



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:06 AM JST

PDB ID : 7EH1  
Title : Thermus thermophilus transcription initiation complex containing a template-strand purine at position TSS-2, GpG RNA primer, and CMPcPP  
Authors : Li, L.; Zhang, Y.  
Deposited on : 2021-03-27  
Resolution : 2.90 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

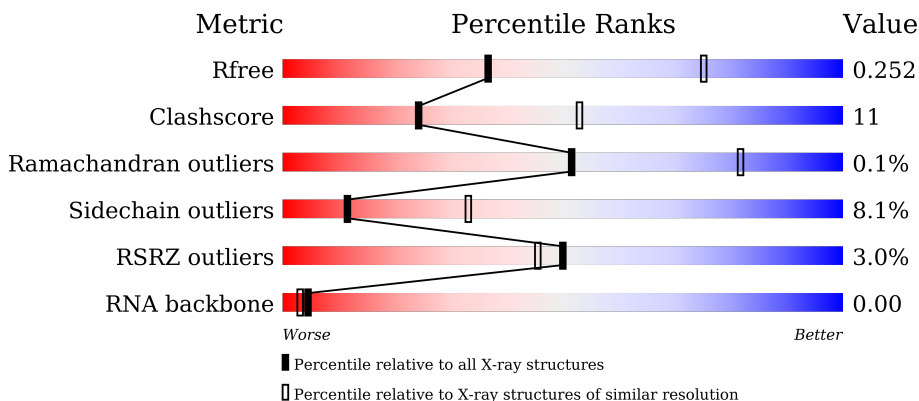
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	 2% 50% 21% 27%
1	B	315	 % 48% 23% 28%
2	C	1119	 2% 68% 29%
3	D	1524	 4% 68% 27%

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Mol	Chain	Length	Quality of chain
4	E	99	 68% 23% 5%
5	F	443	 56% 21% 22%
6	G	27	 44% 44% 7%
7	H	19	 58% 26% 5% 11%
8	I	2	 100%

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28630 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
			Total	C	N	O	S			
1	A	231	Total	C	N	O	S	0	0	0
			1803	1152	312	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1758	1124	301	331	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1112	Total	C	N	O	S	0	0	0
			8750	5538	1553	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1486	Total	C	N	O	S	0	1	0
			11714	7428	2061	2190	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	Total	C	N	O	S	0	0	0
			759	484	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	Total	C	N	O	S	0	0	0
			2803	1767	508	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	25	516	246	99	147	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	17	346	165	66	99	16	0	0	0

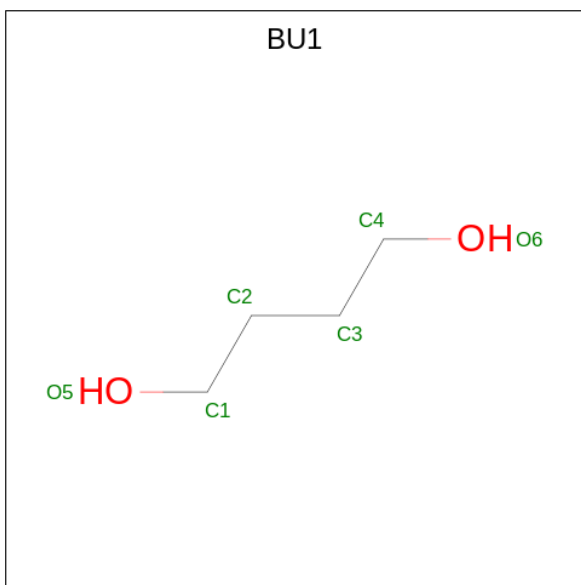
- Molecule 8 is a RNA chain called RNA (5'-R(\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	2	43	20	10	12	1	0	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Mg 2 2	0	0
9	C	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).

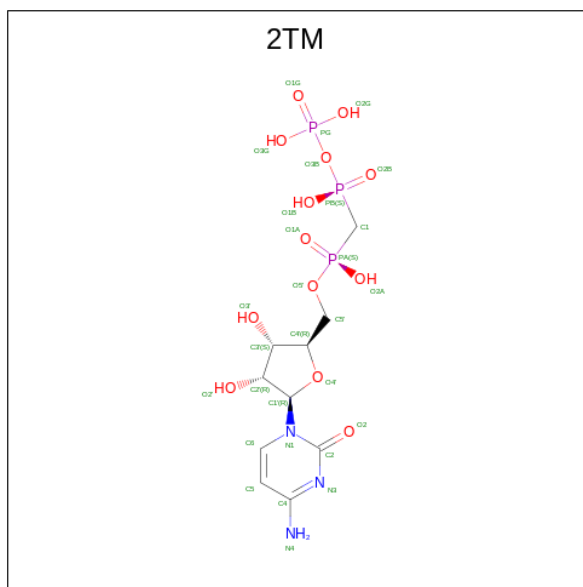


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 6 4 2	0	0
10	D	1	Total C O 6 4 2	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonoxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	I	1	29	10	3	13	3	0	0

- Molecule 13 is water.

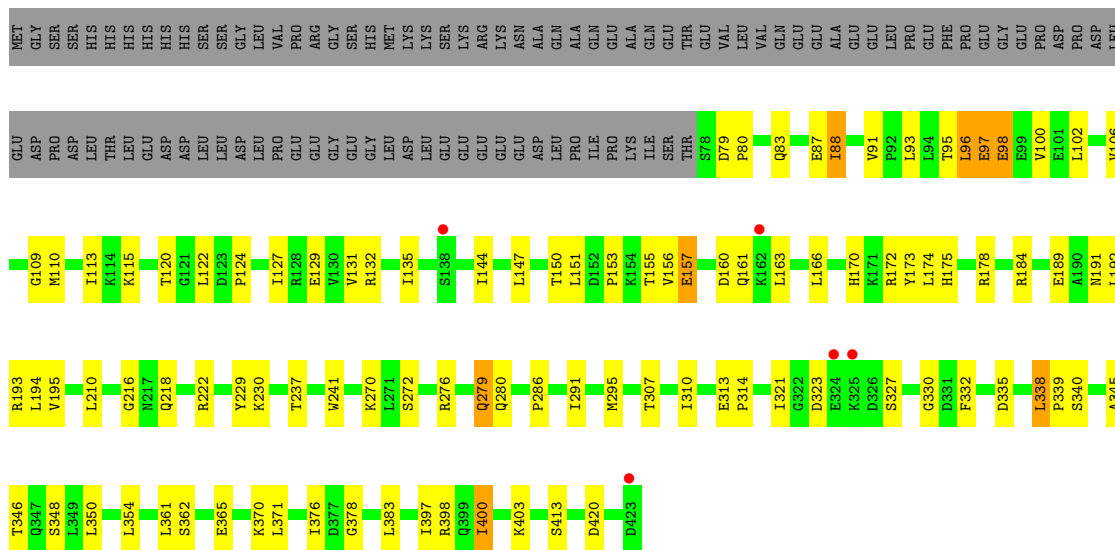
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	4	Total	O	0	0
			4	4		
13	B	4	Total	O	0	0
			4	4		
13	C	28	Total	O	0	0
			28	28		
13	D	42	Total	O	0	0
			42	42		
13	E	3	Total	O	0	0
			3	3		
13	F	5	Total	O	0	0
			5	5		
13	H	1	Total	O	0	0
			1	1		
13	I	3	Total	O	0	0
			3	3		











- Molecule 6: DNA (27-MER)



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



- Molecule 8: RNA (5'-R(\*GP\*G)-3')



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.12Å 103.32Å 295.65Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	25.27 – 2.90 48.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.1 (25.27-2.90) 82.1 (48.88-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.191 , 0.253 0.191 , 0.252	Depositor DCC
$R_{free}$ test set	1971 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.019 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-1$ 0.024 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-1$	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: 2TM, MG, BU1, ZN

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	0.45	0/1835	0.64	0/2497
1	B	0.43	0/1790	0.62	0/2440
2	C	0.48	0/8917	0.63	0/12064
3	D	0.49	1/11923 (0.0%)	0.66	3/16126 (0.0%)
4	E	0.48	0/773	0.65	0/1042
5	F	0.43	0/2848	0.55	0/3833
6	G	1.03	0/580	1.03	1/895 (0.1%)
7	H	0.94	0/388	0.99	2/597 (0.3%)
8	I	0.79	0/48	1.26	0/74
All	All	0.50	1/29102 (0.0%)	0.65	6/39568 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	3
5	F	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1039	CYS	CB-SG	-5.85	1.72	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	16	DC	O4'-C4'-C3'	-7.19	101.62	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	783	ARG	NE-CZ-NH1	-6.26	117.17	120.30
3	D	1108	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	D	1108	ARG	NE-CZ-NH2	-5.91	117.35	120.30
7	H	13	DA	O4'-C4'-C3'	-5.70	102.22	104.50
6	G	15	DT	O4'-C1'-N1	5.07	111.55	108.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1207	TYR	Peptide
3	D	782	SER	Peptide
3	D	829	VAL	Peptide
5	F	330	GLY	Peptide

## 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	1803	0	1852	47	0
1	B	1758	0	1778	50	0
2	C	8750	0	8833	229	0
3	D	11714	0	11926	275	0
4	E	759	0	771	18	0
5	F	2803	0	2871	67	0
6	G	516	0	283	14	0
7	H	346	0	192	3	0
8	I	43	0	23	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
10	B	6	0	10	3	0
10	D	6	0	10	1	0
11	D	2	0	0	0	0
12	I	29	0	14	0	0
13	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	4	0	0	0	0
13	C	28	0	0	3	0
13	D	42	0	0	2	0
13	E	3	0	0	0	0
13	F	5	0	0	1	0
13	H	1	0	0	0	0
13	I	3	0	0	0	0
All	All	28630	0	28563	628	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 11.

