



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:16 PM UTC

PDB ID : 7EH1 / pdb_00007eh1
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

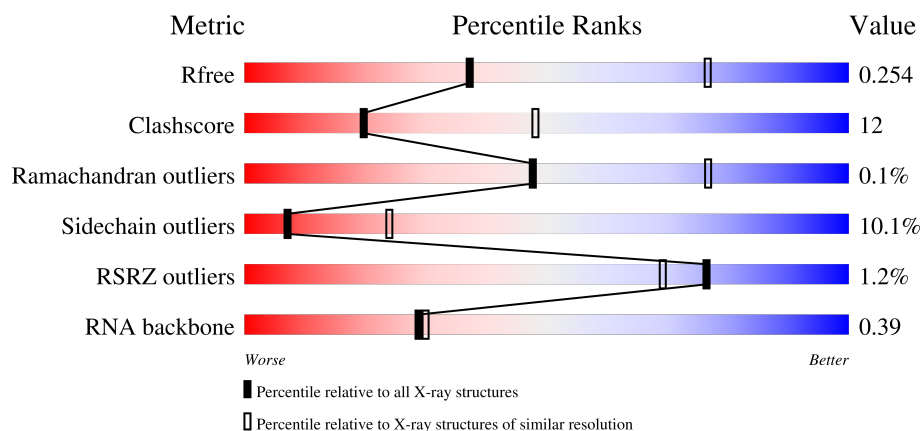
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 $\leq 5\%$. 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	
1	B	315	
2	C	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
4	E	99	68%23%5%
5	F	443	% 54%21%22%
6	G	27	4% 41%52%7%
7	H	19	63%26%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
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
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
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
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
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
6	G	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

- Molecule 7 is a DNA chain called DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*CP*CP*AP*AP*G)-3').

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

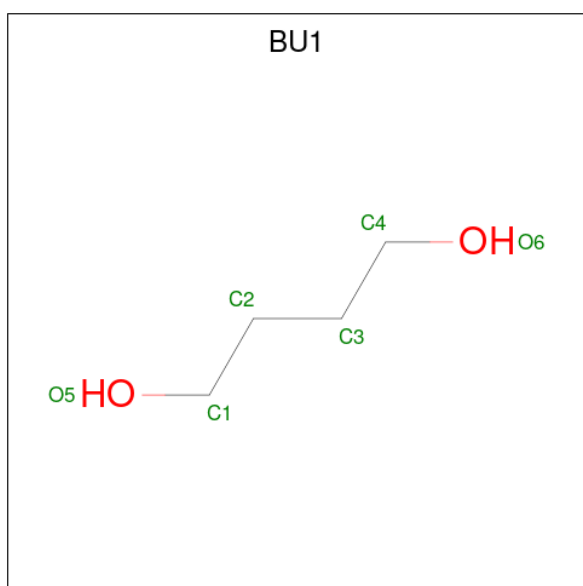
- Molecule 8 is a RNA chain called RNA (5'-R(*GP*G)-3').

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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 10 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula: $C_4H_{10}O_2$).

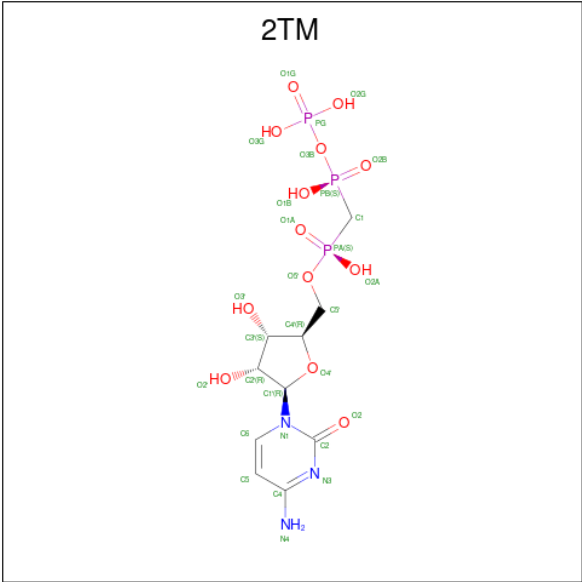


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	4	2		
10	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 12 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: $C_{10}H_{18}N_3O_{13}P_3$).



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

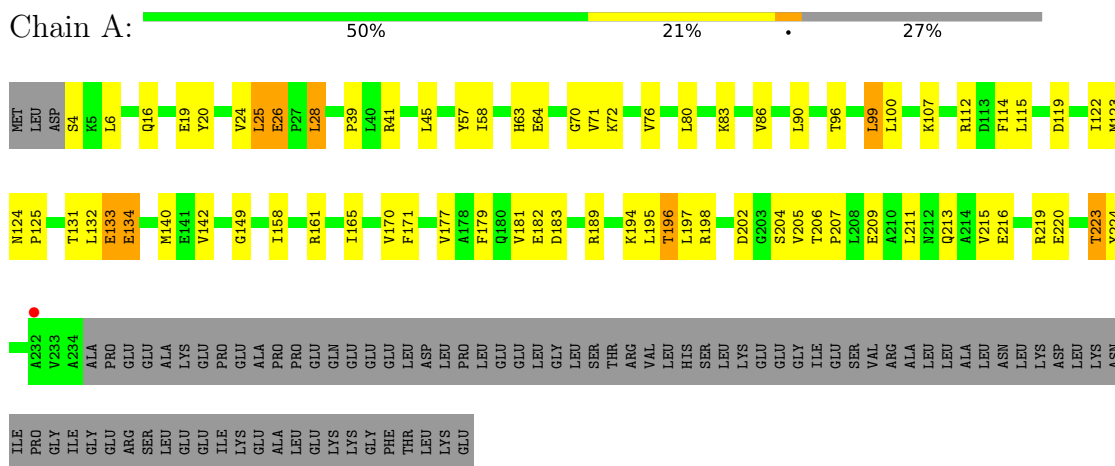
- Molecule 13 is water.

