Full wwPDB X-ray Structure Validation Report (i)

Jul 25, 2016 – 10:14 PM EDT

PDB ID	:	5D4E
Title	:	Crystal structure of Thermus thermophilus product complex for transcription initiation with 3'-dephosphate-CoA and CTP
Authors	:	Zhang, Y.; Ebright, R.H.
Deposited on	:	2015-08-07
Resolution	:	3.08 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

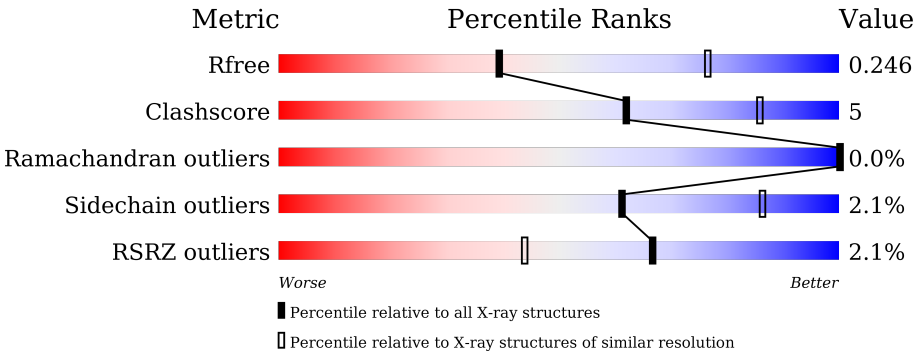
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 61% 12% • 27%
1	B	315	% 61% 10% 29%
1	K	315	2% 61% 12% 27%
1	L	315	60% 11% 29%
2	C	1119	4% 81% 18% ••
2	M	1119	% 85% 14% ••

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Mol	Chain	Length	Quality of chain
3	D	1524	2% 81% 16%
3	N	1524	2% 82% 15%
4	E	99	2% 82% 13% 5%
4	O	99	2% 82% 13% 5%
5	F	443	6% 62% 14% 22%
5	P	443	2% 67% 10% 22%
6	H	27	11% 59% 19% 22%
6	S	27	11% 41% 37% 22%
7	G	19	5% 74% 11% 16%
7	R	19	11% 63% 21% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	C	D	2005	-	-	-	X
12	COD	D	2008	-	-	-	X
8	MG	D	2004	-	-	-	X
8	MG	N	1601	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 57723 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
			1809	1155	315	337	2			
1	B	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	2			
1	K	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	L	223	Total	C	N	O	S	0	0	0
			1758	1124	305	327	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
			8774	5550	1565	1635	24			
2	M	1112	Total	C	N	O	S	0	1	0
			8783	5558	1565	1636	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	0	0
			11738	7441	2067	2195	35			
3	N	1486	Total	C	N	O	S	0	0	0
			11738	7441	2067	2195	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
			758	483	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			758	483	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
			2807	1770	509	524	4			
5	P	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q72L95
F	-18	GLY	-	expression tag	UNP Q72L95
F	-17	SER	-	expression tag	UNP Q72L95
F	-16	SER	-	expression tag	UNP Q72L95
F	-15	HIS	-	expression tag	UNP Q72L95
F	-14	HIS	-	expression tag	UNP Q72L95
F	-13	HIS	-	expression tag	UNP Q72L95
F	-12	HIS	-	expression tag	UNP Q72L95
F	-11	HIS	-	expression tag	UNP Q72L95
F	-10	HIS	-	expression tag	UNP Q72L95
F	-9	SER	-	expression tag	UNP Q72L95
F	-8	SER	-	expression tag	UNP Q72L95
F	-7	GLY	-	expression tag	UNP Q72L95
F	-6	LEU	-	expression tag	UNP Q72L95
F	-5	VAL	-	expression tag	UNP Q72L95
F	-4	PRO	-	expression tag	UNP Q72L95
F	-3	ARG	-	expression tag	UNP Q72L95
F	-2	GLY	-	expression tag	UNP Q72L95
F	-1	SER	-	expression tag	UNP Q72L95
F	0	HIS	-	expression tag	UNP Q72L95
F	46	THR	ALA	conflict	UNP Q72L95
P	-19	MET	-	initiating methionine	UNP Q72L95
P	-18	GLY	-	expression tag	UNP Q72L95
P	-17	SER	-	expression tag	UNP Q72L95
P	-16	SER	-	expression tag	UNP Q72L95
P	-15	HIS	-	expression tag	UNP Q72L95
P	-14	HIS	-	expression tag	UNP Q72L95
P	-13	HIS	-	expression tag	UNP Q72L95
P	-12	HIS	-	expression tag	UNP Q72L95
P	-11	HIS	-	expression tag	UNP Q72L95
P	-10	HIS	-	expression tag	UNP Q72L95
P	-9	SER	-	expression tag	UNP Q72L95
P	-8	SER	-	expression tag	UNP Q72L95
P	-7	GLY	-	expression tag	UNP Q72L95

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-6	LEU	-	expression tag	UNP Q72L95
P	-5	VAL	-	expression tag	UNP Q72L95
P	-4	PRO	-	expression tag	UNP Q72L95
P	-3	ARG	-	expression tag	UNP Q72L95
P	-2	GLY	-	expression tag	UNP Q72L95
P	-1	SER	-	expression tag	UNP Q72L95
P	0	HIS	-	expression tag	UNP Q72L95
P	46	THR	ALA	conflict	UNP Q72L95

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	21	Total	C	N	O	P	0	0	0
			435	207	87	121	20			
6	S	21	Total	C	N	O	P	0	0	0
			435	207	87	121	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	16	Total	C	N	O	P	0	0	0
			327	156	62	94	15			
7	R	16	Total	C	N	O	P	0	0	0
			328	157	62	94	15			

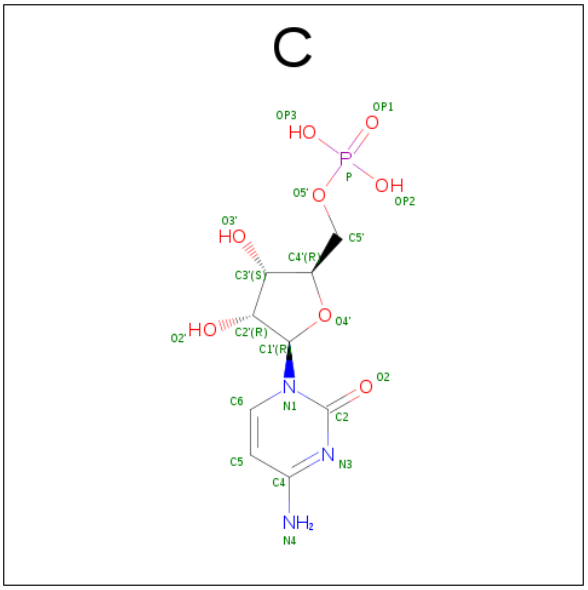
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	D	3	Total	Mg	0	0
			3	3		
8	N	3	Total	Mg	0	0
			3	3		
8	F	1	Total	Mg	0	0
			1	1		

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

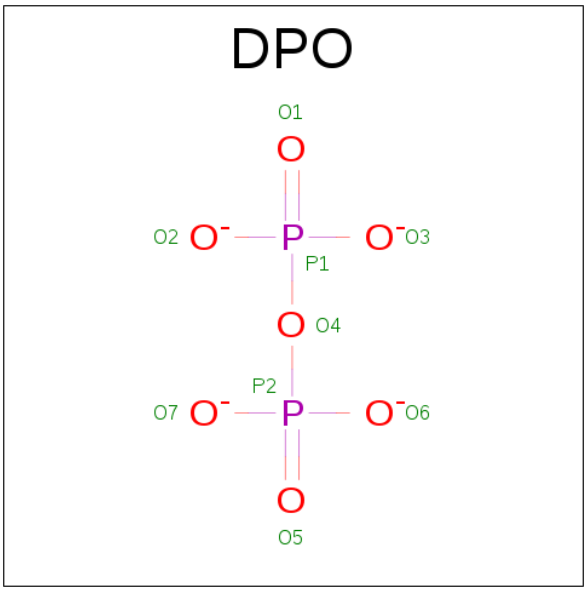
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Zn 2 2	0	0
9	N	2	Total Zn 2 2	0	0

- Molecule 10 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C) (formula: $C_9H_{14}N_3O_8P$).



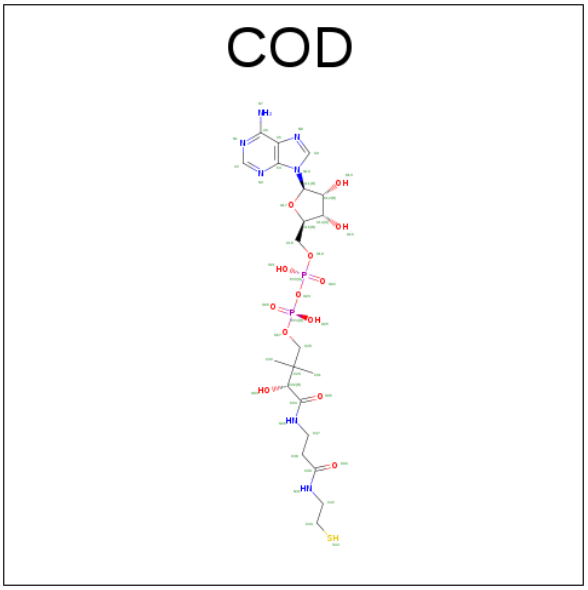
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total C N O P 20 9 3 7 1	0	0
10	N	1	Total C N O P 20 9 3 7 1	0	0

- Molecule 11 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total O P 9 7 2	0	0
11	N	1	Total O P 9 7 2	0	0

- Molecule 12 is DEPHOSPHO COENZYME A (three-letter code: COD) (formula: $C_{21}H_{35}N_7O_{13}P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	1	Total C N O P 28 11 5 10 2	0	0
12	N	1	Total C N O P 27 10 5 10 2	0	0

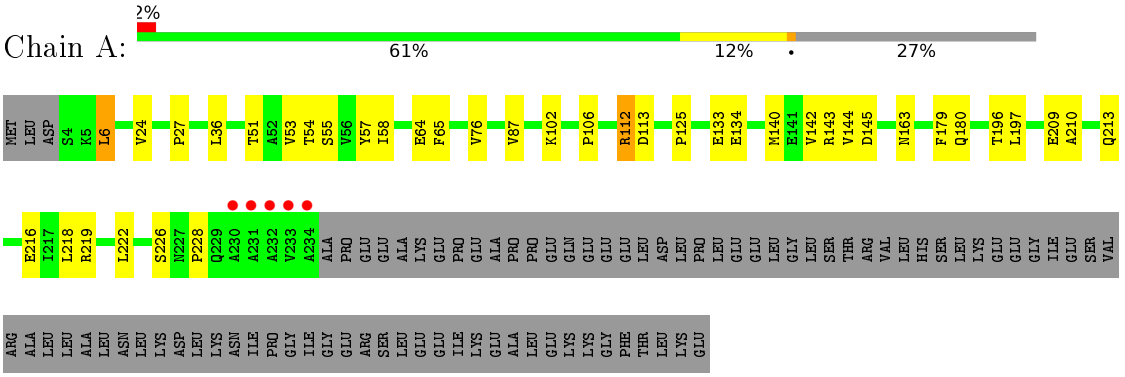
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	17	Total O 17 17	0	0
13	B	10	Total O 10 10	0	0
13	C	74	Total O 74 74	0	0
13	D	144	Total O 144 144	0	0
13	E	8	Total O 8 8	0	0
13	F	17	Total O 17 17	0	0
13	H	6	Total O 6 6	0	0
13	G	3	Total O 3 3	0	0
13	K	16	Total O 16 16	0	0
13	L	14	Total O 14 14	0	0
13	M	178	Total O 178 178	0	0
13	N	217	Total O 217 217	0	0
13	O	16	Total O 16 16	0	0
13	P	41	Total O 41 41	0	0
13	R	9	Total O 9 9	0	0
13	S	5	Total O 5 5	0	0

