



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2017 – 04:42 AM EST

PDB ID : 5UHB  
Title : Crystal structure of Mycobacterium tuberculosis transcription initiation complex in complex with Rifampin  
Authors : Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.  
Deposited on : unknown  
Resolution : 4.29 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345



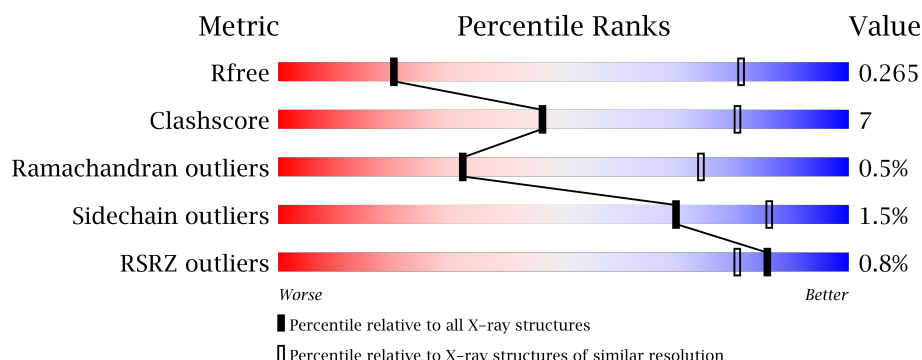
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.29 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))
$R_{free}$	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

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	347	
1	B	347	
2	C	1178	
3	D	1316	
4	E	110	

*Continued on next page...*



Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	528	<div><div><div></div><div></div><div></div><div></div></div><div><div>47%</div><div>13%</div><div></div><div>39%</div></div></div>
6	H	23	<div><div><div></div><div></div></div><div><div>57%</div><div>43%</div></div></div>
7	G	16	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>19%</div><div>44%</div><div>25%</div><div>6%</div><div>25%</div></div></div>



## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25979 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1704	1072	295	335	2			
1	B	227	Total	C	N	O	S	0	0	0
			1715	1080	291	342	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1126	Total	C	N	O	S	0	0	0
			8714	5454	1528	1693	39			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1265	Total	C	N	O	S	0	0	0
			9887	6188	1793	1866	40			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	81	Total	C	N	O	0	0	0
			637	408	106	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	320	Total	C	N	O	S	0	0	0
			2543	1583	459	492	9			

- Molecule 6 is a DNA chain called DNA (5'-D(\*TP\*AP\*TP\*AP\*AP\*TP\*GP\*GP\*GP\*AP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*CP\*GP\*GP\*AP\*TP\*G)-3').

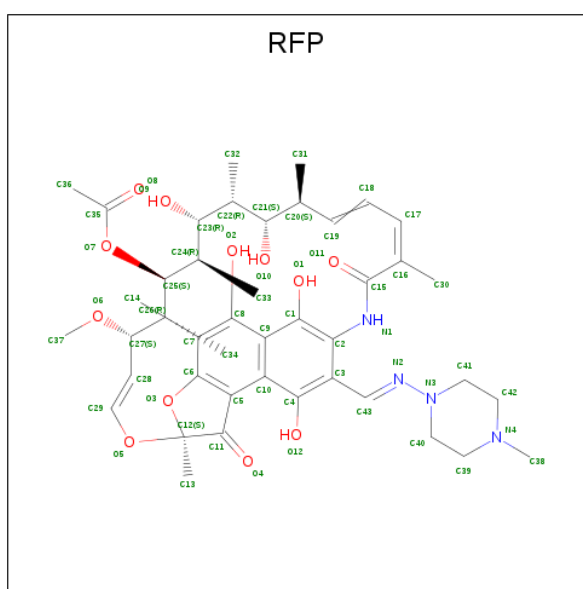


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	23	Total	C	N	O	P	0	0	0
			476	227	91	136	22			

- Molecule 7 is a DNA chain called DNA (5'-D(\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*GP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			

- Molecule 8 is RIFAMPICIN (three-letter code: RFP) (formula: C<sub>43</sub>H<sub>58</sub>N<sub>4</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			59	43	4	12		

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

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

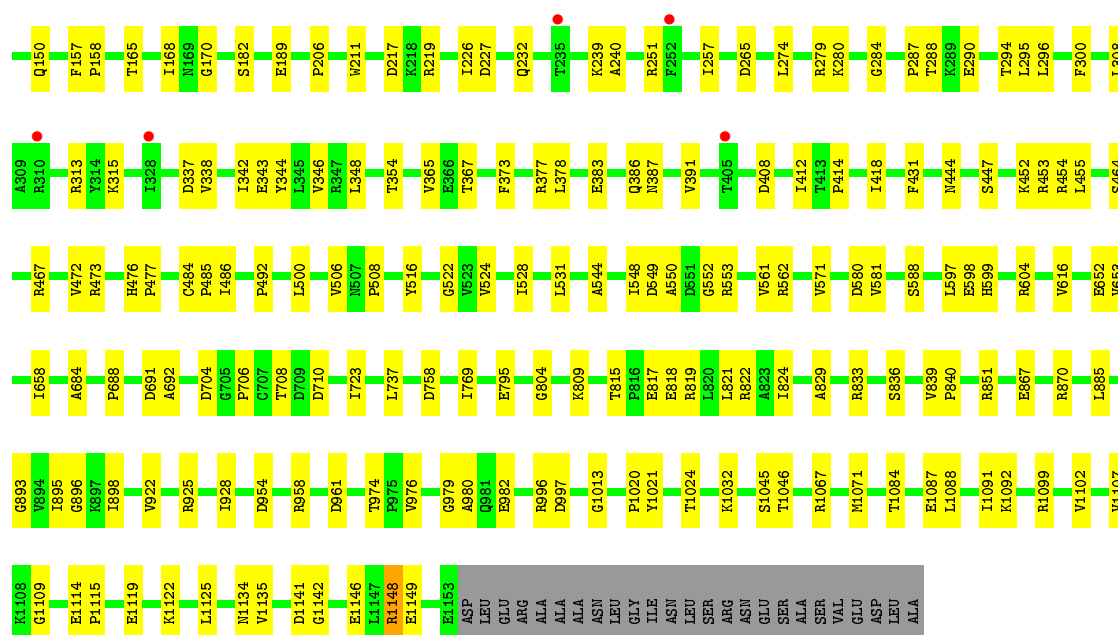
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