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		

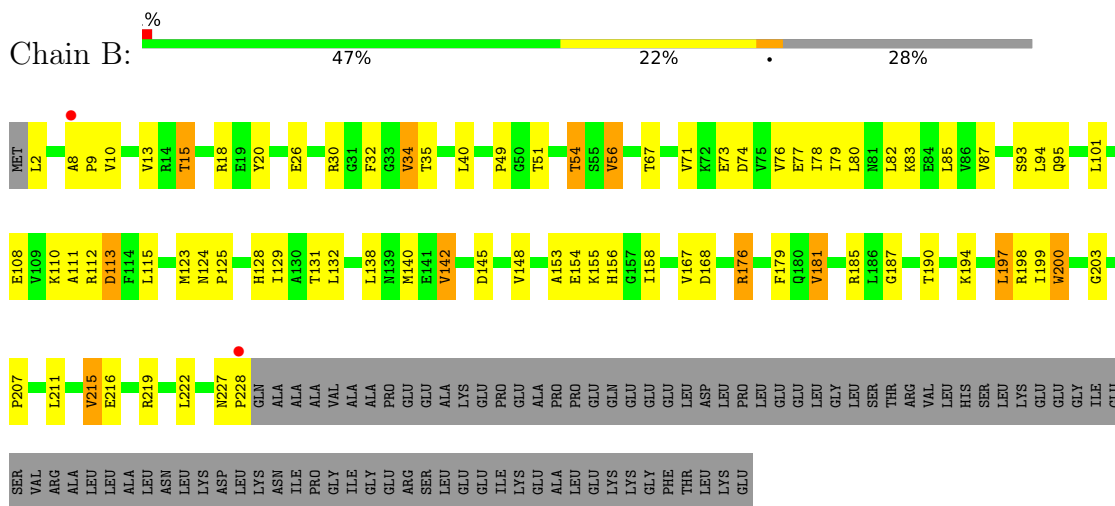
3 Residue-property plots [i](#)

