Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:44 PM GMT

PDB ID	:	4MEY
Title	:	Crystal structure of Escherichia coli RNA polymerase holoenzyme
Authors	:	Feng, Y.; Zhang, Y.; Arnold, E.; Ebright, R.H.
Deposited on	:	2013-08-27
Resolution	:	3.95 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:

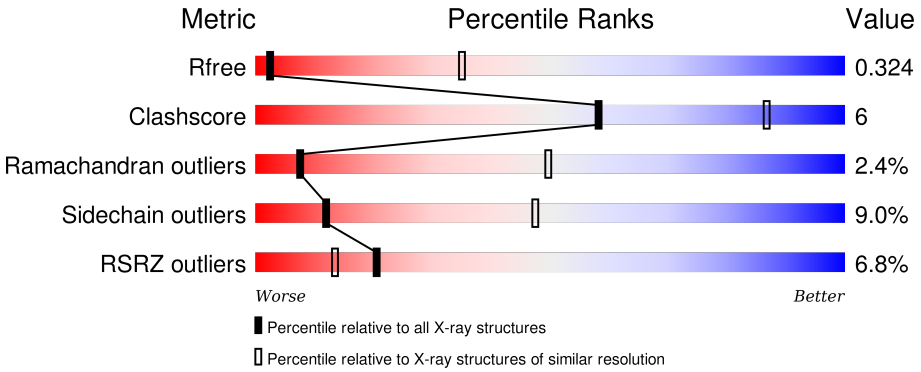
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.95 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	1007 (4.34-3.54)
Clashscore	102246	1042 (4.30-3.58)
Ramachandran outliers	100387	1000 (4.30-3.58)
Sidechain outliers	100360	1021 (4.32-3.56)
RSRZ outliers	91569	1011 (4.34-3.54)

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	335	7% 69% 17% • 11%
1	B	335	12% 65% 17% • 14%
1	G	335	3% 52% 11% • 36%
1	H	335	10% 49% 13% • 36%
2	C	1342	7% 82% 17% •

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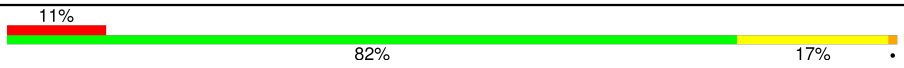
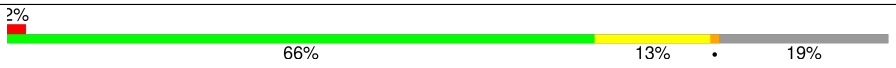
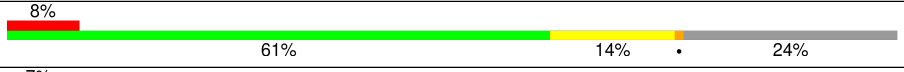
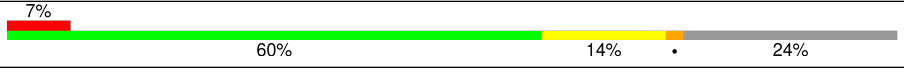
Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49826 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	298	Total	C	N	O	S	0	0	0
			2236	1405	391	432	8			
1	B	287	Total	C	N	O	S	0	0	0
			2160	1359	374	419	8			
1	G	216	Total	C	N	O	S	0	0	0
			1618	1013	282	317	6			
1	H	215	Total	C	N	O	S	0	0	0
			1605	1005	278	316	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	3	0	0
			9522	5999	1675	1829	19			
2	I	1340	Total	C	N	O	S	3	0	0
			9544	6013	1676	1835	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1147	Total	C	N	O	S	0	0	0
			7549	4756	1355	1411	27			
3	J	1140	Total	C	N	O	S	0	0	0
			7512	4733	1348	1404	27			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	0	0	0
			482	299	93	90			
4	K	75	Total	C	N	O	0	0	0
			408	253	79	76			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	464	Total	C	N	O	S	0	0	0
			3592	2253	643	682	14			
5	L	464	Total	C	N	O	S	0	0	0
			3592	2253	643	682	14			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

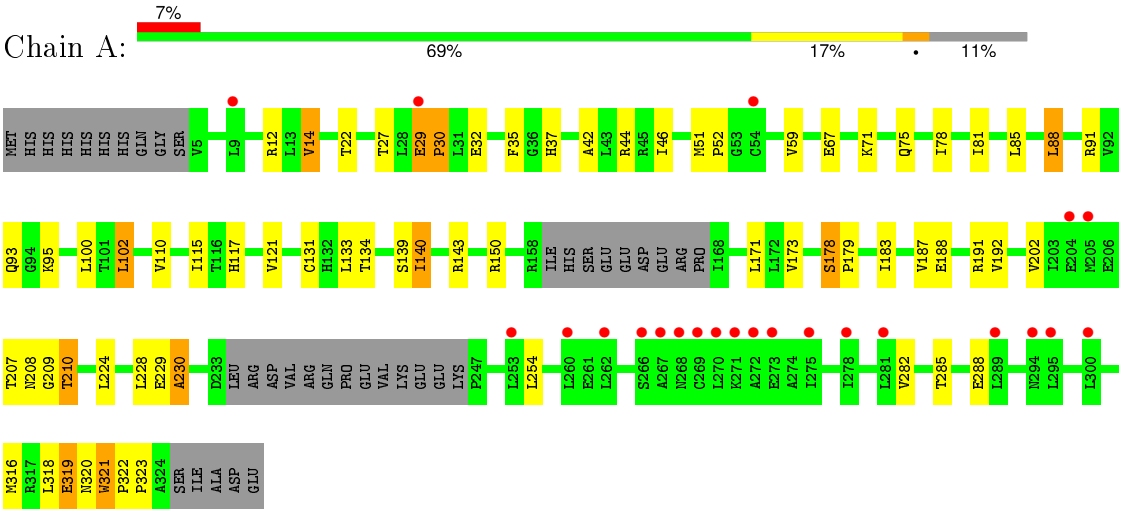
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	2	Total Zn 2 2	0	0
7	D	2	Total Zn 2 2	0	0

3 Residue-property plots (i)

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.

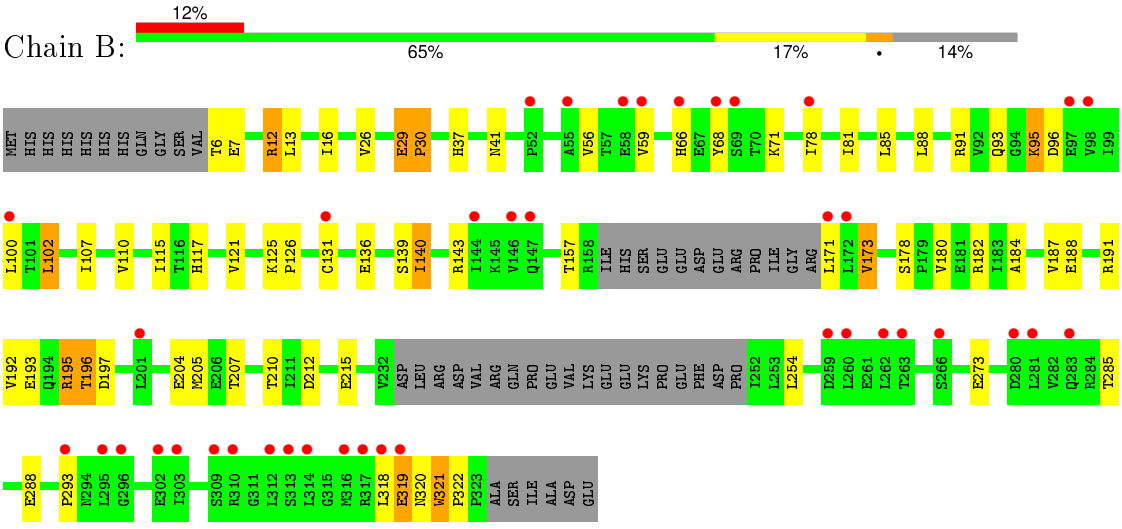
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



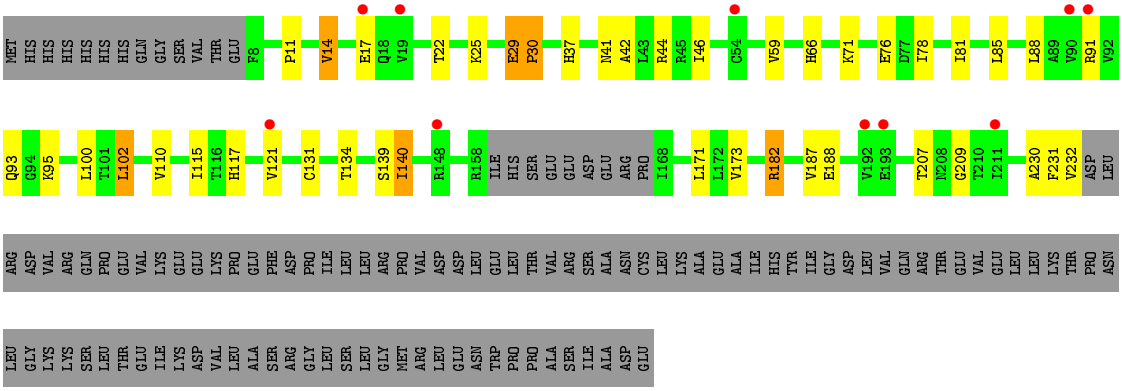
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