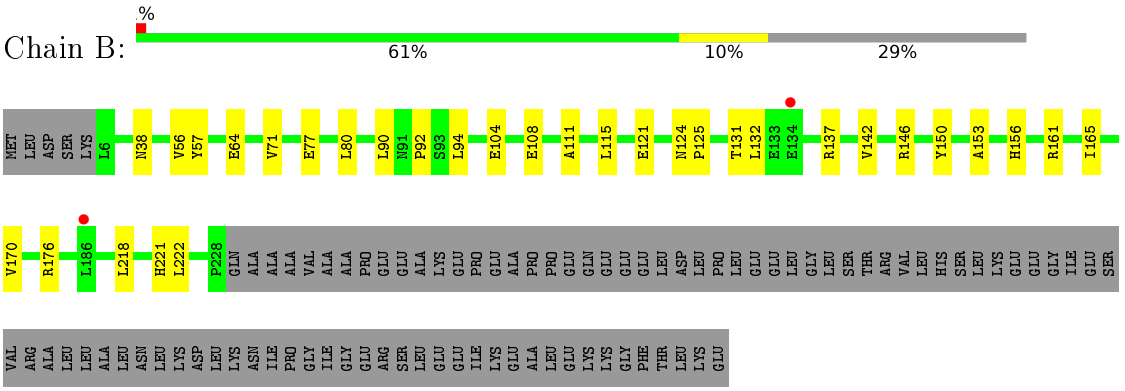
3 Residue-property plots

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

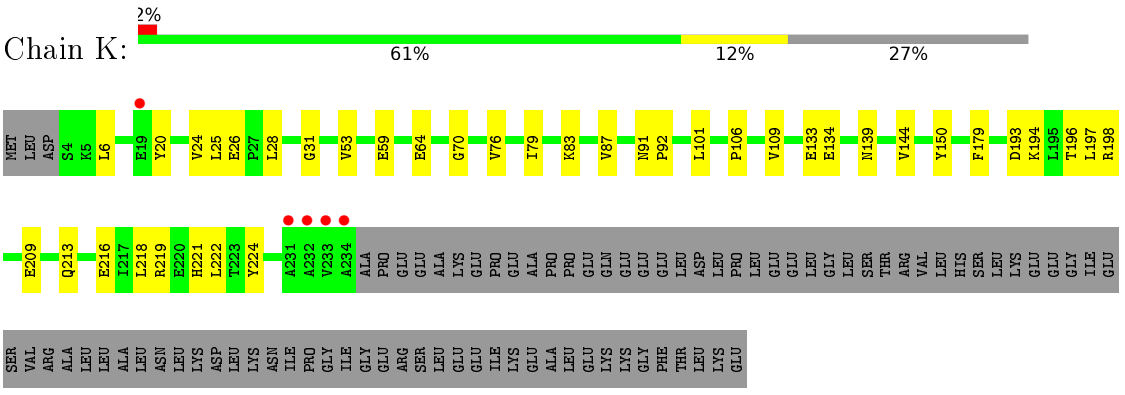
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

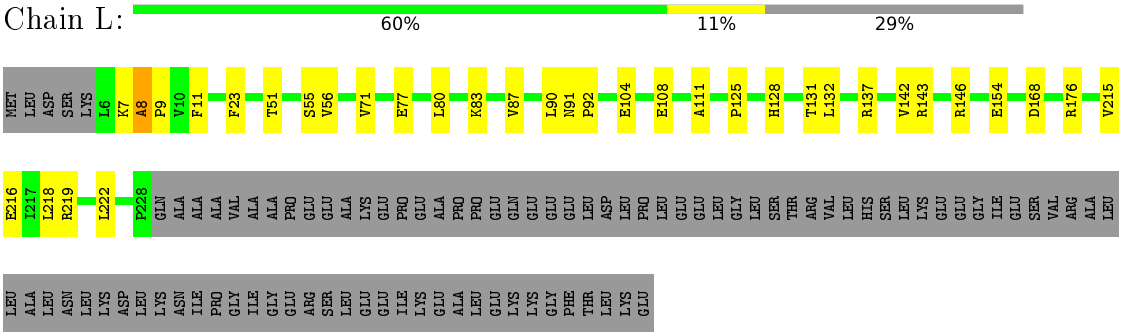


- Molecule 1: DNA-directed RNA polymerase subunit alpha



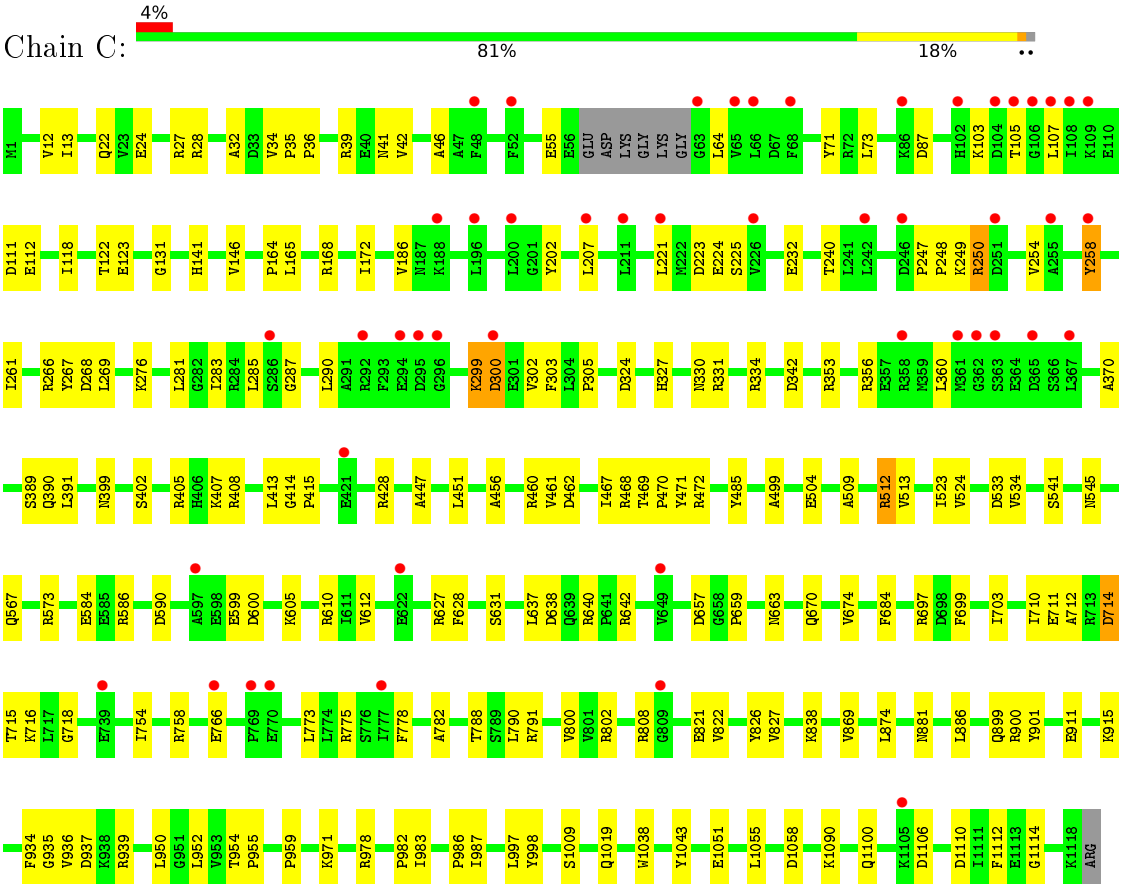
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain L:



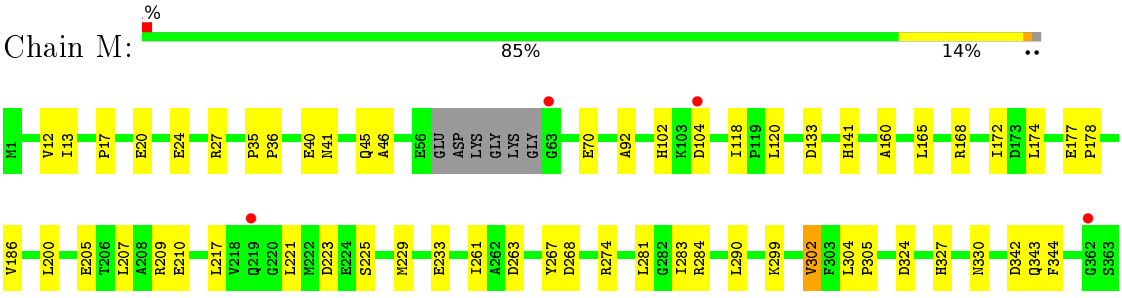
• Molecule 2: DNA-directed RNA polymerase subunit beta

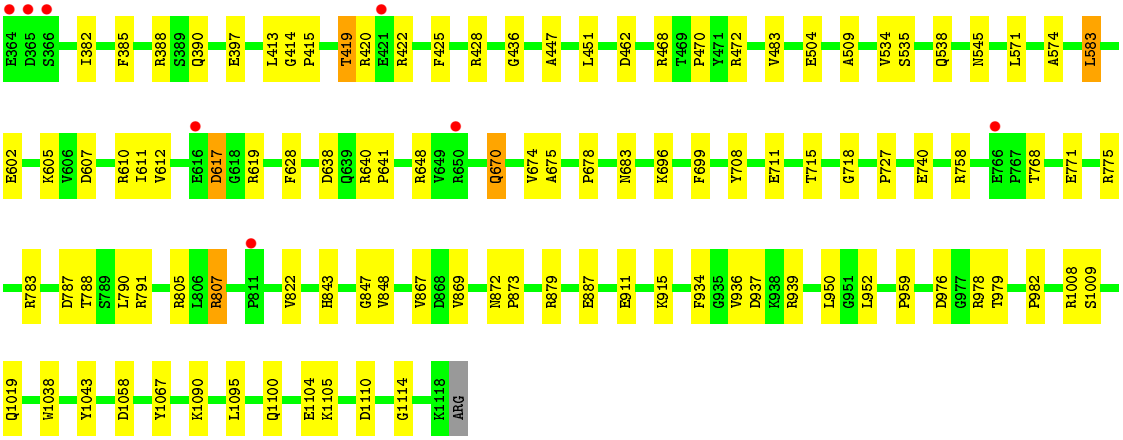
Chain C:



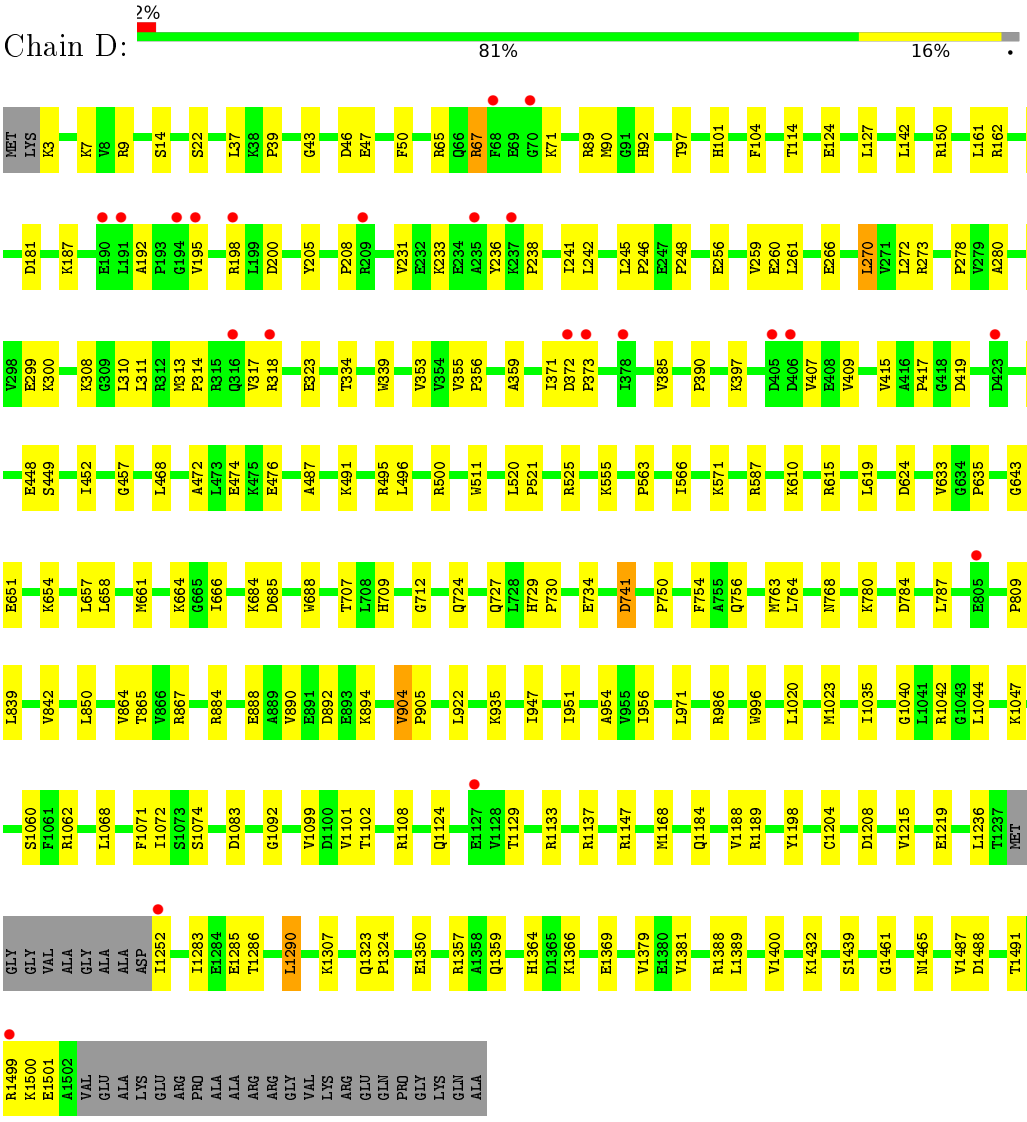
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain M:

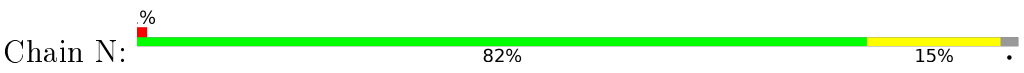


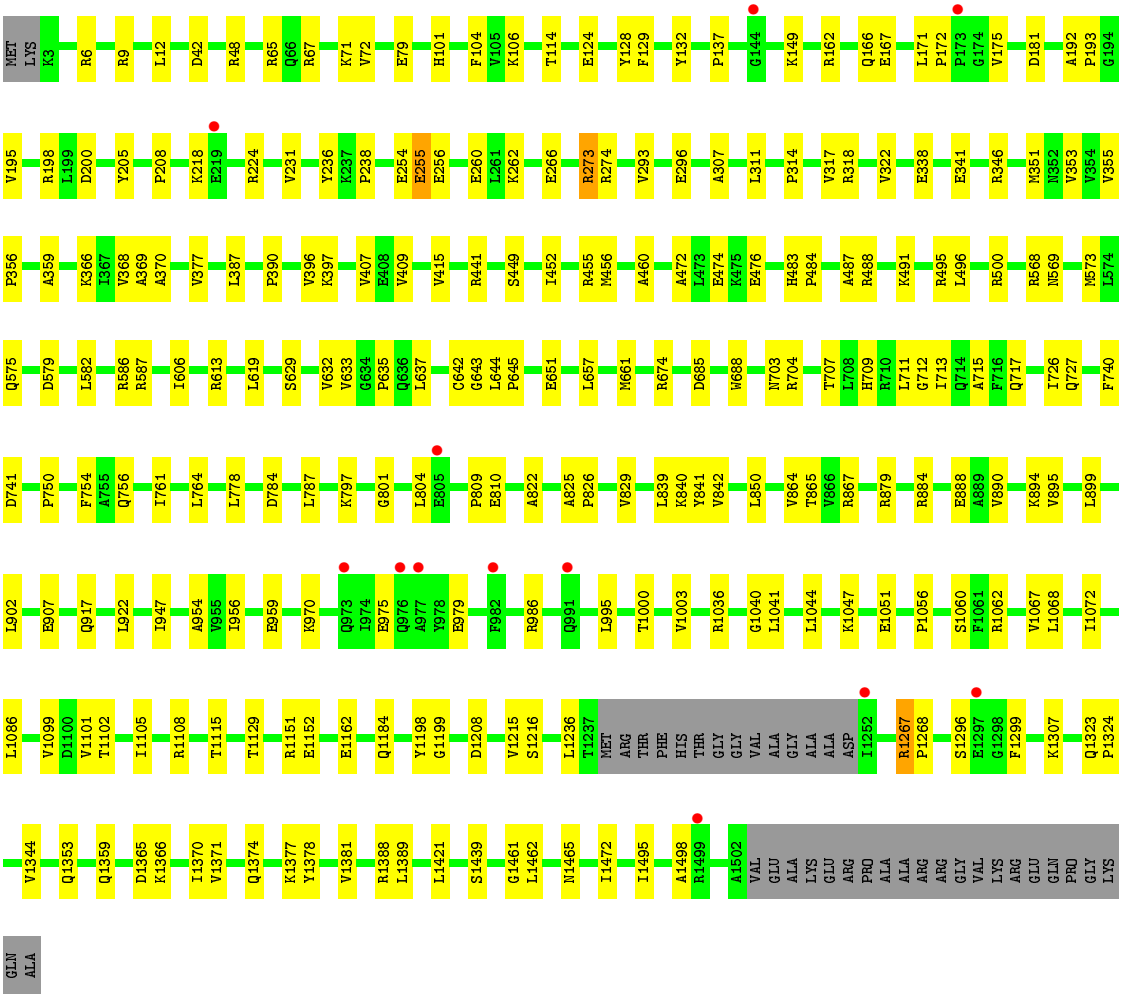


• Molecule 3: DNA-directed RNA polymerase subunit beta'

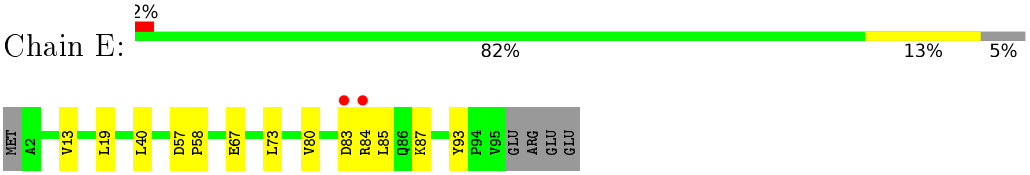


• Molecule 3: DNA-directed RNA polymerase subunit beta'

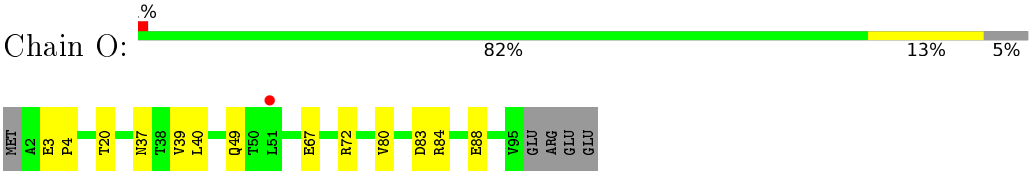




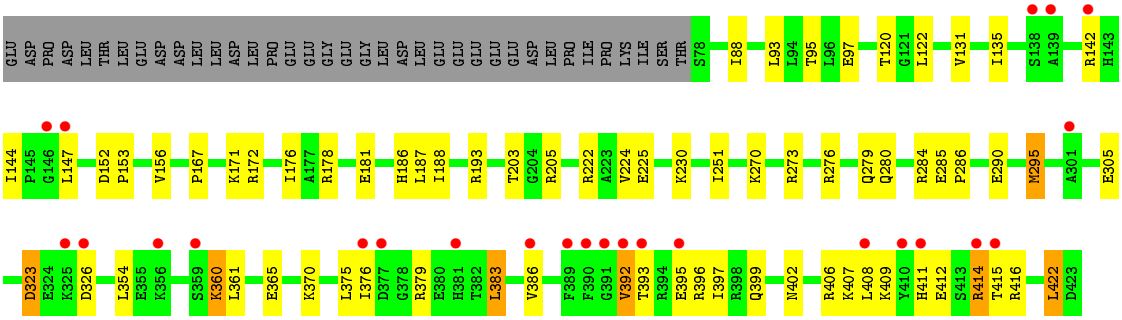
• Molecule 4: DNA-directed RNA polymerase subunit omega



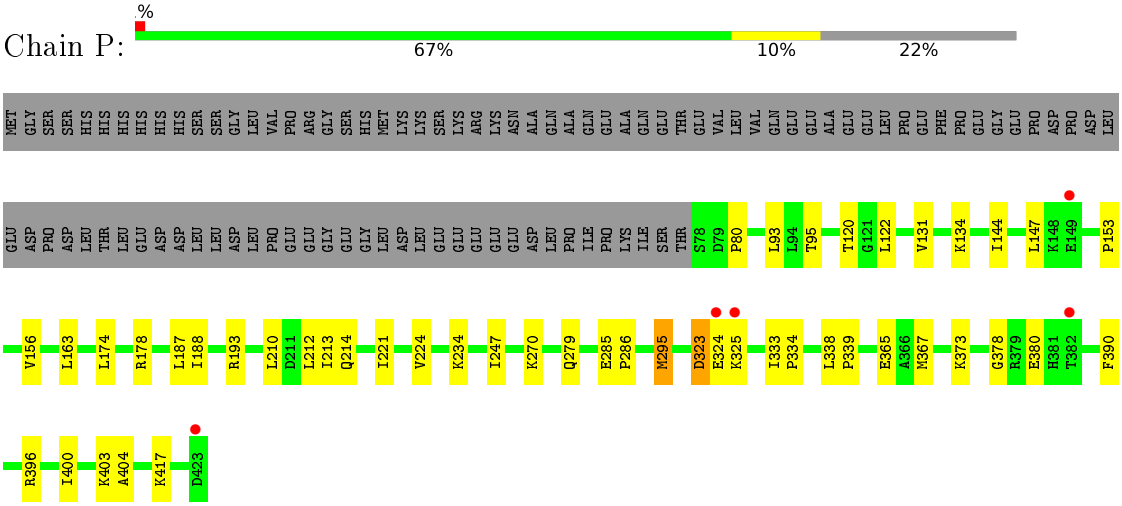
• Molecule 4: DNA-directed RNA polymerase subunit omega



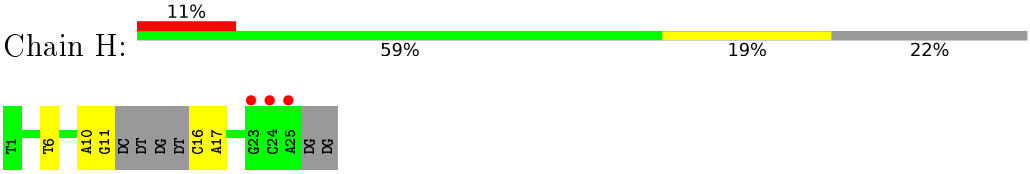
• Molecule 5: RNA polymerase sigma factor SigA



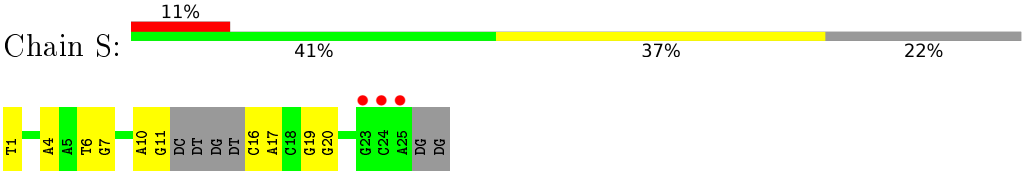
• Molecule 5: RNA polymerase sigma factor SigA



