

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 24, 2023 – 01:37 PM EDT

PDB ID	:	5UHD
Title	:	Crystal structure of Mycobacterium tuberculosis transcription initiation com-
		plex containing 4nt RNA in complex with Rifampin
Authors	:	Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on	:	2017-01-11
Resolution	:	4.01 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 4.01 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	$1098 \ (4.34-3.70)$
Clashscore	141614	1159 (4.34-3.70)
Ramachandran outliers	138981	1118 (4.34-3.70)
Sidechain outliers	138945	1108 (4.34-3.70)
RSRZ outliers	127900	1034 (4.38-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	Qual	ity of chain		
1	А	347	52%	13%	35%	
1	В	347	% • 55%	11%	35%	
2	С	1178	76%		19%	·
3	D	1316	75%		20%	•••
4	Е	110	55%	19%	26%	



Mol	Chain	Length	Quality of	' chain		
5	F	528	48% 12	% •	39%	
6	Н	23	35%	57%		9%
7	G	16	56%	25%	6%	12%



#### 5 UHD

# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 26022 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		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	224	Total	С	Ν	0	S	0	0	0
	A	224	1704	1072	295	335	2	0	0	0
1	р	227	Total	С	Ν	0	S	0	0	0
	D	221	1715	1080	291	342	2	0	0	0

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

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

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

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

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

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
4	Е	81	Total 637	C 408	N 106	O 123	0	0	0

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

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

• 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	Н	23	Total 476	C 227	N 91	O 136	Р 22	0	0	0

• 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	14	Total 284	C 136	N 53	0 82	Р 13	0	0	0

• Molecule 8 is RIFAMPICIN (three-letter code: RFP) (formula:  $C_{43}H_{58}N_4O_{12}$ ).



Mol	Chain	Residues	I	Ator	ns		ZeroOcc	AltConf
8	С	1	Total 59	C 43	N 4	0 12	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	TotalZn22	0	0

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

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



# 3 Residue-property plots (i)

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



• Molecule 1: DNA-directed RNA polymerase subunit alpha







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

Chain D:	75%	20%	•••
MET LEU LEU 13 134 134 135 137 137 137 141 141	L46 P47 P47 P57 P57 P56 P56 P66 P66 P66 P66 P66 P66	H103 1104 F107 R113 L114	L117 L118 D119 L125 E126 E126 K127
1130 1137 1137 1137 1137 1137 1137 1138 1158 1184	K190 A191 A191 C197 C197 C197 C197 C197 C197 C196 C264 C264 C264 C264 C264 C264 C264 C26	S305 S305 P309 M310 V313	P321 P322 R325 N341 N341
1343 1344 1348 1348 1348 1348 1348 1348	E370 1373 1373 1375 1375 1375 1375 1375 1375	K420 L438 G442 M447	K453 M457 K458 R458 R459
K473 R478 A492 T503 G523 G523 H525 H525	D537 S548 R556 R556 R556 L566 L566 L566 L566 R566 L568 R566 L579 F583 L588 R581 L588 R580 R580 R580 R580 R580 R580 R580 R	600 600 600 600 600 603 603	T638 0639 P642 E647
H653 P658 R670 L676 L676 P678 P678 P678 P678 P678	L716 K717 K717 K724 K724 L737 L737 L736 F740 F746 F760 F760 F760 F760 F770 K770 K770 K770 K771 E775 F776 F776	T782 D783 E784 V785 G786 Q787 H792	Y793 N797 P798 T801 L817
1823 1823 1834 1834 1834 1834 1834 1837 1841 1841	E348 1874 1875 1877 1877 1876 1876 1876 1877 1876 1876	1900 1911 1911 1911 1914 1914 1916	A920 Y921 A922 A922 L925 C926 T927
V930 V936 0945 1949 1949 V960 V960 V962 V962 S964	1965           1970           1970           1971           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1977           1978           1979           1977           1977           1978           1903           11003           11003           1115           11003           1115           1115           1115           1115           1115           1115           1115           1115           1115           1115           1115           1115           1115           1115           1115           1115 <tr td=""></tr>	VAL VAL GLV GLV ASP ILE THR THR <b>C1026</b>	R1030 E1033 G1051 R1054 R1054 L1055



# 11065 P1066 V1076 R1065 R1076 R1091 R1092 R1093 R1094 R1094 R1094 R1109 R1110 R1123 R1123 R1123 R1123 R1123 R1124 R1123 R1123 R1124 R1123 R1143 P1101 R1123 R1143 R1123 R1143 R1123 R1143 R1143 R1150 R1151 R1151 R1152 R1154 R1175 R1176 R1177 R1177 R1176 R1177 R1176 R1177 R1176 R1177 R1176 R1177</

E1228	T1229	T1230 R1231	L1245	N1246	G1247	L1248	-	N1251	V1252	T 1 0E 2	11254	01273	P1274	-	A1281	ALA	TYR	THR	ILE	DRO	CED	NEK	TYR	GLU	ASP	GLN	TYR	TYR	SER	PRO	ASP	PHE	GLY	ALA	ALA	THR	GLY	ALA	ALA	VAL	PRO	LEU	ASP	ASP	TYR	GLY	TYR	SER	ASP	TYR	ARG
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• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:		55%		19%	26%	6	I
MET SER SER SER GLN SER ALA	SER LEU ALA ALA VAL PRO PRO ALA ASP GLN	PHE ASP SER SER GLY GLY GLY G28	P32 I35	P38 P39 R46 V47 S48 L53	q70 G74 I75 L82 L82 V83	Lot K90 A95 L96	R97 E98 199 D102



• Molecule 5: RNA polymerase sigma factor SigA



Chain H:	35%	57%	9%
A A E	6 7 7 8 8 8 8 8 8 9 7 7 7 7 7 7 7 7 7 7 7		

• Molecule 7: DNA (5'-D(\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*GP\*AP\*GP\*G)-3')







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	152.08Å 163.10Å 197.90Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	49.48 - 4.01	Depositor
Resolution (A)	49.83 - 4.01	EDS
% Data completeness	90.8 (49.48-4.01)	Depositor
(in resolution range)	90.9(49.83-4.01)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.97 (at 4.00 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
P. P.	0.211 , $0.264$	Depositor
$n, n_{free}$	0.216 , $0.267$	DCC
$R_{free}$ test set	1991 reflections $(5.22\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	30.9	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27 , -13.1	EDS
L-test for $twinning^2$	$ < L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	26022	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, RFP

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).