All (628) 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:12:VAL:HG21	2:C:472:ARG:HD3	1.46	0.97
2:C:805:ARG:HH21	2:C:807:ARG:HD3	1.26	0.97
2:C:628:PHE:H	2:C:638:ASP:HB2	1.32	0.93
1:B:176:ARG:NH1	3:D:888:GLU:OE2	2.04	0.88
2:C:715:THR:HG22	2:C:717:LEU:H	1.35	0.88
3:D:683:ILE:HG22	3:D:687:VAL:HG11	1.58	0.86
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.58	0.85
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.62	0.81
2:C:200:LEU:HG	2:C:300:ASP:HB2	1.61	0.80
2:C:198:ARG:HE	2:C:227:PHE:HA	1.48	0.79
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.66	0.77
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.65	0.77
2:C:101:ILE:HG12	2:C:108:ILE:HG12	1.67	0.77
2:C:1019:GLN:HG3	2:C:1058:ASP:HB3	1.67	0.77
1:A:70:GLY:N	2:C:607:ASP:OD1	2.19	0.76
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.66	0.76
6:G:8:DG:H2 <sup>''</sup>	6:G:9:DG:H5 <sup>''</sup>	1.68	0.75
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.69	0.75
3:D:65:ARG:NH1	5:F:378:GLY:O	2.20	0.75
2:C:1020:PRO:HD3	2:C:1057:SER:HB2	1.69	0.74
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.69	0.74
2:C:588:VAL:HG13	2:C:593:ALA:HB3	1.69	0.74
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.69	0.74
4:E:37:ASN:OD1	4:E:37:ASN:N	2.21	0.74
3:D:131:LYS:HE2	3:D:154:THR:HG22	1.70	0.73
3:D:780:LYS:HD2	3:D:912:LYS:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.73	0.71
3:D:399:ARG:HE	3:D:431:VAL:HG11	1.55	0.71
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.24	0.71
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.56	0.70
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.25	0.69
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.73	0.69
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.75	0.69
3:D:274:ARG:HH21	3:D:279:VAL:HG21	1.58	0.69
1:A:209:GLU:O	1:A:213:GLN:HG3	1.93	0.69
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.75	0.69
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.75	0.68
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.73	0.68
2:C:805:ARG:NH2	2:C:807:ARG:HD3	2.04	0.68
3:D:573:MET:SD	5:F:210:LEU:HB3	2.34	0.68
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.30	0.67
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.76	0.67
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.76	0.66
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.78	0.66
2:C:266:ARG:NH1	6:G:11:DG:O6	2.19	0.66
3:D:142:LEU:HD23	3:D:143:ASN:HB2	1.76	0.66
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.78	0.66
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.77	0.66
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.78	0.66
5:F:362:SER:OG	5:F:365:GLU:HG2	1.94	0.66
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.24	0.66
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.77	0.65
1:B:18:ARG:NH1	1:B:203:GLY:O	2.29	0.65
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.77	0.65
4:E:51:LEU:HD23	4:E:51:LEU:H	1.62	0.65
5:F:370:LYS:HB3	5:F:376:ILE:HG12	1.79	0.64
10:B:2002:BU1:H22	10:D:2004:BU1:H31	1.79	0.64
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.79	0.64
3:D:45:PHE:O	3:D:86:ARG:NH2	2.30	0.64
2:C:768:THR:O	2:C:771:GLU:N	2.30	0.64
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.80	0.64
3:D:787:LEU:HD11	3:D:947:ILE:HD12	1.80	0.64
5:F:163:LEU:HB3	5:F:174:LEU:HD22	1.80	0.64
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.79	0.63
2:C:760:SER:HB2	2:C:788:THR:HG21	1.80	0.63
3:D:514:LEU:HD13	3:D:517:VAL:HG22	1.81	0.63
2:C:294:GLU:HB3	2:C:299:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.25	0.63
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.79	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.81	0.63
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.81	0.63
1:B:34:VAL:HG12	1:B:181:VAL:HG21	1.81	0.62
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.29	0.62
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.29	0.62
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.80	0.62
2:C:768:THR:HB	2:C:771:GLU:OE1	1.99	0.62
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.82	0.62
3:D:1111:ASP:OD1	3:D:1113:GLY:N	2.30	0.61
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.81	0.61
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.34	0.61
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.82	0.61
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.36	0.61
2:C:118:ILE:HD11	2:C:344:PHE:CE1	2.35	0.60
2:C:205:GLU:O	2:C:209:ARG:HG2	2.01	0.60
3:D:260:GLU:HB3	3:D:271:VAL:HB	1.82	0.60
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.36	0.60
2:C:657:ASP:OD2	2:C:663:ASN:N	2.30	0.60
3:D:479:GLU:HA	3:D:482:LYS:HE2	1.83	0.60
1:B:94:LEU:HD12	1:B:95:GLN:H	1.67	0.60
2:C:428:ARG:NH2	2:C:447:ALA:O	2.34	0.60
5:F:88:ILE:HG23	5:F:193:ARG:HG2	1.84	0.60
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.02	0.60
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.37	0.60
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.37	0.60
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.84	0.59
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.84	0.59
1:A:206:THR:OG1	1:A:209:GLU:HG3	2.02	0.59
2:C:210:GLU:HB3	2:C:211:LEU:HD13	1.84	0.59
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.37	0.59
3:D:134:VAL:CG2	3:D:151:GLN:H	2.16	0.59
3:D:477:LEU:HB2	3:D:496:LEU:HD13	1.84	0.59
2:C:251:ASP:N	2:C:251:ASP:OD1	2.33	0.58
2:C:626:ARG:HG3	2:C:629:TYR:CD1	2.37	0.58
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.35	0.58
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.84	0.58
2:C:409:ARG:HD2	13:C:2102:HOH:O	2.02	0.58
2:C:580:MET:HB3	2:C:584:GLU:CD	2.24	0.58
2:C:607:ASP:HB3	2:C:610:ARG:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.39	0.58
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.85	0.58
3:D:1106:VAL:HB	3:D:1108:ARG:NH2	2.17	0.58
2:C:1067:TYR:OH	3:D:674[A]:ARG:NH1	2.37	0.58
2:C:890:LEU:HD12	2:C:914:ILE:HG23	1.86	0.58
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.16	0.58
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	1.84	0.58
3:D:1263:PHE:HD1	3:D:1375:MET:HE2	1.69	0.58
1:A:224:TYR:CE2	1:B:9:PRO:HG2	2.39	0.58
2:C:774:LEU:HD22	5:F:350:LEU:HD11	1.86	0.57
2:C:468:ARG:HA	2:C:486:MET:O	2.03	0.57
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.44	0.57
3:D:1281:VAL:HG23	3:D:1317:ASP:H	1.69	0.57
4:E:50:THR:HG1	4:E:55:PHE:HD2	1.53	0.57
5:F:96:LEU:O	5:F:100:VAL:HG23	2.05	0.57
2:C:937:ASP:OD2	2:C:939:ARG:NH1	2.37	0.57
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.20	0.57
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.87	0.57
3:D:1274:ILE:HD12	3:D:1322:GLY:HA2	1.85	0.57
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.85	0.57
3:D:1236:LEU:HD22	3:D:1359:GLN:HG3	1.87	0.57
1:A:133:GLU:HG2	1:A:134:GLU:N	2.18	0.57
3:D:1159:ARG:HG3	13:D:2114:HOH:O	2.03	0.57
1:A:181:VAL:HG12	2:C:938:LYS:HD2	1.86	0.57
3:D:1286:THR:HB	3:D:1289:LYS:H	1.69	0.56
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.86	0.56
2:C:984:GLU:HB2	3:D:944:THR:O	2.05	0.56
3:D:473:LEU:HD21	3:D:495:ARG:NH2	2.20	0.56
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.87	0.56
3:D:801:GLY:HA3	3:D:821:VAL:HG13	1.88	0.56
1:B:13:VAL:HG12	1:B:15:THR:HG22	1.87	0.56
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.38	0.56
1:A:211:LEU:O	1:A:215:VAL:HG23	2.06	0.56
3:D:236:TYR:CE1	3:D:242:LEU:HA	2.41	0.56
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.05	0.56
1:A:4:SER:HA	1:A:189:ARG:HH22	1.71	0.56
2:C:563:ASN:O	2:C:566:THR:HB	2.06	0.56
2:C:853:LEU:HB2	2:C:858:MET:CE	2.36	0.56
2:C:923:GLU:OE2	2:C:964:LYS:NZ	2.39	0.56
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.88	0.56
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:227:LEU:HD22	3:D:326:GLU:OE1	2.06	0.55
3:D:657:LEU:HG	3:D:661:MET:HE2	1.88	0.55
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.88	0.55
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.06	0.55
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.41	0.55
3:D:255:GLU:OE1	3:D:274:ARG:NH2	2.39	0.55
1:B:211:LEU:O	1:B:215:VAL:HG13	2.06	0.55
2:C:1019:GLN:HG3	2:C:1058:ASP:CB	2.37	0.55
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.88	0.55
2:C:118:ILE:HD11	2:C:344:PHE:HE1	1.72	0.55
3:D:1122:LEU:HD22	3:D:1140:ILE:HD13	1.89	0.55
2:C:536:PRO:HB3	3:D:1067:VAL:HG21	1.89	0.55
3:D:158:TYR:HE1	3:D:454:ALA:HB3	1.71	0.55
2:C:607:ASP:HB2	2:C:610:ARG:HH11	1.72	0.55
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.89	0.55
1:B:74:ASP:O	1:B:78:ILE:HG13	2.07	0.54
1:A:99:LEU:HB3	1:A:114:PHE:HD2	1.72	0.54
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.88	0.54
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.89	0.54
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.90	0.54
3:D:988:ARG:O	3:D:992:ILE:HG13	2.08	0.54
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.90	0.54
3:D:214:GLU:HB2	3:D:384:VAL:HG23	1.90	0.54
3:D:972:LEU:HA	3:D:975:GLU:HB2	1.90	0.54
3:D:1197:ARG:HD2	3:D:1398:TRP:CZ2	2.43	0.54
5:F:109:GLY:O	5:F:113:ILE:HG13	2.08	0.54
3:D:828:LYS:HA	3:D:833:GLU:HA	1.88	0.54
3:D:1031:ASN:OD1	3:D:1034:GLN:HG3	2.08	0.53
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.41	0.53
2:C:246:ASP:OD1	2:C:252:LYS:NZ	2.40	0.53
3:D:117:ASP:HB2	3:D:495:ARG:NH1	2.23	0.53
5:F:93:LEU:HD11	6:G:6:DT:H2 <sup>''</sup>	1.90	0.53
5:F:191:ASN:OD1	6:G:6:DT:N3	2.31	0.53
2:C:150:PRO:HG3	2:C:322:VAL:HG11	1.91	0.53
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.44	0.53
2:C:195:LEU:HD21	2:C:237:ARG:HG3	1.90	0.53
2:C:687:ALA:HB1	2:C:850:ALA:HB2	1.91	0.53
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.34	0.53
1:A:158:ILE:HD11	1:B:2:LEU:HD13	1.90	0.52
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.23	0.52
3:D:572:ARG:NH1	5:F:83:GLN:HB3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:959:GLU:HB3	3:D:963:TYR:HE2	1.74	0.52
2:C:99:GLN:HB3	2:C:110:GLU:HG3	1.92	0.52
2:C:167:LYS:HD3	6:G:12:DC:C5	2.45	0.52
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.45	0.52
3:D:881:LEU:O	3:D:885:ILE:HG13	2.09	0.52
2:C:872:ASN:OD1	2:C:874:LEU:HD12	2.09	0.52
3:D:53:ILE:HG22	3:D:54:LYS:HG3	1.92	0.52
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.90	0.52
5:F:132:ARG:HH21	5:F:184:ARG:NH1	2.08	0.52
2:C:224:GLU:CD	2:C:224:GLU:H	2.13	0.52
3:D:479:GLU:OE1	3:D:482:LYS:NZ	2.33	0.52