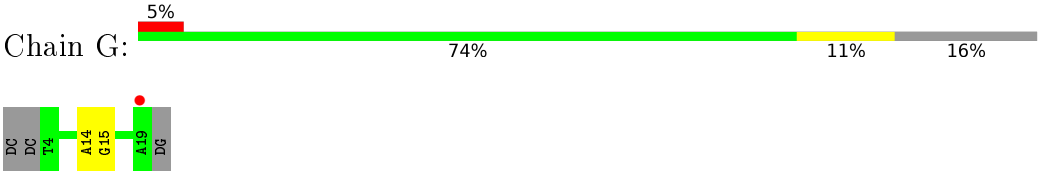
• Molecule 6: DNA (27-MER)



• Molecule 6: DNA (27-MER)

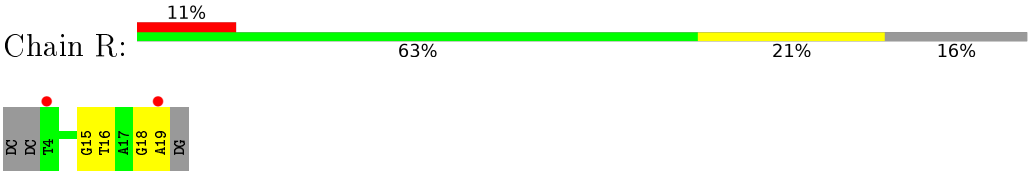


• Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*AP*GP*AP*G)-3')



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

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	185.81Å 103.95Å 297.14Å 90.00° 98.47° 90.00°	Depositor
Resolution (Å)	39.68 – 3.08 39.68 – 3.08	Depositor EDS
% Data completeness (in resolution range)	89.9 (39.68-3.08) 90.0 (39.68-3.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.210 , 0.246 0.209 , 0.246	Depositor DCC
R_{free} test set	9373 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	57723	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.93 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0674e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DPO, MG, ZN, COD

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	0.21	0/1841	0.41	0/2504
1	B	0.26	0/1790	0.45	0/2435
1	K	0.22	0/1841	0.42	0/2504
1	L	0.26	0/1790	0.46	1/2435 (0.0%)
2	C	0.22	0/8941	0.41	0/12092
2	M	0.23	0/8954	0.42	0/12110
3	D	0.21	0/11944	0.40	0/16149
3	N	0.22	0/11944	0.41	0/16149
4	E	0.21	0/772	0.37	0/1040
4	O	0.22	0/772	0.39	0/1040
5	F	0.22	0/2852	0.39	0/3837
5	P	0.21	0/2852	0.38	0/3837
6	H	0.45	0/489	0.99	0/752
6	S	0.45	0/489	1.02	1/752 (0.1%)
7	G	0.44	0/367	0.93	0/565
7	R	0.44	0/368	0.99	1/567 (0.2%)
All	All	0.23	0/58006	0.44	3/78768 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	1	DT	O4'-C1'-N1	5.44	111.81	108.00
7	R	16	DT	O4'-C4'-C3'	-5.28	102.39	104.50
1	L	91	ASN	C-N-CD	5.11	139.13	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1809	0	1863	24	0
1	B	1758	0	1808	22	0
1	K	1809	0	1863	25	0
1	L	1758	0	1808	21	0
2	C	8774	0	8877	121	0
2	M	8783	0	8886	94	0
3	D	11738	0	11971	136	0
3	N	11738	0	11971	133	0
4	E	758	0	770	6	0
4	O	758	0	770	9	0
5	F	2807	0	2882	42	0
5	P	2807	0	2882	29	0
6	H	435	0	238	4	0
6	S	435	0	238	6	0
7	G	327	0	179	2	0
7	R	328	0	182	2	0
8	B	1	0	0	0	0
8	D	3	0	0	0	0
8	F	1	0	0	0	0
8	N	3	0	0	0	0
8	P	1	0	0	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	20	0	11	0	0
10	N	20	0	11	2	0
11	D	9	0	0	0	0
11	N	9	0	0	0	0
12	D	28	0	11	0	0
12	N	27	0	11	0	0
13	A	17	0	0	0	0
13	B	10	0	0	0	0
13	C	74	0	0	2	0
13	D	144	0	0	0	0
13	E	8	0	0	0	0
13	F	17	0	0	0	0
13	G	3	0	0	0	0
13	H	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	K	16	0	0	0	0
13	L	14	0	0	0	0
13	M	178	0	0	3	0
13	N	217	0	0	2	0
13	O	16	0	0	0	0
13	P	41	0	0	0	0
13	R	9	0	0	0	0
13	S	5	0	0	0	0
All	All	57723	0	57232	614	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 5.