Mal	Chain	Bo	ond lengths	Bo	ond angles			
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5			
1	А	0.23	0/1730	0.44	0/2354			
1	В	0.23	0/1741	0.45	0/2371			
2	С	0.25	0/8873	0.43	1/12031~(0.0%)			
3	D	0.26	0/10052	0.43	0/13591			
4	Е	0.30	0/650	0.43	0/886			
5	F	0.25	0/2572	0.41	0/3466			
6	Н	0.69	1/535~(0.2%)	1.03	2/826~(0.2%)			
7	G	0.61	0/318	1.01	1/489~(0.2%)			
All	All	0.27	1/26471 (0.0%)	0.46	4/36014~(0.0%)			

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Н	16	DC	O3'-P	8.16	1.71	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	Н	18	DC	P-O3'-C3'	10.69	132.53	119.70
7	G	8	DC	P-O3'-C3'	10.23	131.97	119.70
6	Н	16	DC	OP1-P-O3'	5.57	117.44	105.20
2	С	48	LEU	CA-CB-CG	5.25	127.38	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	А	1704	0	1741	26	0
1	В	1715	0	1739	23	0
2	С	8714	0	8636	143	0
3	D	9887	0	9943	188	0
4	Е	637	0	635	13	0
5	F	2543	0	2571	54	0
6	Н	476	0	261	32	0
7	G	284	0	159	11	0
8	С	59	0	58	6	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	26022	0	25743	432	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 8.

All (432) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:H:20:DG:O6	7:G:8:DC:N4	1.99	0.95
6:H:20:DG:N1	7:G:8:DC:N3	2.18	0.90
3:D:353:ARG:HH21	5:F:323:GLU:HG2	1.38	0.88
3:D:353:ARG:HH21	5:F:323:GLU:CG	1.88	0.86
6:H:15:DT:C2	6:H:16:DC:C5	2.63	0.86
6:H:16:DC:O2	7:G:12:DG:N2	2.08	0.85
3:D:913:ASP:OD1	3:D:914:PRO:HD2	1.78	0.82
3:D:908:GLY:O	3:D:909:THR:OG1	1.99	0.80
3:D:910:LEU:HD12	3:D:910:LEU:O	1.81	0.80
3:D:354:LEU:O	3:D:354:LEU:HD12	1.81	0.80
6:H:15:DT:C2	6:H:16:DC:C6	2.71	0.79
3:D:901:LEU:HD13	3:D:901:LEU:O	1.82	0.79
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.48	0.78
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.64	0.77
3:D:913:ASP:OD1	3:D:914:PRO:CD	2.33	0.77
3:D:905:ALA:HB3	3:D:908:GLY:O	1.84	0.77



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:907:ASP:OD1	3:D:908:GLY:N	2.16	0.77
3:D:891:CYS:SG	3:D:970:THR:OG1	2.44	0.75
3:D:240:LEU:HD12	3:D:240:LEU:O	1.86	0.75
3:D:62:CYS:HB3	3:D:78:CYS:SG	2.28	0.74
6:H:15:DT:C4	6:H:16:DC:N4	2.56	0.74
2:C:1024:THR:H	3:D:730:THR:HG21	1.54	0.73
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.71	0.72
3:D:353:ARG:NH2	5:F:323:GLU:HG2	2.04	0.72
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.71	0.72
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.23	0.72
6:H:15:DT:N3	6:H:16:DC:C4	2.58	0.71
2:C:737:LEU:HB2	2:C:898:ILE:HG12	1.73	0.71
5:F:470:ARG:HB3	5:F:506:ILE:HD13	1.75	0.69
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.74	0.69
6:H:15:DT:C4	6:H:16:DC:C4	2.80	0.69
2:C:401:ARG:HA	2:C:404:MET:HE2	1.74	0.69
1:B:75:GLU:O	1:B:79:ASN:ND2	2.26	0.69
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.74	0.69
5:F:401:LYS:HA	5:F:405:ILE:HA	1.75	0.68
3:D:353:ARG:HD2	3:D:370:GLU:OE1	1.94	0.68
6:H:20:DG:N2	7:G:8:DC:O2	2.26	0.67
3:D:240:LEU:HD12	3:D:240:LEU:C	2.15	0.67
3:D:473:LYS:HD2	5:F:448:VAL:HG21	1.77	0.67
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.75	0.66
2:C:815:THR:HG22	2:C:817:GLU:H	1.60	0.66
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.78	0.66
2:C:101:GLY:O	2:C:142:ASN:ND2	2.29	0.65
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.77	0.65
4:E:38:PRO:HD2	4:E:96:LEU:HD23	1.79	0.65
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.78	0.65
1:A:87:SER:O	1:A:142:ARG:NH1	2.29	0.64
5:F:470:ARG:HH11	5:F:506:ILE:HD11	1.61	0.64
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.79	0.64
5:F:242:ASN:OD1	5:F:243:ALA:N	2.31	0.64
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.30	0.64
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.78	0.63
6:H:15:DT:H2"	6:H:16:DC:H6	1.63	0.63
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	1.80	0.62
3:D:241:TYR:OH	3:D:254:GLY:HA3	1.99	0.62
3:D:589:THR:HG21	3:D:688:MET:HG2	1.81	0.62
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.82	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.82	0.62
3:D:365:ILE:HG21	5:F:297:GLU:HG2	1.82	0.61
3:D:913:ASP:OD1	3:D:914:PRO:N	2.33	0.61
3:D:600:GLN:HB2	3:D:609:THR:HB	1.80	0.61
2:C:43:LYS:NZ	2:C:544:ALA:O	2.34	0.60
3:D:492:ALA:HB3	4:E:90:LYS:HE2	1.82	0.60
3:D:921:TYR:O	3:D:981:ARG:NH2	2.34	0.60
2:C:762:THR:HG23	2:C:764:LEU:H	1.67	0.60
3:D:738:VAL:HG13	3:D:841:ARG:HD3	1.84	0.60
6:H:20:DG:H1	7:G:8:DC:N4	2.00	0.60
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.82	0.60
3:D:901:LEU:HD13	3:D:901:LEU:C	2.23	0.60
3:D:1273:GLN:O	4:E:105:GLU:N	2.30	0.60
3:D:373:MET:O	3:D:377:SER:OG	2.18	0.59
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.85	0.59
3:D:241:TYR:CE2	3:D:245:VAL:CG2	2.85	0.59
3:D:1274:PRO:HB3	4:E:82:LEU:HD11	1.85	0.59
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.83	0.59
6:H:15:DT:H2"	6:H:16:DC:H5'	1.85	0.58
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.85	0.58
3:D:473:LYS:HZ3	5:F:448:VAL:HG11	1.67	0.58
6:H:18:DC:H2"	6:H:19:DG:C8	2.39	0.58
2:C:561:VAL:HG21	2:C:571:VAL:HB	1.85	0.58
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.84	0.58
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.21	0.58
6:H:20:DG:C6	7:G:8:DC:N4	2.60	0.58
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.67	0.58
3:D:873:LEU:HA	3:D:876:ARG:HE	1.69	0.57
4:E:47:VAL:HG11	4:E:53:LEU:HB2	1.86	0.57
2:C:102:SER:O	2:C:141:ASN:ND2	2.38	0.57
2:C:230:ARG:NH1	7:G:8:DC:OP1	2.38	0.57
3:D:137:THR:OG1	3:D:253:THR:O	2.22	0.57
2:C:318:LYS:NZ	2:C:534:ASP:OD2	2.37	0.57
1:A:214:THR:HA	1:B:230:GLU:HG2	1.87	0.57
2:C:1067:ARG:NH2	3:D:415:GLN:O	2.35	0.57
3:D:997:ILE:HD11	3:D:1248:LEU:HD13	1.87	0.57
3:D:1030:ARG:HH21	3:D:1137:GLU:HG2	1.70	0.57
2:C:48:LEU:HD12	2:C:528:ILE:HD13	1.86	0.56
8:C:1201:RFP:H28C	8:C:1201:RFP:C5	2.35	0.56
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.87	0.56
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.37	0.56