3:D:629:SER:OG	3:D:630:VAL:N	2.42	0.52
3:D:1047:LYS:HD3	3:D:1051:GLU:HG3	1.92	0.52
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.10	0.52
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.92	0.52
2:C:1067:TYR:OH	3:D:674[B]:ARG:NH1	2.42	0.52
3:D:142:LEU:HD11	3:D:157:GLU:HB3	1.92	0.52
3:D:1164:ARG:HE	3:D:1170:ASP:CG	2.13	0.52
5:F:95:THR:HB	5:F:98:GLU:HG3	1.92	0.52
2:C:640:ARG:HE	2:C:642:ARG:NH2	2.08	0.51
6:G:15:DT:H2''	6:G:16:DC:H6	1.76	0.51
1:A:220:GLU:O	1:A:223:THR:HB	2.11	0.51
2:C:358:ARG:HH12	2:C:374:ASN:HB2	1.75	0.51
3:D:176:ASP:OD2	3:D:388:HIS:HB3	2.09	0.51
3:D:968:ASP:O	3:D:971:LEU:HB2	2.10	0.51
3:D:1366:LYS:HA	3:D:1369:GLU:OE1	2.10	0.51
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.14	0.51
2:C:920:GLN:O	2:C:924:VAL:HG23	2.11	0.51
3:D:353:VAL:HG12	3:D:355:VAL:H	1.74	0.51
2:C:172:ILE:HD13	2:C:184:MET:HE2	1.92	0.51
2:C:1020:PRO:CD	2:C:1057:SER:HB2	2.38	0.51
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.41	0.51
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.45	0.51
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.92	0.51
2:C:730:SER:OG	2:C:732:ALA:HB3	2.11	0.51
3:D:1444:THR:O	3:D:1448:THR:HG23	2.11	0.51
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.46	0.51
1:A:25:LEU:HD23	1:A:28:LEU:HD21	1.92	0.51
3:D:432:TYR:O	3:D:448:GLU:HA	2.10	0.51
3:D:1093:TYR:CZ	3:D:1097:LYS:HE3	2.45	0.51
2:C:212:GLY:HA2	2:C:218:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:82:LYS:HB3	3:D:84:ILE:HG22	1.93	0.51
3:D:366:LYS:HD3	3:D:369:ALA:HB2	1.92	0.50
3:D:932:ASP:OD1	3:D:935:LYS:HE2	2.11	0.50
3:D:1053:PHE:CE2	3:D:1072:ILE:HD12	2.45	0.50
2:C:63:GLY:N	2:C:103:LYS:HD2	2.26	0.50
3:D:960:LYS:NZ	3:D:1063:GLU:OE1	2.44	0.50
3:D:984:THR:HG23	3:D:987:GLU:OE2	2.11	0.50
6:G:15:DT:H2''	6:G:16:DC:C6	2.46	0.50
2:C:358:ARG:NH1	2:C:374:ASN:HB2	2.27	0.50
2:C:263:ASP:HB3	2:C:266:ARG:HB2	1.94	0.50
2:C:680:ASP:H	3:D:943:THR:HG1	1.59	0.50
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.93	0.50
3:D:669:ASN:ND2	5:F:420:ASP:OD2	2.31	0.50
3:D:846:PRO:HB3	3:D:880:ILE:CG2	2.41	0.50
3:D:98:PRO:HG3	3:D:515:GLU:HG2	1.94	0.50
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.92	0.50
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.40	0.49
2:C:1056:LYS:HE3	3:D:751:LEU:HG	1.94	0.49
5:F:127:ILE:O	5:F:131:VAL:HG23	2.12	0.49
1:A:133:GLU:HB2	2:C:645:VAL:HG21	1.93	0.49
2:C:579:VAL:HG22	2:C:890:LEU:HD23	1.94	0.49
1:B:79:ILE:HG23	1:B:167:VAL:HG22	1.94	0.49
1:A:39:PRO:HB3	1:B:35:THR:HG23	1.93	0.49
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.95	0.49
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.95	0.49
10:B:2002:BU1:O6	10:B:2002:BU1:H12	2.11	0.49
3:D:654:LYS:HD3	3:D:674[A]:ARG:NH1	2.28	0.49
2:C:1073:GLY:N	3:D:659:LYS:HD3	2.28	0.49
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.93	0.49
2:C:611:ILE:HG21	2:C:655:LEU:HD22	1.95	0.49
3:D:941:PHE:O	3:D:945:SER:HB3	2.13	0.49
1:B:185:ARG:NH1	1:B:187:GLY:O	2.46	0.49
3:D:181:ASP:HB2	3:D:205:TYR:HD2	1.78	0.49
3:D:885:ILE:HD13	3:D:937:TYR:CG	2.48	0.49
2:C:133:ASP:HB3	2:C:395:LYS:HD2	1.95	0.49
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.13	0.49
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.27	0.49
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.95	0.49
2:C:838:LYS:HE3	3:D:741:ASP:O	2.13	0.48
3:D:796:ARG:NH1	3:D:862:ASP:OD1	2.39	0.48
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LYS:NZ	3:D:842:VAL:O	2.46	0.48
2:C:992:MET:HG2	2:C:994:ILE:HG13	1.95	0.48
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.95	0.48
3:D:1192:LEU:HD22	3:D:1345:GLU:CD	2.34	0.48
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.95	0.48
5:F:129:GLU:HB3	5:F:151:LEU:HD21	1.95	0.48
1:B:32:PHE:HA	1:B:35:THR:HB	1.95	0.48
1:B:77:GLU:OE1	3:D:867:ARG:NH1	2.46	0.48
3:D:373:PRO:HA	3:D:376:GLU:HG3	1.95	0.48
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.96	0.48
2:C:805:ARG:O	2:C:806:LEU:HD23	2.13	0.48
5:F:102:LEU:O	5:F:106:VAL:HG23	2.13	0.48
2:C:1071:ILE:HD11	5:F:345:ALA:HB1	1.96	0.48
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.95	0.48
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.94	0.48
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.95	0.48
1:B:113:ASP:OD1	1:B:113:ASP:N	2.47	0.48
3:D:492:ALA:O	3:D:496:LEU:HB2	2.14	0.48
3:D:1087:ARG:O	3:D:1090:ASP:N	2.47	0.48
1:A:198:ARG:HD3	2:C:934:PHE:CE2	2.49	0.48
2:C:173:ASP:O	2:C:184:MET:HA	2.14	0.48
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.95	0.48
3:D:689:ASP:HB3	4:E:51:LEU:HD21	1.96	0.48
3:D:1364:HIS:CE1	3:D:1366:LYS:HD2	2.49	0.48
2:C:937:ASP:OD1	2:C:938:LYS:N	2.47	0.48
3:D:508:ARG:HD3	3:D:510:GLU:OE2	2.13	0.48
4:E:50:THR:HG22	4:E:51:LEU:N	2.29	0.48
2:C:473:ARG:HG3	2:C:474:VAL:N	2.29	0.48
2:C:1102:LEU:HD11	3:D:9:ARG:NH1	2.29	0.48
3:D:791:TYR:CZ	3:D:945:SER:HB2	2.49	0.48
3:D:1205:TYR:CZ	3:D:1366:LYS:HE2	2.48	0.48
3:D:1492:LEU:HD23	3:D:1493:LYS:HE2	1.96	0.48
5:F:321:ILE:O	5:F:327:SER:HB3	2.14	0.48
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.96	0.48
5:F:95:THR:H	5:F:98:GLU:HG3	1.78	0.48
6:G:19:DG:H2''	6:G:20:DG:C8	2.49	0.48
2:C:1067:TYR:CE1	3:D:655:PRO:HG3	2.49	0.47
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.96	0.47
2:C:748:GLU:HA	2:C:799:ILE:HD13	1.96	0.47
3:D:417:PRO:HA	3:D:429:SER:O	2.14	0.47
3:D:696:HIS:CD2	4:E:48:MET:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:157:GLU:O	5:F:161:GLN:HG2	2.13	0.47
1:A:70:GLY:HA2	1:A:133:GLU:OE1	2.14	0.47
3:D:140:ALA:HA	3:D:450:TYR:CG	2.49	0.47
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.97	0.47
3:D:215:TYR:O	3:D:340:THR:HA	2.14	0.47
3:D:1493:LYS:HA	3:D:1493:LYS:HD3	1.58	0.47
1:B:8:ALA:N	1:B:9:PRO:HD3	2.29	0.47
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.50	0.47
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.15	0.47
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.96	0.47
3:D:1200:VAL:HG12	3:D:1373:ARG:NH1	2.29	0.47
4:E:46:PRO:HB2	4:E:57:ASP:HB2	1.96	0.47
1:A:26:GLU:HG2	1:A:194:LYS:HG3	1.96	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.47
3:D:613:ARG:HG3	3:D:618:LEU:HD23	1.96	0.47
3:D:791:TYR:CE1	3:D:945:SER:HB2	2.50	0.47
2:C:348:LEU:HD13	2:C:378:LEU:HD13	1.96	0.47
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.79	0.47
3:D:1293:PHE:CE1	3:D:1302:GLU:HG3	2.50	0.47
1:A:90:LEU:HD12	1:A:119:ASP:HA	1.97	0.47
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.30	0.46
2:C:910:LYS:O	2:C:914:ILE:HG13	2.15	0.46
2:C:1102:LEU:HD11	3:D:9:ARG:HH11	1.80	0.46
3:D:74:GLU:CD	3:D:74:GLU:H	2.19	0.46
3:D:418:GLY:N	3:D:429:SER:O	2.34	0.46
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.45	0.46
3:D:675:ARG:HH22	5:F:420:ASP:HB3	1.80	0.46
2:C:976:ASP:CG	2:C:978:ARG:HH11	2.19	0.46
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.29	0.46
3:D:181:ASP:OD1	3:D:205:TYR:HB2	2.15	0.46
3:D:478:LEU:HD21	3:D:500:ARG:HH21	1.80	0.46
1:B:198:ARG:HB3	1:B:200:TRP:CZ3	2.50	0.46
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.31	0.46
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.50	0.46
3:D:967:ALA:O	3:D:971:LEU:N	2.49	0.46
2:C:20:GLU:O	2:C:24:GLU:HB2	2.16	0.46
2:C:154:ARG:NH1	2:C:178:PRO:HG3	2.30	0.46
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.98	0.46
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.50	0.46
3:D:106:LYS:O	3:D:586:ARG:NH1	2.49	0.46
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.80	0.46
3:D:783:ARG:HD3	3:D:1028:ALA:O	2.15	0.46
3:D:1438:ALA:O	3:D:1443:THR:HG23	2.15	0.46
3:D:1438:ALA:N	3:D:1446:VAL:HG11	2.31	0.46
3:D:529:GLN:HG3	3:D:535:PHE:CZ	2.51	0.46
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.81	0.46
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.49	0.46
5:F:383:LEU:HD13	5:F:398:ARG:HB2	1.97	0.46
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.97	0.46
2:C:267:TYR:HB3	2:C:289:THR:HG22	1.98	0.46
3:D:299:GLU:O	3:D:302:GLN:HG2	2.15	0.46
3:D:534:ARG:NH2	5:F:313:GLU:O	2.48	0.45
5:F:194:LEU:HB2	6:G:6:DT:O2	2.16	0.45
5:F:400:ILE:HG22	5:F:403:LYS:CE	2.45	0.45
2:C:409:ARG:NH2	2:C:442:GLU:OE2	2.49	0.45
2:C:734:LEU:HD23	2:C:737:LEU:HD12	1.98	0.45
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.51	0.45
3:D:438:ASP:HB2	3:D:445:ARG:NH2	2.31	0.45
5:F:93:LEU:HA	5:F:93:LEU:HD23	1.69	0.45
5:F:241:TRP:CE2	6:G:1:DT:H4'	2.51	0.45
2:C:1086:ARG:HG2	2:C:1111:ILE:HD12	1.99	0.45
3:D:135:LEU:CD2	3:D:463:GLN:HG2	2.47	0.45
3:D:1348:LEU:O	3:D:1352:ILE:HG13	2.16	0.45
3:D:1389:LEU:O	3:D:1390:LEU:HD23	2.16	0.45
2:C:281:LEU:HD23	2:C:309:TYR:HD2	1.82	0.45
2:C:1092:LEU:HD23	2:C:1092:LEU:HA	1.72	0.45
3:D:103:TRP:O	3:D:107:ASP:HB3	2.16	0.45
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.97	0.45
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.16	0.45
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.99	0.45
1:B:94:LEU:HD12	1:B:95:GLN:N	2.31	0.45
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.98	0.45
3:D:314:PRO:HD2	3:D:317:VAL:HG13	1.98	0.45
5:F:279:GLN:HG3	5:F:280:GLN:N	2.31	0.45
1:B:179:PHE:CE1	10:B:2002:BU1:H41	2.52	0.45
2:C:1054:THR:O	2:C:1059:ASP:HB3	2.17	0.45
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.82	0.45
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.48	0.45
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.62	0.45
3:D:633:VAL:O	3:D:728:LEU:O	2.34	0.45
3:D:1290:LEU:HD12	3:D:1291:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:16:DC:H2'	7:H:17:DA:C8	2.52	0.45
2:C:310:LEU:O	2:C:314:THR:OG1	2.35	0.45
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.52	0.45
3:D:607:LEU:HD23	3:D:607:LEU:HA	1.65	0.45
3:D:885:ILE:HD13	3:D:937:TYR:CD2	2.52	0.45
4:E:50:THR:HG22	4:E:52:GLU:H	1.82	0.45
1:A:63:HIS:HB2	2:C:799:ILE:HG21	1.97	0.45
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.99	0.45
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.98	0.44
2:C:904:PRO:HD2	2:C:907:ASP:O	2.18	0.44
2:C:1015:LEU:HD23	5:F:335:ASP:HB2	1.99	0.44
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.98	0.44
6:G:23:DG:H2''	6:G:24:DC:H5''	1.99	0.44
2:C:17:PRO:HG2	2:C:20:GLU:HB3	1.98	0.44
2:C:195:LEU:O	2:C:199:VAL:HG23	2.17	0.44
2:C:1009:SER:OG	2:C:1010:THR:N	2.50	0.44
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.46	0.44
5:F:120:THR:HB	5:F:122:LEU:HD13	1.99	0.44
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.51	0.44
2:C:605:LYS:HB2	2:C:612:VAL:HG23	1.98	0.44