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

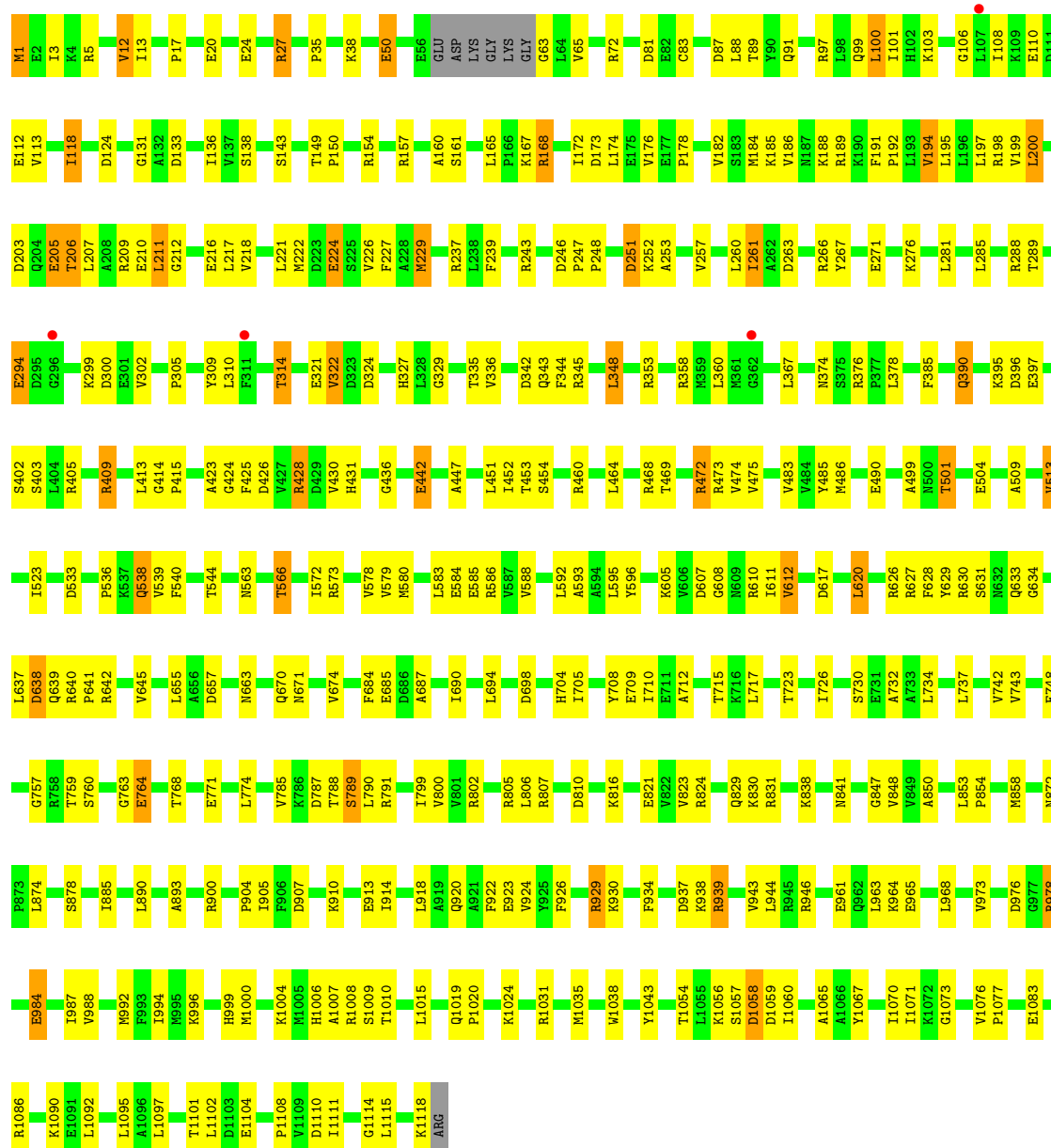


• Molecule 1: DNA-directed RNA polymerase subunit alpha

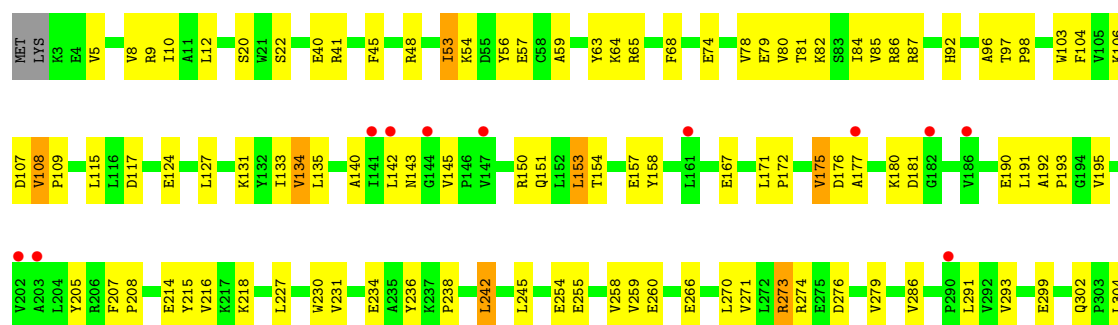


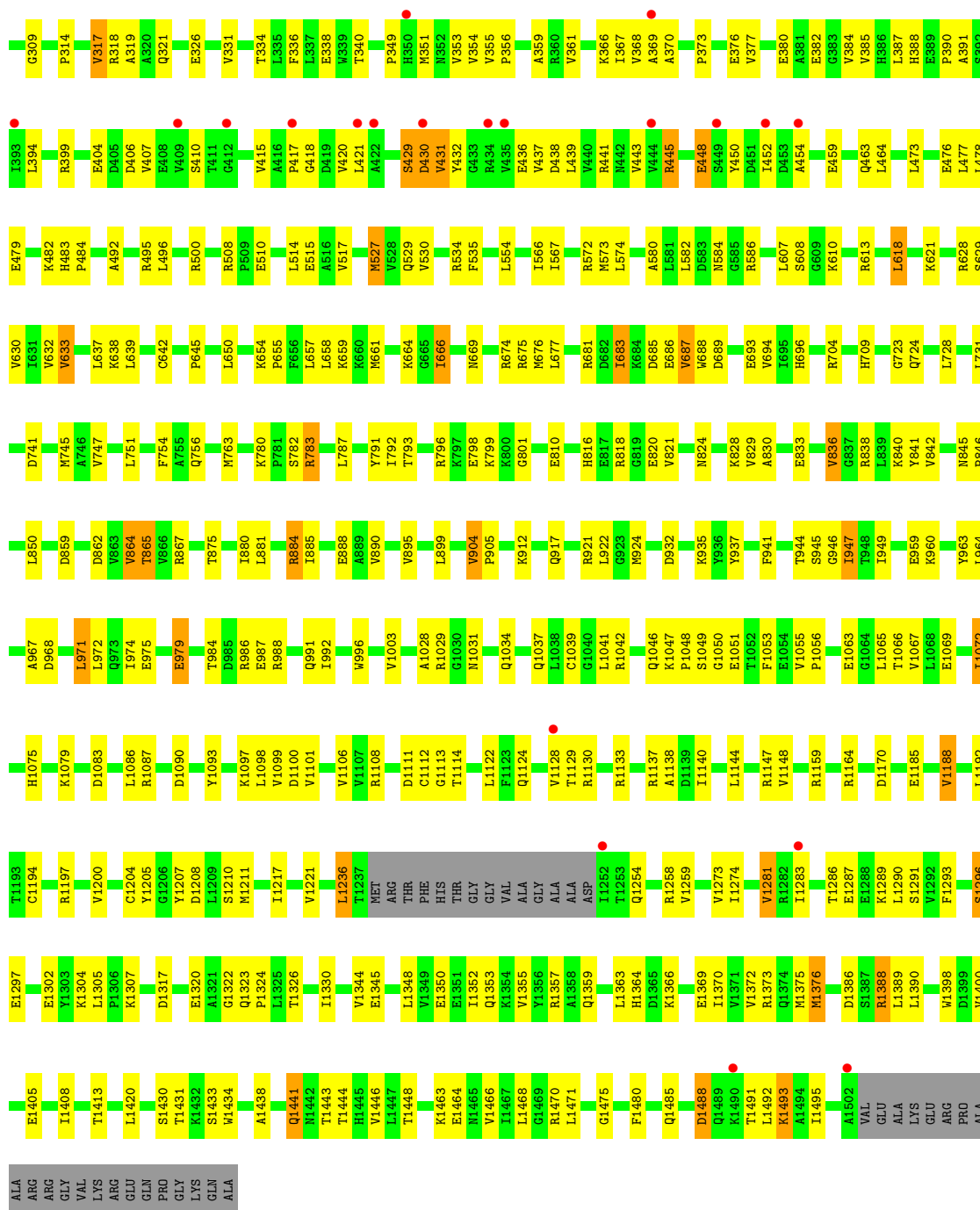
• Molecule 2: DNA-directed RNA polymerase subunit beta