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:757:ILE:HD12	2:C:837:LEU:HB2	1.88	0.56
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.88	0.56
4:E:70:GLN:O	4:E:74:GLY:N	2.34	0.56
1:B:72:ASP:OD1	1:B:73:VAL:N	2.38	0.56
3:D:241:TYR:CE2	3:D:245:VAL:HG21	2.41	0.56
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.87	0.56
3:D:45:GLY:H	3:D:48:CYS:HB2	1.72	0.55
1:A:105:VAL:HG13	1:A:125:ILE:HB	1.88	0.55
3:D:903:GLU:O	3:D:911:ILE:N	2.31	0.55
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.88	0.55
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.38	0.55
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.38	0.55
2:C:441:ASP:OD2	2:C:443:ASN:ND2	2.40	0.55
2:C:1045:SER:OG	2:C:1046:THR:N	2.37	0.55
8:C:1201:RFP:HN1	8:C:1201:RFP:C18	2.20	0.55
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.87	0.55
3:D:1030:ARG:NH1	3:D:1033:GLU:OE1	2.39	0.55
1:B:84:VAL:HG12	1:B:199:LYS:HD3	1.89	0.55
1:A:64:THR:OG1	1:A:65:THR:N	2.40	0.55
3:D:676:LEU:HD23	3:D:716:LEU:HD23	1.87	0.55
2:C:150:GLN:HG2	2:C:414:PRO:HG2	1.89	0.54
2:C:473:ARG:NH2	2:C:492:PRO:O	2.40	0.54
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.90	0.54
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.88	0.54
2:C:475:VAL:O	3:D:854:HIS:ND1	2.35	0.54
3:D:707:ILE:HD11	4:E:32:PRO:HB3	1.89	0.54
2:C:597:LEU:HB3	2:C:976:VAL:HG13	1.88	0.54
3:D:1065:THR:HG23	3:D:1076:VAL:HB	1.90	0.54
5:F:499:THR:OG1	5:F:500:ARG:N	2.39	0.54
2:C:516:TYR:HD2	2:C:531:LEU:HD13	1.71	0.54
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.89	0.54
6:H:15:DT:N3	6:H:16:DC:C5	2.76	0.54
2:C:885:LEU:HD12	2:C:895:ILE:HD11	1.90	0.54
5:F:364:ARG:HG3	5:F:368:ILE:HG12	1.90	0.54
2:C:959:LEU:HD12	2:C:960:PRO:HD2	1.90	0.53
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.90	0.53
2:C:182:SER:HB2	2:C:377:ARG:HB2	1.89	0.53
2:C:211:TRP:NE1	6:H:13:DT:O2	2.41	0.53
2:C:821:LEU:HD22	5:F:456:LEU:HD11	1.90	0.53
7:G:15:DT:H2'	7:G:16:DC:C6	2.44	0.53
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.24	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:353:ARG:HD2	3:D:370:GLU:CD	2.30	0.53
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.91	0.53
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.39	0.53
1:B:178:VAL:HG22	1:B:192:LEU:HD13	1.91	0.52
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.92	0.52
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.91	0.52
3:D:353:ARG:HH21	5:F:323:GLU:CD	2.13	0.52
5:F:499:THR:HG23	5:F:500:ARG:HD2	1.92	0.52
2:C:317:ASN:O	2:C:321:GLY:N	2.38	0.52
5:F:345:THR:HB	6:H:4:DA:H8	1.75	0.52
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.45	0.51
1:A:175:THR:OG1	1:A:176:TYR:N	2.42	0.51
3:D:459:ARG:HA	3:D:462:ASP:HB2	1.92	0.51
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.91	0.51
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.09	0.51
6:H:20:DG:N1	7:G:8:DC:N4	2.56	0.51
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.25	0.51
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.93	0.51
3:D:384:ASN:HB2	3:D:401:SER:HB3	1.93	0.51
5:F:474:VAL:HA	5:F:477:LEU:HD12	1.92	0.51
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.75	0.51
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.93	0.51
2:C:472:VAL:HG22	6:H:14:DG:N2	2.25	0.51
3:D:353:ARG:CD	3:D:370:GLU:OE2	2.58	0.51
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.11	0.50
2:C:599:HIS:ND1	3:D:840:PHE:O	2.38	0.50
2:C:185:VAL:HG12	2:C:316:VAL:HG22	1.93	0.50
2:C:1055:GLN:HG2	2:C:1094:ASP:HB3	1.92	0.50
3:D:438:LEU:O	3:D:561:SER:OG	2.27	0.50
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.26	0.50
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.45	0.50
3:D:373:MET:SD	5:F:318:LEU:HB3	2.52	0.50
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.94	0.50
3:D:798:PRO:HA	3:D:801:THR:HB	1.94	0.50
5:F:344:SER:OG	6:H:5:DA:OP2	2.24	0.50
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.93	0.50
5:F:467:LEU:HD21	5:F:514:LEU:HD21	1.93	0.49