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.82	0.44
1:B:197:LEU:HD23	1:B:199:ILE:HD11	1.99	0.44
2:C:1:MET:HE3	2:C:3:ILE:HD11	1.97	0.44
2:C:65:VAL:O	2:C:100:LEU:HD23	2.18	0.44
3:D:236:TYR:CD1	3:D:242:LEU:HD12	2.53	0.44
5:F:83:GLN:O	5:F:87:GLU:HG3	2.17	0.44
1:A:171:PHE:HZ	1:B:2:LEU:HD11	1.83	0.44
1:B:77:GLU:OE1	3:D:867:ARG:HD3	2.18	0.44
2:C:690:ILE:HB	2:C:694:LEU:HD12	2.00	0.44
2:C:929:ARG:HG2	2:C:930:LYS:N	2.33	0.44
1:A:149:GLY:O	1:A:171:PHE:HB2	2.17	0.44
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.99	0.44
1:B:155:LYS:HD3	1:B:155:LYS:HA	1.77	0.44
2:C:225:SER:O	2:C:229:MET:HE2	2.17	0.44
3:D:367:ILE:HB	3:D:377:VAL:HG12	2.00	0.44
5:F:397:ILE:HA	5:F:400:ILE:HG12	1.99	0.44
3:D:483:HIS:CD2	3:D:484:PRO:HD2	2.52	0.44
3:D:731:LEU:HD23	3:D:731:LEU:HA	1.63	0.44
3:D:1148:VAL:HA	3:D:1164:ARG:O	2.17	0.44
3:D:1468:LEU:HB3	3:D:1470:ARG:HG3	1.98	0.44
5:F:156:VAL:O	5:F:160:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.52	0.44
2:C:630:ARG:HG2	2:C:634:GLY:HA2	2.00	0.44
3:D:816:HIS:HB2	3:D:836:VAL:HG11	1.99	0.44
5:F:210:LEU:HD23	5:F:210:LEU:HA	1.83	0.44
5:F:338:LEU:HD23	5:F:339:PRO:HD2	2.00	0.44
2:C:207:LEU:HD13	2:C:221:LEU:HD21	2.00	0.44
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.18	0.44
3:D:1485:GLN:O	4:E:75:PHE:HA	2.18	0.44
1:A:64:GLU:HA	1:A:165:ILE:HD13	1.99	0.43
2:C:961:GLU:O	2:C:965:GLU:HG3	2.18	0.43
5:F:124:PRO:HA	5:F:127:ILE:HD12	2.00	0.43
7:H:3:DT:H2'	7:H:4:DG:C8	2.52	0.43
2:C:106:GLY:O	2:C:108:ILE:HG13	2.18	0.43
2:C:136:ILE:HB	2:C:336:VAL:HG13	2.00	0.43
2:C:943:VAL:HG11	2:C:973:VAL:HG22	2.00	0.43
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.82	0.43
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.99	0.43
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.50	0.43
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.84	0.43
2:C:1097:LEU:HA	2:C:1097:LEU:HD23	1.77	0.43
3:D:97:THR:HG22	3:D:98:PRO:O	2.18	0.43
3:D:245:LEU:HB2	3:D:309:GLY:O	2.19	0.43
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.52	0.43
3:D:1259:VAL:HG23	3:D:1355:VAL:HG11	2.00	0.43
2:C:376:ARG:HE	5:F:276:ARG:HG3	1.83	0.43
2:C:874:LEU:O	3:D:1029:ARG:HG3	2.18	0.43
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.67	0.43
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.54	0.43
3:D:1463:LYS:HB3	3:D:1463:LYS:HE2	1.81	0.43
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.34	0.43
1:B:73:GLU:OE1	1:B:73:GLU:N	2.43	0.43
2:C:88:LEU:O	2:C:131:GLY:N	2.52	0.43
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.00	0.43
2:C:281:LEU:HD23	2:C:309:TYR:CD2	2.54	0.43
3:D:78:VAL:HG12	3:D:79:GLU:O	2.18	0.43
3:D:270:LEU:HD13	3:D:304:LEU:HD13	2.00	0.43
3:D:1296:SER:OG	3:D:1297:GLU:N	2.51	0.43
1:B:153:ALA:HB2	1:B:168:ASP:N	2.33	0.43
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.39	0.43
3:D:190:GLU:HG3	3:D:190:GLU:O	2.18	0.43
3:D:436:GLU:HB3	3:D:445:ARG:HE	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1031:ARG:NH2	13:C:2101:HOH:O	2.51	0.43
3:D:818:ARG:NE	3:D:820:GLU:OE2	2.41	0.43
3:D:1475:GLY:HA2	4:E:17:TYR:CG	2.54	0.43
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.01	0.43
2:C:191:PHE:HB2	2:C:192:PRO:HD2	2.01	0.42
3:D:167:GLU:O	3:D:394:LEU:HD12	2.20	0.42
3:D:567:ILE:HD13	3:D:567:ILE:HA	1.82	0.42
1:A:16:GLN:HG3	1:A:20:TYR:HD2	1.84	0.42
1:B:156:HIS:ND1	1:B:158:ILE:HG23	2.34	0.42
3:D:1066:THR:HG23	3:D:1069:GLU:OE1	2.18	0.42
3:D:610:LYS:NZ	7:H:14:DG:OP1	2.52	0.42
3:D:974:ILE:HD13	3:D:991:GLN:HB3	2.01	0.42
3:D:1053:PHE:CD2	3:D:1072:ILE:HG23	2.55	0.42
5:F:88:ILE:HD13	5:F:193:ARG:HA	2.01	0.42
5:F:237:THR:OG1	6:G:4:DA:H8	2.02	0.42
2:C:436:GLY:HA2	2:C:538:GLN:O	2.19	0.42
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.84	0.42
5:F:354:LEU:HD23	5:F:354:LEU:HA	1.82	0.42
1:A:170:VAL:HG12	1:A:170:VAL:O	2.18	0.42
1:A:202:ASP:OD1	1:A:204:SER:HB3	2.20	0.42
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.54	0.42
3:D:1079:LYS:HB2	3:D:1079:LYS:HE2	1.77	0.42
2:C:83:CYS:HA	2:C:88:LEU:HB2	2.01	0.42
2:C:905:ILE:C	2:C:907:ASP:H	2.23	0.42
3:D:22:SER:HB2	3:D:92:HIS:HB3	2.00	0.42
3:D:1124:GLN:HE21	3:D:1133:ARG:HH22	1.66	0.42
3:D:1350:GLU:CD	3:D:1357:ARG:HH22	2.23	0.42
2:C:89:THR:HG22	2:C:91:GLN:HB3	2.01	0.42
2:C:572:ILE:HG13	2:C:573:ARG:HG3	2.00	0.42
2:C:987:ILE:HD11	3:D:946:GLY:HA2	2.02	0.42
2:C:1019:GLN:NE2	3:D:621:LYS:HG2	2.35	0.42
3:D:135:LEU:HD23	3:D:463:GLN:HG2	2.00	0.42
3:D:361:VAL:O	3:D:382:GLU:HA	2.20	0.42
1:A:71:VAL:O	2:C:608:GLY:N	2.53	0.42
2:C:726:ILE:HD11	2:C:757:GLY:CA	2.50	0.42
3:D:134:VAL:CG1	3:D:153:LEU:HD21	2.50	0.42
3:D:258:VAL:HG12	3:D:273:ARG:O	2.20	0.42
3:D:349:PRO:HB3	5:F:97:GLU:HG3	2.01	0.42
3:D:1441:GLN:HE21	3:D:1441:GLN:HB2	1.58	0.42
5:F:270:LYS:HE2	5:F:295:MET:HE2	2.00	0.42
2:C:50:GLU:OE2	2:C:345:ARG:NE	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:ALA:O	3:D:584:ASN:HB2	2.19	0.42
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	2.01	0.42
3:D:1376:MET:HE2	3:D:1376:MET:HB3	1.81	0.42
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.81	0.42
2:C:27:ARG:HB3	2:C:27:ARG:CZ	2.50	0.42
3:D:1197:ARG:HD2	3:D:1398:TRP:CE2	2.55	0.42
2:C:260:LEU:O	2:C:261:ILE:HD12	2.20	0.41
2:C:946:ARG:HD2	13:D:2112:HOH:O	2.20	0.41
2:C:1118:LYS:HE2	3:D:20:SER:O	2.19	0.41
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.02	0.41
3:D:1098:LEU:HD23	3:D:1098:LEU:HA	1.80	0.41
1:A:45:LEU:HA	1:A:45:LEU:HD23	1.80	0.41
1:A:107:LYS:NZ	1:A:113:ASP:OD1	2.33	0.41
2:C:620:LEU:HD12	2:C:620:LEU:HA	1.84	0.41
2:C:1006:HIS:ND1	2:C:1007:ALA:N	2.68	0.41
5:F:91:VAL:HG21	5:F:189:GLU:HB3	2.02	0.41
2:C:425:PHE:CE1	3:D:1086:LEU:HD12	2.54	0.41
2:C:743:VAL:HG11	2:C:800:VAL:HG21	2.01	0.41
3:D:59:ALA:HB2	3:D:78:VAL:HG21	2.02	0.41
3:D:207:PHE:HD2	3:D:391:ALA:HB3	1.86	0.41
3:D:1236:LEU:HD22	3:D:1359:GLN:CG	2.50	0.41
4:E:43:GLU:HG2	4:E:44:GLU:N	2.35	0.41
1:B:40:LEU:HA	1:B:40:LEU:HD23	1.78	0.41
2:C:423:ALA:O	2:C:428:ARG:NH1	2.54	0.41
2:C:424:GLY:O	2:C:428:ARG:HD2	2.19	0.41
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	2.01	0.41
3:D:172:PRO:HG2	3:D:175:VAL:HG21	2.03	0.41
3:D:846:PRO:HB3	3:D:880:ILE:HG21	2.02	0.41
3:D:864:VAL:CG1	3:D:865:THR:N	2.83	0.41
5:F:132:ARG:NH2	5:F:184:ARG:HH12	2.17	0.41
5:F:222:ARG:HA	5:F:222:ARG:NE	2.34	0.41
1:B:71:VAL:HG13	1:B:131:THR:O	2.21	0.41
3:D:191:LEU:N	3:D:195:VAL:O	2.53	0.41
3:D:949:ILE:HD13	3:D:949:ILE:HA	1.89	0.41
1:A:86:VAL:HG23	1:A:124:ASN:ND2	2.35	0.41
1:B:56:VAL:HG22	1:B:142:VAL:HG12	2.02	0.41
2:C:563:ASN:HB3	13:C:2107:HOH:O	2.20	0.41
2:C:627:ARG:HD3	2:C:638:ASP:OD1	2.20	0.41
2:C:1067:TYR:HE1	3:D:655:PRO:HG3	1.86	0.41
3:D:430:ASP:OD1	3:D:431:VAL:HG13	2.21	0.41
3:D:792:ILE:HD13	3:D:941:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1302:GLU:OE1	3:D:1304:LYS:HE3	2.20	0.41
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.85	0.41
1:B:124:ASN:OD1	1:B:124:ASN:N	2.53	0.41
2:C:226:VAL:O	2:C:229:MET:HG3	2.21	0.41
2:C:501:THR:HG21	2:C:513:VAL:HB	2.03	0.41
3:D:796:ARG:NH1	3:D:859:ASP:HB2	2.34	0.41
3:D:921:ARG:O	3:D:922:LEU:HD23	2.21	0.41
5:F:314:PRO:HD2	13:F:2101:HOH:O	2.20	0.41
1:A:72:LYS:HG3	2:C:641:PRO:HG2	2.02	0.41
2:C:203:ASP:O	2:C:206:THR:N	2.54	0.41
2:C:742:VAL:HG22	2:C:823:VAL:HG11	2.03	0.41
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.55	0.41
3:D:79:GLU:HG2	3:D:80:VAL:N	2.35	0.41
3:D:176:ASP:OD1	3:D:177:ALA:N	2.48	0.41
5:F:115:LYS:HG2	5:F:173:TYR:CE2	2.56	0.41
5:F:194:LEU:HB2	6:G:6:DT:C2	2.56	0.41
1:B:132:LEU:HD21	1:B:138:LEU:CB	2.47	0.41
2:C:72:ARG:NE	2:C:112:GLU:OE2	2.49	0.41
2:C:185:LYS:HA	2:C:189:ARG:O	2.20	0.41
2:C:376:ARG:HE	5:F:276:ARG:CG	2.33	0.41
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.36	0.41
2:C:595:LEU:HD21	2:C:639:GLN:HE22	1.84	0.41
3:D:127:LEU:HD23	3:D:127:LEU:HA	1.89	0.41
3:D:448:GLU:H	3:D:448:GLU:HG2	1.55	0.41
3:D:464:LEU:HD23	3:D:464:LEU:HA	1.84	0.41
3:D:801:GLY:HA2	3:D:821:VAL:HG22	2.03	0.41
3:D:845:ASN:HA	3:D:867:ARG:O	2.21	0.41
3:D:979:GLU:H	3:D:979:GLU:HG2	1.55	0.41
3:D:1194:CYS:HB2	3:D:1204:CYS:SG	2.60	0.41
4:E:80:VAL:HG22	4:E:81:PRO:O	2.21	0.41
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.95	0.41
5:F:286:PRO:HB2	5:F:291:ILE:HG13	2.03	0.41
5:F:332:PHE:CD1	5:F:332:PHE:N	2.87	0.41
2:C:631:SER:HB3	2:C:637:LEU:HG	2.02	0.41
2:C:757:GLY:HA2	2:C:789:SER:HB3	2.02	0.41
3:D:10:ILE:O	3:D:10:ILE:HG23	2.20	0.41
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.90	0.40
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.03	0.40
2:C:395:LYS:HD3	2:C:397:GLU:HB3	2.03	0.40
2:C:807:ARG:HG2	2:C:821:GLU:HB3	2.02	0.40
2:C:847:GLY:HA2	3:D:741:ASP:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HA	1:A:195:LEU:O	2.21	0.40
1:B:58:ILE:HD11	1:B:140:MET:HE1	2.02	0.40
2:C:97:ARG:HA	2:C:112:GLU:HA	2.04	0.40
2:C:430:VAL:O	3:D:1075:HIS:CE1	2.74	0.40
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.21	0.40
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.85	0.40
1:B:176:ARG:HG2	1:B:200:TRP:CE3	2.56	0.40
2:C:885:ILE:HD13	2:C:885:ILE:HA	1.80	0.40
2:C:926:PHE:CE1	2:C:930:LYS:HE2	2.56	0.40
3:D:529:GLN:HG3	3:D:535:PHE:CE1	2.56	0.40
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.47	0.40
1:A:41:ARG:HG3	1:A:177:VAL:HB	2.02	0.40
1:A:131:THR:O	1:A:132:LEU:HD12	2.22	0.40
2:C:157:ARG:NH1	2:C:176:VAL:HG12	2.36	0.40
2:C:243:ARG:NH1	6:G:9:DG:O6	2.33	0.40
3:D:134:VAL:HG23	3:D:150:ARG:N	2.36	0.40
3:D:236:TYR:HE1	3:D:242:LEU:HA	1.84	0.40
3:D:645:PRO:HB3	3:D:723:GLY:O	2.21	0.40
5:F:195:VAL:HG13	5:F:216:GLY:HA3	2.03	0.40
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.87	0.40
2:C:302:VAL:C	2:C:305:PRO:HD2	2.42	0.40
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.02	0.40
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.56	0.40
3:D:56:TYR:HA	3:D:80:VAL:HG13	2.04	0.40
3:D:959:GLU:HB3	3:D:963:TYR:CD2	2.56	0.40
3:D:1046:GLN:NE2	3:D:1050:GLY:O	2.54	0.40
3:D:1205:TYR:CE2	3:D:1366:LYS:HE2	2.56	0.40
5:F:307:THR:O	5:F:310:ILE:HG22	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	229/315 (73%)	211 (92%)	18 (8%)	0	100	100
1	B	225/315 (71%)	212 (94%)	13 (6%)	0	100	100
2	C	1108/1119 (99%)	1034 (93%)	74 (7%)	0	100	100
3	D	1483/1524 (97%)	1389 (94%)	92 (6%)	2 (0%)	51	82
4	E	92/99 (93%)	86 (94%)	6 (6%)	0	100	100
5	F	344/443 (78%)	335 (97%)	9 (3%)	0	100	100
All	All	3481/3815 (91%)	3267 (94%)	212 (6%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	830	ALA
3	D	783	ARG