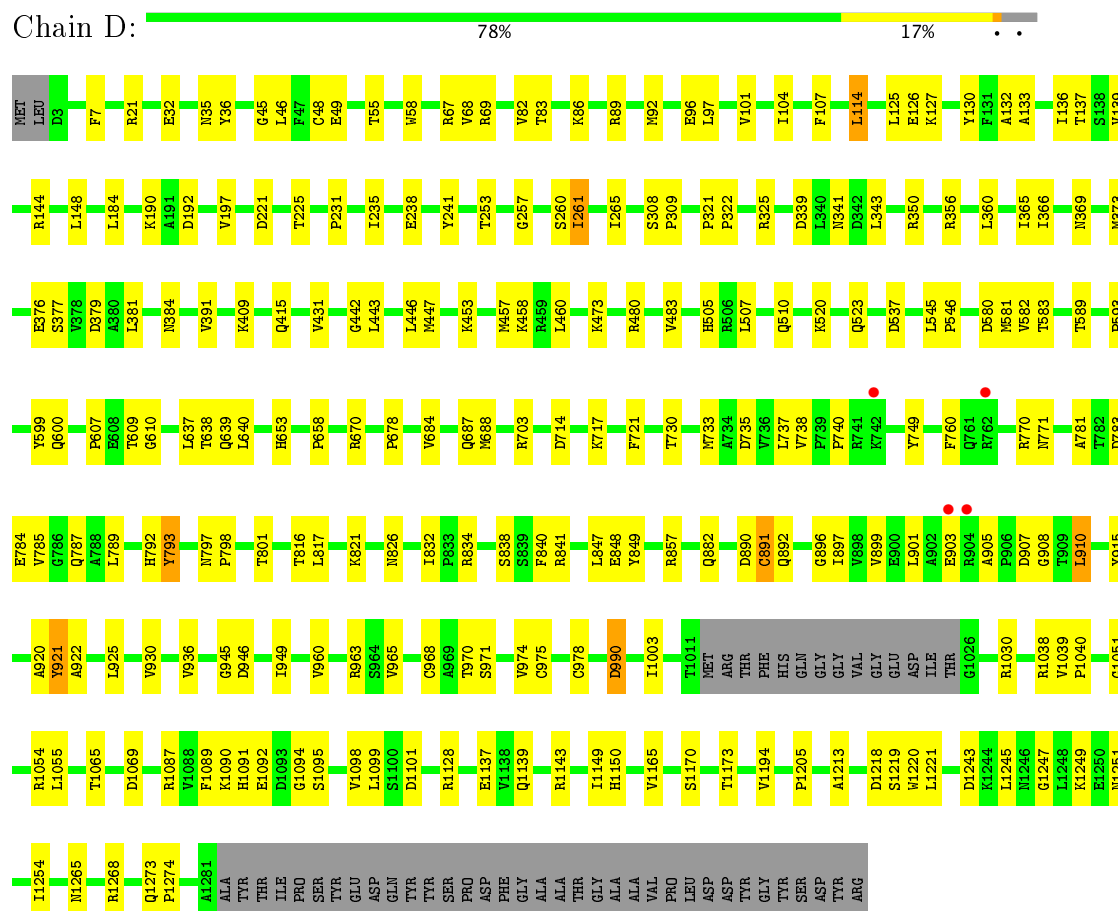








• Molecule 3: DNA-directed RNA polymerase subunit beta'



• Molecule 4: DNA-directed RNA polymerase subunit omega

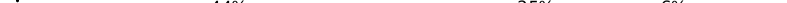


GLU

- Chain F: 

V448  
D449  
A450  
V451  
S452  
F453  
L456  
R470  
V474  
L477  
Q485  
P486  
R487  
T488  
L489  
I492  
V495  
Y496  
T499  
R500  
E501  
R502  
R503  
R504  
Q505  
I506  
—  
—  
K509  
L514  
R515  
—  
R519  
S520  
Q521  
V522  
L523  
—  
L527  
E528