2:C:540:VAL:HG13	2:C:561:VAL:HG13	1.94	0.49
6:H:15:DT:C2'	6:H:16:DC:H6	2.25	0.49
2:C:587:VAL:HB	2:C:591:THR:HB	1.94	0.49
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.48	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:1164:ARG:HD2	3:D:1208:MET:HE1	1.95	0.49
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.94	0.49
3:D:1170:SER:O	3:D:1173:THR:OG1	2.28	0.49
2:C:1112:ILE:HG13	3:D:548:SER:HA	1.94	0.49
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.95	0.49
3:D:95:ILE:HD13	3:D:348:ILE:HG12	1.95	0.48
3:D:834:ARG:HH22	3:D:848:GLU:HA	1.77	0.48
3:D:925:LEU:HD12	3:D:962:VAL:HG12	1.96	0.48
5:F:386:LEU:HD12	5:F:399:LEU:HD23	1.95	0.48
2:C:944:TRP:NE1	2:C:963:LEU:O	2.45	0.48
3:D:354:LEU:HD12	3:D:354:LEU:C	2.32	0.48
4:E:46:ARG:NE	4:E:102:ASP:OD1	2.36	0.48
6:H:20:DG:C2	7:G:8:DC:N3	2.81	0.48
1:B:173:LYS:HE3	1:B:175:THR:HG23	1.94	0.48
3:D:341:ASN:O	3:D:345:ARG:HB2	2.13	0.48
2:C:598:GLU:HA	3:D:849:TYR:CE1	2.49	0.48
3:D:889:HIS:O	3:D:977:THR:OG1	2.25	0.48
1:A:97:LEU:HD21	1:A:105:VAL:HG21	1.96	0.48
3:D:184:LEU:HD12	3:D:197:VAL:HG21	1.95	0.48
2:C:40:SER:HB2	2:C:973:SER:HB2	1.96	0.47
2:C:549:ASP:HB3	2:C:553:ARG:H	1.80	0.47
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.95	0.47
3:D:1228:GLU:OE2	3:D:1231:ARG:NH1	2.47	0.47
3:D:215:GLU:OE1	3:D:218:ARG:NH1	2.44	0.47
3:D:884:VAL:HG11	3:D:1156:VAL:HG13	1.96	0.47
6:H:22:DT:H1'	6:H:23:DG:H5'	1.95	0.47
2:C:88:GLU:CD	2:C:310:ARG:HH12	2.18	0.47
2:C:447:SER:HA	2:C:613:ARG:HG3	1.96	0.47
3:D:407:LYS:HE2	3:D:1230:THR:HG21	1.96	0.47
3:D:910:LEU:HD12	3:D:910:LEU:C	2.34	0.47
4:E:95:ALA:O	4:E:99:ILE:HG13	2.14	0.47
2:C:809:LYS:HD2	2:C:833:ARG:HD3	1.96	0.47
2:C:1051:MET:HA	5:F:441:ASP:HB2	1.96	0.47
3:D:190:LYS:HE3	3:D:192:ASP:HB3	1.95	0.47
3:D:369:ASN:O	3:D:373:MET:HG3	2.13	0.47
6:H:11:DG:H5"	6:H:12:DC:C4	2.50	0.47
2:C:615:ALA:HB3	2:C:715:LEU:HD22	1.97	0.47
3:D:724:ALA:O	3:D:727:SER:OG	2.28	0.47
1:A:225:LEU:HD13	1:A:225:LEU:H	1.80	0.47
1:B:42:LEU:HD23	1:B:211:ALA:CB	2.45	0.47
2:C:653:VAL:HG23	2:C:658:ILE:HG12	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:1119:GLU:OE2	3:D:89:ARG:NH2	2.48	0.47
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.96	0.47
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.96	0.47
8:C:1201:RFP:O4	8:C:1201:RFP:O12	2.29	0.47
3:D:353:ARG:HD3	5:F:322:GLN:HB3	1.97	0.47
8:C:1201:RFP:H28C	8:C:1201:RFP:H341	1.59	0.47
2:C:598:GLU:HA	3:D:849:TYR:HE1	1.80	0.46
3:D:823:LEU:HD13	3:D:831:PHE:HB3	1.96	0.46
5:F:342:LYS:HE2	5:F:342:LYS:HB3	1.70	0.46
3:D:308:SER:HA	3:D:309:PRO:HD3	1.80	0.46
1:A:62:GLU:HG3	1:A:77:ILE:HD12	1.96	0.46
2:C:818:GLU:OE2	2:C:822:ARG:NH1	2.48	0.46
5:F:317:PHE:O	5:F:321:ILE:HG13	2.15	0.46
5:F:515:ARG:O	5:F:519:ARG:N	2.46	0.46
1:B:90:ASP:HA	1:B:142:ARG:HD3	1.96	0.46
2:C:723:ILE:O	3:D:730:THR:HG23	2.16	0.46
3:D:101:VAL:HG23	3:D:375:GLN:CD	2.36	0.46
3:D:745:ILE:HD13	3:D:784:GLU:HG2	1.97	0.46
8:C:1201:RFP:H24C	8:C:1201:RFP:H342	1.61	0.46
3:D:235:ILE:HD12	3:D:241:TYR:HD1	1.80	0.46
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.80	0.46
3:D:915:TYR:HA	3:D:1143:ARG:HH12	1.79	0.46
6:H:15:DT:N1	6:H:16:DC:C5	2.82	0.46
3:D:891:CYS:O	3:D:892:GLN:HB2	2.15	0.46
2:C:758:ASP:N	2:C:758:ASP:OD1	2.49	0.46
5:F:231:TYR:O	5:F:235:ILE:HG13	2.15	0.46
2:C:1137:VAL:HG21	2:C:1147:LEU:HD11	1.97	0.46
2:C:974:THR:HG23	2:C:980:ALA:H	1.81	0.45
3:D:473:LYS:NZ	5:F:448:VAL:HG11	2.31	0.45
1:A:149:ALA:N	1:A:165:ASP:OD2	2.44	0.45
2:C:877:ARG:HH12	2:C:1039:ASP:CG	2.20	0.45
3:D:67:ARG:HB3	3:D:69:ARG:HG2	1.97	0.45
3:D:127:LYS:HA	3:D:132:ALA:HB3	1.98	0.45
3:D:834:ARG:NH2	3:D:847:LEU:HG	2.31	0.45
1:B:212:GLY:O	1:B:216:VAL:HG23	2.16	0.45
3:D:1245:LEU:HD13	3:D:1254:ILE:HD13	1.98	0.45
5:F:378:LYS:HD3	5:F:381:ARG:HH11	1.82	0.45
1:A:185:GLN:HG2	1:A:186:ARG:H	1.82	0.45
3:D:457:MET:HB2	3:D:457:MET:HE3	1.78	0.45
5:F:262:LEU:O	5:F:266:LEU:HG	2.16	0.45
2:C:104:SER:HB3	2:C:140:ILE:HB	1.98	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:158:GLU:OE2	3:D:247:ARG:NH2	2.47	0.45