### 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	Percentiles	
1	A	199/273 (73%)	182 (92%)	17 (8%)	10	31
1	B	193/273 (71%)	177 (92%)	16 (8%)	11	32
2	C	932/941 (99%)	851 (91%)	81 (9%)	10	30
3	D	1247/1279 (98%)	1151 (92%)	96 (8%)	13	35
4	E	82/88 (93%)	73 (89%)	9 (11%)	6	19
5	F	300/388 (77%)	280 (93%)	20 (7%)	16	43
All	All	2953/3242 (91%)	2714 (92%)	239 (8%)	11	33

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	19	GLU
1	A	28	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	32	PHE
1	A	83	LYS
1	A	96	THR
1	A	99	LEU
1	A	115	LEU
1	A	122	ILE
1	A	126	ASP
1	A	133	GLU
1	A	134	GLU
1	A	142	VAL
1	A	182	GLU
1	A	196	THR
1	A	205	VAL
1	A	223	THR
1	B	10	VAL
1	B	15	THR
1	B	51	THR
1	B	54	THR
1	B	56	VAL
1	B	67	THR
1	B	93	SER
1	B	112	ARG
1	B	113	ASP
1	B	129	ILE
1	B	146	ARG
1	B	154	GLU
1	B	190	THR
1	B	197	LEU
1	B	200	TRP
1	B	215	VAL
2	C	1	MET
2	C	5	ARG
2	C	12	VAL
2	C	26	TYR
2	C	27	ARG
2	C	81	ASP
2	C	100	LEU
2	C	118	ILE
2	C	133	ASP
2	C	138	SER
2	C	143	SER
2	C	149	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	161	SER
2	C	168	ARG
2	C	188	LYS
2	C	200	LEU
2	C	205	GLU
2	C	206	THR
2	C	211	LEU
2	C	216	GLU
2	C	217	LEU
2	C	229	MET
2	C	251	ASP
2	C	257	VAL
2	C	276	LYS
2	C	284	ARG
2	C	285	LEU
2	C	294	GLU
2	C	309	TYR
2	C	314	THR
2	C	321	GLU
2	C	322	VAL
2	C	335	THR
2	C	342	ASP
2	C	348	LEU
2	C	353	ARG
2	C	360	LEU
2	C	390	GLN
2	C	402	SER
2	C	403	SER
2	C	409	ARG
2	C	426	ASP
2	C	434	HIS
2	C	439	CYS
2	C	442	GLU
2	C	452	ILE
2	C	454	SER
2	C	464	LEU
2	C	501	THR
2	C	513	VAL
2	C	538	GLN
2	C	566	THR
2	C	583	LEU
2	C	585	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	610	ARG
2	C	617	ASP
2	C	638	ASP
2	C	661	SER
2	C	670	GLN
2	C	698	ASP
2	C	723	THR
2	C	759	THR
2	C	764	GLU
2	C	785	VAL
2	C	789	SER
2	C	802	ARG
2	C	805	ARG
2	C	816	LYS
2	C	829	GLN
2	C	848	VAL
2	C	929	ARG
2	C	968	LEU
2	C	978	ARG
2	C	984	GLU
2	C	996	LYS
2	C	1024	LYS
2	C	1058	ASP
2	C	1060	ILE
2	C	1076	VAL
2	C	1101	THR
2	C	1104	GLU
3	D	5	VAL
3	D	40	GLU
3	D	68	PHE
3	D	81	THR
3	D	108	VAL
3	D	115	LEU
3	D	133	ILE
3	D	145	VAL
3	D	153	LEU
3	D	171	LEU
3	D	180	LYS
3	D	216	VAL
3	D	234	GLU
3	D	242	LEU
3	D	273	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	276	ASP
3	D	286	VAL
3	D	291	LEU
3	D	331	VAL
3	D	380	GLU
3	D	404	GLU
3	D	406	ASP
3	D	407	VAL
3	D	410	SER
3	D	415	VAL
3	D	420	VAL
3	D	421	LEU
3	D	429	SER
3	D	430	ASP
3	D	443	VAL
3	D	445	ARG
3	D	448	GLU
3	D	476	GLU
3	D	508	ARG
3	D	608	SER
3	D	618	LEU
3	D	628	ARG
3	D	633	VAL
3	D	681	ARG
3	D	683	ILE
3	D	686	GLU
3	D	687	VAL
3	D	709	HIS
3	D	743	ASP
3	D	754	PHE
3	D	783	ARG
3	D	784	ASP
3	D	799	LYS
3	D	810	GLU
3	D	832	ARG
3	D	836	VAL
3	D	865	THR
3	D	875	THR
3	D	904	VAL
3	D	947	ILE
3	D	971	LEU
3	D	979	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	1039	CYS
3	D	1041	LEU
3	D	1055	VAL
3	D	1072	ILE
3	D	1083	ASP
3	D	1100	ASP
3	D	1101	VAL
3	D	1128	VAL
3	D	1129	THR
3	D	1130	ARG
3	D	1133	ARG
3	D	1185	GLU
3	D	1188	VAL
3	D	1210	SER
3	D	1221	VAL
3	D	1287	GLU
3	D	1296	SER
3	D	1305	LEU
3	D	1307	LYS
3	D	1320	GLU
3	D	1326	THR
3	D	1344	VAL
3	D	1363	LEU
3	D	1366	LYS
3	D	1370	ILE
3	D	1376	MET
3	D	1386	ASP
3	D	1388	ARG
3	D	1400	VAL
3	D	1405	GLU
3	D	1408	ILE
3	D	1413	THR
3	D	1430	SER
3	D	1431	THR
3	D	1433	SER
3	D	1441	GLN
3	D	1471	LEU
3	D	1488	ASP
3	D	1493	LYS
4	E	15	SER
4	E	32	ARG
4	E	37	ASN