- |    |    |    |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| T1 | A4 | A5 | G11 | G12 | T13 | G14 | T15 | C16 | A17 | C18 | G19 | G20 | G23 |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Chain G: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.19 Å   164.23 Å   200.20 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.78 – 4.29 49.78 – 4.29	Depositor EDS
% Data completeness (in resolution range)	83.4 (49.78-4.29) 83.4 (49.78-4.29)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 4.29 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.208   ,   0.267 0.209   ,   0.265	Depositor DCC
$R_{free}$ test set	2004 reflections (6.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 16.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	25979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, RFP, 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	0.23	0/1730	0.44	0/2354
1	B	0.23	0/1741	0.44	0/2371
2	C	0.23	0/8873	0.42	1/12031 (0.0%)
3	D	0.24	0/10052	0.45	5/13591 (0.0%)
4	E	0.25	0/650	0.42	0/886
5	F	0.25	0/2572	0.41	0/3466
6	H	0.55	0/535	0.89	0/826
7	G	0.55	0/269	1.11	1/413 (0.2%)
All	All	0.25	0/26422	0.46	7/35938 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	12	DG	P-O3'-C3'	11.67	133.70	119.70
3	D	910	LEU	O-C-N	11.09	140.44	122.70
3	D	910	LEU	CA-C-N	-8.90	97.62	117.20
3	D	910	LEU	C-N-CA	-7.78	102.25	121.70
3	D	1213	ALA	N-CA-CB	6.34	118.97	110.10
3	D	903	GLU	O-C-N	-6.12	112.91	122.70
2	C	48	LEU	CA-CB-CG	5.41	127.74	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	1704	0	1741	30	0
1	B	1715	0	1739	22	0
2	C	8714	0	8636	129	0
3	D	9887	0	9943	159	0
4	E	637	0	635	9	0
5	F	2543	0	2571	55	0
6	H	476	0	261	10	0
7	G	241	0	137	8	0
8	C	59	0	58	6	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	25979	0	25721	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:562:ARG:NH2	3:D:847:LEU:CD1	2.05	1.19
2:C:562:ARG:NH2	3:D:847:LEU:HD11	1.62	1.11
3:D:891:CYS:SG	3:D:970:THR:OG1	2.09	1.09
2:C:562:ARG:HH22	3:D:847:LEU:HD11	1.23	0.93
7:G:11:DT:H2"	7:G:12:DG:H8	1.32	0.92
3:D:968:CYS:SG	3:D:978:CYS:HB3	2.11	0.90
2:C:562:ARG:HH21	3:D:847:LEU:CD1	1.83	0.87
3:D:970:THR:HG22	3:D:971:SER:H	1.38	0.86
7:G:11:DT:H2"	7:G:12:DG:C8	2.11	0.84
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.69	0.75
2:C:562:ARG:HH21	3:D:847:LEU:HD13	1.50	0.75
2:C:284:GLY:H	5:F:219:ALA:HB1	1.53	0.74
3:D:970:THR:HG22	3:D:971:SER:N	2.02	0.72
2:C:454:ARG:HH22	8:C:1201:RFP:H19C	1.55	0.72
1:A:11:GLU:HB2	1:A:22:VAL:HB	1.74	0.70
2:C:562:ARG:HH22	3:D:847:LEU:CD1	1.87	0.70
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.74	0.69
3:D:46:LEU:O	3:D:325:ARG:NH2	2.20	0.69
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.75	0.69
1:B:75:GLU:O	1:B:79:ASN:ND2	2.26	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:470:ARG:HB3	5:F:506:ILE:HD13	1.76	0.68
2:C:101:GLY:O	2:C:142:ASN:ND2	2.27	0.68
2:C:1024:THR:H	3:D:730:THR:HG21	1.59	0.67
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.28	0.66
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.79	0.65
5:F:401:LYS:HA	5:F:405:ILE:HA	1.79	0.65
7:G:11:DT:C2'	7:G:12:DG:C8	2.79	0.65
3:D:356:ARG:HH21	3:D:360:LEU:HD11	1.62	0.64
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.63	0.64
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.80	0.64
3:D:637:LEU:HD13	3:D:640:LEU:HD12	1.80	0.63
2:C:561:VAL:HG21	2:C:571:VAL:HB	1.80	0.63
3:D:832:ILE:HG22	3:D:834:ARG:H	1.63	0.63
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.79	0.63
2:C:104:SER:HB3	2:C:140:ILE:HB	1.80	0.63
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.80	0.62
6:H:15:DT:H2''	6:H:16:DC:H5'	1.81	0.62
3:D:473:LYS:HD2	5:F:448:VAL:HG21	1.82	0.62
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.64	0.62
1:A:40:ARG:NH1	2:C:1013:GLY:O	2.31	0.62
2:C:48:LEU:HD12	2:C:528:ILE:HD13	1.81	0.62
3:D:238:GLU:OE1	5:F:237:LYS:NZ	2.32	0.62
2:C:815:THR:HG22	2:C:817:GLU:H	1.65	0.61
2:C:562:ARG:NH2	3:D:847:LEU:HD13	2.04	0.61
3:D:589:THR:HG21	3:D:688:MET:HG2	1.83	0.61
3:D:891:CYS:O	3:D:892:GLN:HB2	1.99	0.61
1:A:87:SER:O	1:A:142:ARG:NH1	2.31	0.60
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.82	0.60
5:F:499:THR:OG1	5:F:500:ARG:N	2.31	0.60
3:D:737:LEU:N	3:D:793:TYR:OH	2.32	0.60
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.83	0.60
7:G:11:DT:C1'	7:G:12:DG:C8	2.85	0.60
3:D:365:ILE:HG21	5:F:297:GLU:HG2	1.84	0.59
3:D:1265:ASN:OD1	3:D:1268:ARG:NH2	2.35	0.59
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.85	0.59
1:A:214:THR:HA	1:B:230:GLU:HG2	1.83	0.59
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.84	0.59
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.85	0.58
2:C:821:LEU:HD22	5:F:456:LEU:HD11	1.85	0.58
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.67	0.58
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.36	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:137:THR:OG1	3:D:253:THR:O	2.18	0.58