3:D:899:VAL:HG11	3:D:920:ALA:HB2	1.97	0.45
2:C:233:PRO:HB2	2:C:236:VAL:HG23	1.99	0.45
2:C:1055:GLN:NE2	3:D:420:LYS:HG2	2.32	0.45
1:A:98:ARG:HG2	1:A:135:GLU:HG3	1.99	0.45
2:C:220:ASP:HB3	2:C:257:ILE:HG22	1.98	0.45
3:D:266:GLU:HA	3:D:310:MET:HE1	1.97	0.45
3:D:353:ARG:NH2	5:F:323:GLU:OE2	2.49	0.45
6:H:15:DT:C2'	6:H:16:DC:C6	3.00	0.45
2:C:46:GLU:N	2:C:47:PRO:HD3	2.31	0.45
2:C:50:VAL:O	2:C:633:ARG:NH1	2.47	0.45
2:C:183:PRO:HB2	2:C:312:GLY:HA2	1.98	0.45
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.81	0.45
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.49	0.45
3:D:1120:GLU:HA	3:D:1123:ARG:HG2	1.98	0.45
1:A:37:SER:O	1:A:41:THR:OG1	2.33	0.45
2:C:165:THR:HG22	2:C:452:LYS:HE2	1.99	0.45
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.75	0.45
2:C:1119:GLU:O	2:C:1123:VAL:HG23	2.17	0.45
1:B:45:SER:OG	1:B:214:THR:HG21	2.16	0.44
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.53	0.44
5:F:299:ASN:OD1	6:H:6:DT:N3	2.39	0.44
1:A:5:GLN:HG2	1:B:144:ARG:HH21	1.82	0.44
1:A:42:LEU:HA	1:A:46:ILE:HG12	1.99	0.44
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.52	0.44
2:C:658:ILE:HG21	2:C:702:ILE:HD12	2.00	0.44
3:D:588:LEU:HD12	3:D:589:THR:HG23	1.99	0.44
5:F:468:SER:HB3	5:F:471:GLU:HG3	2.00	0.44
3:D:36:TYR:CZ	3:D:37:ARG:HG3	2.52	0.44
1:A:45:SER:HG	1:B:30:PHE:HE2	1.65	0.44
2:C:344:TYR:OH	2:C:364:PRO:O	2.34	0.44
2:C:1088:LEU:HD22	2:C:1092:LYS:HD2	1.98	0.44
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.99	0.44
3:D:1176:LEU:H	3:D:1176:LEU:HD12	1.81	0.44
2:C:206:PRO:HA	2:C:308:LEU:HD23	1.98	0.44
2:C:641:VAL:HG11	2:C:708:THR:HG21	1.98	0.44
2:C:922:VAL:H	2:C:923:PRO:HD2	1.83	0.44
2:C:928:ILE:H	2:C:928:ILE:HG13	1.52	0.44
2:C:1041:ILE:HD11	3:D:447:MET:HG3	1.99	0.44
3:D:927:THR:OG1	3:D:961:LYS:HD3	2.17	0.44
2:C:704:ASP:HB2	2:C:708:THR:HB	1.99	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:319:LYS:HE3	2:C:344:TYR:CZ	2.53	0.43
2:C:600:ASP:OD2	2:C:889:HIS:ND1	2.41	0.43
2:C:1050:SER:N	2:C:1055:GLN:O	2.36	0.43
2:C:314:TYR:CZ	2:C:318:LYS:HD3	2.53	0.43
2:C:1042:HIS:HB2	2:C:1060:LYS:HG3	2.00	0.43
2:C:1089:LEU:HD12	3:D:1252:VAL:HG13	1.99	0.43
3:D:107:PHE:CZ	3:D:126:GLU:HG2	2.39	0.43
4:E:84:GLU:CD	4:E:84:GLU:H	2.21	0.43
2:C:927:ASN:O	2:C:930:GLN:HG2	2.18	0.43
3:D:525:HIS:O	3:D:528:VAL:HG22	2.18	0.43
3:D:580:ASP:OD1	3:D:580:ASP:N	2.51	0.43
3:D:642:PRO:HG2	3:D:647:GLU:HB2	1.99	0.43
4:E:84:GLU:O	4:E:97:ARG:NH2	2.49	0.43
5:F:347:ALA:O	5:F:351:ILE:HG13	2.17	0.43
5:F:474:VAL:HA	5:F:477:LEU:HB2	1.99	0.43
1:A:56:ILE:HB	1:A:59:VAL:HB	2.00	0.43
6:H:20:DG:H2"	6:H:21:DA:C8	2.53	0.43
7:G:11:DT:H2"	7:G:12:DG:C8	2.54	0.43
2:C:408:ASP:O	2:C:412:ILE:HG13	2.18	0.43
2:C:544:ALA:HB2	2:C:580:ASP:HB2	2.00	0.43
2:C:1079:TYR:CD2	3:D:559:MET:HG2	2.54	0.43
3:D:901:LEU:C	3:D:901:LEU:CD1	2.86	0.43
1:B:110:ILE:O	1:B:112:PRO:HD3	2.19	0.43
2:C:387:ASN:O	2:C:391:VAL:HG23	2.18	0.43
2:C:815:THR:O	2:C:819:ARG:N	2.42	0.43
2:C:936:LEU:HB2	2:C:985:LEU:HD11	1.99	0.43
5:F:489:LEU:H	5:F:489:LEU:HD23	1.83	0.43
3:D:1003:ILE:O	3:D:1006:PRO:HD2	2.19	0.43
1:A:100:GLN:HG2	1:A:101:GLY:H	1.84	0.43
1:A:181:THR:O	1:A:188:ASP:HA	2.19	0.43
1:B:182:ARG:HA	1:B:187:THR:HA	2.01	0.43
3:D:353:ARG:NH2	5:F:323:GLU:CG	2.66	0.43
5:F:345:THR:HA	6:H:5:DA:N7	2.34	0.43
1:B:11:GLU:HB2	1:B:22:VAL:HB	2.01	0.43
2:C:122:CYS:HA	2:C:127:MET:HG2	2.01	0.43
6:H:15:DT:H2"	6:H:16:DC:C6	2.47	0.43
2:C:1107:VAL:HG21	5:F:451:VAL:HG11	2.00	0.42
3:D:1099:LEU:HD23	3:D:1099:LEU:HA	1.83	0.42
6:H:15:DT:O2	6:H:16:DC:C6	2.72	0.42
3:D:945:GLY:O	3:D:949:ILE:HG12	2.18	0.42
2:C:522:GLY:O	2:C:553:ARG:HA	2.20	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:C:549:ASP:HB3	2:C:553:ARG:N	2.35	0.42
3:D:1172:SER:N	3:D:1199:GLU:O	2.33	0.42
2:C:396:MET:HE1	2:C:418:ILE:HG12	2.00	0.42
1:B:112:PRO:HA	1:B:113:PRO:HD3	1.92	0.42
2:C:47:PRO:HB2	2:C:581:VAL:HG13	2.02	0.42
2:C:313:ARG:HH22	2:C:337:ASP:CG	2.22	0.42
3:D:922:ALA:HB3	3:D:1150:HIS:CE1	2.54	0.42
1:A:136:VAL:HG12	1:A:137:GLU:H	1.85	0.42
3:D:117:LEU:HD12	3:D:299:VAL:HG22	2.02	0.42