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





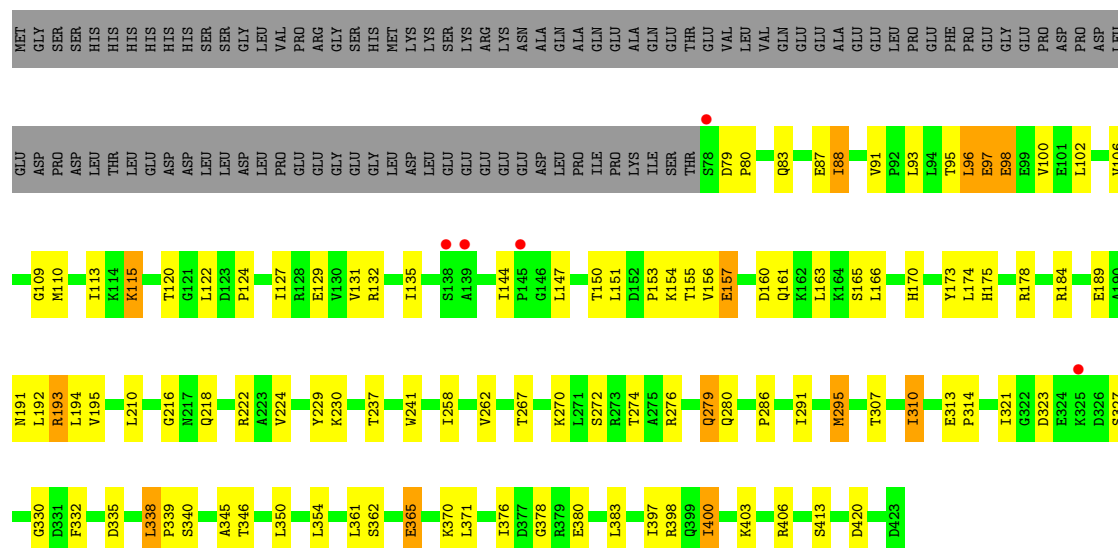
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 68% 23% 5%

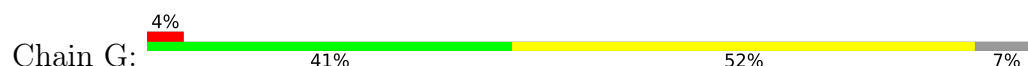


- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 54% 21% 22%



• 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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.12Å 103.32Å 295.65Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	25.27 – 2.90 25.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.1 (25.27-2.90) 82.1 (25.27-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.191 , 0.253 0.193 , 0.254	Depositor DCC
R_{free} test set	1971 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.024 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28630	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 2TM, BU1

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	0.39	0/1835	0.62	0/2497
1	B	0.36	0/1790	0.60	0/2440
2	C	0.41	0/8917	0.62	0/12064
3	D	0.43	0/11923	0.65	0/16126
4	E	0.43	0/773	0.60	0/1042
5	F	0.37	0/2848	0.55	0/3833
6	G	0.47	0/580	0.60	0/895
7	H	0.40	0/388	0.53	0/597
8	I	0.35	0/48	0.47	0/74
All	All	0.41	0/29102	0.62	0/39568

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

There are no bond length outliers.

There are no bond angle outliers.