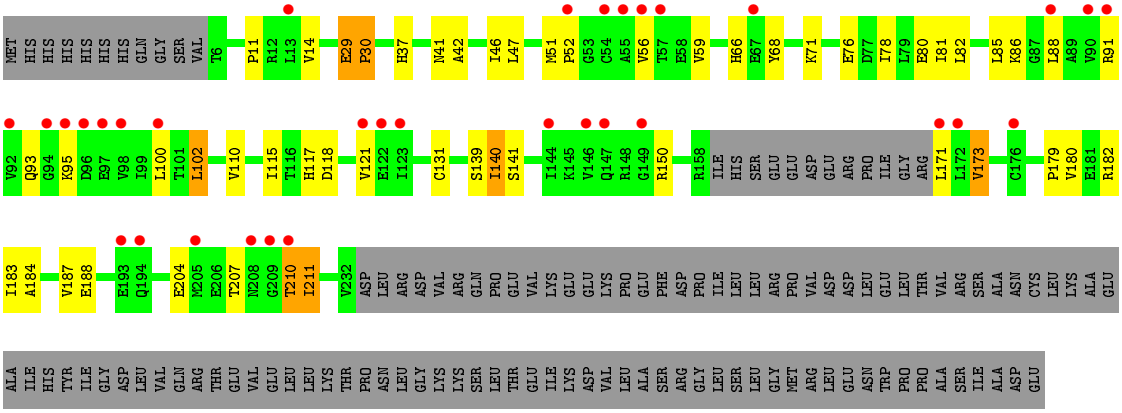
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



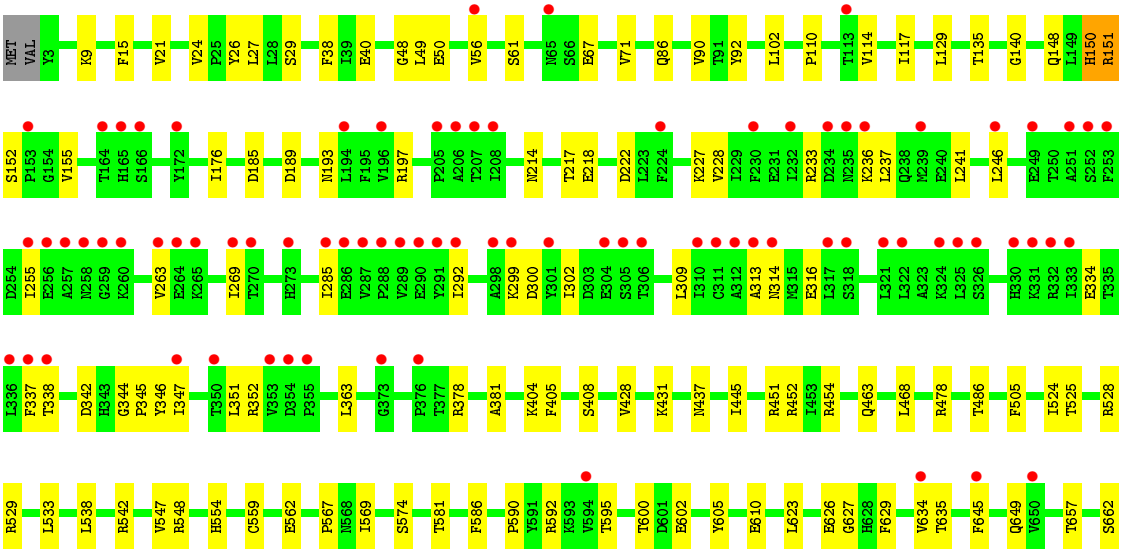
• Molecule 1: DNA-directed RNA polymerase subunit alpha

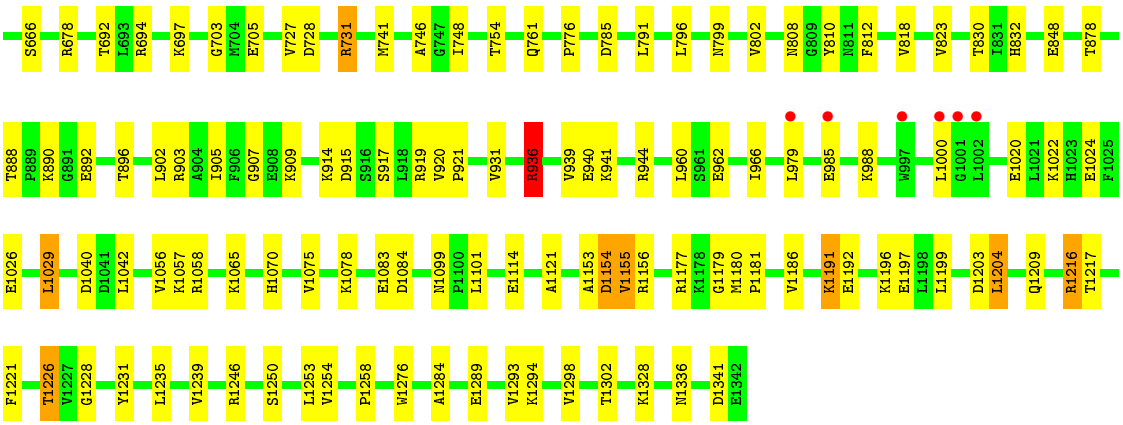
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

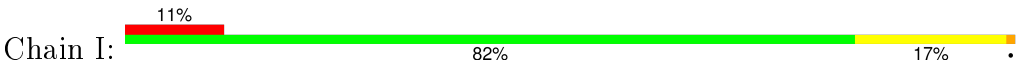
Chain C:

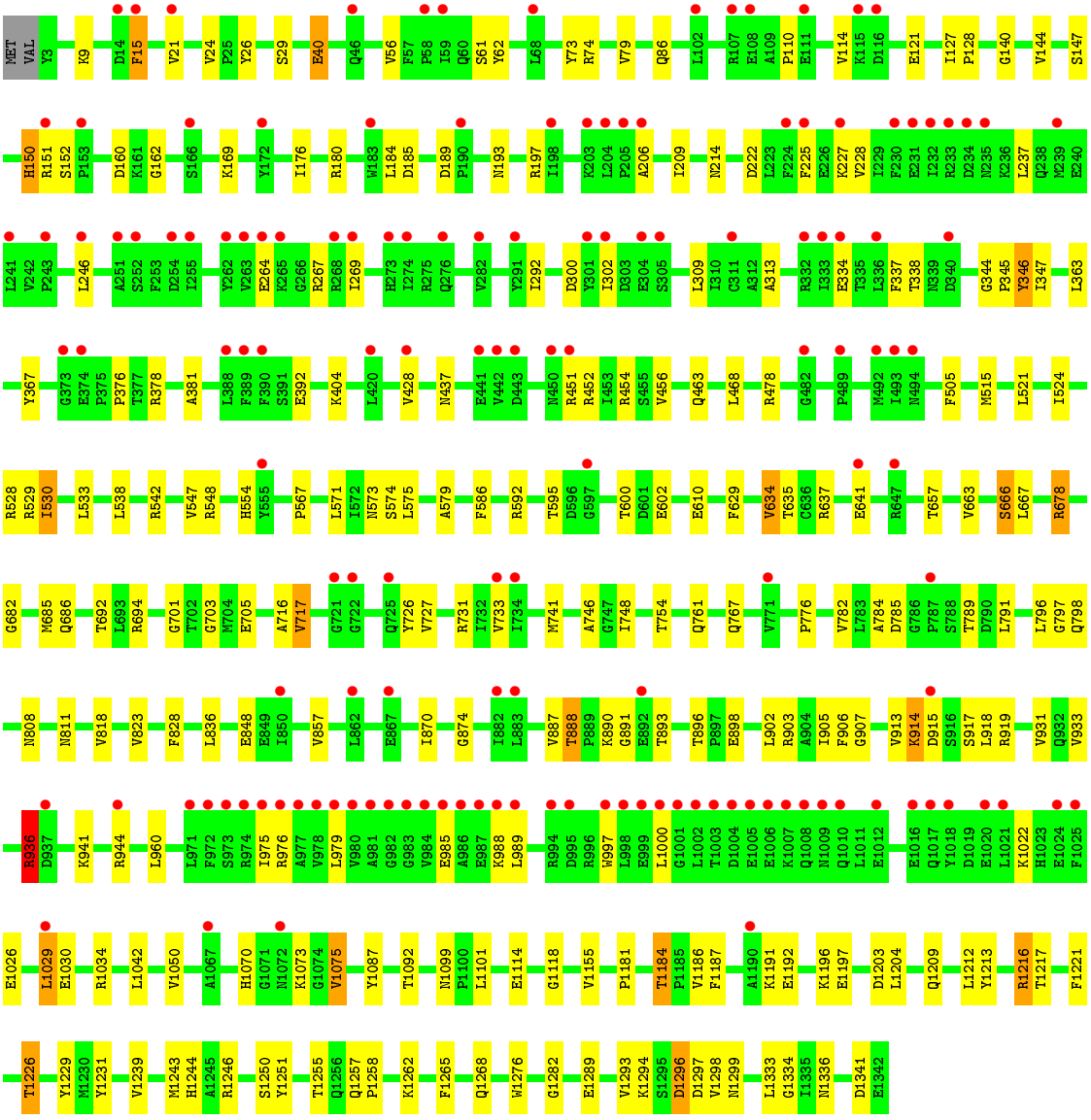




• Molecule 2: DNA-directed RNA polymerase subunit beta

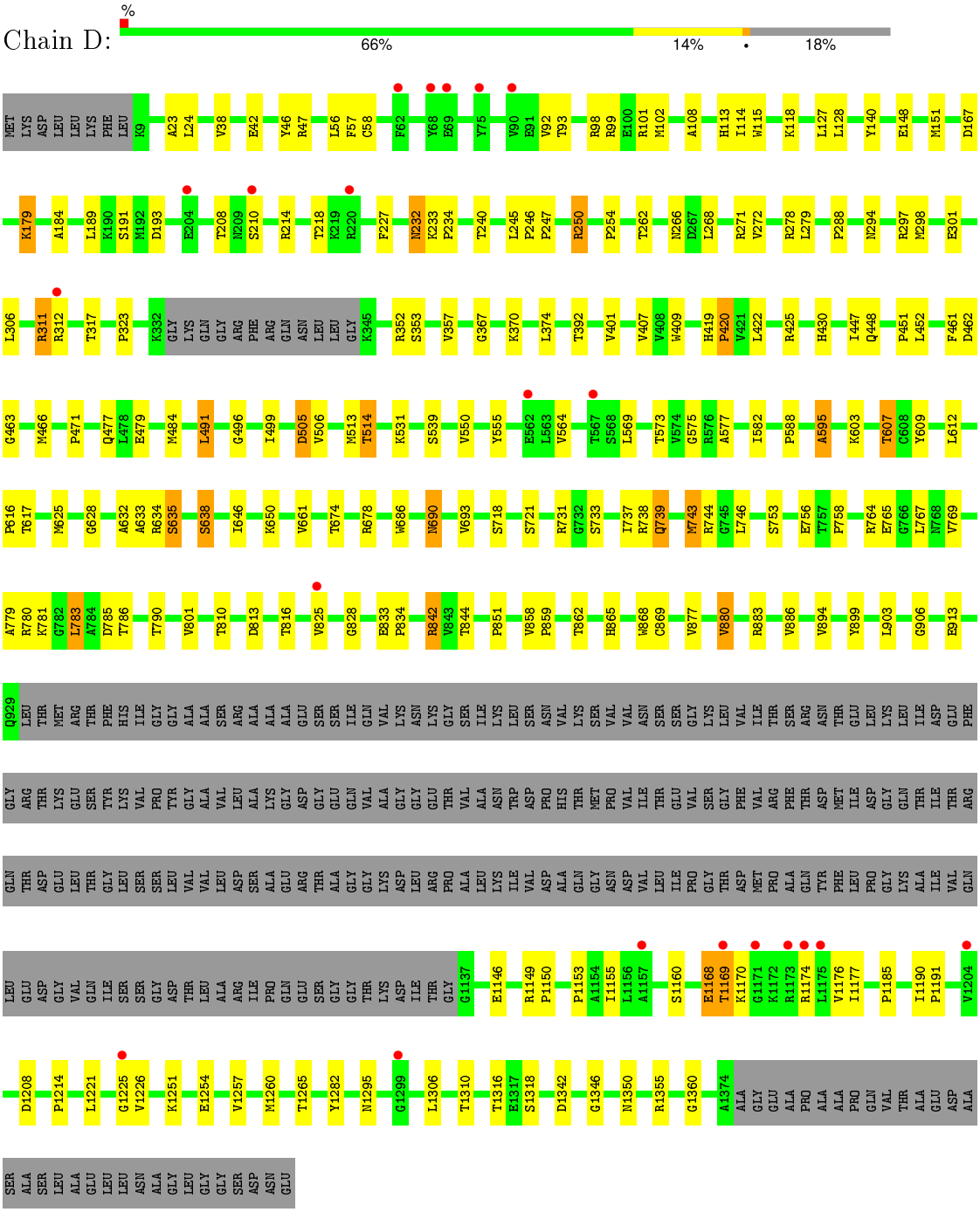
Chain I:





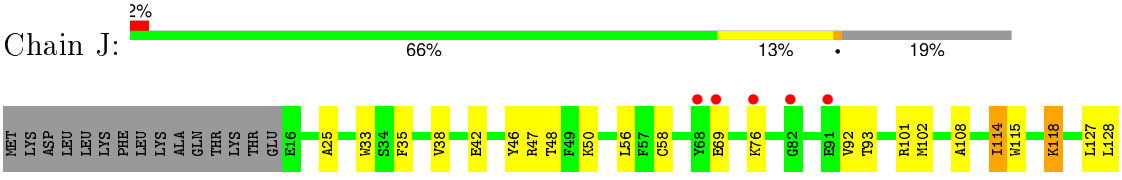
• Molecule 3: DNA-directed RNA polymerase subunit beta'

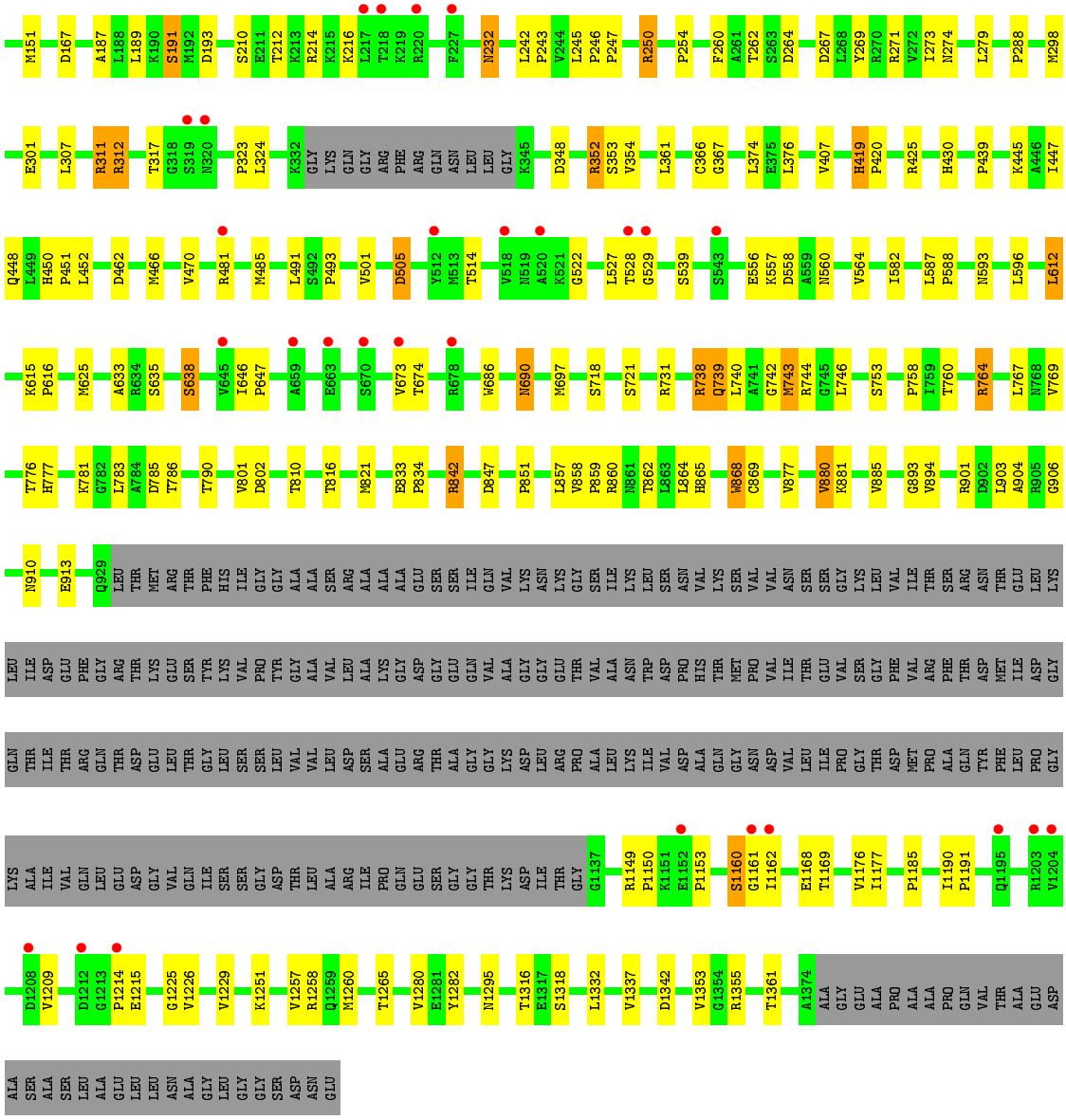
Chain D:



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

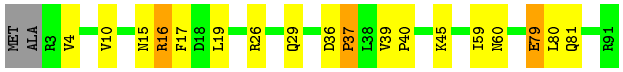
Chain J:





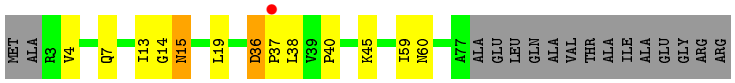
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