3:D:409:LYS:O	3:D:415:GLN:HB2	2.19	0.42
2:C:252:PHE:HB3	2:C:258:MET:HG3	2.01	0.42
2:C:721:VAL:HG23	2:C:915:ILE:HG23	2.02	0.42
3:D:797:ASN:HA	3:D:798:PRO:HD3	1.74	0.42
3:D:913:ASP:HB3	3:D:916:ILE:HG13	2.01	0.42
2:C:909:ASP:OD1	2:C:909:ASP:N	2.43	0.42
1:B:42:LEU:HD23	1:B:211:ALA:HB2	2.02	0.42
2:C:38:ARG:HA	2:C:971:ILE:HG13	2.01	0.42
3:D:750:GLU:OE1	3:D:837:LYS:NZ	2.46	0.42
1:B:147:VAL:HA	1:B:148:PRO:HD3	1.92	0.42
3:D:153:ALA:O	3:D:157:VAL:HG23	2.19	0.42
3:D:567:SER:HA	3:D:568:PRO:HD3	1.90	0.42
3:D:756:VAL:HG21	3:D:777:ILE:HD11	2.01	0.42
2:C:974:THR:HG23	2:C:979:GLY:HA3	2.02	0.41
3:D:240:LEU:C	3:D:240:LEU:CD1	2.85	0.41
3:D:353:ARG:CD	3:D:370:GLU:CD	2.89	0.41
3:D:737:LEU:N	3:D:793:TYR:OH	2.32	0.41
3:D:925:LEU:HD11	3:D:960:VAL:HG11	2.02	0.41
2:C:253:GLY:HA2	2:C:259:ARG:HE	1.84	0.41
2:C:687:CYS:HA	2:C:688:PRO:HD3	1.87	0.41
2:C:954:ASP:O	2:C:958:ARG:NH1	2.53	0.41
4:E:38:PRO:HA	4:E:39:PRO:HD3	1.98	0.41
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.52	0.41
2:C:893:GLY:HA2	3:D:537:ASP:HA	2.02	0.41
3:D:1166:THR:HB	3:D:1206:VAL:HG21	2.02	0.41
1:A:130:ASP:O	1:A:131:LYS:HG2	2.20	0.41
2:C:216:VAL:HG11	2:C:349:HIS:CD2	2.56	0.41
2:C:928:ILE:HG12	3:D:817:LEU:CD1	2.51	0.41
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.36	0.41
1:A:120:ASN:OD1	1:A:120:ASN:N	2.53	0.41
1:A:223:ARG:HD3	1:B:213:LYS:HB2	2.01	0.41
3:D:353:ARG:HD3	3:D:370:GLU:OE2	2.20	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
3:D:589:THR:HG22	3:D:670:ARG:HG2	2.01	0.41
5:F:446:VAL:HB	5:F:449:ASP:HB2	2.02	0.41
2:C:557:PRO:O	2:C:573:SER:N	2.53	0.41
2:C:817:GLU:N	2:C:817:GLU:OE1	2.53	0.41
3:D:823:LEU:HB3	3:D:831:PHE:HD1	1.85	0.41
2:C:899:LEU:HB3	2:C:903:ASP:HB2	2.03	0.41
3:D:353:ARG:HD2	3:D:370:GLU:OE2	2.20	0.41
3:D:556:ARG:HG3	4:E:35:ILE:HG12	2.02	0.41
1:B:97:LEU:HD22	1:B:110:ILE:HG12	2.01	0.41
2:C:70:TRP:CH2	2:C:82:PRO:HB2	2.56	0.41
2:C:597:LEU:HD23	2:C:976:VAL:HG11	2.03	0.41
2:C:1091:ILE:HB	2:C:1102:VAL:HG21	2.02	0.41
3:D:119:ASP:HB2	3:D:295:ARG:CZ	2.51	0.41
3:D:391:VAL:O	3:D:399:LEU:HG	2.21	0.41
3:D:453:LYS:O	3:D:457:MET:HG3	2.20	0.41
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.56	0.41
2:C:720:LEU:HD23	2:C:913:VAL:HA	2.03	0.41
3:D:104:ILE:HB	3:D:379:ASP:OD1	2.20	0.41
3:D:114:LEU:HB3	3:D:125:LEU:HD21	2.03	0.41
3:D:478:ARG:HD3	3:D:478:ARG:HA	1.91	0.41
3:D:772:GLU:O	3:D:776:GLU:HG2	2.21	0.41
3:D:781:ALA:O	3:D:785:VAL:HG23	2.21	0.41
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.53	0.41
5:F:231:TYR:HE2	5:F:321:ILE:HG21	1.86	0.41
5:F:278:ARG:O	5:F:282:MET:HB2	2.21	0.41
5:F:335:PHE:CE1	5:F:343:PHE:HA	2.55	0.41
5:F:503:ILE:HD12	5:F:503:ILE:HA	1.91	0.41
2:C:515:PRO:HB2	2:C:581:VAL:HG21	2.02	0.41
3:D:46:LEU:O	3:D:325:ARG:NH2	2.34	0.41
3:D:57:ASP:HB3	3:D:58:TRP:CE3	2.56	0.41
3:D:1110:GLN:NE2	3:D:1112:MET:O	2.51	0.41
2:C:773:ILE:HD11	2:C:804:GLY:HA2	2.03	0.40
2:C:464:SER:HB3	2:C:467:ARG:HG3	2.02	0.40
2:C:690:VAL:HG11	2:C:696:VAL:HG11	2.02	0.40
2:C:1078:ALA:HB1	3:D:998:VAL:HG22	2.03	0.40
3:D:350:ARG:NE	5:F:319:ASP:OD1	2.54	0.40
3:D:888:GLU:HG2	3:D:889:HIS:H	1.86	0.40
2:C:123:LYS:HA	2:C:170:GLY:HA2	2.02	0.40
2:C:444:ASN:O	2:C:447:SER:HB3	2.22	0.40
2:C:458:LEU:HD13	8:C:1201:RFP:H133	2.03	0.40
3:D:113:ARG:N	3:D:113:ARG:HD2	2.37	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:392:THR:HB	3:D:396:ASN:HA	2.03	0.40
3:D:877:LEU:O	3:D:880:VAL:HG12	2.22	0.40
6:H:15:DT:O4	6:H:16:DC:N4	2.55	0.40
2:C:344:TYR:OH	2:C:365:VAL:HA	2.22	0.40
3:D:403:SER:O	3:D:407:LYS:HG3	2.21	0.40
3:D:783:ASP:O	3:D:787:GLN:HG2	2.22	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	Perce	ntiles
1	А	222/347~(64%)	210 (95%)	11 (5%)	1 (0%)	29	67
1	В	225/347~(65%)	208 (92%)	16 (7%)	1 (0%)	34	71
2	С	1124/1178~(95%)	1050 (93%)	68 (6%)	6~(0%)	29	67
3	D	1261/1316~(96%)	1194 (95%)	61 (5%)	6 (0%)	29	67
4	Е	79/110~(72%)	76~(96%)	3 (4%)	0	100	100
5	F	316/528~(60%)	299~(95%)	16 (5%)	1 (0%)	41	75
All	All	3227/3826~(84%)	3037 (94%)	175 (5%)	15 (0%)	29	67