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Mol	Chain	Res	Type
4	E	51	LEU
4	E	74	VAL
4	E	80	VAL
4	E	84	ARG
4	E	89	MET
4	E	93	TYR
5	F	88	ILE
5	F	96	LEU
5	F	97	GLU
5	F	98	GLU
5	F	110	MET
5	F	150	THR
5	F	155	THR
5	F	157	GLU
5	F	172	ARG
5	F	218	GLN
5	F	272	SER
5	F	279	GLN
5	F	323	ASP
5	F	338	LEU
5	F	340	SER
5	F	346	THR
5	F	348	SER
5	F	371	LEU
5	F	400	ILE
5	F	413	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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
12	2TM	I	2101	-	27,30,30	5.01	18 (66%)	39,47,47	1.21	2 (5%)
10	BU1	D	2004	-	5,5,5	0.38	0	4,4,4	0.17	0
10	BU1	B	2002	-	5,5,5	0.43	0	4,4,4	0.30	0

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
12	2TM	I	2101	-	-	6/19/38/38	0/2/2/2
10	BU1	D	2004	-	-	1/3/3/3	-
10	BU1	B	2002	-	-	1/3/3/3	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2101	2TM	PB-O3B	15.00	1.75	1.58
12	I	2101	2TM	C2'-C3'	-7.91	1.31	1.53
12	I	2101	2TM	O4'-C4'	-7.42	1.28	1.45
12	I	2101	2TM	C2-N3	7.30	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2101	2TM	C6-C5	6.84	1.51	1.35
12	I	2101	2TM	O4'-C1'	6.16	1.56	1.42
12	I	2101	2TM	C2-N1	5.81	1.52	1.40
12	I	2101	2TM	C4-N3	5.47	1.45	1.34
12	I	2101	2TM	PA-O5'	4.60	1.64	1.57
12	I	2101	2TM	C5-C4	4.07	1.52	1.42
12	I	2101	2TM	O2-C2	-3.98	1.16	1.23
12	I	2101	2TM	C1'-N1	-3.46	1.37	1.47
12	I	2101	2TM	C3'-C4'	3.43	1.61	1.53
12	I	2101	2TM	O2'-C2'	3.34	1.50	1.43
12	I	2101	2TM	PB-O2B	3.09	1.59	1.51
12	I	2101	2TM	C6-N1	2.93	1.45	1.38
12	I	2101	2TM	C4-N4	2.66	1.40	1.33
12	I	2101	2TM	C5'-C4'	2.40	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	2101	2TM	PB-O3B-PG	-3.16	121.50	132.62
12	I	2101	2TM	C2'-C3'-C4'	2.11	106.75	102.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