All (614) 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:628:PHE:H	2:C:638:ASP:HB3	1.40	0.86
2:M:168:ARG:HD3	2:M:268:ASP:HB3	1.64	0.79
2:M:165:LEU:HB2	2:M:168:ARG:HG3	1.63	0.78
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.66	0.75
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.74
2:M:628:PHE:H	2:M:638:ASP:HB3	1.51	0.74
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.69	0.73
2:M:428:ARG:NH2	2:M:447:ALA:O	2.22	0.72
3:N:351:MET:HG2	3:N:370:ALA:HB2	1.72	0.72
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.73	0.71
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.73	0.71
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.72	0.70
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.25	0.69
2:C:28:ARG:HH22	2:C:42:VAL:HG21	1.58	0.69
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.26	0.68
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.76	0.68
5:F:273:ARG:HG2	5:F:276:ARG:HH12	1.58	0.68
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.77	0.67
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.75	0.66
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.28	0.66
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.29	0.66
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.79	0.65
3:D:208:PRO:HA	3:D:390:PRO:HA	1.78	0.64
2:C:541:SER:O	2:C:545:ASN:ND2	2.27	0.64
1:K:222:LEU:HD22	1:L:215:VAL:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:PRO:HG3	1:K:134:GLU:HG2	1.78	0.64
5:F:392:VAL:HG11	5:F:396:ARG:HD3	1.79	0.64
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.30	0.64
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.80	0.64
3:N:167:GLU:OE2	3:N:198:ARG:NH1	2.30	0.64
2:M:24:GLU:OE2	2:M:27:ARG:NH2	2.31	0.64
7:R:18:DG:H2"	7:R:19:DA:H5'	1.80	0.64
2:M:1100:GLN:HG3	3:N:9:ARG:HH21	1.62	0.63
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.80	0.63
3:N:970:LYS:HD3	3:N:995:LEU:HD13	1.79	0.63
5:F:279:GLN:HB3	5:F:286:PRO:HD3	1.80	0.63
2:M:290:LEU:HD22	2:M:302:VAL:HG11	1.80	0.63
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.32	0.63
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.81	0.62
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.32	0.62
2:M:939:ARG:HG2	2:M:982:PRO:HD3	1.80	0.62
3:N:171:LEU:HD12	3:N:390:PRO:HG2	1.81	0.62
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.80	0.62
2:C:408:ARG:NH2	2:C:456:ALA:O	2.32	0.62
2:M:727:PRO:HB3	2:M:783:ARG:HD3	1.82	0.61
3:N:208:PRO:HA	3:N:390:PRO:HA	1.82	0.61
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.81	0.61
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.83	0.61
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.83	0.61
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.82	0.61
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.82	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.82	0.60
2:M:740:GLU:OE1	2:M:805:ARG:NH1	2.34	0.60
2:M:420:ARG:NH2	5:P:324:GLU:OE2	2.35	0.60
5:P:365:GLU:HB2	5:P:404:ALA:HB2	1.84	0.60
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.82	0.60
3:N:65:ARG:NH1	5:P:378:GLY:O	2.35	0.60
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.83	0.59
2:C:715:THR:OG1	2:C:718:GLY:O	2.19	0.59
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.35	0.59
2:C:586:ARG:NH2	2:C:590:ASP:OD1	2.36	0.59
5:F:193:ARG:HB2	6:H:6:DT:H1'	1.84	0.59
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.84	0.59
2:C:637:LEU:HG	2:C:659:PRO:HG3	1.83	0.59
4:O:39:VAL:O	4:O:72:ARG:NH1	2.31	0.59
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:ARG:NH1	6:H:11:DG:O6	2.35	0.59
3:N:128:TYR:OH	3:N:579:ASP:OD2	2.20	0.59
3:N:569:ASN:ND2	5:P:214:GLN:OE1	2.35	0.59
2:C:64:LEU:HD12	2:C:103:LYS:HB2	1.85	0.59
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.66	0.59
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.36	0.58
2:C:758:ARG:HH21	2:C:788:THR:HB	1.67	0.58
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.35	0.58
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.58
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.85	0.58
2:C:232:GLU:HG3	2:C:250:ARG:HE	1.69	0.58
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.85	0.58
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.86	0.58
2:M:807:ARG:NH1	13:M:1205:HOH:O	2.37	0.58
3:N:704:ARG:NH2	10:N:1605:C:O2'	2.36	0.58
5:P:270:LYS:HG2	5:P:295:MET:HE1	1.84	0.58
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.86	0.58
2:C:202:TYR:OH	2:C:300:ASP:OD1	2.20	0.58
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.85	0.58
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.85	0.58
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.85	0.57
2:M:172:ILE:HG12	2:M:186:VAL:HG22	1.85	0.57
3:N:1047:LYS:HD3	3:N:1051:GLU:HB3	1.87	0.57
2:M:17:PRO:HB2	2:M:20:GLU:HB3	1.86	0.57
3:N:787:LEU:HD21	3:N:947:ILE:HG21	1.87	0.57
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.05	0.57
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.86	0.57
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.86	0.57
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.40	0.57
2:M:324:ASP:O	2:M:330:ASN:ND2	2.29	0.57
2:C:283:ILE:HD13	2:C:305:PRO:HG2	1.86	0.56
3:D:657:LEU:HG	3:D:661:MET:HE2	1.86	0.56
2:C:12:VAL:HG13	2:C:13:ILE:HG23	1.87	0.56
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.88	0.56
1:L:11:PHE:HE1	1:L:23:PHE:HB3	1.69	0.56
1:B:92:PRO:O	1:B:146:ARG:NH2	2.39	0.56
5:P:210:LEU:HD23	5:P:213:ILE:HD12	1.87	0.56
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.89	0.55
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.88	0.55
2:M:768:THR:OG1	2:M:771:GLU:OE1	2.25	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:188:ILE:HD13	5:P:221:ILE:HG12	1.88	0.55
2:C:428:ARG:NH2	2:C:447:ALA:O	2.32	0.55
5:F:360:LYS:HG3	5:F:411:HIS:HB2	1.88	0.55
3:N:266:GLU:HG3	3:N:314:PRO:HB3	1.88	0.55
3:N:1296:SER:HB3	3:N:1299:PHE:HB2	1.88	0.55
5:P:120:THR:HG22	5:P:122:LEU:HD13	1.90	0.54
2:C:24:GLU:HG3	2:C:27:ARG:HH22	1.72	0.54
2:C:399:ASN:O	2:C:402:SER:OG	2.22	0.54
2:M:207:LEU:HD13	2:M:221:LEU:HD21	1.89	0.54
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.88	0.54
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.38	0.54
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.89	0.54
2:M:168:ARG:HA	2:M:168:ARG:HE	1.73	0.54
3:D:1495:ILE:HG21	4:E:80:VAL:HG12	1.90	0.54
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.89	0.54
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.89	0.54
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.90	0.54
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.90	0.54
3:D:658:LEU:HA	3:D:661:MET:HE3	1.88	0.54
1:L:80:LEU:HD21	3:N:842:VAL:HG12	1.90	0.54
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.40	0.54
3:N:1152:GLU:HG2	3:N:1162:GLU:H	1.72	0.54
3:N:172:PRO:HG2	3:N:175:VAL:HB	1.90	0.53
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.89	0.53
2:C:714:ASP:OD2	2:C:808:ARG:NH1	2.41	0.53
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.89	0.53
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.89	0.53
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.72	0.53
2:C:39:ARG:NH1	2:C:71:TYR:O	2.29	0.53
3:D:231:VAL:O	3:D:236:TYR:OH	2.26	0.53
2:C:55:GLU:O	2:C:356:ARG:NH2	2.41	0.53
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.90	0.53
3:D:1047:LYS:HD3	3:D:1051:GLU:HG3	1.90	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.89	0.53
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.91	0.53
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.91	0.53
2:M:283:ILE:HD13	2:M:305:PRO:HG2	1.91	0.53
2:M:758:ARG:HH21	2:M:788:THR:HB	1.72	0.53
3:N:353:VAL:HG11	3:N:387:LEU:HD11	1.90	0.53
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.90	0.53
2:C:754:ILE:HG12	2:C:791:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:238:PRO:HD3	3:N:318:ARG:HG2	1.89	0.53
2:C:900:ARG:NH1	13:C:1206:HOH:O	2.42	0.53
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.90	0.53
3:N:644:LEU:HD12	3:N:645:PRO:HD2	1.89	0.53
3:D:520:LEU:O	3:D:525:ARG:NE	2.39	0.53
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.33	0.53
2:C:370:ALA:O	5:F:280:GLN:NE2	2.38	0.53
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.91	0.53
1:K:59:GLU:OE1	1:K:139:ASN:ND2	2.37	0.53
3:N:1044:LEU:HD23	3:N:1056:PRO:HB3	1.90	0.53
2:M:937:ASP:OD1	2:M:939:ARG:HD3	2.09	0.52
3:N:132:TYR:OH	3:N:568:ARG:NH1	2.43	0.52
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.91	0.52
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.90	0.52
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.90	0.52
2:M:715:THR:OG1	2:M:718:GLY:O	2.23	0.52
3:N:1003:VAL:HG21	3:N:1041:LEU:HG	1.91	0.52
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.44	0.52
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.91	0.52
3:N:351:MET:HG2	3:N:370:ALA:CB	2.39	0.52
2:C:254:VAL:O	2:C:258:TYR:HB3	2.10	0.52
2:M:13:ILE:HD13	2:M:483:VAL:HG11	1.91	0.52
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.90	0.52
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.91	0.52
3:N:356:PRO:HB3	3:N:441:ARG:HA	1.92	0.52
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.92	0.52
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.92	0.51
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.91	0.51
5:F:361:LEU:HD13	5:F:407:LYS:HD2	1.92	0.51
1:L:108:GLU:HG2	1:L:131:THR:HG22	1.92	0.51
2:M:571:LEU:HB2	2:M:574:ALA:HB2	1.92	0.51
3:N:1374:GLN:NE2	13:N:2104:HOH:O	2.42	0.51
2:C:657:ASP:OD2	2:C:663:ASN:N	2.44	0.51
3:N:956:ILE:HD11	3:N:1062:ARG:HG2	1.90	0.51
3:N:575:GLN:NE2	3:N:579:ASP:OD1	2.43	0.51
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.92	0.51
5:F:370:LYS:HG2	5:F:375:LEU:HD22	1.93	0.51
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.91	0.51
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.40	0.51
3:D:256:GLU:HG2	3:D:299:GLU:HA	1.92	0.51
3:D:647:ARG:HH21	3:D:724:GLN:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:ASN:O	2:M:46:ALA:HB2	2.11	0.51
3:N:633:VAL:HB	3:N:740:PHE:CE2	2.45	0.51
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.44	0.51
2:C:460:ARG:HD3	2:C:485:TYR:CE2	2.46	0.51
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.93	0.51
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.93	0.51
7:G:14:DA:H2'	7:G:15:DG:C8	2.45	0.51
3:N:1236:LEU:HA	3:N:1359:GLN:HG3	1.93	0.51
3:N:895:VAL:HG11	3:N:922:LEU:HD21	1.93	0.51
2:C:800:VAL:HG22	2:C:827:VAL:HG22	1.92	0.51
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.93	0.51
2:M:1008:ARG:NH2	13:M:1203:HOH:O	2.33	0.51
3:N:455:ARG:HB2	3:N:460:ALA:HB2	1.92	0.51
2:C:168:ARG:O	2:C:267:TYR:HA	2.11	0.50
2:M:1038:TRP:CE2	3:N:1099:VAL:HG11	2.46	0.50
2:M:847:GLY:HA2	3:N:741:ASP:HA	1.93	0.50
5:F:152:ASP:OD1	5:F:152:ASP:N	2.43	0.50
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.92	0.50
2:M:787:ASP:OD2	2:M:791:ARG:NH2	2.40	0.50
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.12	0.50
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.93	0.50
5:P:188:ILE:HG12	5:P:224:VAL:HG21	1.94	0.50
3:N:809:PRO:HB3	3:N:839:LEU:HD13	1.93	0.50
5:F:135:ILE:HG13	5:F:181:GLU:HB2	1.93	0.50
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.47	0.50
3:N:314:PRO:HB2	3:N:317:VAL:HG12	1.94	0.50
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.94	0.50
3:D:407:VAL:HG22	3:D:409:VAL:H	1.77	0.49
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.45	0.49
2:M:670:GLN:HG2	2:M:699:PHE:CD2	2.47	0.49
3:N:899:LEU:HD22	3:N:917:GLN:HB3	1.93	0.49
2:C:122:THR:HG22	2:C:123:GLU:H	1.76	0.49
1:K:196:THR:HG21	2:M:934:PHE:HE1	1.77	0.49
3:N:637:LEU:HD13	3:N:642:CYS:HA	1.94	0.49
2:C:111:ASP:OD1	2:C:112:GLU:N	2.45	0.49
2:C:223:ASP:OD1	2:C:225:SER:OG	2.25	0.49
2:C:513:VAL:HG13	2:C:524:VAL:HG23	1.94	0.49
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.95	0.49
3:N:890:VAL:HB	3:N:922:LEU:HD13	1.93	0.49
2:M:1067:TYR:OH	3:N:674:ARG:NH1	2.42	0.49
2:M:168:ARG:O	2:M:267:TYR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:LEU:HD21	2:C:302:VAL:HG22	1.95	0.49
3:N:500:ARG:NH1	3:N:1388:ARG:O	2.44	0.49
3:D:241:ILE:HG12	3:D:310:LEU:HD21	1.95	0.49
2:M:843:HIS:NE2	2:M:887:GLU:OE2	2.41	0.49
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.95	0.49
2:C:331:ARG:NH1	13:C:1205:HOH:O	2.37	0.49
1:A:65:PHE:HE1	2:C:703:ILE:HD12	1.78	0.49
3:D:664:LYS:HB2	3:D:666:ILE:HD12	1.94	0.49
3:N:975:GLU:O	3:N:979:GLU:HG2	2.12	0.49
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.95	0.48
2:M:1009:SER:HB3	3:N:651:GLU:O	2.12	0.48
2:C:299:LYS:HE3	2:C:300:ASP:H	1.77	0.48
2:M:390:GLN:HB3	2:M:415:PRO:HD3	1.96	0.48
2:C:886:LEU:HD21	3:D:951:ILE:HG12	1.95	0.48
3:D:261:LEU:HD13	3:D:270:LEU:HD12	1.95	0.48
2:M:229:MET:HB2	2:M:233:GLU:HB2	1.96	0.48
2:M:674:VAL:HG12	2:M:869:VAL:HB	1.96	0.48
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.95	0.48
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.94	0.48
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.96	0.48
2:M:223:ASP:OD1	2:M:225:SER:OG	2.26	0.48
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.13	0.48
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.96	0.48
3:N:106:LYS:O	3:N:586:ARG:NH1	2.46	0.48
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.14	0.48
10:N:1605:C:O2	7:R:15:DG:N2	2.37	0.48
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.95	0.48
2:M:911:GLU:O	2:M:915:LYS:HG2	2.14	0.48
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.96	0.48
1:K:25:LEU:HD23	1:K:28:LEU:HD11	1.96	0.48
1:L:92:PRO:O	1:L:146:ARG:NH2	2.46	0.48
3:N:162:ARG:O	3:N:449:SER:HB2	2.14	0.48
2:C:41:ASN:O	2:C:46:ALA:HB2	2.14	0.48
3:D:50:PHE:O	3:D:89:ARG:HD2	2.14	0.48
1:B:38:ASN:ND2	2:C:978:ARG:O	2.46	0.48
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.96	0.48
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.96	0.47
2:M:281:LEU:HD13	2:M:305:PRO:HB2	1.96	0.47
3:N:307:ALA:HB1	3:N:311:LEU:HD11	1.96	0.47
5:F:370:LYS:HB3	5:F:375:LEU:HB2	1.96	0.47
2:C:324:ASP:O	2:C:330:ASN:ND2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:383:LEU:H	5:F:383:LEU:HD22	1.79	0.47
2:M:711:GLU:O	2:M:758:ARG:NH1	2.46	0.47
3:N:1353:GLN:NE2	3:N:1365:ASP:OD1	2.46	0.47
5:P:93:LEU:HD21	5:P:193:ARG:HD2	1.95	0.47
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.96	0.47
2:C:599:GLU:HG3	2:C:600:ASP:H	1.79	0.47
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.95	0.47
1:L:8:ALA:HB1	1:L:9:PRO:HA	1.97	0.47
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.96	0.47
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.48	0.47
3:N:368:VAL:HB	3:N:377:VAL:HB	1.96	0.47
5:P:212:LEU:HD22	5:P:247:ILE:HG23	1.95	0.47
2:C:261:ILE:HD11	2:C:303:PHE:CZ	2.48	0.47
2:C:773:LEU:HD23	5:F:354:LEU:HD13	1.96	0.47
2:M:1104:GLU:HG2	3:N:6:ARG:HG3	1.97	0.47
3:N:954:ALA:O	3:N:1062:ARG:NH2	2.47	0.47
3:N:1105:ILE:HG23	3:N:1199:GLY:HA2	1.96	0.47
5:P:144:ILE:HB	5:P:147:LEU:HD13	1.96	0.47
2:C:470:PRO:HG3	2:C:485:TYR:CE2	2.50	0.47
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.43	0.47
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.96	0.47
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.79	0.47
3:N:166:GLN:HB3	3:N:396:VAL:HG13	1.97	0.47
3:D:1285:GLU:HG3	3:D:1290:LEU:HG	1.97	0.47
1:K:218:LEU:HD23	1:L:222:LEU:HD21	1.96	0.47
1:A:210:ALA:HA	1:A:213:GLN:HE21	1.80	0.46
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.97	0.46
1:L:128:HIS:CE1	1:L:131:THR:HG23	2.51	0.46
3:N:797:LYS:HE3	3:N:826:PRO:HG3	1.98	0.46
3:D:162:ARG:O	3:D:449:SER:HB2	2.15	0.46
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.97	0.46
3:D:1168:MET:HA	3:D:1168:MET:HE3	1.98	0.46