8:C:1201:RFP:C18	8:C:1201:RFP:HN1	2.17	0.58
8:C:1201:RFP:H28C	8:C:1201:RFP:C5	2.32	0.58
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.37	0.58
2:C:737:LEU:HB2	2:C:898:ILE:HG12	1.85	0.58
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.36	0.57
2:C:43:LYS:NZ	2:C:544:ALA:O	2.36	0.57
2:C:604:ARG:HG3	2:C:925:ARG:HB3	1.86	0.57
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.69	0.57
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.87	0.57
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.85	0.57
5:F:320:LEU:HD21	5:F:359:MET:HE3	1.87	0.57
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.87	0.56
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.88	0.56
2:C:485:PRO:O	3:D:857:ARG:NH2	2.38	0.56
2:C:758:ASP:N	2:C:758:ASP:OD1	2.36	0.56
2:C:1087:GLU:HG2	2:C:1092:LYS:HG3	1.87	0.55
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.89	0.55
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.88	0.55
2:C:974:THR:HG23	2:C:980:ALA:H	1.71	0.55
1:B:100:GLN:HG3	1:B:133:LYS:HA	1.88	0.55
2:C:41:PHE:HB2	2:C:979:GLY:HA2	1.88	0.55
3:D:373:MET:SD	5:F:318:LEU:HB3	2.46	0.55
3:D:921:TYR:HE1	3:D:946:ASP:HA	1.72	0.55
2:C:653:VAL:HG12	2:C:692:ALA:HB2	1.87	0.55
3:D:897:ILE:HD13	3:D:1128:ARG:HH11	1.71	0.55
3:D:915:TYR:HA	3:D:1143:ARG:HH12	1.72	0.55
2:C:1107:VAL:HG21	5:F:451:VAL:HG11	1.89	0.55
3:D:507:LEU:HB3	3:D:510:GLN:HE21	1.71	0.55
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.88	0.55
3:D:970:THR:CG2	3:D:971:SER:H	2.15	0.54
5:F:345:THR:HB	6:H:4:DA:H8	1.73	0.54
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.40	0.54
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.90	0.54
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.89	0.54
2:C:1045:SER:OG	2:C:1046:THR:N	2.41	0.54
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.88	0.54
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.89	0.53
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.90	0.53
2:C:107:PHE:HE1	2:C:418:ILE:HD11	1.73	0.53
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.90	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:NH1	2:C:997:ASP:OD1	2.41	0.53
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.89	0.53
3:D:257:GLY:O	3:D:260:SER:OG	2.23	0.53
3:D:49:GLU:OE2	3:D:55:THR:N	2.40	0.52
1:A:223:ARG:HD3	1:B:213:LYS:HB2	1.91	0.52
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.92	0.52
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.91	0.52
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.91	0.52
5:F:302:LEU:O	5:F:305:SER:OG	2.20	0.52
2:C:1091:ILE:HB	2:C:1102:VAL:HG21	1.91	0.52
3:D:1273:GLN:O	4:E:105:GLU:N	2.36	0.52
4:E:70:GLN:O	4:E:74:GLY:N	2.32	0.51
2:C:378:LEU:HD21	2:C:455:LEU:HD22	1.92	0.51
5:F:515:ARG:O	5:F:519:ARG:N	2.43	0.51
2:C:893:GLY:HA2	3:D:537:ASP:HA	1.92	0.51
3:D:738:VAL:HG13	3:D:841:ARG:HD3	1.92	0.51
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.46	0.51
2:C:704:ASP:HB2	2:C:708:THR:HB	1.93	0.51
2:C:287:PRO:HD2	5:F:216:ARG:HG3	1.93	0.51
2:C:815:THR:O	2:C:819:ARG:N	2.42	0.51
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.46	0.51
2:C:982:GLU:HG3	3:D:841:ARG:HH12	1.76	0.51
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.12	0.50
1:B:97:LEU:HD22	1:B:110:ILE:HG12	1.94	0.50
2:C:524:VAL:HG21	2:C:548:ILE:HD13	1.92	0.50
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.26	0.50
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.92	0.50
5:F:492:ILE:HG22	5:F:503:ILE:HG21	1.93	0.50
3:D:1038:ARG:NH1	6:H:18:DC:O3'	2.44	0.50
3:D:970:THR:CG2	3:D:971:SER:N	2.73	0.50
4:E:33:LEU:H	4:E:33:LEU:HD23	1.77	0.50
3:D:350:ARG:NH1	3:D:373:MET:HB3	2.27	0.50
3:D:990:ASP:N	3:D:990:ASP:OD1	2.45	0.50
2:C:206:PRO:HA	2:C:308:LEU:HD23	1.93	0.50
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.76	0.49
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.93	0.49
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.45	0.49
3:D:376:GLU:OE2	5:F:227:SER:HB3	2.12	0.49
3:D:816:THR:HG23	3:D:821:LYS:HA	1.92	0.49
2:C:896:GLY:HA2	3:D:431:VAL:HG13	1.94	0.49
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.93	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:616:VAL:N	2:C:1032:LYS:O	2.44	0.49
3:D:350:ARG:HH11	3:D:373:MET:HB3	1.78	0.49
5:F:492:ILE:HA	5:F:495:VAL:HG12	1.95	0.49
3:D:735:ASP:O	3:D:797:ASN:ND2	2.40	0.49
6:H:18:DC:H2"	6:H:19:DG:C8	2.47	0.49
1:A:153:ARG:HD3	2:C:795:GLU:CB	2.43	0.49
2:C:822:ARG:NE	2:C:829:ALA:HB2	2.28	0.49
2:C:290:GLU:O	2:C:294:THR:OG1	2.24	0.49
3:D:749:TYR:OH	3:D:784:GLU:OE1	2.24	0.49
3:D:545:LEU:HD12	3:D:546:PRO:HD2	1.95	0.49
3:D:882:GLN:HE22	3:D:1249:LYS:HG3	1.77	0.49
3:D:600:GLN:HB2	3:D:609:THR:HB	1.94	0.48
5:F:266:LEU:HA	5:F:269:ARG:HG2	1.95	0.48
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.95	0.48
2:C:1109:GLY:HA3	3:D:458:LYS:HE3	1.95	0.48
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.29	0.48
1:A:37:SER:O	1:A:41:THR:OG1	2.30	0.48