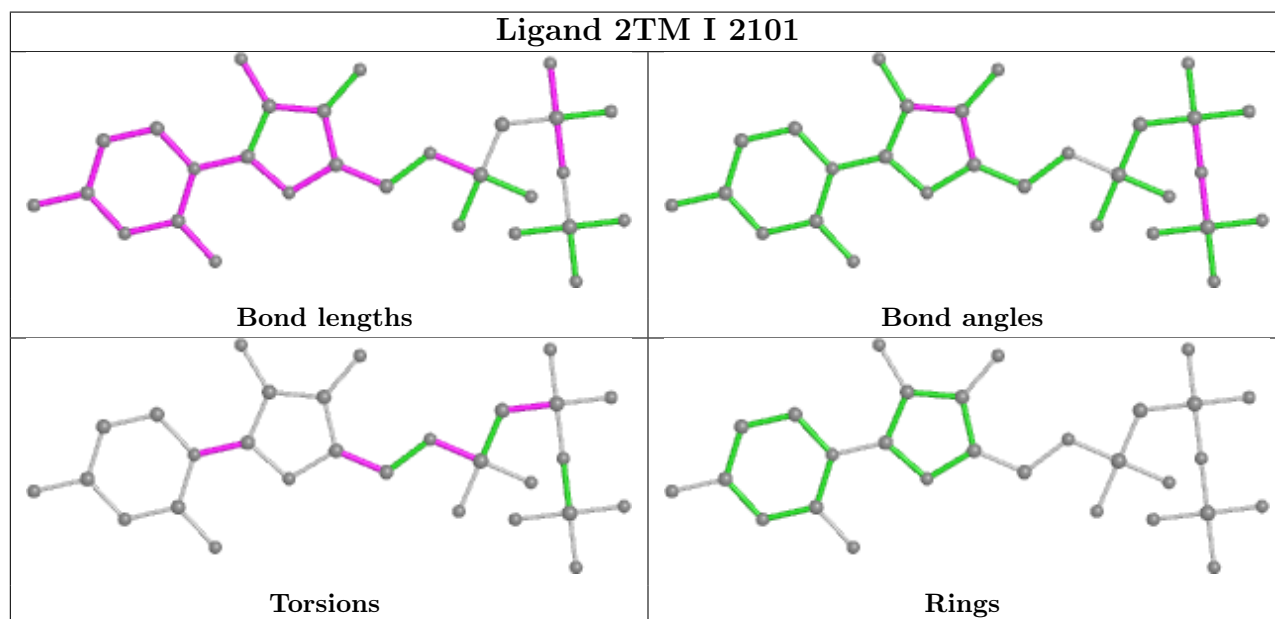
Mol	Chain	Res	Type	Atoms
12	I	2101	2TM	C5'-O5'-PA-O2A
12	I	2101	2TM	PA-C1-PB-O3B
12	I	2101	2TM	PA-C1-PB-O1B
12	I	2101	2TM	PA-C1-PB-O2B
10	B	2002	BU1	O5-C1-C2-C3
10	D	2004	BU1	O5-C1-C2-C3
12	I	2101	2TM	C2'-C1'-N1-C2
12	I	2101	2TM	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	2004	BU1	1	0
10	B	2002	BU1	3	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 than 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