5:F:386:VAL:HG13	5:F:397:ILE:HG21	1.98	0.46
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.30	0.46
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.81	0.46
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.97	0.46
5:F:414:ARG:HG2	5:F:415:THR:HG23	1.98	0.46
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.50	0.46
5:F:412:GLU:O	5:F:416:ARG:N	2.43	0.46
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.98	0.46
1:K:209:GLU:O	1:K:213:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:SER:HB3	1:L:143:ARG:HB3	1.96	0.46
3:N:822:ALA:HB3	3:N:825:ALA:HB2	1.98	0.46
2:C:105:THR:HG22	2:C:107:LEU:H	1.81	0.46
1:K:26:GLU:HB3	1:K:194:LYS:HG3	1.97	0.46
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.98	0.46
3:N:606:ILE:O	3:N:613:ARG:N	2.49	0.46
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.98	0.46
5:F:392:VAL:HG12	5:F:393:THR:H	1.81	0.46
2:M:419:THR:HG23	2:M:422:ARG:HG3	1.98	0.45
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	1.98	0.45
3:N:707:THR:HG23	3:N:712:GLY:HA3	1.99	0.45
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.98	0.45
1:K:70:GLY:N	2:M:607:ASP:OD1	2.50	0.45
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.31	0.45
5:P:373:LYS:HD3	5:P:373:LYS:HA	1.85	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
3:D:633:VAL:C	3:D:635:PRO:HD3	2.37	0.45
5:F:93:LEU:HD21	5:F:193:ARG:HD2	1.97	0.45
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.99	0.45
3:D:834:THR:OG1	3:D:835:SER:N	2.49	0.45
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.40	0.45
1:B:77:GLU:OE1	3:D:867:ARG:NH2	2.44	0.45
3:D:1364:HIS:ND1	3:D:1366:LYS:HG2	2.32	0.45
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.99	0.45
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.50	0.45
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.82	0.45
1:K:133:GLU:HG2	1:K:134:GLU:H	1.81	0.45
3:N:1216:SER:N	13:N:2117:HOH:O	2.50	0.45
5:P:80:PRO:HB2	5:P:210:LEU:HD11	1.99	0.45
3:D:248:PRO:HG3	3:D:308:LYS:HE3	1.98	0.45
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.98	0.45
1:L:90:LEU:HD13	1:L:90:LEU:HA	1.75	0.45
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.99	0.45
2:M:390:GLN:HG2	2:M:414:GLY:HA2	1.98	0.45
2:M:425:PHE:CE1	3:N:1086:LEU:HD12	2.52	0.45
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.99	0.45
5:P:187:LEU:HD23	5:P:224:VAL:HG13	1.97	0.45
3:D:890:VAL:HG23	3:D:892:ASP:H	1.81	0.45
3:N:633:VAL:O	3:N:635:PRO:HD3	2.17	0.45
5:P:193:ARG:HB2	6:S:6:DT:H1'	1.98	0.45
3:D:285:PRO:HD2	3:D:288:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:205:ARG:HG3	5:F:251:ILE:HD13	1.99	0.45
2:M:708:TYR:HB3	2:M:790:LEU:HD21	1.99	0.45
2:M:950:LEU:HB3	2:M:952:LEU:HD13	1.99	0.44
3:N:685:ASP:HA	3:N:688:TRP:CD1	2.52	0.44
5:P:153:PRO:HA	5:P:156:VAL:HG22	1.98	0.44
2:C:469:THR:HA	2:C:470:PRO:HD3	1.88	0.44
2:C:1009:SER:HB3	3:D:651:GLU:O	2.17	0.44
3:D:67:ARG:CZ	5:F:379:ARG:HD2	2.47	0.44
1:K:53:VAL:HG22	1:K:144:VAL:HG22	1.99	0.44
2:M:678:PRO:HA	2:M:683:ASN:HD21	1.82	0.44
3:N:657:LEU:HG	3:N:661:MET:HE2	2.00	0.44
3:N:629:SER:HB3	3:N:726:ILE:HG13	1.99	0.44
5:P:193:ARG:HB3	6:S:7:DG:H5"	1.98	0.44
3:D:1500:LYS:HB3	3:D:1500:LYS:HE2	1.79	0.44
6:H:10:DA:H2"	6:H:11:DG:C8	2.53	0.44
3:N:407:VAL:HG22	3:N:409:VAL:H	1.81	0.44
3:N:42:ASP:OD1	3:N:48:ARG:NH1	2.50	0.44
2:C:353:ARG:NH2	5:F:203:THR:OG1	2.50	0.44
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.98	0.44
1:L:77:GLU:OE1	3:N:867:ARG:NH2	2.41	0.44
2:M:535:SER:O	2:M:538:GLN:HG2	2.17	0.44
5:P:234:LYS:HG3	6:S:4:DA:H3'	1.99	0.44
3:D:397:LYS:HB3	3:D:397:LYS:HE2	1.86	0.44
2:M:177:GLU:HG3	2:M:178:PRO:HD2	2.00	0.44
2:M:40:GLU:O	2:M:45:GLN:HG2	2.17	0.44
2:M:607:ASP:HB2	2:M:610:ARG:HH11	1.82	0.44
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.52	0.44
3:D:864:VAL:HG22	3:D:865:THR:H	1.83	0.44
1:A:53:VAL:HG22	1:A:144:VAL:HG22	2.00	0.44
2:C:22:GLN:HG3	2:C:407:LYS:HB3	2.00	0.44
3:D:171:LEU:HD12	3:D:390:PRO:HG2	2.00	0.44
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.99	0.44
1:L:111:ALA:HB3	1:L:125:PRO:HA	1.98	0.44
2:M:610:ARG:HG2	2:M:611:ILE:N	2.33	0.44
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.32	0.43
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.00	0.43
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.00	0.43
3:D:555:LYS:HA	5:F:142:ARG:HH12	1.83	0.43
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.53	0.43
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.99	0.43
3:N:1377:LYS:HE3	3:N:1378:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1071:PHE:O	3:D:1074:SER:OG	2.35	0.43
3:D:1283:ILE:HG13	3:D:1283:ILE:H	1.70	0.43
6:H:16:DC:H2"	6:H:17:DA:H5'	1.99	0.43
1:K:91:ASN:HA	1:K:92:PRO:HD3	1.85	0.43
3:N:101:HIS:HB3	3:N:104:PHE:HD2	1.82	0.43
5:P:163:LEU:HD13	5:P:174:LEU:HD13	2.00	0.43
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.01	0.43
3:D:39:PRO:HG2	3:D:47:GLU:HG3	2.00	0.43
2:C:766:GLU:HG2	3:D:65:ARG:HE	1.83	0.43
3:N:569:ASN:O	3:N:573:MET:HG3	2.19	0.43
3:N:619:LEU:HD11	3:N:1439:SER:HB2	2.00	0.43
5:P:279:GLN:HB3	5:P:286:PRO:HD3	1.99	0.43
1:L:71:VAL:HG22	1:L:132:LEU:HG	2.00	0.43
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.99	0.43
3:N:864:VAL:HG22	3:N:865:THR:H	1.82	0.43
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.89	0.43
1:A:112:ARG:HG3	1:A:125:PRO:HB2	2.01	0.43
3:D:200:ASP:O	3:D:397:LYS:HG2	2.17	0.43
3:D:610:LYS:HA	3:D:615:ARG:HD3	2.00	0.43
2:C:389:SER:OG	2:C:390:GLN:N	2.52	0.43
2:C:1051:GLU:HG3	2:C:1055:LEU:HD12	2.01	0.43
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.99	0.43
3:D:142:LEU:HB2	3:D:161:LEU:HD11	2.00	0.43
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.01	0.43
5:F:144:ILE:HB	5:F:147:LEU:HD13	2.00	0.43
5:F:270:LYS:HG2	5:F:295:MET:HE1	2.01	0.43
5:F:414:ARG:HG2	5:F:415:THR:N	2.34	0.43
3:N:114:THR:HG23	3:N:495:ARG:HG2	2.01	0.43
3:N:472:ALA:O	3:N:476:GLU:HG2	2.18	0.43
2:C:12:VAL:HG11	2:C:472:ARG:HD3	2.01	0.43
2:C:584:GLU:N	2:C:584:GLU:OE2	2.52	0.43
4:E:83:ASP:O	4:E:87:LYS:HG2	2.19	0.43
5:F:323:ASP:N	5:F:323:ASP:OD1	2.52	0.43
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.00	0.43
2:M:210:GLU:HG2	2:M:304:LEU:HD21	2.00	0.43
3:N:483:HIS:CG	3:N:484:PRO:HD2	2.53	0.43
5:P:323:ASP:N	5:P:323:ASP:OD1	2.31	0.43
1:A:133:GLU:HG2	1:A:134:GLU:H	1.84	0.42
1:A:209:GLU:O	1:A:213:GLN:HG2	2.19	0.42
1:B:124:ASN:N	1:B:124:ASN:OD1	2.52	0.42
1:B:150:TYR:CE2	1:B:170:VAL:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:187:LYS:N	3:D:200:ASP:OD2	2.43	0.42
3:D:236:TYR:HB3	3:D:313:MET:HG3	2.01	0.42
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.93	0.42
3:D:741:ASP:N	3:D:741:ASP:OD1	2.48	0.42
3:D:935:LYS:HB3	3:D:935:LYS:HE2	1.88	0.42
1:K:87:VAL:HG21	1:K:144:VAL:HG21	2.00	0.42
2:M:848:VAL:HG22	3:N:740:PHE:O	2.19	0.42
1:A:226:SER:O	1:A:228:PRO:HD3	2.19	0.42
2:C:146:VAL:HG21	2:C:281:LEU:HD11	2.01	0.42
2:C:249:LYS:HE2	2:C:249:LYS:HB3	1.85	0.42
2:C:911:GLU:O	2:C:915:LYS:HG2	2.19	0.42
2:M:35:PRO:HA	2:M:36:PRO:HD3	1.89	0.42
3:N:137:PRO:HD3	3:N:149:LYS:HG3	2.01	0.42
3:N:715:ALA:HB3	3:N:764:LEU:HA	2.00	0.42
5:P:285:GLU:HA	5:P:286:PRO:HD3	1.81	0.42
1:B:94:LEU:O	1:B:146:ARG:NH2	2.49	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.75	0.42
3:D:1124:GLN:OE1	3:D:1133:ARG:NH1	2.52	0.42
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.00	0.42
1:L:104:GLU:OE2	1:L:137:ARG:NH1	2.53	0.42
2:M:12:VAL:HG21	2:M:472:ARG:HD3	2.01	0.42
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.19	0.42
3:N:1462:LEU:HD22	3:N:1472:ILE:HB	2.01	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.86	0.42
2:C:1106:ASP:OD1	3:D:7:LYS:NZ	2.44	0.42
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.41	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.54	0.42
3:D:259:VAL:HG22	3:D:272:LEU:HD11	2.01	0.42
3:D:764:LEU:O	3:D:768:ASN:ND2	2.53	0.42
2:M:879:ARG:NH1	13:M:1216:HOH:O	2.52	0.42
3:N:1344:VAL:HG11	3:N:1421:LEU:HD22	2.01	0.42
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.35	0.42
5:F:222:ARG:NH2	5:F:225:GLU:OE1	2.52	0.42
2:M:602:GLU:HB2	2:M:648:ARG:HH21	1.84	0.42
3:N:1000:THR:HG23	3:N:1036:ARG:HD2	2.01	0.42
6:S:10:DA:H2"	6:S:11:DG:C8	2.55	0.42
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.90	0.42
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.53	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.87	0.42
3:D:472:ALA:O	3:D:476:GLU:HG2	2.20	0.42
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:353:VAL:HG12	3:D:355:VAL:H	1.85	0.42
3:D:684:LYS:HB3	3:D:684:LYS:HE2	1.86	0.42
2:M:299:LYS:HB2	2:M:299:LYS:HE3	1.84	0.42
3:N:129:PHE:CD2	3:N:456:MET:HB3	2.54	0.42
3:N:72:VAL:HA	3:N:79:GLU:HA	2.02	0.42
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.82	0.42
6:S:19:DG:H2'	6:S:20:DG:C8	2.55	0.42
2:C:631:SER:HB3	2:C:637:LEU:HD13	2.02	0.42
2:M:118:ILE:HD11	2:M:344:PHE:CE1	2.55	0.42
2:M:611:ILE:HD11	2:M:641:PRO:HB3	2.02	0.42
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.19	0.42
3:N:1115:THR:O	3:N:1151:ARG:NH1	2.53	0.42
3:N:633:VAL:HB	3:N:740:PHE:CZ	2.54	0.42
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.85	0.42
1:L:11:PHE:CE1	1:L:23:PHE:HB3	2.52	0.42
1:L:51:THR:OG1	1:L:87:VAL:O	2.35	0.42
2:M:976:ASP:HB3	2:M:979:THR:OG1	2.20	0.42
3:N:1366:LYS:O	3:N:1370:ILE:HG12	2.19	0.42
3:N:1498:ALA:HB1	4:O:84:ARG:HH21	1.84	0.42
3:N:256:GLU:OE1	3:N:274:ARG:NH1	2.53	0.42
3:N:200:ASP:O	3:N:397:LYS:HG2	2.20	0.42
1:B:90:LEU:HA	1:B:90:LEU:HD13	1.79	0.42
1:A:180:GLN:NE2	2:C:935:GLY:O	2.53	0.42
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.02	0.42
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.02	0.42
1:K:198:ARG:HD3	2:M:934:PHE:CZ	2.55	0.42
2:M:436:GLY:HA2	2:M:538:GLN:O	2.20	0.42
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	2.02	0.42
3:N:1267:ARG:HA	3:N:1268:PRO:HD3	1.92	0.42
3:N:236:TYR:CD2	3:N:322:VAL:HG21	2.55	0.42
3:N:750:PRO:HG2	3:N:756:GLN:NE2	2.35	0.42
1:A:51:THR:OG1	1:A:87:VAL:O	2.29	0.41
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.56	0.41
2:C:285:LEU:HB3	2:C:287:GLY:O	2.20	0.41
2:C:469:THR:HG23	2:C:471:TYR:CE2	2.55	0.41
3:D:1487:VAL:HG22	3:D:1491:THR:HB	2.02	0.41
3:D:238:PRO:HD3	3:D:318:ARG:HG3	2.01	0.41
3:D:245:LEU:HA	3:D:246:PRO:HD3	1.89	0.41
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.41
1:K:79:ILE:O	1:K:83:LYS:HG3	2.20	0.41
3:N:801:GLY:O	3:N:804:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:809:PRO:HG3	3:N:829:VAL:HG11	2.02	0.41
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.87	0.41
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.85	0.41
2:C:567:GLN:O	2:C:998:TYR:N	2.53	0.41
3:D:43:GLY:H	3:D:46:ASP:HB2	1.85	0.41
3:D:90:MET:SD	3:D:521:PRO:HD3	2.61	0.41
2:M:36:PRO:HB3	2:M:70:GLU:HB2	2.02	0.41
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.84	0.41
2:C:573:ARG:NH1	2:C:697:ARG:O	2.42	0.41
5:F:276:ARG:O	5:F:279:GLN:HG3	2.20	0.41
3:N:12:LEU:HD21	3:N:104:PHE:CZ	2.54	0.41
3:N:487:ALA:O	3:N:491:LYS:HG2	2.21	0.41
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.53	0.41
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.55	0.41
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.54	0.41
2:C:838:LYS:HE2	2:C:997:LEU:HD12	2.00	0.41
3:D:241:ILE:HD13	3:D:310:LEU:HD11	2.01	0.41
5:P:400:ILE:HA	5:P:403:LYS:HG2	2.02	0.41
2:C:168:ARG:HE	2:C:168:ARG:HA	1.85	0.41
2:C:954:THR:HA	2:C:955:PRO:HD3	1.88	0.41
3:D:65:ARG:HA	3:D:65:ARG:HD3	1.83	0.41
2:M:470:PRO:HB2	2:M:534:VAL:HG21	2.02	0.41
3:N:1381:VAL:HG21	3:N:1389:LEU:HD23	2.03	0.41
3:N:353:VAL:HG12	3:N:355:VAL:H	1.86	0.41
2:C:642:ARG:HA	2:C:642:ARG:HD2	1.84	0.41
3:D:428:LYS:HB3	3:D:428:LYS:HE2	1.92	0.41
2:M:545:ASN:HB3	2:M:583:LEU:HD22	2.02	0.41
3:N:452:ILE:H	3:N:452:ILE:HG13	1.53	0.41
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.84	0.41
2:C:24:GLU:HG3	2:C:27:ARG:NH2	2.35	0.41
2:C:276:LYS:HB3	2:C:276:LYS:HE3	1.92	0.41
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	2.01	0.41
4:O:37:ASN:OD1	4:O:37:ASN:N	2.49	0.41
2:C:461:VAL:HG22	2:C:467:ILE:HG12	2.03	0.41
2:C:881:ASN:OD1	2:C:881:ASN:N	2.53	0.41
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.47	0.41
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.90	0.41
5:F:187:LEU:HD23	5:F:224:VAL:HG13	2.03	0.41
2:M:205:GLU:O	2:M:209:ARG:HG2	2.21	0.41
3:N:761:ILE:HD12	4:O:20:THR:HA	2.03	0.41
1:B:153:ALA:HA	1:B:156:HIS:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:899:GLN:NE2	2:C:901:TYR:OH	2.54	0.41
2:C:778:PHE:CD2	5:F:422:LEU:HD13	2.56	0.41
1:L:216:GLU:OE1	1:L:219:ARG:NH2	2.42	0.41
2:M:172:ILE:HD11	2:M:261:ILE:HD11	2.03	0.41
3:N:293:VAL:HG22	3:N:296:GLU:HG3	2.03	0.41
3:N:879:ARG:HD3	3:N:902:LEU:O	2.21	0.41
1:B:71:VAL:HG22	1:B:132:LEU:HG	2.01	0.41
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.41
5:F:167:PRO:O	5:F:171:LYS:N	2.53	0.41
1:K:221:HIS:HA	1:K:224:TYR:CD2	2.56	0.41
3:N:262:LYS:HE2	3:N:341:GLU:OE2	2.21	0.41
5:P:134:LYS:HA	5:P:134:LYS:HD3	1.93	0.41
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.03	0.41
3:D:1092:GLY:HA3	7:G:14:DA:O4'	2.21	0.41
1:K:101:LEU:HD21	1:K:109:VAL:HG11	2.03	0.41
1:K:64:GLU:HG2	1:K:76:VAL:HG22	2.03	0.41
2:M:1090:LYS:HD3	2:M:1090:LYS:HA	1.78	0.41
3:N:1323:GLN:HA	3:N:1324:PRO:HD3	1.93	0.41
3:N:181:ASP:HB2	3:N:205:TYR:CD2	2.56	0.41
3:N:711:LEU:HD12	3:N:778:LEU:HD23	2.02	0.41
4:O:40:LEU:HG	4:O:67:GLU:HG2	2.03	0.41
3:N:1151:ARG:HA	3:N:1151:ARG:HD3	1.95	0.40
1:A:54:THR:OG1	1:A:145:ASP:OD1	2.36	0.40
2:C:512:ARG:HB2	2:C:523:ILE:HD11	2.02	0.40
3:D:323:GLU:HB2	3:D:334:THR:HB	2.02	0.40
3:D:654:LYS:O	3:D:658:LEU:HG	2.21	0.40
5:F:172:ARG:O	5:F:176:ILE:HG12	2.21	0.40
1:K:31:GLY:N	1:K:193:ASP:OD2	2.54	0.40
1:K:20:TYR:OH	1:K:198:ARG:HD2	2.20	0.40
2:M:1019:GLN:HG2	2:M:1058:ASP:HB3	2.02	0.40
4:O:83:ASP:OD1	4:O:83:ASP:N	2.55	0.40
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.96	0.40
2:C:983:ILE:HG21	2:C:987:ILE:HD11	2.02	0.40
4:E:80:VAL:HG21	4:E:85:LEU:HD13	2.02	0.40
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.79	0.40
5:F:402:ASN:O	5:F:406:ARG:N	2.54	0.40
2:M:118:ILE:HG12	2:M:382:ILE:HD13	2.03	0.40
3:N:192:ALA:HB1	3:N:193:PRO:HD2	2.02	0.40
3:N:255:GLU:HG2	3:N:274:ARG:HH12	1.87	0.40
4:O:3:GLU:HA	4:O:4:PRO:HD3	1.93	0.40
6:S:16:DC:H2"	6:S:17:DA:H5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.56	0.40
1:B:90:LEU:HD21	1:B:121:GLU:HB2	2.03	0.40
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.02	0.40
3:D:233:LYS:HB2	3:D:236:TYR:CZ	2.57	0.40
3:D:431:VAL:HG21	3:D:448:GLU:HG2	2.03	0.40
5:F:326:ASP:OD1	5:F:326:ASP:N	2.54	0.40
3:N:483:HIS:CE1	3:N:488:ARG:HD3	2.56	0.40
2:C:775:ARG:HH11	2:C:782:ALA:HA	1.86	0.40
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.62	0.40
2:C:716:LYS:HE3	3:D:37:LEU:HG	2.03	0.40
3:D:150:ARG:HH22	3:D:468:LEU:HD21	1.85	0.40
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.04	0.40
2:M:263:ASP:O	2:M:267:TYR:N	2.53	0.40
2:M:872:ASN:HA	2:M:873:PRO:HD2	1.95	0.40
3:N:959:GLU:OE1	3:N:959:GLU:N	2.54	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%)	224 (98%)	5 (2%)	0	100	100
1	B	221/315 (70%)	216 (98%)	5 (2%)	0	100	100
1	K	229/315 (73%)	225 (98%)	4 (2%)	0	100	100
1	L	221/315 (70%)	217 (98%)	3 (1%)	1 (0%)	34	72
2	C	1108/1119 (99%)	1075 (97%)	33 (3%)	0	100	100
2	M	1109/1119 (99%)	1080 (97%)	29 (3%)	0	100	100
3	D	1482/1524 (97%)	1445 (98%)	37 (2%)	0	100	100
3	N	1482/1524 (97%)	1447 (98%)	35 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
4	O	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	334 (97%)	9 (3%)	1 (0%)	46	80
5	P	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	6953/7630 (91%)	6782 (98%)	169 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	376	ILE
1	L	8	ALA