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
2	С	47	PRO
3	D	971	SER
2	С	922	VAL
2	С	1134	ASN
3	D	593	PRO



Mol	Chain	Res	Type
1	А	184	GLU
2	С	33	PRO
1	В	35	GLY
2	С	1148	ARG
3	D	607	PRO
3	D	658	PRO
5	F	405	ILE
2	С	46	GLU
3	D	835	PRO

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	192/297~(65%)	189 (98%)	3~(2%)	62	79
1	В	192/297~(65%)	192 (100%)	0	100	100
2	С	948/998~(95%)	934 (98%)	14 (2%)	65	80
3	D	1048/1095~(96%)	1027 (98%)	21 (2%)	55	74
4	Ε	68/90~(76%)	65~(96%)	3(4%)	28	55
5	F	270/427~(63%)	262~(97%)	8 (3%)	41	64
All	All	2718/3204 (85%)	2669 (98%)	49 (2%)	59	77

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	159	ILE
1	А	182	ARG
1	А	225	LEU
2	С	44	LEU
2	С	48	LEU
2	С	180	VAL
2	С	185	VAL
2	С	380	THR
2	С	456	SER



Mol	Chain	Res	Type
2	С	621	SER
2	С	691	ASP
2	С	835	THR
2	С	854	SER
2	С	1034	HIS
2	С	1037	VAL
2	С	1099	ARG
2	С	1148	ARG
3	D	7	PHE
3	D	60	CYS
3	D	75	CYS
3	D	78	CYS
3	D	82	VAL
3	D	83	THR
3	D	101	VAL
3	D	240	LEU
3	D	305	SER
3	D	377	SER
3	D	503	THR
3	D	582	VAL
3	D	583	THR
3	D	653	HIS
3	D	793	TYR
3	D	849	TYR
3	D	921	TYR
3	D	968	CYS
3	D	978	CYS
3	D	1194	VAL
3	D	1246	ASN
4	Ε	48	SER
4	Е	75	ILE
4	E	106	HIS
5	F	258	TYR
5	F	269	ARG
5	F	361	ASP
5	F	367	ARG
5	F	402	GLU
5	F	425	GLN
5	F	442	SER
5	F	448	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such side chains are listed below:



Mol	Chain	Res	Type
2	С	142	ASN
2	С	443	ASN
2	С	543	GLN
2	С	941	HIS
2	С	969	ASN
2	С	1034	HIS
3	D	465	HIS
5	F	415	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 monosaccharides 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	Chain	Dec	Link Bond le		ond leng	gths	Bond angles			
	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2		
8	RFP	С	1201	-	63,63,63	2.61	11 (17%)	94,94,94	2.26	21 (22%)

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	С	1201	-	-	24/60/85/85	0/5/5/5

All (	(11)	bond	length	outliers	are	listed	below:
1111	()	bonu	nongun	outilities	$a_{1}c$	moucu	DC10W.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	С	1201	RFP	O4-C11	11.48	1.40	1.21
8	С	1201	RFP	C43-N2	8.15	1.50	1.27
8	С	1201	RFP	C17-C16	7.11	1.55	1.34
8	С	1201	RFP	C3-C43	5.35	1.56	1.46
8	С	1201	RFP	O7-C25	-4.99	1.37	1.44
8	С	1201	RFP	C15-N1	4.97	1.46	1.35
8	С	1201	RFP	C12-C11	-3.60	1.40	1.54
8	С	1201	RFP	C18-C17	3.41	1.54	1.43
8	С	1201	RFP	C6-C7	3.13	1.45	1.39
8	С	1201	RFP	O9-C23	-2.24	1.37	1.43
8	C	1201	RFP	C29-C28	2.10	1.41	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	С	1201	RFP	C38-N4-C42	8.65	123.60	110.66
8	С	1201	RFP	C30-C16-C17	-7.56	105.12	123.42
8	С	1201	RFP	C43-N2-N3	-7.54	109.85	120.43
8	С	1201	RFP	C2-C3-C43	-7.28	116.77	124.17
8	С	1201	RFP	O3-C6-C7	5.40	130.43	121.14
8	С	1201	RFP	O4-C11-C5	-4.46	123.30	131.81
8	С	1201	RFP	O7-C35-C36	4.14	118.70	111.09
8	С	1201	RFP	C23-C24-C25	4.09	118.60	110.61
8	С	1201	RFP	C12-O5-C29	3.61	126.76	117.84
8	С	1201	RFP	C37-O6-C27	2.79	119.70	113.01
8	С	1201	RFP	C4-C3-C43	2.63	119.66	116.52
8	С	1201	RFP	C33-C24-C25	-2.56	106.81	111.40
8	С	1201	RFP	C25-O7-C35	2.53	121.64	117.72
8	С	1201	RFP	O5-C12-C13	2.53	113.60	106.99
8	С	1201	RFP	C34-C26-C25	-2.41	107.09	111.40
8	С	1201	RFP	C3-C2-C1	2.38	122.40	120.70
8	С	1201	RFP	C3-C43-N2	-2.37	118.09	121.54
8	С	1201	RFP	C5-C10-C4	-2.34	121.57	124.03
8	С	1201	RFP	C5-C6-C7	-2.34	119.58	125.29
8	С	1201	RFP	C25-C26-C27	2.31	118.31	112.02
8	С	1201	RFP	C20-C19-C18	-2.09	121.76	126.16

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
8	С	1201	RFP	C4-C3-C43-N2
8	С	1201	RFP	C26-C27-C28-C29
8	С	1201	RFP	O6-C27-C28-C29
8	С	1201	RFP	C43-N2-N3-C40
8	С	1201	RFP	C36-C35-O7-C25
8	С	1201	RFP	C3-C43-N2-N3
8	С	1201	RFP	C16-C17-C18-C19
8	С	1201	RFP	C15-C16-C17-C18
8	С	1201	RFP	C34-C26-C27-C28
8	С	1201	RFP	C34-C26-C27-O6
8	С	1201	RFP	C25-C26-C27-O6
8	С	1201	RFP	C18-C19-C20-C31
8	С	1201	RFP	C27-C28-C29-O5
8	С	1201	RFP	C11-C12-O5-C29
8	С	1201	RFP	O3-C12-O5-C29
8	С	1201	RFP	C32-C22-C23-C24
8	С	1201	RFP	C28-C27-O6-C37
8	С	1201	RFP	C33-C24-C25-C26
8	С	1201	RFP	C2-C3-C43-N2
8	С	1201	RFP	C21-C22-C23-C24
8	С	1201	RFP	C23-C24-C25-C26
8	С	1201	RFP	C18-C19-C20-C21
8	С	1201	RFP	C30-C16-C17-C18
8	С	1201	RFP	C33-C24-C25-O7

All (24) torsion outliers are listed below:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient





equivalents in the CSD to analyse the geometry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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>	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	224/347~(64%)	-0.26	0 100 100	18,62,126,158	0
1	В	227/347~(65%)	0.26	3 (1%) 77 68	59,102,143,167	0
2	С	1126/1178~(95%)	-0.41	1 (0%) 95 94	5, 38, 126, 161	0
3	D	1265/1316~(96%)	-0.53	0 100 100	3, 38, 109, 144	0
4	E	81/110 (73%)	-0.44	0 100 100	24, 53, 89, 110	0
5	F	320/528~(60%)	-0.35	2 (0%) 89 84	7,63,157,185	0
6	Н	23/23~(100%)	0.17	0 100 100	33, 122, 194, 200	0
7	G	14/16~(87%)	0.96	2 (14%) 2 3	104, 162, 240, 304	0
All	All	3280/3865~(84%)	-0.38	8 (0%) 95 93	3, 48, 131, 304	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	6	DA	3.5
5	F	487	ARG	3.1
7	G	5	DC	2.8
1	В	135	GLU	2.7
5	F	500	ARG	2.5
1	В	62	GLU	2.4
2	С	252	PHE	2.1
1	В	66	VAL	2.1

## 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 monosaccharides in this entry.

#### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
10	MG	D	1403	1/1	0.91	0.10	3,3,3,3	0
8	RFP	С	1201	59/59	0.96	0.24	12,23,53,58	0
9	ZN	D	1402	1/1	0.99	0.10	44,44,44,44	0
9	ZN	D	1401	1/1	0.99	0.07	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





# 6.5 Other polymers (i)

There are no such residues in this entry.