1:B:72:ASP:OD1	1:B:73:VAL:N	2.45	0.48
2:C:885:LEU:HD12	2:C:895:ILE:HD11	1.95	0.48
3:D:589:THR:HG22	3:D:670:ARG:HG2	1.96	0.48
2:C:549:ASP:HB3	2:C:553:ARG:H	1.78	0.48
1:A:136:VAL:HG12	1:A:137:GLU:H	1.78	0.48
5:F:242:ASN:OD1	5:F:243:ALA:N	2.47	0.48
3:D:907:ASP:N	3:D:907:ASP:OD1	2.47	0.47
7:G:11:DT:H1'	7:G:12:DG:C8	2.49	0.47
2:C:344:TYR:OH	2:C:365:VAL:HA	2.13	0.47
3:D:1170:SER:O	3:D:1173:THR:OG1	2.31	0.47
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.29	0.47
5:F:499:THR:HG23	5:F:500:ARG:HD2	1.96	0.47
5:F:470:ARG:HH11	5:F:506:ILE:HD11	1.80	0.47
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.48	0.47
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.97	0.47
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.29	0.47
5:F:446:VAL:HB	5:F:449:ASP:HB2	1.97	0.47
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.50	0.47
3:D:144:ARG:O	3:D:148:LEU:HB2	2.15	0.47
5:F:345:THR:HA	6:H:5:DA:N7	2.30	0.47
3:D:896:GLY:O	3:D:1128:ARG:NH1	2.35	0.47
3:D:922:ALA:HB3	3:D:1150:HIS:CE1	2.50	0.47
3:D:325:ARG:NH1	3:D:341:ASN:OD1	2.46	0.47
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.32	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:409:LYS:NZ	7:G:15:DT:OP2	2.40	0.47
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.98	0.46
1:B:77:ILE:HG22	1:B:81:LYS:HE3	1.97	0.46
3:D:580:ASP:HB2	3:D:721:PHE:CE1	2.50	0.46
3:D:580:ASP:HB2	3:D:721:PHE:HE1	1.80	0.46
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.49	0.46
1:A:18:ARG:NH2	1:A:195:ASP:OD1	2.41	0.46
1:A:62:GLU:HG3	1:A:77:ILE:HD12	1.97	0.46
3:D:261:ILE:O	3:D:265:ILE:HG13	2.15	0.46
3:D:369:ASN:O	3:D:373:MET:HG3	2.16	0.46
5:F:489:LEU:HD23	5:F:489:LEU:H	1.80	0.46
1:A:97:LEU:HD21	1:A:105:VAL:HG21	1.98	0.46
2:C:522:GLY:O	2:C:553:ARG:HA	2.16	0.46
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	1.98	0.46
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.15	0.46
3:D:35:ASN:OD1	3:D:36:TYR:N	2.49	0.46
3:D:453:LYS:O	3:D:457:MET:HG3	2.16	0.46
1:B:95:MET:HB3	1:B:113:PRO:HD3	1.98	0.46
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.48	0.46
3:D:221:ASP:O	3:D:225:THR:OG1	2.32	0.46
1:B:171:VAL:HG22	1:B:198:THR:HG22	1.98	0.45
8:C:1201:RFP:O12	8:C:1201:RFP:O4	2.33	0.45
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.99	0.45
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.98	0.45
6:H:19:DG:H2"	6:H:20:DG:C8	2.51	0.45
3:D:783:ASP:O	3:D:787:GLN:HG2	2.17	0.45
5:F:342:LYS:HB3	5:F:342:LYS:HE2	1.79	0.45
2:C:544:ALA:HB2	2:C:580:ASP:HB2	1.99	0.45
1:A:120:ASN:N	1:A:120:ASN:OD1	2.48	0.45
1:A:175:THR:OG1	1:A:176:TYR:N	2.50	0.45
8:C:1201:RFP:H342	8:C:1201:RFP:H24C	1.67	0.45
2:C:817:GLU:OE1	2:C:817:GLU:N	2.50	0.45
3:D:365:ILE:HG23	3:D:366:ILE:HG13	1.98	0.45
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.98	0.45
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.71	0.45
3:D:905:ALA:HB3	3:D:908:GLY:O	2.16	0.45
6:H:19:DG:O6	7:G:8:DC:N4	2.49	0.44
2:C:41:PHE:O	2:C:979:GLY:HA2	2.17	0.44
2:C:444:ASN:H	2:C:447:SER:HB3	1.83	0.44
3:D:58:TRP:CD2	3:D:68:VAL:HG13	2.53	0.44
7:G:15:DT:H2'	7:G:16:DC:C6	2.53	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:LYS:HA	2:C:315:LYS:HD2	1.85	0.44
2:C:1067:ARG:NH2	3:D:415:GLN:O	2.50	0.44
3:D:581:MET:HG3	3:D:721:PHE:CE1	2.52	0.44
1:B:39:ARG:HH21	1:B:173:LYS:NZ	2.14	0.44
2:C:928:ILE:H	2:C:928:ILE:HG13	1.50	0.44
2:C:954:ASP:O	2:C:958:ARG:NH1	2.51	0.44
1:A:130:ASP:O	1:A:131:LYS:HG2	2.18	0.44
2:C:288:THR:HG22	2:C:290:GLU:H	1.82	0.44
3:D:798:PRO:HA	3:D:801:THR:HB	1.98	0.44
5:F:364:ARG:HG3	5:F:368:ILE:HG12	1.99	0.44
2:C:824:ILE:HG12	5:F:514:LEU:HD13	2.00	0.44
3:D:1219:SER:OG	3:D:1243:ASP:OD2	2.32	0.44
5:F:347:ALA:O	5:F:351:ILE:HG13	2.18	0.44
1:A:181:THR:O	1:A:188:ASP:HA	2.17	0.44
1:A:208:LEU:O	1:B:222:ALA:HB1	2.18	0.44
1:A:100:GLN:HG2	1:A:101:GLY:H	1.83	0.44
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.53	0.44
2:C:851:ARG:HB3	2:C:870:ARG:HB2	2.00	0.44
3:D:1220:TRP:CD1	3:D:1243:ASP:HB2	2.52	0.44
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.99	0.44
3:D:446:LEU:HD12	3:D:520:LYS:HG2	1.99	0.44
3:D:945:GLY:O	3:D:949:ILE:HG12	2.18	0.44
3:D:127:LYS:O	3:D:133:ALA:N	2.47	0.43
3:D:235:ILE:HD12	3:D:241:TYR:HD1	1.83	0.43
2:C:928:ILE:HG12	3:D:817:LEU:CD1	2.48	0.43
3:D:21:ARG:NH2	3:D:96:GLU:OE2	2.50	0.43
6:H:11:DG:H5"	6:H:12:DC:C4	2.53	0.43
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	2.01	0.43
3:D:443:LEU:HD11	3:D:447:MET:HE2	1.99	0.43
3:D:899:VAL:HG11	3:D:920:ALA:HB2	2.01	0.43
3:D:925:LEU:HD11	3:D:960:VAL:HG11	2.01	0.43
1:B:45:SER:OG	1:B:214:THR:HG21	2.18	0.43
2:C:47:PRO:HB2	2:C:581:VAL:HG13	2.01	0.43
5:F:474:VAL:HA	5:F:477:LEU:HB2	1.99	0.43
3:D:45:GLY:H	3:D:48:CYS:HB2	1.84	0.43
5:F:262:LEU:O	5:F:266:LEU:HG	2.18	0.43
8:C:1201:RFP:H28C	8:C:1201:RFP:H341	1.58	0.43
2:C:815:THR:HG21	5:F:453:PHE:CE1	2.54	0.43
3:D:104:ILE:HB	3:D:379:ASP:OD1	2.19	0.43
3:D:733:MET:HB3	3:D:733:MET:HE2	1.83	0.43