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

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Mol	Chain	Res	Type	Group
3	D	829	VAL	Peptide
5	F	330	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1803	0	1852	48	0
1	B	1758	0	1778	54	0
2	C	8750	0	8833	240	0
3	D	11714	0	11926	288	0
4	E	759	0	771	18	0
5	F	2803	0	2871	68	0
6	G	516	0	283	15	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
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	658	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (658) 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
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.54	0.88
3:D:657:LEU:HG	3:D:661:MET:HE2	1.58	0.86
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"	6:G:9:DG:H5"	1.68	0.75
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.69	0.75
2:C:226:VAL:HA	2:C:229:MET:HE3	1.67	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
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
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.73	0.70
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:184:MET:HE2	2:C:186:VAL:HG21	1.77	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
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.32	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
2:C:580:MET:HB3	2:C:584:GLU:CD	2.24	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
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.81	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:230:TRP:CD1	3:D:231:VAL:H	2.21	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
5:F:295:MET:HA	5:F:295:MET:HE2	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:607:ASP:HB3	2:C:610:ARG:H	1.67	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	1.84	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
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
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
2:C:224:GLU:CD	2:C:224:GLU:H	2.13	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
3:D:1164:ARG:HE	3:D:1170:ASP:CG	2.13	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
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.14	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: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
3:D:227:LEU:HD22	3:D:326:GLU:OE1	2.06	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
3:D:479:GLU:OE1	3:D:482:LYS:NZ	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:218:VAL:HG22	2:C:222:MET:HE2	1.88	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
6:G:12:DC:H1'	6:G:13:DT:H72	1.90	0.54
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.89	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
3:D:1192:LEU:HD22	3:D:1345:GLU:CD	2.34	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''	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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:74:GLU:CD	3:D:74:GLU:H	2.19	0.51
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.45	0.51
2:C:976:ASP:CG	2:C:978:ARG:HH11	2.19	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
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:1:MET:HE3	2:C:3:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:578:VAL:HG23	2:C:671:ASN:CG	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:157:GLU:O	5:F:161:GLN:HG2	2.13	0.47
2:C:853:LEU:HB2	2:C:858:MET:CE	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:1350:GLU:CD	3:D:1357:ARG:HH22	2.23	0.47
2:C:348:LEU:HD13	2:C:378:LEU:HD13	1.96	0.47
2:C:905:ILE:C	2:C:907:ASP:H	2.23	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:418:GLY:N	3:D:429:SER:O	2.34	0.46
3:D:527:MET:HB2	3:D:527:MET:HE2	1.63	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: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
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.80	0.46
3:D:658:LEU:HA	3:D:661:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
5:F:274:THR:OG1	5:F:295:MET:HE3	2.17	0.45
7:H:16:DC:H2'	7:H:17:DA:C8	2.52	0.45
2:C:302:VAL:C	2:C:305:PRO:HD2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:1208:ASP:OD2	3:D:1211:MET:HE2	2.17	0.44
4:E:9:LEU:CD1	4:E:65:MET:HE2	2.47	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
1:B:123:MET:HE3	1:B:123:MET:HB3	1.88	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:65:VAL:O	2:C:100:LEU:HD23	2.18	0.44
2:C:805:ARG:C	2:C:806:LEU:HD23	2.43	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
3:D:650:LEU:C	3:D:650:LEU:HD23	2.42	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:666:ILE:HG22	3:D:676:MET:HE1	2.00	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:327:HIS:C	2:C:329:GLY:H	2.26	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:596:TYR:C	2:C:655:LEU:HD12	2.44	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:924:MET:HB3	3:D:924:MET:HE2	1.61	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:1147:ARG:HH22	3:D:1369:GLU:CD	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.37	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
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:1463:LYS:O	3:D:1464:GLU:C	2.62	0.42
3:D:108:VAL:HA	3:D:109:PRO:C	2.44	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
3:D:1137:ARG:O	3:D:1138:ALA:C	2.62	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:246:ASP:OD1	2:C:252:LYS:NZ	2.40	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:50:GLU:OE2	2:C:345:ARG:NE	2.53	0.42
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
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:841:ASN:OD1	2:C:841:ASN:C	2.62	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:20:TYR:C	1:A:207:PRO:HG2	2.45	0.41
1:A:45:LEU:HA	1:A:45:LEU:HD23	1.80	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
2:C:988:VAL:HG21	3:D:949:ILE:C	2.45	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
2:C:327:HIS:C	2:C:329:GLY:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TYR:C	1:B:207:PRO:HG2	2.46	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:661:MET:HE1	3:D:677:LEU:HD11	2.03	0.41
3:D:792:ILE:HD13	3:D:941:PHE:CE2	2.55	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:HH12	3:D:888:GLU:CD	2.23	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:54:THR:OG1	1:B:145:ASP:OD2	2.31	0.40
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
1:A:24:VAL:HA	1:A:195:LEU:O	2.21	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:763:GLY:C	2:C:764:GLU:HG2	2.47	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
2:C:324:ASP:CG	2:C:431:HIS:HE2	2.30	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:638:LYS:O	3:D:639:LEU:C	2.65	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
1:A:123:MET:HE3	1:A:123:MET:HB3	1.86	0.40
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.87	0.40
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.02	0.40
2:C:684:PHE:O	2:C:685:GLU:C	2.65	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
3:D:1376:MET:HE2	3:D:1376:MET:HB3	1.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	48	77
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%)	48	77

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%)	179 (90%)	20 (10%)	7	24
1	B	193/273 (71%)	173 (90%)	20 (10%)	7	23
2	C	932/941 (99%)	840 (90%)	92 (10%)	7	24
3	D	1247/1279 (98%)	1121 (90%)	126 (10%)	7	24
4	E	82/88 (93%)	74 (90%)	8 (10%)	7	25
5	F	300/388 (77%)	269 (90%)	31 (10%)	7	23
All	All	2953/3242 (91%)	2656 (90%)	297 (10%)	7	24

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	19	GLU
1	A	25	LEU
1	A	26	GLU
1	A	28	LEU
1	A	76	VAL
1	A	83	LYS
1	A	96	THR
1	A	99	LEU
1	A	100	LEU
1	A	107	LYS
1	A	115	LEU
1	A	122	ILE
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	34	VAL
1	B	51	THR
1	B	54	THR
1	B	56	VAL
1	B	67	THR
1	B	76	VAL
1	B	93	SER
1	B	112	ARG

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Mol	Chain	Res	Type
1	B	113	ASP
1	B	129	ILE
1	B	142	VAL
1	B	154	GLU
1	B	176	ARG
1	B	181	VAL
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	27	ARG
2	C	50	GLU
2	C	81	ASP
2	C	100	LEU
2	C	113	VAL
2	C	118	ILE
2	C	138	SER
2	C	143	SER
2	C	149	THR
2	C	161	SER
2	C	168	ARG
2	C	182	VAL
2	C	188	LYS
2	C	194	VAL
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	224	GLU
2	C	229	MET
2	C	251	ASP
2	C	257	VAL
2	C	261	ILE
2	C	276	LYS
2	C	285	LEU
2	C	294	GLU
2	C	314	THR

