499	ASN
2	B	516	ASN
2	B	538	ASN
2	B	590	HIS
2	B	657	HIS
2	B	744	HIS
2	B	842	ASN
2	B	862	GLN
2	B	1015	HIS
2	B	1062	HIS
2	B	1161	HIS
2	B	1178	ASN
3	C	24	ASN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	184	ASN
3	C	195	GLN
3	C	203	GLN
3	C	231	ASN
4	D	41	GLN
5	E	5	ASN
5	E	61	GLN
5	E	113	GLN
5	E	147	HIS
7	G	57	GLN
7	G	122	ASN
7	G	131	GLN
8	H	21	ASN
9	I	11	ASN
9	I	12	ASN
11	K	29	ASN
11	K	44	ASN
11	K	65	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	K	92	ASN
12	L	66	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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, 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	1416/1733 (81%)	0.22	55 (3%) 43 36	118, 185, 242, 274	0
2	B	1097/1224 (89%)	0.19	21 (1%) 70 62	111, 200, 254, 282	0
3	C	266/318 (83%)	0.21	6 (2%) 64 55	139, 193, 237, 271	0
4	D	177/221 (80%)	0.19	5 (2%) 56 48	149, 199, 250, 261	0
5	E	214/215 (99%)	0.38	8 (3%) 45 37	153, 223, 267, 279	0
6	F	84/155 (54%)	0.17	0 100 100	113, 165, 217, 239	0
7	G	171/171 (100%)	0.26	6 (3%) 48 40	157, 188, 230, 261	0
8	H	133/146 (91%)	0.56	9 (6%) 20 16	185, 229, 254, 261	0
9	I	119/122 (97%)	0.62	13 (10%) 7 8	185, 233, 264, 271	0
10	J	65/70 (92%)	0.04	0 100 100	148, 173, 225, 245	0
11	K	115/120 (95%)	0.23	1 (0%) 85 80	140, 182, 230, 246	0
12	L	46/70 (65%)	0.30	0 100 100	153, 242, 260, 266	0
13	X	113/594 (19%)	0.33	3 (2%) 58 49	232, 271, 294, 295	0
All	All	4016/5159 (77%)	0.24	127 (3%) 51 42	111, 196, 260, 295	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	3.9
1	A	114	LEU	3.5
1	A	164	ARG	3.4
1	A	145	LYS	3.3
2	B	132	VAL	3.3
1	A	112	LYS	3.2
2	B	915	THR	3.1
1	A	149	GLU	3.1
2	B	918	ILE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
11	K	115	ALA	3.1
9	I	18	GLU	3.1
7	G	51	TYR	3.0
5	E	88	VAL	2.9
3	C	13	ALA	2.9
2	B	345	LYS	2.9
8	H	127	GLY	2.8
1	A	344	ARG	2.8
2	B	1127	GLY	2.8
2	B	591	ARG	2.7
3	C	97	VAL	2.7
1	A	148	CYS	2.7
2	B	577	ALA	2.7
1	A	1284	MET	2.7
8	H	112	ILE	2.7
9	I	76	PRO	2.7
1	A	199	LEU	2.7
2	B	935	ARG	2.7
4	D	37	GLN	2.6
7	G	115	MET	2.6
1	A	146	MET	2.6
1	A	1126	ALA	2.6
1	A	108	MET	2.6
1	A	257	ARG	2.6
5	E	89	GLY	2.6
2	B	569	TYR	2.6
7	G	94	CYS	2.6
2	B	916	THR	2.6
1	A	118	HIS	2.6
1	A	1108	ALA	2.6
4	D	66	ARG	2.6
1	A	1303	GLU	2.6
1	A	147	VAL	2.6
1	A	919	ILE	2.6
9	I	102	VAL	2.5
2	B	917	PRO	2.5
9	I	15	TYR	2.5
7	G	137	ILE	2.5
9	I	73	ARG	2.5
1	A	197	PRO	2.5
2	B	590	HIS	2.5
1	A	981	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	116	ASN	2.5
7	G	130	TYR	2.5
1	A	1282	VAL	2.5
8	H	35	GLN	2.5
1	A	200	ARG	2.5
2	B	102	VAL	2.5
8	H	126	GLU	2.5
4	D	4	SER	2.5
7	G	128	PRO	2.5
1	A	115	LEU	2.5
1	A	901	LEU	2.5
5	E	114	ASN	2.5
5	E	30	ILE	2.4
1	A	259	GLU	2.4
1	A	908	LEU	2.4
9	I	77	LYS	2.4
1	A	1095	THR	2.4
1	A	893	PHE	2.4
1	A	983	ILE	2.3
1	A	1283	VAL	2.3
3	C	4	GLU	2.3
1	A	1036	ARG	2.3
5	E	106	GLN	2.3
8	H	140	ALA	2.3
1	A	1081	LEU	2.3
1	A	1120	LEU	2.3
9	I	105	SER	2.3
1	A	49	LYS	2.3
1	A	323	LYS	2.3
2	B	130	VAL	2.3
13	X	283	GLU	2.2
13	X	284	GLU	2.2
2	B	866	TYR	2.2
1	A	104	GLU	2.2
1	A	1304	TRP	2.2
8	H	130	ARG	2.2
1	A	111	GLY	2.2
1	A	202	LEU	2.2
1	A	155	GLU	2.2
3	C	77	ILE	2.2
9	I	104	LEU	2.2
1	A	171	GLN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	120	GLN	2.2
1	A	402	ALA	2.2
2	B	936	ASP	2.2
1	A	1241	ARG	2.2
1	A	944	ARG	2.1
9	I	83	ASN	2.1
2	B	466	TRP	2.1
9	I	27	PHE	2.1
1	A	763	ALA	2.1
8	H	139	ASN	2.1
5	E	28	TYR	2.1
1	A	900	ASP	2.1
9	I	14	LEU	2.1
1	A	60	SER	2.1
5	E	82	PHE	2.1
5	E	123	LEU	2.1
4	D	44	GLU	2.1
3	C	160	LYS	2.1
4	D	35	LEU	2.1
1	A	116	ASP	2.1
1	A	113	LEU	2.1
3	C	44	LEU	2.1
1	A	73	GLY	2.1
1	A	258	GLY	2.1
2	B	650	GLU	2.1
1	A	1112	LYS	2.0
2	B	654	ARG	2.0
8	H	111	LEU	2.0
1	A	806	ARG	2.0
8	H	129	TYR	2.0
2	B	729	ILE	2.0
1	A	126	LEU	2.0
1	A	1256	GLU	2.0
13	X	337	ASN	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 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( $\text{\AA}^2$ )	Q<0.9
14	ZN	J	1066	1/1	0.99	0.30	0.03	192,192,192,192	0
14	ZN	B	2225	1/1	0.99	0.18	-1.35	96,96,96,96	0
14	ZN	I	1121	1/1	0.97	0.09	-1.68	230,230,230,230	0
14	ZN	A	2456	1/1	0.94	0.09	-1.91	181,181,181,181	0
14	ZN	L	1071	1/1	0.84	0.07	-1.96	266,266,266,266	0
14	ZN	I	1122	1/1	0.97	0.25	-2.05	245,245,245,245	0
14	ZN	A	2457	1/1	0.97	0.15	-2.07	105,105,105,105	0
14	ZN	C	1269	1/1	0.98	0.08	-2.07	140,140,140,140	0
15	MG	A	2458	1/1	-0.04	1.05	-	130,130,130,130	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.