3:D:127:LYS:HA	3:D:132:ALA:HB3	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:599:TYR:HA	3:D:610:GLY:HA3	2.00	0.43
3:D:781:ALA:O	3:D:785:VAL:HG23	2.18	0.43
3:D:834:ARG:NH2	3:D:847:LEU:HG	2.34	0.43
2:C:251:ARG:NH2	2:C:343:GLU:OE1	2.46	0.43
3:D:1247:GLY:H	3:D:1251:ASN:ND2	2.16	0.43
5:F:231:TYR:O	5:F:235:ILE:HG13	2.19	0.43
4:E:32:PRO:HB2	4:E:37:ASN:HB2	2.00	0.43
4:E:40:ILE:O	4:E:44:LEU:HG	2.19	0.43
4:E:56:TYR:HE2	4:E:99:ILE:HG12	1.84	0.43
2:C:150:GLN:HG2	2:C:414:PRO:HG2	2.01	0.43
2:C:598:GLU:HA	3:D:849:TYR:CE1	2.53	0.43
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.86	0.43
2:C:211:TRP:HH2	6:H:14:DG:OP1	2.02	0.43
2:C:809:LYS:HD2	2:C:833:ARG:HD3	2.00	0.42
1:A:56:ILE:HG12	1:A:136:VAL:HG13	2.01	0.42
2:C:295:LEU:HD12	2:C:296:LEU:HD12	2.02	0.42
3:D:69:ARG:HE	5:F:485:GLN:HB2	1.84	0.42
3:D:1221:LEU:HD12	3:D:1221:LEU:HA	1.91	0.42
1:A:100:GLN:HG3	1:A:133:LYS:HB2	2.02	0.42
1:A:14:LEU:HD23	1:A:19:SER:HB2	2.00	0.42
5:F:371:HIS:O	5:F:375:VAL:HG23	2.20	0.42
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.49	0.42
2:C:549:ASP:OD2	2:C:550:ALA:N	2.52	0.42
3:D:760:PHE:CD2	3:D:770:ARG:HD2	2.54	0.42
3:D:832:ILE:HG22	3:D:834:ARG:N	2.33	0.42
1:A:10:SER:HA	1:A:23:ILE:HG12	2.02	0.42
2:C:769:ILE:HD12	2:C:867:GLU:HB3	2.02	0.42
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.35	0.42
2:C:599:HIS:ND1	3:D:840:PHE:O	2.46	0.42
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.53	0.42
2:C:408:ASP:O	2:C:412:ILE:HG13	2.19	0.42
2:C:604:ARG:NH1	2:C:925:ARG:HD2	2.35	0.42
2:C:47:PRO:HG2	2:C:581:VAL:O	2.20	0.42
3:D:1218:ASP:N	3:D:1218:ASP:OD1	2.44	0.42
3:D:32:GLU:HG3	5:F:367:ARG:HB2	2.02	0.42
5:F:330:ARG:HH21	5:F:350:TRP:HZ3	1.67	0.42
1:A:107:ALA:HB2	1:A:123:MET:HE1	2.02	0.42
1:A:11:GLU:N	1:A:22:VAL:O	2.42	0.42
1:B:182:ARG:HA	1:B:187:THR:HA	2.01	0.42
2:C:257:ILE:HD11	2:C:346:VAL:HG23	2.01	0.42
2:C:46:GLU:N	2:C:47:PRO:HD3	2.35	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:308:SER:HA	3:D:309:PRO:HD3	1.82	0.41
2:C:104:SER:N	2:C:140:ILE:O	2.52	0.41
2:C:804:GLY:HA2	2:C:836:SER:OG	2.20	0.41
2:C:818:GLU:OE2	2:C:822:ARG:NH1	2.51	0.41
2:C:839:VAL:HA	2:C:840:PRO:HD3	1.95	0.41
3:D:136:ILE:HD11	3:D:235:ILE:HD11	2.02	0.41
3:D:457:MET:HE3	3:D:457:MET:HB2	1.81	0.41
1:B:42:LEU:HD22	1:B:171:VAL:HG21	2.01	0.41
2:C:1114:GLU:HA	2:C:1115:PRO:HD3	1.93	0.41
2:C:338:VAL:O	2:C:342:ILE:HG13	2.20	0.41
2:C:464:SER:HB3	2:C:467:ARG:HG3	2.02	0.41
3:D:139:VAL:HG12	3:D:231:PRO:HD3	2.02	0.41
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.55	0.41
1:B:208:LEU:O	1:B:212:GLY:N	2.53	0.41
5:F:503:ILE:HA	5:F:503:ILE:HD12	1.80	0.41
2:C:157:PHE:HA	2:C:158:PRO:HD3	1.96	0.41
3:D:589:THR:HB	3:D:687:GLN:HA	2.02	0.41
2:C:472:VAL:HG22	6:H:14:DG:N2	2.35	0.41
2:C:165:THR:HG22	2:C:452:LYS:HE2	2.02	0.41
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.78	0.41
5:F:378:LYS:HD3	5:F:381:ARG:HH11	1.85	0.41
3:D:384:ASN:HD21	3:D:391:VAL:H	1.68	0.41
3:D:789:LEU:HA	3:D:789:LEU:HD23	1.93	0.41
5:F:273:LEU:HD13	5:F:277:GLN:HB3	2.03	0.41
2:C:1084:THR:O	2:C:1088:LEU:HG	2.21	0.41
2:C:597:LEU:HB3	2:C:976:VAL:HG13	2.02	0.41
3:D:1003:ILE:HA	3:D:1149:ILE:HD13	2.03	0.41
2:C:723:ILE:O	3:D:730:THR:HG23	2.20	0.41
5:F:474:VAL:HA	5:F:477:LEU:HD12	2.03	0.41
2:C:226:ILE:HG23	2:C:300:PHE:HZ	1.86	0.41
2:C:383:GLU:HA	2:C:386:GLN:HB3	2.02	0.41
3:D:125:LEU:HA	3:D:125:LEU:HD12	1.84	0.41
3:D:184:LEU:HD12	3:D:197:VAL:HG21	2.02	0.41
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.86	0.41
3:D:990:ASP:HB3	4:E:49:SER:HB2	2.03	0.41
5:F:392:ARG:NH1	5:F:398:GLU:OE2	2.53	0.41
1:B:147:VAL:HA	1:B:148:PRO:HD3	1.91	0.41
2:C:473:ARG:NH2	2:C:492:PRO:O	2.54	0.41
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.24	0.40
2:C:32:VAL:H	2:C:33:PRO:HD3	1.85	0.40
3:D:826:ASN:HD22	3:D:832:ILE:HD11	1.86	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:502:ARG:O	5:F:506:ILE:HG13	2.20	0.40
2:C:387:ASN:O	2:C:391:VAL:HG23	2.21	0.40
3:D:1054:ARG:HB3	3:D:1065:THR:HB	2.02	0.40
3:D:480:ARG:O	3:D:483:VAL:HG22	2.21	0.40
1:A:105:VAL:HG12	1:A:126:ALA:O	2.22	0.40
1:B:212:GLY:O	1:B:216:VAL:HG23	2.21	0.40
2:C:102:SER:O	2:C:141:ASN:ND2	2.54	0.40
2:C:217:ASP:HB3	2:C:219:ARG:H	1.86	0.40
3:D:460:LEU:HD23	3:D:460:LEU:HA	1.94	0.40
3:D:365:ILE:HD11	5:F:234:GLN:HB3	2.04	0.40
5:F:496:TYR:CD1	5:F:503:ILE:HD13	2.56	0.40
1:A:173:LYS:HD2	2:C:996:ARG:HH11	1.85	0.40
2:C:240:ALA:HB1	2:C:274:LEU:HD23	2.04	0.40
2:C:453:ARG:NH2	2:C:500:LEU:HD23	2.37	0.40
3:D:339:ASP:OD1	5:F:422:SER:OG	2.27	0.40
3:D:67:ARG:HB3	3:D:69:ARG:HG2	2.02	0.40
3:D:797:ASN:HA	3:D:798:PRO:HD3	1.78	0.40
3:D:834:ARG:HH21	3:D:848:GLU:HA	1.87	0.40
1:B:157:ALA:C	1:B:159:ILE:H	2.25	0.40
2:C:1146:GLU:HB2	2:C:1149:GLU:O	2.21	0.40
3:D:350:ARG:HD2	3:D:377:SER:OG	2.21	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	222/347 (64%)	210 (95%)	11 (5%)	1 (0%)	32	74
1	B	225/347 (65%)	208 (92%)	15 (7%)	2 (1%)	20	63
2	C	1124/1178 (95%)	1053 (94%)	63 (6%)	8 (1%)	25	68
3	D	1261/1316 (96%)	1197 (95%)	59 (5%)	5 (0%)	38	77