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Mol	Chain	Res	Type
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	367	LEU
2	C	390	GLN
2	C	402	SER
2	C	403	SER
2	C	409	ARG
2	C	426	ASP
2	C	428	ARG
2	C	442	GLU
2	C	452	ILE
2	C	453	THR
2	C	454	SER
2	C	464	LEU
2	C	472	ARG
2	C	475	VAL
2	C	501	THR
2	C	513	VAL
2	C	523	ILE
2	C	538	GLN
2	C	539	VAL
2	C	566	THR
2	C	583	LEU
2	C	585	GLU
2	C	612	VAL
2	C	617	ASP
2	C	620	LEU
2	C	638	ASP
2	C	670	GLN
2	C	674	VAL
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

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Mol	Chain	Res	Type
2	C	816	LYS
2	C	829	GLN
2	C	830	LYS
2	C	848	VAL
2	C	878	SER
2	C	913	GLU
2	C	929	ARG
2	C	939	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	53	ILE
3	D	68	PHE
3	D	81	THR
3	D	108	VAL
3	D	115	LEU
3	D	124	GLU
3	D	133	ILE
3	D	134	VAL
3	D	145	VAL
3	D	153	LEU
3	D	171	LEU
3	D	175	VAL
3	D	180	LYS
3	D	216	VAL
3	D	234	GLU
3	D	242	LEU
3	D	254	GLU
3	D	259	VAL
3	D	273	ARG
3	D	276	ASP
3	D	286	VAL
3	D	291	LEU

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Mol	Chain	Res	Type
3	D	293	VAL
3	D	317	VAL
3	D	331	VAL
3	D	334	THR
3	D	354	VAL
3	D	380	GLU
3	D	387	LEU
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	431	VAL
3	D	439	LEU
3	D	443	VAL
3	D	445	ARG
3	D	448	GLU
3	D	452	ILE
3	D	459	GLU
3	D	476	GLU
3	D	527	MET
3	D	530	VAL
3	D	574	LEU
3	D	608	SER
3	D	618	LEU
3	D	628	ARG
3	D	632	VAL
3	D	633	VAL
3	D	666	ILE
3	D	681	ARG
3	D	683	ILE
3	D	686	GLU
3	D	687	VAL
3	D	694	VAL
3	D	709	HIS
3	D	724	GLN
3	D	747	VAL
3	D	754	PHE

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Mol	Chain	Res	Type
3	D	756	GLN
3	D	799	LYS
3	D	810	GLU
3	D	836	VAL
3	D	838	ARG
3	D	864	VAL
3	D	865	THR
3	D	875	THR
3	D	884	ARG
3	D	904	VAL
3	D	947	ILE
3	D	964	LEU
3	D	971	LEU
3	D	979	GLU
3	D	986	ARG
3	D	1003	VAL
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	1185	GLU
3	D	1188	VAL
3	D	1210	SER
3	D	1217	ILE
3	D	1221	VAL
3	D	1236	LEU
3	D	1273	VAL
3	D	1281	VAL
3	D	1283	ILE
3	D	1287	GLU
3	D	1296	SER
3	D	1305	LEU
3	D	1307	LYS
3	D	1320	GLU
3	D	1323	GLN
3	D	1326	THR

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Mol	Chain	Res	Type
3	D	1344	VAL
3	D	1363	LEU
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	1466	VAL
3	D	1471	LEU
3	D	1488	ASP
3	D	1493	LYS
4	E	15	SER
4	E	37	ASN
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	115	LYS
5	F	150	THR
5	F	154	LYS
5	F	155	THR
5	F	157	GLU
5	F	165	SER
5	F	193	ARG
5	F	218	GLN
5	F	224	VAL
5	F	258	ILE
5	F	262	VAL

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Mol	Chain	Res	Type
5	F	267	THR
5	F	272	SER
5	F	279	GLN
5	F	295	MET
5	F	310	ILE
5	F	323	ASP
5	F	338	LEU
5	F	340	SER
5	F	346	THR
5	F	365	GLU
5	F	371	LEU
5	F	380	GLU
5	F	400	ILE
5	F	406	ARG
5	F	413	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	212	ASN
2	C	187	ASN
2	C	390	GLN
2	C	498	GLN
2	C	663	ASN
2	C	1064	ASN
3	D	388	HIS
3	D	442	ASN
3	D	703	ASN
3	D	717	GLN
3	D	737	ASN
3	D	744	GLN
3	D	994	GLN
3	D	1046	GLN
3	D	1227	GLN
4	E	33	HIS
5	F	312	GLN

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 oligosaccharides 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	-	26,30,30	5.05	17 (65%)	39,47,47	1.22	2 (5%)
10	BU1	D	2004	-	5,5,5	0.37	0	4,4,4	0.16	0
10	BU1	B	2002	-	5,5,5	0.43	0	4,4,4	0.33	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	-	-	5/19/38/38	0/2/2/2
10	BU1	D	2004	-	-	1/3/3/3	-
10	BU1	B	2002	-	-	1/3/3/3	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2101	2TM	PB-O3B	15.01	1.75	1.58
12	I	2101	2TM	C2'-C3'	-8.00	1.31	1.53
12	I	2101	2TM	C2-N3	7.47	1.51	1.36
12	I	2101	2TM	O4'-C4'	-7.46	1.28	1.45
12	I	2101	2TM	C6-C5	6.85	1.51	1.35
12	I	2101	2TM	O4'-C1'	6.31	1.56	1.42
12	I	2101	2TM	C2-N1	5.98	1.52	1.40
12	I	2101	2TM	C4-N3	5.55	1.45	1.34
12	I	2101	2TM	C5-C4	4.00	1.52	1.42
12	I	2101	2TM	O2-C2	-3.96	1.16	1.23
12	I	2101	2TM	C1'-N1	-3.51	1.37	1.47
12	I	2101	2TM	C3'-C4'	3.45	1.61	1.53
12	I	2101	2TM	O2'-C2'	3.18	1.50	1.43
12	I	2101	2TM	PB-O2B	3.15	1.59	1.51
12	I	2101	2TM	C6-N1	2.93	1.45	1.38
12	I	2101	2TM	C4-N4	2.58	1.40	1.33
12	I	2101	2TM	C5'-C4'	2.50	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	-3.05	121.50	132.45
12	I	2101	2TM	C2'-C3'-C4'	2.14	106.75	102.61