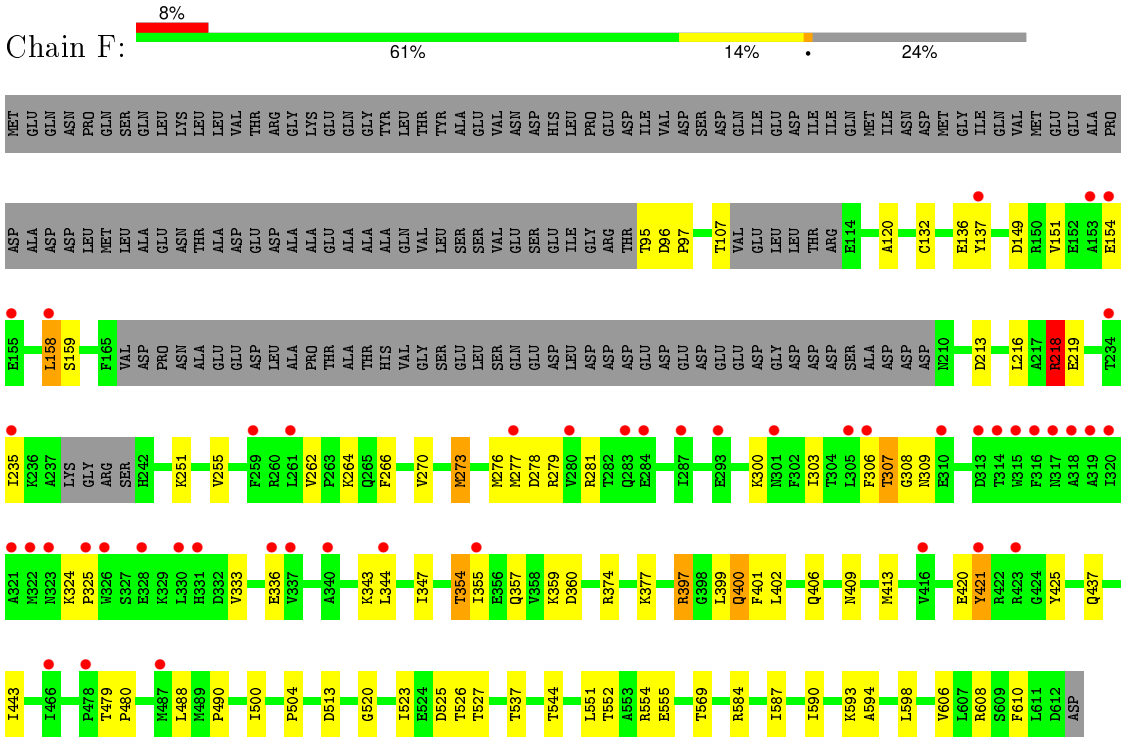
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



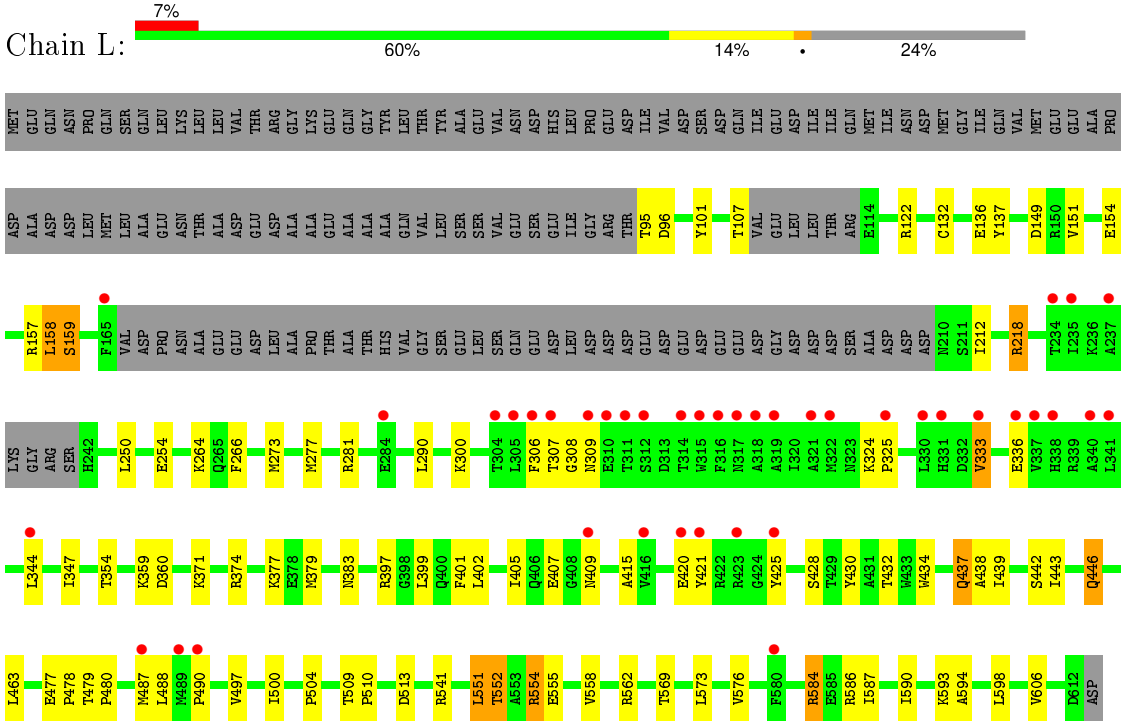
- Molecule 5: RNA polymerase sigma factor RpoD

Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	186.39Å 207.24Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.95 49.92 – 3.95	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.92-3.95) 96.2 (49.92-3.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.276 , 0.325 0.273 , 0.324	Depositor DCC
R_{free} test set	2022 reflections (1.99%)	DCC
Wilson B-factor (Å^2)	142.5	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 153.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 103788 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	49826	wwPDB-VP
Average B, all atoms (Å^2)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.25	0/2263	0.49	0/3073
1	B	0.25	0/2185	0.49	0/2967
1	G	0.24	0/1636	0.47	0/2221
1	H	0.23	0/1623	0.46	0/2205
2	C	0.26	0/9653	0.47	1/13062 (0.0%)
2	I	0.25	0/9676	0.45	1/13089 (0.0%)
3	D	0.28	0/7644	0.50	0/10385
3	J	0.25	0/7607	0.47	0/10334
4	E	0.33	0/482	0.63	1/662 (0.2%)
4	K	0.24	0/407	0.48	0/558
5	F	0.25	0/3636	0.47	2/4892 (0.0%)
5	L	0.25	0/3636	0.47	2/4892 (0.0%)
All	All	0.26	0/50448	0.48	7/68340 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	39	VAL	C-N-CA	7.62	153.99	122.00
2	I	936	ARG	NE-CZ-NH2	6.31	123.45	120.30
2	C	936	ARG	NE-CZ-NH2	5.72	123.16	120.30
5	F	149	ASP	CB-CG-OD2	5.23	123.00	118.30
5	L	149	ASP	CB-CG-OD2	5.17	122.96	118.30
5	F	218	ARG	NE-CZ-NH1	5.07	122.83	120.30
5	L	551	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2236	0	2254	31	0
1	B	2160	0	2184	30	0
1	G	1618	0	1622	22	0
1	H	1605	0	1599	28	0
2	C	9522	0	8569	113	0
2	I	9544	0	8601	125	0
3	D	7549	0	6266	88	0
3	J	7512	0	6245	87	0
4	E	482	0	301	7	0
4	K	408	0	255	9	0
5	F	3592	0	3433	40	0
5	L	3592	0	3433	46	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	49826	0	44762	558	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 6.