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	79/110 (72%)	77 (98%)	2 (2%)	0	100	100
5	F	316/528 (60%)	302 (96%)	13 (4%)	1 (0%)	44	81
All	All	3227/3826 (84%)	3047 (94%)	163 (5%)	17 (0%)	32	74

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
1	A	184	GLU
2	C	1148	ARG
5	F	405	ILE
1	B	158	GLU
2	C	47	PRO
2	C	922	VAL
2	C	1134	ASN
3	D	607	PRO
3	D	658	PRO
3	D	703	ARG
1	B	35	GLY
2	C	508	PRO
3	D	593	PRO
2	C	32	VAL
2	C	33	PRO
2	C	552	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	192/297 (65%)	190 (99%)	2 (1%)	80	90
1	B	192/297 (65%)	192 (100%)	0	100	100
2	C	948/998 (95%)	939 (99%)	9 (1%)	82	91
3	D	1048/1095 (96%)	1025 (98%)	23 (2%)	57	80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	68/90 (76%)	65 (96%)	3 (4%)	33	65
5	F	270/427 (63%)	265 (98%)	5 (2%)	62	83
All	All	2718/3204 (85%)	2676 (98%)	42 (2%)	70	86

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ARG
1	A	225	LEU
2	C	48	LEU
2	C	354	THR
2	C	373	PHE
2	C	506	VAL
2	C	691	ASP
2	C	710	ASP
2	C	961	ASP
2	C	1071	MET
2	C	1099	ARG
3	D	7	PHE
3	D	82	VAL
3	D	83	THR
3	D	92	MET
3	D	97	LEU
3	D	101	VAL
3	D	114	LEU
3	D	261	ILE
3	D	582	VAL
3	D	583	THR
3	D	653	HIS
3	D	684	VAL
3	D	714	ASP
3	D	793	TYR
3	D	838	SER
3	D	891	CYS
3	D	901	LEU
3	D	910	LEU
3	D	921	TYR
3	D	975	CYS
3	D	990	ASP
3	D	1099	LEU
3	D	1194	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	E	48	SER
4	E	75	ILE
4	E	106	HIS
5	F	269	ARG
5	F	361	ASP
5	F	367	ARG
5	F	402	GLU
5	F	527	LEU