There are no chirality outliers.

All (7) torsion outliers are listed below:

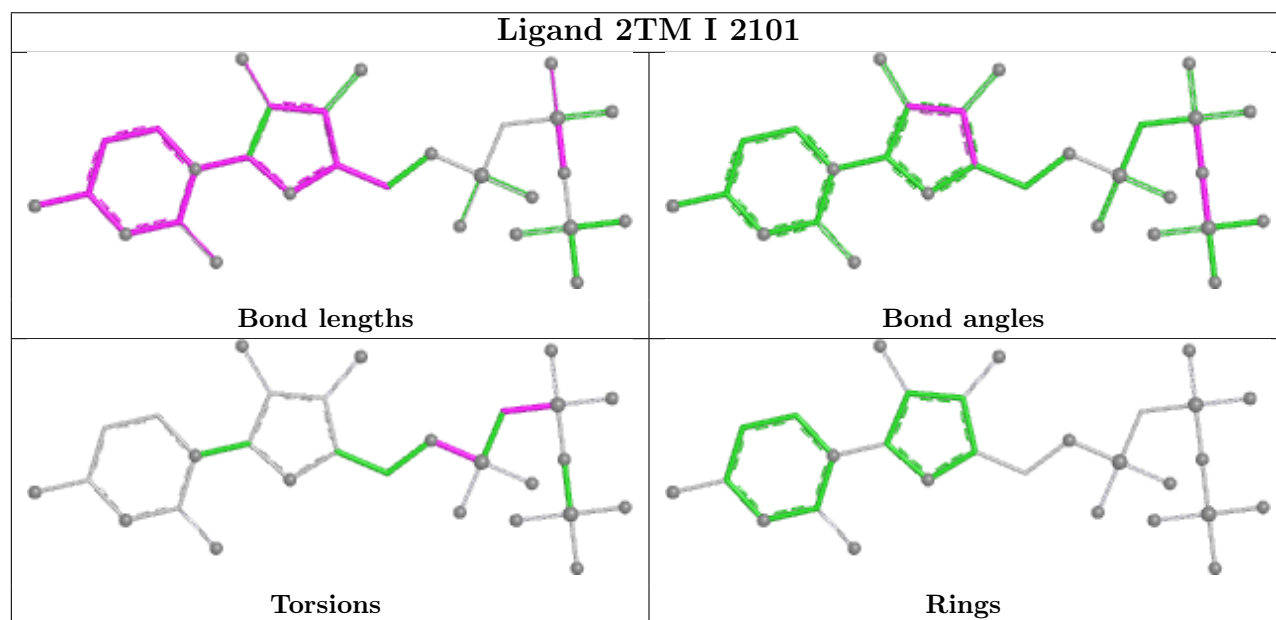
Mol	Chain	Res	Type	Atoms
12	I	2101	2TM	C5'-O5'-PA-O2A
12	I	2101	2TM	PA-C1-PB-O3B
12	I	2101	2TM	PA-C1-PB-O1B
12	I	2101	2TM	PA-C1-PB-O2B
10	B	2002	BU1	O5-C1-C2-C3
10	D	2004	BU1	O5-C1-C2-C3
12	I	2101	2TM	C5'-O5'-PA-O1A

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, 95th 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 ²)	Q<0.9
1	A	231/315 (73%)	-0.27	1 (0%) 88 85	23, 43, 65, 96	0
1	B	227/315 (72%)	-0.04	2 (0%) 81 75	27, 53, 82, 118	0
2	C	1112/1119 (99%)	-0.39	4 (0%) 88 85	12, 37, 87, 121	0
3	D	1486/1524 (97%)	-0.15	31 (2%) 63 54	8, 41, 97, 125	1 (0%)
4	E	94/99 (94%)	-0.41	0 100 100	20, 40, 71, 82	0
5	F	346/443 (78%)	0.03	5 (1%) 73 65	24, 56, 94, 114	0
6	G	25/27 (92%)	0.53	1 (4%) 42 34	57, 74, 136, 146	0
7	H	17/19 (89%)	0.03	0 100 100	31, 60, 140, 144	0
8	I	2/2 (100%)	-0.50	0 100 100	24, 24, 24, 25	2 (100%)
All	All	3540/3863 (91%)	-0.21	44 (1%) 76 69	8, 43, 94, 146	3 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	325	LYS	4.0
3	D	177	ALA	3.7
3	D	203	ALA	3.5
5	F	139	ALA	3.5
3	D	422	ALA	3.5
3	D	142	LEU	3.3
2	C	107	LEU	3.1
6	G	25	DA	3.0
3	D	161	LEU	2.9
3	D	393	ILE	2.8
2	C	311	PHE	2.8
3	D	449	SER	2.8
3	D	369	ALA	2.7
3	D	141	ILE	2.7
3	D	1128	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	1283	ILE	2.6
1	A	232	ALA	2.5
1	B	8	ALA	2.5
5	F	138	SER	2.5
5	F	145	PRO	2.4
3	D	444	VAL	2.4
3	D	186	VAL	2.4
3	D	290	PRO	2.3
2	C	362	GLY	2.3
3	D	144	GLY	2.3
3	D	435	VAL	2.3
3	D	1252	ILE	2.3
3	D	147	VAL	2.3
3	D	409	VAL	2.2
3	D	421	LEU	2.2
3	D	350	HIS	2.2
3	D	452	ILE	2.2
3	D	182	GLY	2.1
3	D	434	ARG	2.1
3	D	430	ASP	2.1
3	D	1490	LYS	2.1
3	D	417	PRO	2.1
2	C	296	GLY	2.1
3	D	454	ALA	2.1
3	D	202	VAL	2.0
3	D	412	GLY	2.0
3	D	1502	ALA	2.0
5	F	78	SER	2.0
1	B	228	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