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	200/273 (73%)	196 (98%)	4 (2%)	63	87
1	B	196/273 (72%)	195 (100%)	1 (0%)	92	96
1	K	200/273 (73%)	199 (100%)	1 (0%)	92	96
1	L	196/273 (72%)	194 (99%)	2 (1%)	82	93
2	C	936/941 (100%)	919 (98%)	17 (2%)	66	88
2	M	937/941 (100%)	916 (98%)	21 (2%)	60	86
3	D	1253/1279 (98%)	1223 (98%)	30 (2%)	57	84
3	N	1253/1279 (98%)	1232 (98%)	21 (2%)	68	89
4	E	82/88 (93%)	79 (96%)	3 (4%)	41	77
4	O	82/88 (93%)	81 (99%)	1 (1%)	78	92
5	F	301/388 (78%)	285 (95%)	16 (5%)	28	64
5	P	301/388 (78%)	294 (98%)	7 (2%)	58	84
All	All	5937/6484 (92%)	5813 (98%)	124 (2%)	61	86

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	112	ARG
1	A	113	ASP
1	A	142	VAL
1	B	115	LEU
2	C	34	VAL
2	C	118	ILE
2	C	141	HIS
2	C	224	GLU
2	C	240	THR
2	C	250	ARG
2	C	258	TYR
2	C	299	LYS
2	C	300	ASP
2	C	360	LEU
2	C	391	LEU
2	C	405	ARG
2	C	512	ARG
2	C	610	ARG
2	C	627	ARG
2	C	640	ARG
2	C	714	ASP
3	D	3	LYS
3	D	67	ARG
3	D	71	LYS
3	D	175	VAL
3	D	270	LEU
3	D	297	ILE
3	D	452	ILE
3	D	709	HIS
3	D	741	ASP
3	D	754	PHE
3	D	784	ASP
3	D	810	GLU
3	D	894	LYS
3	D	904	VAL
3	D	971	LEU
3	D	986	ARG
3	D	1083	ASP
3	D	1129	THR
3	D	1137	ARG
3	D	1184	GLN

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Mol	Chain	Res	Type
3	D	1188	VAL
3	D	1219	GLU
3	D	1252	ILE
3	D	1286	THR
3	D	1290	LEU
3	D	1307	LYS
3	D	1488	ASP
3	D	1493	LYS
3	D	1499	ARG
3	D	1501	GLU
4	E	73	LEU
4	E	84	ARG
4	E	93	TYR
5	F	88	ILE
5	F	95	THR
5	F	97	GLU
5	F	186	HIS
5	F	295	MET
5	F	323	ASP
5	F	360	LYS
5	F	365	GLU
5	F	383	LEU
5	F	392	VAL
5	F	395	GLU
5	F	399	GLN
5	F	408	LEU
5	F	409	LYS
5	F	414	ARG
5	F	422	LEU
1	K	6	LEU
1	L	7	LYS
1	L	154	GLU
2	M	102	HIS
2	M	104	ASP
2	M	133	ASP
2	M	141	HIS
2	M	200	LEU
2	M	217	LEU
2	M	274	ARG
2	M	284	ARG
2	M	302	VAL
2	M	342	ASP