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

Mol	Chain	Res	Type
2	C	969	ASN
3	D	465	HIS

### 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 4 ligands modelled in this entry, 3 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
8	RFP	C	1201	-	62,63,63	2.64	11 (17%)	91,94,94	1.96	16 (17%)

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
8	RFP	C	1201	-	-	0/60/85/85	0/1/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1201	RFP	O7-C25	-4.90	1.37	1.44
8	C	1201	RFP	C12-C11	-2.86	1.40	1.54
8	C	1201	RFP	O9-C23	-2.23	1.37	1.43
8	C	1201	RFP	O10-C21	-2.09	1.38	1.43
8	C	1201	RFP	C6-C7	3.02	1.45	1.39
8	C	1201	RFP	C18-C17	3.45	1.54	1.43
8	C	1201	RFP	C15-N1	4.86	1.46	1.35
8	C	1201	RFP	C3-C43	5.71	1.56	1.46
8	C	1201	RFP	C17-C16	6.38	1.55	1.34
8	C	1201	RFP	C43-N2	10.43	1.50	1.27
8	C	1201	RFP	O4-C11	10.80	1.40	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1201	RFP	C30-C16-C17	-6.76	105.63	123.44
8	C	1201	RFP	C43-N2-N3	-6.71	108.44	120.40
8	C	1201	RFP	C2-C3-C43	-4.21	117.33	123.29
8	C	1201	RFP	O4-C11-C5	-3.70	123.37	131.84
8	C	1201	RFP	C20-C19-C18	-2.37	120.50	126.06
8	C	1201	RFP	C33-C24-C25	-2.11	107.53	111.43
8	C	1201	RFP	C5-C10-C4	-2.06	121.44	124.21
8	C	1201	RFP	C34-C26-C25	-2.00	107.74	111.43
8	C	1201	RFP	C42-N4-C39	2.07	112.23	109.47
8	C	1201	RFP	C37-O6-C27	2.65	119.89	112.98
8	C	1201	RFP	C25-O7-C35	2.69	121.94	117.72
8	C	1201	RFP	C12-O5-C29	2.82	126.26	118.10
8	C	1201	RFP	C23-C24-C25	3.72	118.54	110.88
8	C	1201	RFP	O7-C35-C36	4.06	118.73	111.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1201	RFP	O3-C6-C7	4.26	130.03	121.31
8	C	1201	RFP	C38-N4-C42	8.36	123.28	110.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1201	RFP	6	0

## 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	224/347 (64%)	-0.12	1 (0%) 92 88	23, 64, 126, 150	0
1	B	227/347 (65%)	0.32	9 (3%) 39 31	48, 102, 161, 204	0
2	C	1126/1178 (95%)	-0.24	5 (0%) 92 88	8, 47, 127, 163	0
3	D	1265/1316 (96%)	-0.39	4 (0%) 93 91	7, 39, 111, 155	0
4	E	81/110 (73%)	-0.13	0 100 100	28, 59, 94, 129	0
5	F	320/528 (60%)	-0.18	5 (1%) 72 64	10, 64, 159, 190	0
6	H	23/23 (100%)	0.04	0 100 100	21, 139, 179, 194	0
7	G	12/16 (75%)	1.19	3 (25%) 1 2	130, 169, 396, 396	0
All	All	3278/3865 (84%)	-0.23	27 (0%) 86 80	7, 51, 135, 396	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	500	ARG	5.4
7	G	16	DC	3.7
7	G	15	DT	3.3
7	G	14	DG	3.2
1	B	60	LEU	3.1
1	B	59	VAL	3.1
5	F	520	SER	2.9
2	C	252	PHE	2.9
5	F	207	ASP	2.5
1	B	155	SER	2.5
1	B	90	ASP	2.5
3	D	904	ARG	2.5
1	B	61	HIS	2.5
3	D	903	GLU	2.4
2	C	235	THR	2.4
2	C	310	ARG	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	70	LYS	2.3
1	B	71	GLU	2.3
5	F	503	ILE	2.3
5	F	487	ARG	2.2
3	D	762	ARG	2.2
3	D	742	LYS	2.2
1	B	116	VAL	2.1
1	A	3	ILE	2.1
2	C	405	THR	2.1
1	B	151	GLN	2.0
2	C	328	ILE	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
8	RFP	C	1201	59/59	0.95	0.31	1.91	13,27,57,81	0
9	ZN	D	1401	1/1	0.98	0.08	-1.57	33,33,33,33	0
9	ZN	D	1402	1/1	0.99	0.10	-2.50	28,28,28,28	0
10	MG	D	1403	1/1	0.98	0.10	-	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.