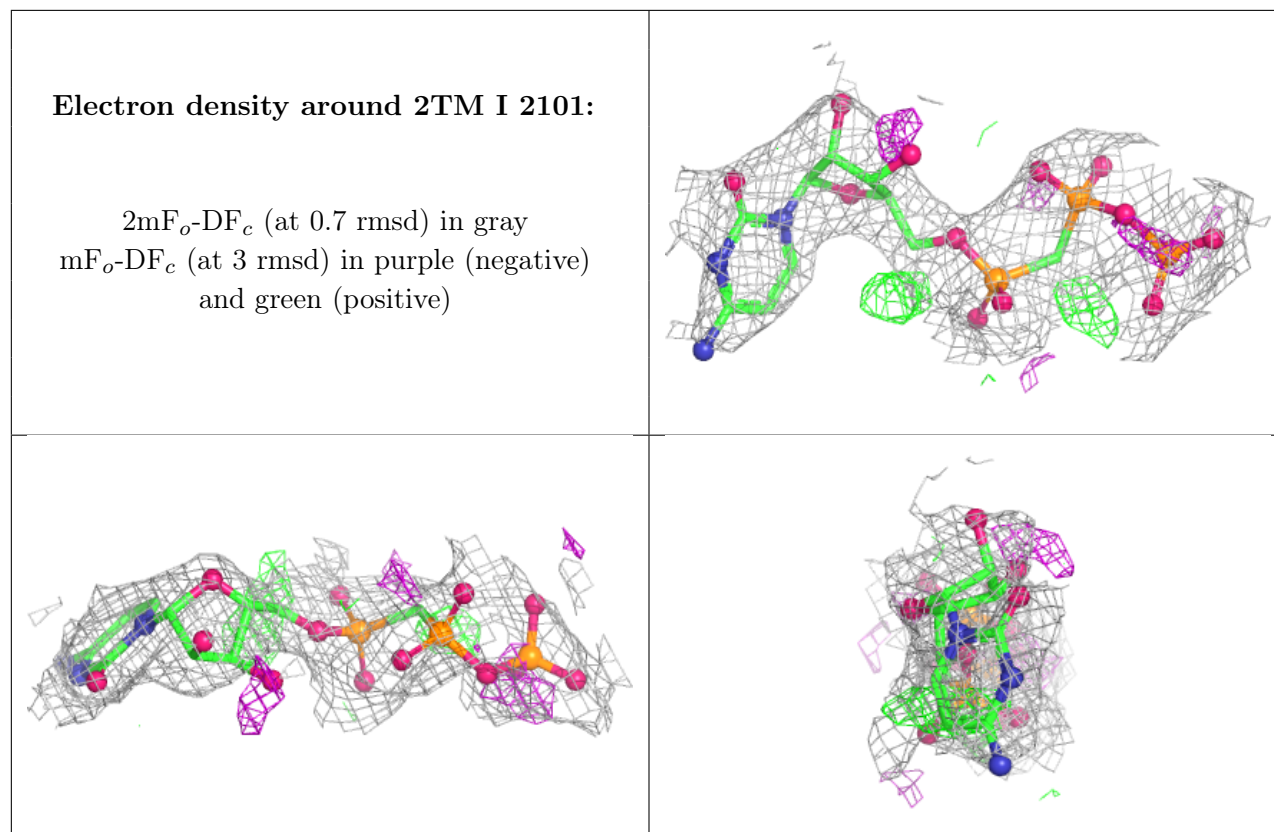
There are no oligosaccharides in this entry.

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, 95th 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($\text{\AA}^2$)	Q<0.9
10	BU1	B	2002	6/6	0.71	0.16	34,40,48,49	0
10	BU1	D	2004	6/6	0.82	0.20	27,30,37,39	0
12	2TM	I	2101	29/29	0.85	0.13	21,38,72,76	29
9	MG	B	2001	1/1	0.88	0.10	57,57,57,57	0
9	MG	C	2001	1/1	0.92	0.21	20,20,20,20	0
9	MG	B	2003	1/1	0.93	0.23	41,41,41,41	0
9	MG	F	2001	1/1	0.96	0.05	28,28,28,28	0
9	MG	D	2003	1/1	0.99	0.08	8,8,8,8	0
11	ZN	D	2002	1/1	1.00	0.02	61,61,61,61	0
11	ZN	D	2001	1/1	1.00	0.01	24,24,24,24	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.