All (558) 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)
3:J:910:ASN:CG	4:K:15:ASN:HB2	1.65	1.17
2:I:936:ARG:HH21	2:I:936:ARG:HG3	1.29	0.98
2:C:936:ARG:HG3	2:C:936:ARG:HH21	1.33	0.92
2:C:808:ASN:H	3:D:633:ALA:HB2	1.44	0.82
1:G:11:PRO:HA	1:G:30:PRO:HD2	1.65	0.79
2:I:185:ASP:HB2	2:I:197:ARG:HB2	1.65	0.76
5:L:218:ARG:HH11	5:L:218:ARG:HG2	1.51	0.76
5:F:218:ARG:HG2	5:F:218:ARG:HH11	1.50	0.75
3:J:288:PRO:HA	5:L:377:LYS:HE3	1.69	0.74
1:A:228:LEU:O	1:A:230:ALA:N	2.20	0.73
2:I:345:PRO:O	2:I:347:ILE:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:26:TYR:HB2	2:I:29:SER:HB3	1.70	0.72
3:J:317:THR:HA	3:J:323:PRO:HA	1.71	0.72
1:G:44:ARG:NH1	2:I:1087:TYR:OH	2.23	0.71
2:I:1101:LEU:HB3	3:J:731:ARG:HG3	1.73	0.70
3:D:452:LEU:HG	3:D:625:MET:HE3	1.74	0.70
1:H:71:LYS:NZ	1:H:139:SER:O	2.24	0.70
2:C:345:PRO:O	2:C:347:ILE:N	2.23	0.70
2:I:931:VAL:HB	2:I:944:ARG:HH22	1.57	0.69
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.26	0.69
3:J:910:ASN:HB2	4:K:15:ASN:HA	1.76	0.68
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.75	0.68
2:C:931:VAL:HB	2:C:944:ARG:HH22	1.58	0.67
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.77	0.67
2:C:832:HIS:HE1	2:C:1058:ARG:HB2	1.59	0.67
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.27	0.67
1:G:230:ALA:O	1:G:232:VAL:N	2.28	0.67
5:F:276:MET:SD	5:F:279:ARG:NH2	2.69	0.66
3:J:910:ASN:CG	4:K:15:ASN:CB	2.56	0.66
2:C:408:SER:O	2:C:431:LYS:NZ	2.28	0.66
5:L:399:LEU:HD13	5:L:446:GLN:HG2	1.79	0.65
5:F:397:ARG:HG2	5:F:443:ILE:HD12	1.77	0.65
2:I:147:SER:HB2	2:I:530:ILE:HG22	1.78	0.65
2:C:404:LYS:HE2	2:C:586:PHE:HZ	1.62	0.65
3:J:114:ILE:HD11	3:J:307:LEU:HB2	1.79	0.65
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.78	0.65
3:D:102:MET:HG2	3:D:246:PRO:HD3	1.79	0.64
3:J:245:LEU:O	3:J:250:ARG:NH1	2.30	0.64
1:A:208:ASN:OD1	1:A:210:THR:OG1	2.13	0.64
1:H:11:PRO:HA	1:H:30:PRO:HD2	1.80	0.64
1:H:78:ILE:HD13	1:H:81:ILE:HD12	1.79	0.64
5:F:587:ILE:HD12	5:F:590:ILE:HD11	1.79	0.64
5:L:428:SER:O	5:L:432:THR:OG1	2.14	0.63
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.81	0.63
2:C:979:LEU:HD21	2:C:1000:LEU:HD23	1.81	0.63
3:J:901:ARG:O	3:J:1251:LYS:NZ	2.32	0.63
5:L:151:VAL:HG11	5:L:158:LEU:HG	1.81	0.62
1:B:110:VAL:HG21	1:B:140:ILE:HD11	1.80	0.62
2:C:890:LYS:HG2	2:C:914:LYS:HB2	1.79	0.62
2:C:548:ARG:NH2	2:C:567:PRO:O	2.33	0.62
5:L:587:ILE:HD12	5:L:590:ILE:HD11	1.82	0.62
2:C:148:GLN:NE2	2:C:533:LEU:O	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:898:GLU:HG2	5:L:541:ARG:HA	1.83	0.61
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.82	0.61
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.35	0.61
2:C:56:VAL:HG21	2:C:468:LEU:HB3	1.81	0.61
2:C:222:ASP:OD1	2:C:227:LYS:NZ	2.28	0.61
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.82	0.61
2:I:74:ARG:NE	2:I:121:GLU:OE2	2.32	0.61
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.83	0.60
5:L:551:LEU:HD11	5:L:555:GLU:HG3	1.84	0.60
3:J:821:MET:HA	3:J:881:LYS:HA	1.82	0.60
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.84	0.60
1:A:150:ARG:HE	1:B:6:THR:HA	1.65	0.60
2:C:189:ASP:OD1	2:C:193:ASN:N	2.34	0.60
1:G:102:LEU:HG	1:G:115:ILE:HG12	1.84	0.60
5:F:590:ILE:HA	5:F:593:LYS:HG2	1.82	0.60
2:I:915:ASP:OD2	2:I:919:ARG:NH2	2.34	0.60
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.85	0.59
3:D:693:VAL:HG21	3:D:743:MET:HG3	1.84	0.59
1:H:100:LEU:HD21	1:H:121:VAL:HG21	1.85	0.59
3:D:491:LEU:HA	3:D:499:ILE:H	1.68	0.58
2:C:703:GLY:N	2:C:705:GLU:OE2	2.37	0.58
3:D:506:VAL:HG13	3:D:628:GLY:HA3	1.85	0.58
3:D:288:PRO:HA	5:F:377:LYS:HE3	1.84	0.58
2:I:808:ASN:H	3:J:633:ALA:HB2	1.68	0.58
2:C:152:SER:OG	2:C:452:ARG:HG2	2.04	0.58
2:I:548:ARG:NH2	2:I:567:PRO:O	2.37	0.58
2:C:1209:GLN:HA	2:C:1226:THR:HA	1.85	0.58
5:F:213:ASP:OD1	5:F:213:ASP:N	2.33	0.58
1:H:102:LEU:HG	1:H:115:ILE:HG12	1.84	0.57
3:D:271:ARG:NH1	5:F:400:GLN:OE1	2.38	0.57
5:L:590:ILE:HA	5:L:593:LYS:HG2	1.85	0.57
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.85	0.57
2:I:1209:GLN:HA	2:I:1226:THR:HA	1.86	0.57
1:G:110:VAL:HG21	1:G:140:ILE:HD11	1.85	0.57
3:D:746:LEU:HD22	3:D:758:PRO:HB3	1.86	0.57
2:C:21:VAL:HG21	2:C:592:ARG:HD3	1.85	0.57
1:G:71:LYS:NZ	1:G:139:SER:O	2.37	0.57
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.87	0.57
2:C:150:HIS:CE1	2:C:454:ARG:HD2	2.40	0.57
3:J:118:LYS:HE3	3:J:312:ARG:HG2	1.87	0.57
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:HIS:CE1	1:B:187:VAL:HG21	2.39	0.56
2:C:915:ASP:OD2	2:C:919:ARG:NH2	2.37	0.56
2:C:1289:GLU:HB3	2:C:1294:LYS:HD2	1.87	0.56
2:I:222:ASP:OD1	2:I:227:LYS:NZ	2.39	0.56
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.87	0.55
1:A:285:THR:HG23	1:A:288:GLU:H	1.71	0.55
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.36	0.55
3:D:108:ALA:HB3	3:D:279:LEU:HD23	1.88	0.55
2:I:936:ARG:HG3	2:I:936:ARG:NH2	2.05	0.55
3:D:210:SER:O	3:D:214:ARG:NH2	2.40	0.55
2:I:887:VAL:HB	2:I:913:VAL:HB	1.88	0.55
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.40	0.55
2:I:21:VAL:HG21	2:I:592:ARG:HD3	1.89	0.55
2:C:314:ASN:O	2:C:352:ARG:NH2	2.41	0.54
5:F:120:ALA:HB1	5:F:421:TYR:HB2	1.88	0.54
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.88	0.54
3:J:481:ARG:HA	3:J:485:MET:HG2	1.89	0.54
3:J:527:LEU:O	3:J:529:GLY:N	2.39	0.54
3:J:452:LEU:HG	3:J:625:MET:HE3	1.89	0.54
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.42	0.54
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.89	0.54
2:I:960:LEU:HD22	2:I:1029:LEU:HD12	1.89	0.54
2:C:1153:ALA:O	2:C:1155:VAL:N	2.41	0.54
1:G:78:ILE:HD13	1:G:81:ILE:HD12	1.88	0.54
1:B:182:ARG:HD3	3:D:531:LYS:HA	1.90	0.54
2:C:1101:LEU:HB3	3:D:731:ARG:HG3	1.90	0.54
5:L:551:LEU:HD22	5:L:552:THR:H	1.73	0.54
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.87	0.54
1:A:102:LEU:HG	1:A:115:ILE:HG12	1.89	0.54
1:H:91:ARG:NH2	1:H:210:THR:O	2.40	0.54
2:C:960:LEU:HD22	2:C:1029:LEU:HG	1.90	0.53