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Mol	Chain	Res	Type
2	M	388	ARG
2	M	397	GLU
2	M	419	THR
2	M	583	LEU
2	M	617	ASP
2	M	640	ARG
2	M	670	GLN
2	M	775	ARG
2	M	807	ARG
2	M	1043	TYR
2	M	1105	LYS
3	N	67	ARG
3	N	71	LYS
3	N	231	VAL
3	N	255	GLU
3	N	273	ARG
3	N	346	ARG
3	N	415	VAL
3	N	632	VAL
3	N	709	HIS
3	N	717	GLN
3	N	754	PHE
3	N	784	ASP
3	N	810	GLU
3	N	894	LYS
3	N	907	GLU
3	N	986	ARG
3	N	1067	VAL
3	N	1129	THR
3	N	1184	GLN
3	N	1267	ARG
3	N	1307	LYS
4	O	49	GLN
5	P	95	THR
5	P	295	MET
5	P	323	ASP
5	P	325	LYS
5	P	380	GLU
5	P	396	ARG
5	P	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
2	C	99	GLN
2	C	102	HIS
2	C	390	GLN
2	C	434	HIS
2	C	538	GLN
2	C	899	GLN
2	C	1026	GLN
3	D	66	GLN
3	D	560	GLN
3	D	669	ASN
3	D	724	GLN
3	D	976	GLN
3	D	1046	GLN
3	D	1172	HIS
3	D	1184	GLN
3	D	1195	GLN
5	F	83	GLN
5	F	411	HIS
2	M	219	GLN
3	N	66	GLN
3	N	724	GLN
3	N	994	GLN
3	N	1184	GLN
3	N	1254	GLN
3	N	1359	GLN
3	N	1374	GLN
4	O	33	HIS
4	O	49	GLN
5	P	83	GLN
5	P	402	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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	$\#\|Z\|>2$
10	C	D	2005	8,12	14,21,22	0.74	0	18,30,33	0.49	0
11	DPO	D	2006	8	8,8,8	1.83	1 (12%)	12,13,13	1.31	0
12	COD	D	2008	10	25,30,46	1.61	6 (24%)	26,46,68	2.31	3 (11%)
10	C	N	1605	8,12	14,21,22	0.74	0	18,30,33	0.54	0
11	DPO	N	1606	8	8,8,8	1.84	1 (12%)	12,13,13	1.29	0
12	COD	N	1608	10	24,29,46	1.66	5 (20%)	23,45,68	2.39	1 (4%)

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
10	C	D	2005	8,12	-	0/3/25/26	0/2/2/2
11	DPO	D	2006	8	-	0/6/6/6	0/0/0/0
12	COD	D	2008	10	-	0/15/35/59	0/3/3/3
10	C	N	1605	8,12	-	0/3/25/26	0/2/2/2
11	DPO	N	1606	8	-	0/6/6/6	0/0/0/0
12	COD	N	1608	10	-	0/12/32/59	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	1608	COD	O13-C12	-2.37	1.37	1.43
12	D	2008	COD	O13-C12	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2008	COD	O15-C14	-2.01	1.38	1.43
12	D	2008	COD	C6-N7	2.36	1.43	1.34
12	N	1608	COD	C6-N7	2.37	1.43	1.34
12	D	2008	COD	C2-N1	2.58	1.38	1.33
12	N	1608	COD	C2-N1	2.61	1.38	1.33
12	D	2008	COD	C18-C16	2.91	1.61	1.51
12	N	1608	COD	C18-C16	2.95	1.61	1.51
12	N	1608	COD	C2-N3	4.10	1.39	1.32
12	D	2008	COD	C2-N3	4.23	1.39	1.32
11	D	2006	DPO	P1-O2	5.02	1.61	1.51
11	N	1606	DPO	P1-O2	5.06	1.61	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	1608	COD	N3-C2-N1	-10.56	120.57	128.87
12	D	2008	COD	N3-C2-N1	-10.51	120.61	128.87
12	D	2008	COD	O17-C16-C18	2.02	116.52	109.29
12	D	2008	COD	O23-P24-O27	2.93	111.59	102.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	1605	C	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	231/315 (73%)	-0.17	5 (2%) 65 42	29, 51, 78, 126	1 (0%)
1	B	223/315 (70%)	-0.27	2 (0%) 85 70	26, 53, 93, 122	0
1	K	231/315 (73%)	-0.39	5 (2%) 65 42	22, 38, 65, 128	1 (0%)
1	L	223/315 (70%)	-0.33	0 100 100	21, 49, 82, 102	0
2	C	1112/1119 (99%)	0.06	49 (4%) 38 17	12, 58, 115, 132	3 (0%)
2	M	1112/1119 (99%)	-0.35	12 (1%) 82 65	5, 32, 82, 118	3 (0%)
3	D	1486/1524 (97%)	-0.17	23 (1%) 76 57	7, 43, 96, 131	4 (0%)
3	N	1486/1524 (97%)	-0.29	12 (0%) 87 74	4, 34, 85, 125	4 (0%)
4	E	94/99 (94%)	-0.24	2 (2%) 67 44	22, 44, 88, 102	0
4	O	94/99 (94%)	-0.44	1 (1%) 82 65	14, 31, 67, 85	0
5	F	346/443 (78%)	0.26	25 (7%) 18 7	33, 70, 134, 152	0
5	P	346/443 (78%)	-0.20	5 (1%) 78 59	14, 43, 93, 112	0
6	H	21/27 (77%)	0.55	3 (14%) 4 1	47, 92, 134, 155	0
6	S	21/27 (77%)	0.29	3 (14%) 4 1	35, 73, 118, 146	0
7	G	16/19 (84%)	0.56	1 (6%) 23 9	49, 77, 129, 134	0
7	R	16/19 (84%)	0.55	2 (12%) 5 2	31, 60, 131, 137	0
All	All	7058/7722 (91%)	-0.18	150 (2%) 67 44	4, 45, 99, 155	16 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	9.4
5	F	391	GLY	7.3
1	A	233	VAL	7.3
5	F	390	PHE	6.0
1	K	233	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
2	M	365	ASP	5.7
1	A	234	ALA	5.4
1	K	232	ALA	5.4
1	K	234	ALA	5.2
1	A	232	ALA	5.2
5	F	377	ASP	4.9
5	F	389	PHE	4.9
5	F	381	HIS	4.7
2	C	362	GLY	4.6
2	C	200	LEU	4.4
2	C	188	LYS	4.3
2	C	363	SER	4.3
3	N	1252	ILE	4.1
3	D	191	LEU	4.0
5	F	410	TYR	3.9
2	C	809	GLY	3.8
3	D	70	GLY	3.7
5	F	392	VAL	3.7
7	G	19	DA	3.7
5	F	411	HIS	3.6
2	C	769	PRO	3.6
2	M	219	GLN	3.6
2	C	86	LYS	3.5
2	C	107	LEU	3.5
3	N	1499	ARG	3.5
6	S	25	DA	3.5
3	D	194	GLY	3.5
6	H	25	DA	3.4
6	H	24	DC	3.4
5	F	414	ARG	3.4
5	F	326	ASP	3.3
2	C	251	ASP	3.3
2	C	104	ASP	3.3
3	D	423	ASP	3.2
2	M	104	ASP	3.2
3	D	372	ASP	3.2
5	F	325	LYS	3.2
3	N	1297	GLU	3.2
2	M	766	GLU	3.1
5	F	359	SER	3.1
2	C	367	LEU	3.0
3	N	991	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	373	PRO	3.0
2	C	770	GLU	3.0
5	F	356	LYS	3.0
2	C	65	VAL	3.0
5	F	415	THR	2.9
7	R	19	DA	2.9
5	F	386	VAL	2.9
3	D	405	ASP	2.9
2	C	48	PHE	2.9
2	C	109	LYS	2.9
5	P	382	THR	2.9
3	D	1127	GLU	2.8
2	C	421	GLU	2.8
2	C	105	THR	2.8
2	C	649	VAL	2.8
3	N	173	PRO	2.8
2	C	294	GLU	2.8
3	D	1499	ARG	2.7
3	D	1495	ILE	2.7
2	M	364	GLU	2.7
2	C	295	ASP	2.7
2	C	68	PHE	2.7
5	F	142	ARG	2.6
6	S	24	DC	2.6
2	C	296	GLY	2.6
5	F	138	SER	2.6
1	A	231	ALA	2.6
3	N	144	GLY	2.6
5	F	376	ILE	2.6
3	D	195	VAL	2.5
6	H	23	DG	2.5
2	C	365	ASP	2.5
5	P	324	GLU	2.5
3	D	235	ALA	2.5
3	D	198	ARG	2.5
2	C	106	GLY	2.5
2	C	597	ALA	2.5
6	S	23	DG	2.5
2	C	196	LEU	2.5
2	C	622	GLU	2.5
3	N	976	GLN	2.4
5	F	393	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	52	PHE	2.4
2	C	358	ARG	2.4
3	D	318	ARG	2.4
2	C	255	ALA	2.4
5	F	147	LEU	2.4
2	C	292	ARG	2.4
2	C	258	TYR	2.4
3	D	209	ARG	2.4
2	C	246	ASP	2.3
2	C	108	ILE	2.3
3	D	378	ILE	2.3
2	M	366	SER	2.3
5	F	139	ALA	2.3
2	C	242	LEU	2.3
1	B	134	GLU	2.3
2	C	286	SER	2.3
5	P	423	ASP	2.3
7	R	4	DT	2.3
4	O	51	LEU	2.3
2	M	650	ARG	2.3
2	C	66	LEU	2.3
3	D	1252	ILE	2.2
5	F	146	GLY	2.2
2	C	361	MET	2.2
3	D	68	PHE	2.2
1	K	231	ALA	2.2
2	C	766	GLU	2.2
2	C	102	HIS	2.2
3	N	805	GLU	2.2
2	M	811	PRO	2.2
3	N	982	PHE	2.2
5	F	301	ALA	2.2
2	M	362	GLY	2.2
2	C	1105	LYS	2.2
3	D	190	GLU	2.2
5	P	149	GLU	2.2
2	C	221	LEU	2.1
2	C	777	ILE	2.1
4	E	83	ASP	2.1
1	A	230	ALA	2.1
2	M	63	GLY	2.1
5	F	395	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	186	LEU	2.1
2	C	300	ASP	2.1
3	N	977	ALA	2.1
2	C	739	GLU	2.1
1	K	19	GLU	2.1
2	M	616	GLU	2.1
3	D	237	LYS	2.1
3	D	805	GLU	2.1
5	P	325	LYS	2.1
3	N	219	GLU	2.1
3	N	973	GLN	2.1
3	D	406	ASP	2.1
4	E	84	ARG	2.0
2	M	421	GLU	2.0
2	C	207	LEU	2.0
2	C	226	VAL	2.0
2	C	211	LEU	2.0
5	F	408	LEU	2.0
3	D	316	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	COD	D	2008	28/44	0.77	0.40	9.88	50,73,102,116	28
8	MG	N	1601	1/1	0.97	0.45	5.64	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	MG	D	2004	1/1	0.97	0.43	4.77	27,27,27,27	0
10	C	D	2005	20/21	0.88	0.25	2.03	43,61,71,80	20
11	DPO	D	2006	9/9	0.93	0.21	1.92	45,68,84,98	0
11	DPO	N	1606	9/9	0.90	0.19	1.36	26,51,74,84	0
8	MG	N	1607	1/1	0.95	0.17	1.34	36,36,36,36	0
10	C	N	1605	20/21	0.90	0.20	1.33	24,34,49,57	20
12	COD	N	1608	27/44	0.89	0.23	1.32	35,43,62,65	27
8	MG	D	2007	1/1	0.92	0.17	0.28	49,49,49,49	0
9	ZN	N	1602	1/1	0.99	0.13	-0.31	16,16,16,16	0
9	ZN	D	2001	1/1	1.00	0.13	-0.88	20,20,20,20	0
8	MG	F	2001	1/1	0.80	0.17	-0.94	92,92,92,92	0
9	ZN	D	2002	1/1	0.97	0.04	-1.47	92,92,92,92	0
9	ZN	N	1603	1/1	0.99	0.04	-2.51	50,50,50,50	0
8	MG	D	2003	1/1	0.96	0.15	-	22,22,22,22	0
8	MG	P	2001	1/1	0.87	0.12	-	38,38,38,38	0
8	MG	B	2001	1/1	0.74	0.29	-	71,71,71,71	0
8	MG	N	1604	1/1	0.99	0.19	-	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.