### 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	231/315 (73%)	-0.25	5 (2%) 62 59	23, 43, 65, 96	0
1	B	227/315 (72%)	-0.17	4 (1%) 68 67	27, 53, 82, 118	0
2	C	1112/1119 (99%)	-0.24	23 (2%) 63 61	12, 37, 87, 121	0
3	D	1486/1524 (97%)	-0.05	67 (4%) 33 29	8, 41, 97, 125	0
4	E	94/99 (94%)	-0.36	0 100 100	20, 40, 71, 82	0
5	F	346/443 (78%)	-0.08	5 (1%) 75 75	24, 56, 94, 114	0
6	G	25/27 (92%)	-0.01	0 100 100	57, 74, 136, 146	0
7	H	17/19 (89%)	0.14	1 (5%) 22 18	31, 60, 140, 144	0
8	I	2/2 (100%)	-0.14	0 100 100	27, 27, 27, 28	2 (100%)
All	All	3540/3863 (91%)	-0.14	105 (2%) 50 45	8, 43, 94, 146	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASP	5.0
2	C	365	ASP	4.9
1	B	2	LEU	4.5
3	D	422	ALA	4.1
2	C	107	LEU	4.1
2	C	221	LEU	4.1
3	D	974	ILE	4.1
3	D	393	ILE	4.0
3	D	406	ASP	3.7
3	D	371	ILE	3.7
1	A	232	ALA	3.7
2	C	228	ALA	3.7
5	F	325	LYS	3.5
2	C	219	GLN	3.5
3	D	368	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	144	GLY	3.4
3	D	186	VAL	3.4
2	C	216	GLU	3.4
3	D	388	HIS	3.4
3	D	173	PRO	3.3
3	D	1319	VAL	3.3
2	C	104	ASP	3.2
2	C	207	LEU	3.2
3	D	310	LEU	3.2
3	D	1127	GLU	3.2
3	D	1130	ARG	3.2
3	D	454	ALA	3.2
1	A	233	VAL	3.1
3	D	241	ILE	3.1
3	D	804	LEU	3.1
3	D	449	SER	3.0
3	D	203	ALA	3.0
3	D	1287	GLU	3.0
2	C	311	PHE	2.9
3	D	409	VAL	2.9
3	D	346	ARG	2.9
3	D	355	VAL	2.8
3	D	213	VAL	2.8
3	D	1300	SER	2.8
3	D	1499	ARG	2.8
3	D	237	LYS	2.7
3	D	1489	GLN	2.7
3	D	201	GLY	2.7
2	C	226	VAL	2.7
3	D	318	ARG	2.7
2	C	222	MET	2.7
2	C	217	LEU	2.7
3	D	324	ALA	2.7
5	F	324	GLU	2.6
3	D	142	LEU	2.6
3	D	1313	VAL	2.6
3	D	345	TYR	2.6
2	C	366	SER	2.5
3	D	1409	ALA	2.5
3	D	1408	ILE	2.5
3	D	435	VAL	2.5
3	D	1297	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	231	ALA	2.5
3	D	410	SER	2.4
2	C	367	LEU	2.4
3	D	322	VAL	2.4
3	D	821	VAL	2.4
3	D	177	ALA	2.4
3	D	1131	SER	2.4
2	C	204	GLN	2.4
3	D	197	SER	2.4
2	C	595	LEU	2.4
3	D	353	VAL	2.3
1	B	6	LEU	2.3
3	D	378	ILE	2.3
3	D	1497	GLU	2.3
3	D	236	TYR	2.3
3	D	1279	GLY	2.3
3	D	245	LEU	2.2
3	D	175	VAL	2.2
3	D	211	VAL	2.2
7	H	5	DC	2.2
2	C	227	PHE	2.2
3	D	174	GLY	2.2
3	D	1318	TYR	2.2
1	A	230	ALA	2.2
3	D	1490	LYS	2.2
3	D	418	GLY	2.1
3	D	178	LEU	2.1
2	C	233	GLU	2.1
3	D	805	GLU	2.1
3	D	994	GLN	2.1
2	C	648	ARG	2.1
3	D	309	GLY	2.1
1	B	138	LEU	2.1
3	D	219	GLU	2.1
3	D	143	ASN	2.1
1	A	234	ALA	2.1
5	F	162	LYS	2.1
5	F	138	SER	2.1
2	C	215	GLY	2.1
2	C	224	GLU	2.1
3	D	377	VAL	2.1
3	D	1299	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
5	F	423	ASP	2.0
2	C	364	GLU	2.0
3	D	68	PHE	2.0
3	D	179	VAL	2.0
3	D	370	ALA	2.0
2	C	181	VAL	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](#)

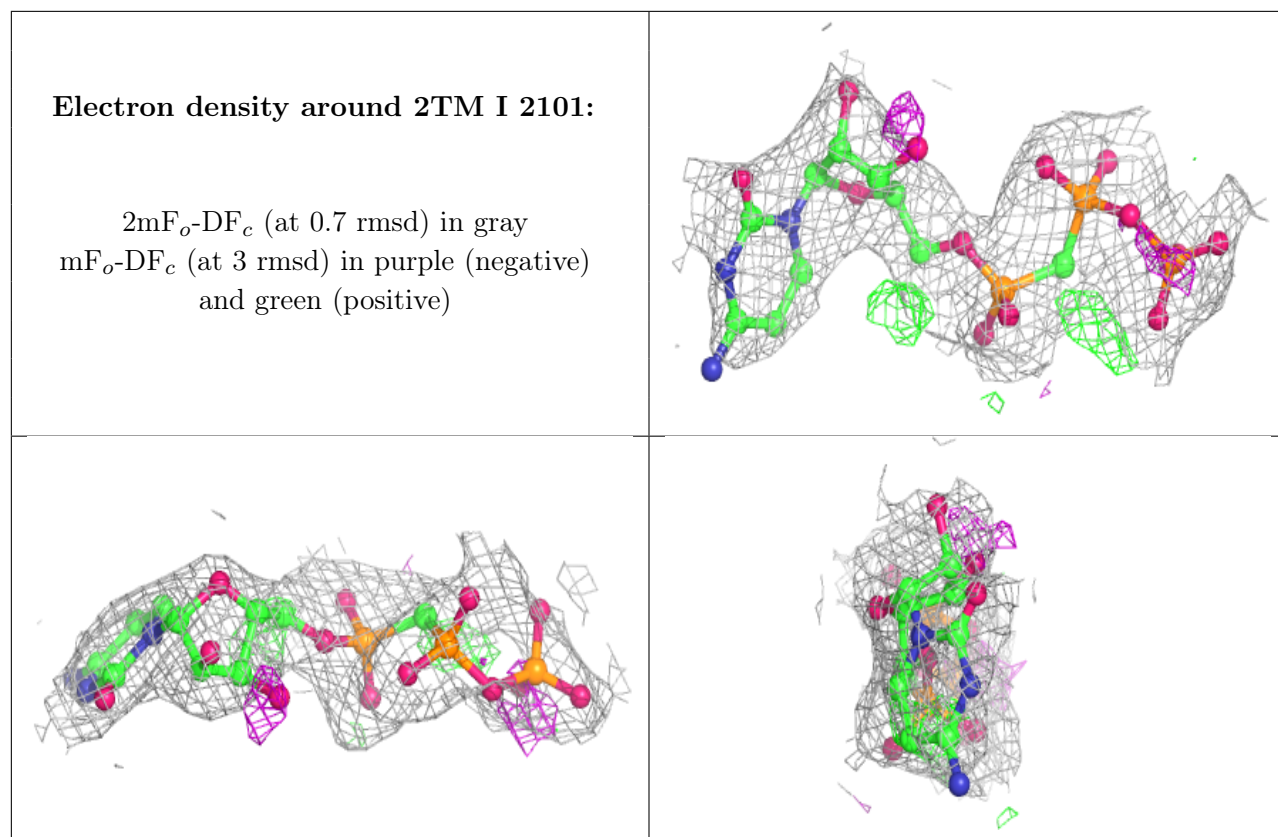
There are no monosaccharides in this entry.

## 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
9	MG	B	2001	1/1	0.87	0.11	57,57,57,57	0
12	2TM	I	2101	29/29	0.87	0.24	21,38,72,76	29
10	BU1	B	2002	6/6	0.88	0.29	34,40,48,49	0
10	BU1	D	2004	6/6	0.91	0.33	27,30,37,39	0
9	MG	B	2003	1/1	0.92	0.23	41,41,41,41	0
9	MG	C	2001	1/1	0.94	0.27	20,20,20,20	0
9	MG	F	2001	1/1	0.98	0.10	28,28,28,28	0
11	ZN	D	2001	1/1	0.99	0.11	24,24,24,24	0
11	ZN	D	2002	1/1	0.99	0.08	61,61,61,61	0
9	MG	D	2003	1/1	0.99	0.22	8,8,8,8	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.