5:L:101:TYR:CE2	5:L:405:ILE:HD13	2.43	0.53
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.37	0.53
5:F:151:VAL:HG11	5:F:158:LEU:HG	1.90	0.53
1:A:75:GLN:HE21	2:C:727:VAL:HG11	1.71	0.53
2:C:316:GLU:HG3	2:C:352:ARG:NH2	2.23	0.53
3:D:609:TYR:HA	3:D:617:THR:OG1	2.09	0.53
3:D:232:ASN:OD1	3:D:232:ASN:N	2.40	0.53
2:C:936:ARG:HG3	2:C:936:ARG:NH2	2.10	0.53
2:C:246:LEU:HB3	2:C:269:ILE:HD13	1.90	0.53
5:F:97:PRO:HB2	5:F:402:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:232:ASN:OD1	3:J:232:ASN:N	2.39	0.53
2:I:228:VAL:HG23	2:I:337:PHE:HB2	1.90	0.53
2:I:150:HIS:CE1	2:I:454:ARG:HD2	2.44	0.53
3:D:245:LEU:O	3:D:250:ARG:NH1	2.41	0.53
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.89	0.53
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.89	0.53
5:L:573:LEU:HD13	5:L:584:ARG:HE	1.73	0.53
2:I:1075:VAL:HG21	3:J:354:VAL:HG11	1.90	0.53
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.90	0.53
2:I:237:LEU:HD13	2:I:292:ILE:HD12	1.91	0.52
2:I:798:GLN:OE1	2:I:828:PHE:N	2.35	0.52
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.91	0.52
3:J:353:SER:HB3	3:J:447:ILE:HG13	1.91	0.52
1:B:184:ALA:HB3	1:B:204:GLU:HB3	1.90	0.52
2:I:979:LEU:HD21	2:I:1000:LEU:HD23	1.91	0.52
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.20	0.52
2:I:1276:TRP:CE2	3:J:801:VAL:HG11	2.44	0.52
1:B:12:ARG:HG3	1:B:30:PRO:HG3	1.91	0.52
1:B:16:ILE:HG12	1:B:26:VAL:HG22	1.92	0.52
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.92	0.52
3:D:1168:GLU:O	3:D:1170:LYS:N	2.42	0.52
2:I:1244:HIS:HB2	2:I:1265:PHE:CG	2.45	0.52
1:G:91:ARG:NH2	1:G:209:GLY:O	2.43	0.52
2:I:933:VAL:HG13	2:I:1050:VAL:HG22	1.92	0.52
3:D:471:PRO:O	3:D:477:GLN:NE2	2.43	0.52
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.91	0.52
3:D:179:LYS:O	3:D:184:ALA:HB2	2.10	0.52
2:C:1154:ASP:O	2:C:1156:ARG:N	2.43	0.52
2:I:836:LEU:HB3	2:I:918:LEU:HD21	1.92	0.52
2:I:811:ASN:HB2	2:I:1099:ASN:HB2	1.90	0.52
5:F:278:ASP:OD1	5:F:281:ARG:NH2	2.43	0.51
3:D:1169:THR:HA	3:D:1174:ARG:HA	1.91	0.51
2:C:785:ASP:OD2	2:C:791:LEU:N	2.42	0.51
1:A:282:VAL:HB	1:A:316:MET:HB2	1.92	0.51
4:K:13:ILE:HG22	4:K:14:GLY:N	2.25	0.51
1:G:182:ARG:NH1	2:I:1092:THR:OG1	2.42	0.51
3:J:48:THR:HG22	3:J:50:LYS:HG2	1.92	0.51
1:B:212:ASP:HB2	1:B:215:GLU:HG2	1.92	0.51
3:J:274:ASN:ND2	5:L:446:GLN:OE1	2.43	0.51
3:D:690:ASN:ND2	3:D:743:MET:SD	2.83	0.51
2:I:344:GLY:H	2:I:437:ASN:HD21	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:VAL:HG11	1:H:183:ILE:HD11	1.92	0.51
1:H:184:ALA:HB3	1:H:204:GLU:HB3	1.91	0.51
4:E:15:ASN:O	4:E:17:PHE:N	2.43	0.51
1:H:179:PRO:HB3	1:H:211:ILE:HG23	1.92	0.51
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.93	0.51
5:F:95:THR:OG1	5:F:96:ASP:N	2.38	0.51
2:C:1070:HIS:NE2	2:C:1114:GLU:OE2	2.44	0.51
1:H:37:HIS:CE1	1:H:187:VAL:HG21	2.45	0.51
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.93	0.51
2:I:796:LEU:N	2:I:1231:TYR:OH	2.44	0.51
2:C:1065:LYS:HE2	2:C:1235:LEU:HD12	1.92	0.51
5:L:218:ARG:HH11	5:L:218:ARG:CG	2.22	0.51
1:B:41:ASN:HD21	2:C:1217:THR:HG22	1.75	0.51
3:D:1257:VAL:HA	3:D:1260:MET:HE3	1.93	0.50
3:J:46:TYR:CZ	3:J:47:ARG:HG3	2.45	0.50
2:C:548:ARG:O	3:D:780:ARG:NH1	2.45	0.50
2:I:227:LYS:NZ	2:I:334:GLU:OE2	2.35	0.50
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.11	0.50
1:A:52:PRO:HG3	1:A:150:ARG:NH1	2.26	0.50
3:D:294:ASN:HD22	5:F:406:GLN:HE21	1.59	0.50
3:D:865:HIS:HB3	3:D:868:TRP:HD1	1.76	0.50
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.94	0.50
4:K:13:ILE:CG1	4:K:19:LEU:HD13	2.41	0.50
2:C:1101:LEU:HD22	3:D:731:ARG:HB2	1.93	0.50
2:I:890:LYS:HG2	2:I:914:LYS:HE3	1.94	0.50
2:C:300:ASP:OD1	2:C:313:ALA:N	2.43	0.50
1:A:71:LYS:NZ	1:A:139:SER:O	2.45	0.50
2:C:796:LEU:N	2:C:1231:TYR:OH	2.45	0.49
4:E:79:GLU:O	4:E:81:GLN:N	2.44	0.49
1:B:71:LYS:NZ	1:B:139:SER:O	2.45	0.49
2:I:338:THR:HB	2:I:345:PRO:HD3	1.93	0.49
3:D:140:TYR:HD1	3:D:297:ARG:HD3	1.77	0.49
2:I:785:ASP:OD2	2:I:791:LEU:N	2.44	0.49
2:I:1268:GLN:NE2	3:J:352:ARG:HB3	2.27	0.49
3:D:370:LYS:HB3	3:D:409:TRP:CZ3	2.47	0.49
2:C:1226:THR:HG23	3:D:638:SER:OG	2.13	0.49
5:F:218:ARG:CG	5:F:218:ARG:HH11	2.22	0.49
2:I:404:LYS:HE2	2:I:586:PHE:HZ	1.77	0.49
5:L:122:ARG:HG2	5:L:371:LYS:HE2	1.94	0.49
1:H:66:HIS:HD2	1:H:68:TYR:HB3	1.77	0.49
3:D:57:PHE:O	3:D:98:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:338:THR:HG21	2:I:345:PRO:HB3	1.95	0.49
3:D:46:TYR:CZ	3:D:47:ARG:HG3	2.48	0.49
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.13	0.49
1:H:42:ALA:O	1:H:46:ILE:HG12	2.13	0.49
2:C:404:LYS:HE2	2:C:586:PHE:CZ	2.47	0.49
2:C:562:GLU:OE1	2:C:662:SER:OG	2.24	0.49
1:A:44:ARG:HG3	1:A:183:ILE:HB	1.95	0.48
3:J:102:MET:HG2	3:J:246:PRO:HD3	1.94	0.48
3:J:865:HIS:H	3:J:868:TRP:HB2	1.78	0.48
2:C:344:GLY:H	2:C:437:ASN:HD21	1.61	0.48
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.96	0.48
2:I:1243:MET:SD	3:J:445:LYS:HB3	2.53	0.48
1:G:182:ARG:HD2	2:I:1092:THR:HA	1.94	0.48
5:L:277:MET:HE2	5:L:281:ARG:HG3	1.95	0.48
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.96	0.48
3:D:1318:SER:HB2	3:D:1342:ASP:OD2	2.13	0.48
2:I:530:ILE:HG12	2:I:573:ASN:O	2.14	0.48
2:C:903:ARG:O	2:C:907:GLY:N	2.46	0.48
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.11	0.48
2:I:629:PHE:CE2	2:I:634:VAL:HG12	2.49	0.48
2:C:26:TYR:HB2	2:C:29:SER:HB3	1.95	0.48
1:B:196:THR:OG1	1:B:197:ASP:OD1	2.31	0.48
5:F:303:ILE:O	5:F:307:THR:OG1	2.21	0.48
1:B:285:THR:HG23	1:B:288:GLU:H	1.79	0.48
3:J:108:ALA:HB3	3:J:279:LEU:HD23	1.96	0.48
2:C:832:HIS:CE1	2:C:1058:ARG:HB2	2.45	0.48
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.28	0.48
2:C:67:GLU:O	2:C:102:LEU:HD12	2.14	0.48
1:B:91:ARG:NH2	1:B:210:THR:O	2.46	0.48
2:I:1255:THR:HB	2:I:1257:GLN:HG3	1.94	0.48
2:I:717:VAL:HG12	2:I:782:VAL:HA	1.95	0.48
2:I:180:ARG:NH2	2:I:392:GLU:O	2.46	0.48
2:I:701:GLY:O	2:I:1184:THR:N	2.33	0.48
1:B:37:HIS:CD2	2:C:1216:ARG:HG2	2.49	0.47
4:E:16:ARG:O	4:E:19:LEU:HB3	2.14	0.47
5:L:439:ILE:O	5:L:443:ILE:HG13	2.15	0.47
3:J:210:SER:O	3:J:214:ARG:NH2	2.46	0.47
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.47
3:D:1295:ASN:O	3:J:1225:GLY:HA3	2.13	0.47
2:I:703:GLY:N	2:I:705:GLU:OE2	2.46	0.47
2:I:1294:LYS:O	3:J:348:ASP:N	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:HG21	2:C:727:VAL:O	2.15	0.47
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.47	0.47
1:B:37:HIS:CG	2:C:1216:ARG:HG2	2.49	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.74	0.47
3:J:739:GLN:HE21	3:J:744:ARG:HG3	1.79	0.47
1:A:133:LEU:HD21	1:A:140:ILE:HG12	1.97	0.47
3:J:690:ASN:ND2	3:J:743:MET:SD	2.88	0.47
5:F:399:LEU:HD23	5:F:443:ILE:HG22	1.97	0.47
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.96	0.47
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.50	0.47
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.39	0.47
1:B:180:VAL:HA	1:B:207:THR:HA	1.97	0.47
2:C:344:GLY:H	2:C:437:ASN:ND2	2.12	0.46
2:C:151:ARG:HH21	2:C:445:ILE:HG21	1.80	0.46
2:C:48:GLY:C	2:C:50:GLU:H	2.18	0.46
3:D:550:VAL:O	3:D:569:LEU:HA	2.15	0.46
3:J:260:PHE:HB3	5:L:504:PRO:HB3	1.98	0.46
5:L:463:LEU:HD13	5:L:487:MET:SD	2.55	0.46
3:D:317:THR:HA	3:D:323:PRO:HA	1.96	0.46
3:J:647:PRO:HG3	3:J:697:MET:HA	1.96	0.46
3:J:127:LEU:HA	3:J:127:LEU:HD23	1.71	0.46
3:J:556:GLU:O	3:J:558:ASP:N	2.48	0.46
5:F:520:GLY:HA2	5:F:523:ILE:HD12	1.97	0.46
1:B:78:ILE:HD13	1:B:81:ILE:HD12	1.98	0.46
1:G:59:VAL:HG21	1:G:85:LEU:HD13	1.97	0.46
5:L:555:GLU:HB2	5:L:594:ALA:HB2	1.97	0.46
1:A:22:THR:HB	1:A:207:THR:O	2.16	0.46
1:H:82:LEU:O	1:H:86:LYS:HG3	2.15	0.46
1:A:224:LEU:O	1:A:228:LEU:HG	2.16	0.46
2:I:1101:LEU:HD22	3:J:731:ARG:HB2	1.98	0.46
2:I:367:TYR:CD1	2:I:376:PRO:HB3	2.51	0.46
1:H:180:VAL:HA	1:H:207:THR:HA	1.97	0.46
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.97	0.46
3:J:419:HIS:O	3:J:439:PRO:HD2	2.15	0.46
2:I:1186:VAL:HG13	2:I:1187:PHE:HD2	1.81	0.46
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.49	0.46
2:I:300:ASP:OD1	2:I:313:ALA:N	2.43	0.46
3:J:615:LYS:H	4:K:7:GLN:CG	2.29	0.46
2:C:848:GLU:HG2	2:C:888:THR:HA	1.98	0.46
1:B:195:ARG:O	1:B:197:ASP:N	2.43	0.46
2:C:48:GLY:O	2:C:50:GLU:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:144:VAL:HG23	2:I:515:MET:HG2	1.97	0.46
3:J:269:TYR:O	3:J:273:ILE:HG13	2.16	0.46
1:A:27:THR:HG22	1:A:202:VAL:HG13	1.97	0.46
5:L:157:ARG:HG3	5:L:159:SER:H	1.80	0.46
3:J:738:ARG:O	3:J:742:GLY:N	2.48	0.46
5:L:407:GLU:HG3	5:L:442:SER:OG	2.16	0.45
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.16	0.45
5:L:562:ARG:HG2	5:L:576:VAL:HG21	1.99	0.45
1:G:37:HIS:CE1	1:G:187:VAL:HG21	2.51	0.45
3:D:842:ARG:HD2	3:D:842:ARG:HA	1.61	0.45
3:J:425:ARG:HB2	3:J:466:MET:HG2	1.98	0.45
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.51	0.45
3:J:262:THR:HG22	5:L:504:PRO:HB2	1.98	0.45
3:D:603:LYS:O	3:D:607:THR:OG1	2.34	0.45
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.51	0.45
1:A:42:ALA:O	1:A:46:ILE:HG12	2.15	0.45
3:D:461:PHE:C	3:D:463:GLY:H	2.20	0.45
2:C:812:PHE:HB3	3:D:357:VAL:HG21	1.98	0.45
3:J:1160:SER:O	3:J:1162:ILE:N	2.50	0.45
3:J:35:PHE:CD2	3:J:101:ARG:HD3	2.52	0.45
5:L:487:MET:HA	5:L:487:MET:HE2	1.99	0.45
3:D:425:ARG:HB2	3:D:466:MET:HG2	1.97	0.45
1:H:56:VAL:HG12	1:H:173:VAL:HG11	1.99	0.45
3:D:739:GLN:HG3	3:D:744:ARG:HG3	1.97	0.45
2:C:728:ASP:HB3	2:C:731:ARG:H	1.82	0.45
2:I:663:VAL:O	2:I:666:SER:HB2	2.17	0.45
5:F:343:LYS:O	5:F:347:ILE:HG13	2.17	0.45
2:I:206:ALA:O	2:I:209:ILE:HG22	2.16	0.45
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.98	0.45
3:D:678:ARG:NH2	3:D:756:GLU:OE1	2.48	0.45
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.99	0.45
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.81	0.45
2:C:92:TYR:CE2	2:C:129:LEU:HB2	2.51	0.45
1:A:37:HIS:CE1	1:A:187:VAL:HG21	2.51	0.45
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.98	0.45
3:J:1257:VAL:HA	3:J:1260:MET:HE3	1.99	0.45
2:I:1087:TYR:CZ	2:I:1213:TYR:HB2	2.52	0.44
2:C:1221:PHE:HD1	3:D:634:ARG:HA	1.82	0.44
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.48	0.44
3:D:422:LEU:HD22	3:D:484:MET:HE2	1.98	0.44
3:J:842:ARG:HD2	3:J:842:ARG:HA	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:250:LEU:O	5:L:254:GLU:HG2	2.18	0.44
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.86	0.44
5:L:379:MET:O	5:L:383:ASN:ND2	2.50	0.44
3:J:847:ASP:HA	3:J:860:ARG:HB2	1.99	0.44
2:I:682:GLY:O	2:I:686:GLN:HG3	2.17	0.44
1:H:51:MET:HA	1:H:52:PRO:HD3	1.76	0.44
2:I:1333:LEU:HD13	3:J:115:TRP:CZ3	2.52	0.44
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.98	0.44
1:B:66:HIS:HD2	1:B:68:TYR:H	1.66	0.44
3:J:376:LEU:HB3	3:J:470:VAL:HG21	2.00	0.44
4:E:26:ARG:HH21	4:E:37:PRO:CB	2.30	0.44
2:I:1226:THR:HG23	3:J:638:SER:OG	2.18	0.44
5:L:290:LEU:HB3	5:L:333:VAL:HG21	2.00	0.44
2:C:228:VAL:HG23	2:C:337:PHE:HB2	2.00	0.44
1:H:41:ASN:ND2	2:I:1217:THR:HG22	2.32	0.44
1:G:134:THR:HG21	2:I:727:VAL:O	2.18	0.44
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.17	0.44
2:C:645:PHE:CG	2:C:649:GLN:HB2	2.52	0.44
1:B:273:GLU:OE2	1:B:293:PRO:HD2	2.17	0.44
5:L:344:LEU:HD12	5:L:347:ILE:HD12	1.98	0.44
3:J:746:LEU:HD22	3:J:758:PRO:HB3	1.99	0.44
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.99	0.44
3:J:114:ILE:HG13	3:J:114:ILE:H	1.41	0.44
2:I:344:GLY:H	2:I:437:ASN:ND2	2.16	0.44
3:J:857:LEU:HA	3:J:858:VAL:HA	1.57	0.44
3:D:496:GLY:HA3	3:D:903:LEU:HD22	2.00	0.44
2:I:1336:ASN:HA	3:J:33:TRP:HH2	1.83	0.44
2:I:152:SER:OG	2:I:452:ARG:HG2	2.18	0.44
2:I:61:SER:OG	2:I:62:TYR:N	2.51	0.44
2:I:685:MET:SD	2:I:1073:LYS:HD3	2.57	0.44
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.99	0.44
2:C:241:LEU:HD22	2:C:285:ILE:HD13	2.00	0.44
3:J:893:GLY:O	3:J:1258:ARG:NH2	2.45	0.44
2:I:363:LEU:HB3	2:I:381:ALA:HB1	2.00	0.44
5:L:101:TYR:OH	5:L:409:ASN:ND2	2.48	0.43
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.99	0.43
3:J:38:VAL:HG11	3:J:56:LEU:HD23	2.00	0.43
1:B:107:ILE:HG13	1:B:136:GLU:HG3	2.00	0.43
5:F:354:THR:HG22	5:F:357:GLN:HE21	1.83	0.43
3:J:118:LYS:HD2	3:J:118:LYS:HA	1.62	0.43
1:H:86:LYS:HG2	1:H:173:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1146:GLU:CD	3:D:1310:THR:HG1	2.20	0.43
3:J:298:MET:HG2	5:L:402:LEU:HD23	2.00	0.43
1:A:91:ARG:NH2	1:A:209:GLY:O	2.51	0.43
2:I:575:LEU:HG	2:I:579:ALA:HB3	2.00	0.43
1:G:17:GLU:HB3	1:G:25:LYS:HB2	2.00	0.43
5:F:270:VAL:HA	5:F:273:MET:HG3	2.00	0.43
3:J:493:PRO:HG3	3:J:904:ALA:HB2	2.00	0.43
2:C:626:GLU:HA	2:C:627:GLY:C	2.39	0.43
3:D:24:LEU:HD23	3:D:24:LEU:HA	1.91	0.43
1:B:95:LYS:NZ	1:B:96:ASP:H	2.16	0.43
2:I:637:ARG:HG3	2:I:641:GLU:O	2.19	0.43
3:J:264:ASP:HB3	3:J:324:LEU:HB3	2.01	0.43
1:G:41:ASN:HD22	1:G:44:ARG:CZ	2.32	0.43
2:I:1070:HIS:NE2	2:I:1114:GLU:OE2	2.42	0.43
3:D:127:LEU:HD11	3:D:227:PHE:CZ	2.54	0.43
2:C:1177:ARG:C	2:C:1179:GLY:H	2.22	0.43
2:I:1297:ASP:OD1	2:I:1299:ASN:N	2.52	0.43
5:F:555:GLU:HB2	5:F:594:ALA:HB2	2.01	0.43
2:I:264:GLU:HB2	2:I:267:ARG:HG3	2.01	0.43
3:J:361:LEU:HD13	3:J:366:CYS:HA	2.01	0.43
2:I:189:ASP:OD1	2:I:193:ASN:N	2.51	0.43
5:L:95:THR:OG1	5:L:96:ASP:N	2.52	0.43
3:D:38:VAL:HG11	3:D:56:LEU:HD23	2.00	0.43
2:I:975:ILE:HD11	2:I:997:TRP:HE3	1.84	0.43
5:L:551:LEU:CD1	5:L:555:GLU:HG3	2.47	0.42
3:D:113:HIS:CD2	3:D:115:TRP:HB2	2.54	0.42
5:F:409:ASN:O	5:F:413:MET:HG3	2.18	0.42
1:B:56:VAL:HG12	1:B:173:VAL:HG11	2.00	0.42
2:I:15:PHE:HA	2:I:15:PHE:HD1	1.69	0.42
3:J:1332:LEU:HA	3:J:1332:LEU:HD23	1.89	0.42
3:D:686:TRP:CD2	3:D:758:PRO:HG3	2.53	0.42
5:F:277:MET:HE1	5:F:359:LYS:HG2	2.01	0.42
1:A:178:SER:HA	1:A:179:PRO:HD3	1.73	0.42
2:I:56:VAL:HG21	2:I:468:LEU:HB3	2.00	0.42
3:D:353:SER:HB3	3:D:447:ILE:HG13	2.01	0.42
2:I:160:ASP:C	2:I:162:GLY:H	2.23	0.42
2:C:810:TYR:CE1	2:C:1078:LYS:HD3	2.54	0.42
5:L:306:PHE:O	5:L:308:GLY:N	2.52	0.42
5:F:132:CYS:O	5:F:136:GLU:HG3	2.20	0.42
2:I:944:ARG:HH21	2:I:1050:VAL:HG13	1.83	0.42
3:D:101:ARG:O	3:D:246:PRO:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:150:HIS:CE1	2:I:152:SER:HA	2.54	0.42
4:K:13:ILE:CG2	4:K:14:GLY:N	2.83	0.42
2:C:155:VAL:HG12	2:C:405:PHE:HA	2.01	0.42
2:C:255:ILE:HB	2:C:263:VAL:HB	2.01	0.42
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.75	0.42
2:I:40:GLU:O	2:I:73:TYR:OH	2.34	0.42
2:I:246:LEU:HB3	2:I:269:ILE:HD13	2.01	0.42
5:L:300:LYS:HB3	5:L:300:LYS:HE3	1.81	0.42
3:D:865:HIS:H	3:D:868:TRP:HB2	1.84	0.42
5:L:554:ARG:O	5:L:558:VAL:HG23	2.19	0.42
3:J:212:THR:O	3:J:216:LYS:HG2	2.20	0.42
1:H:76:GLU:HB2	1:H:80:GLU:HB2	2.01	0.42
2:C:338:THR:HG21	2:C:345:PRO:HB3	2.01	0.42
3:D:298:MET:HG2	5:F:402:LEU:HD23	2.02	0.42
2:I:890:LYS:HE2	2:I:914:LYS:HG3	2.01	0.42
3:J:646:ILE:HA	3:J:647:PRO:HD3	1.81	0.42
2:I:302:ILE:HG22	2:I:309:LEU:HA	2.02	0.42
3:D:250:ARG:O	3:D:266:ASN:ND2	2.39	0.42
2:I:797:GLY:N	2:I:1231:TYR:OH	2.50	0.42
2:I:1257:GLN:HG2	2:I:1296:ASP:HB3	2.02	0.42
1:A:29:GLU:HB3	1:A:30:PRO:HD3	2.02	0.42
3:D:1221:LEU:HD22	3:D:1306:LEU:HB2	2.02	0.42
3:D:1225:GLY:HA3	3:J:1295:ASN:O	2.20	0.42
2:I:905:ILE:HD11	5:L:598:LEU:HD13	2.02	0.42
1:H:51:MET:HB3	1:H:179:PRO:HD2	2.00	0.42
2:C:38:PHE:HA	2:C:48:GLY:HA2	2.02	0.42
1:B:321:TRP:HA	1:B:322:PRO:HA	1.68	0.42
3:D:632:ALA:O	3:D:635:SER:OG	2.38	0.42
5:F:306:PHE:O	5:F:308:GLY:N	2.53	0.42
5:L:430:TYR:O	5:L:434:TRP:HD1	2.02	0.42
1:G:14:VAL:HB	1:G:29:GLU:HB2	2.02	0.42
1:H:118:ASP:HB3	1:H:121:VAL:HB	2.02	0.42
2:I:1289:GLU:HB3	2:I:1294:LYS:HD2	2.02	0.42
3:J:686:TRP:CD2	3:J:758:PRO:HG3	2.55	0.42
2:C:1253:LEU:HA	5:F:525:ASP:HB2	2.01	0.42
5:L:132:CYS:O	5:L:136:GLU:HG3	2.20	0.42
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.53	0.41
2:I:1251:TYR:HE1	2:I:1258:PRO:HG3	1.85	0.41
1:A:14:VAL:HB	1:A:29:GLU:HB2	2.01	0.41
3:D:779:ALA:O	3:D:783:LEU:HD22	2.20	0.41
2:C:1121:ALA:HB1	2:C:1180:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:524:ILE:O	2:C:528:ARG:HG3	2.20	0.41
5:F:300:LYS:HB3	5:F:300:LYS:HE3	1.81	0.41
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.20	0.41
2:C:1083:GLU:HG2	2:C:1084:ASP:OD1	2.20	0.41
2:I:906:PHE:HB3	2:I:907:GLY:H	1.54	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.88	0.41
1:G:76:GLU:H	1:G:76:GLU:CD	2.24	0.41
2:I:1282:GLY:O	3:J:1361:THR:HG23	2.20	0.41
2:I:1212:LEU:HB3	2:I:1221:PHE:HD2	1.85	0.41
2:C:962:GLU:O	2:C:966:ILE:HG13	2.20	0.41
2:C:1191:LYS:NZ	2:C:1191:LYS:HB2	2.36	0.41
5:L:437:GLN:HG3	5:L:438:ALA:N	2.34	0.41
1:A:150:ARG:HH21	1:B:6:THR:CB	2.34	0.41
1:H:52:PRO:HG3	1:H:150:ARG:NH1	2.35	0.41
3:J:35:PHE:HD2	3:J:101:ARG:HD3	1.84	0.41
2:C:1191:LYS:HB2	2:C:1191:LYS:HZ3	1.85	0.41
2:C:1022:LYS:O	2:C:1026:GLU:HG3	2.20	0.41
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.02	0.41
5:F:355:ILE:HG13	5:F:355:ILE:H	1.52	0.41
1:A:51:MET:HA	1:A:52:PRO:HD3	1.69	0.41
2:I:1022:LYS:O	2:I:1026:GLU:HG3	2.21	0.41
3:J:69:GLU:HG3	3:J:76:LYS:HG2	2.02	0.41
2:I:1118:GLY:HA3	2:I:1229:TYR:O	2.20	0.41
5:L:477:GLU:HA	5:L:478:PRO:HD3	1.81	0.41
2:C:1199:LEU:O	2:C:1204:LEU:N	2.44	0.41
2:C:1336:ASN:N	3:D:23:ALA:O	2.54	0.41
3:J:187:ALA:O	3:J:191:SER:HB2	2.21	0.41
2:C:218:GLU:HG2	2:C:299:LYS:HA	2.01	0.41
1:A:282:VAL:O	1:A:316:MET:N	2.45	0.41
4:K:13:ILE:HG21	4:K:19:LEU:HB2	2.02	0.41
3:D:1360:GLY:HA2	4:E:17:PHE:CD2	2.55	0.41
3:D:278:ARG:HD3	5:F:406:GLN:HB3	2.02	0.41
5:L:402:LEU:HA	5:L:402:LEU:HD12	1.76	0.41
5:L:324:LYS:HB3	5:L:325:PRO:HD2	2.03	0.41
2:C:697:LYS:O	2:C:799:ASN:ND2	2.49	0.41
2:I:976:ARG:HG3	2:I:989:LEU:HD23	2.03	0.41
1:G:42:ALA:O	1:G:46:ILE:HG12	2.21	0.41
5:F:216:LEU:O	5:F:219:GLU:HB3	2.21	0.41
2:I:521:LEU:HD22	2:I:667:LEU:HD12	2.02	0.41
2:I:176:ILE:HD11	2:I:428:VAL:HG21	2.03	0.41
3:J:118:LYS:HB3	3:J:311:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:590:PRO:HD3	2:C:605:TYR:CE2	2.56	0.41
2:C:468:LEU:HD12	2:C:468:LEU:HA	1.94	0.41
3:J:312:ARG:HA	3:J:312:ARG:HD3	1.77	0.41
1:H:37:HIS:HB3	2:I:1216:ARG:HB3	2.02	0.41
2:C:342:ASP:HA	2:C:437:ASN:HB3	2.03	0.41
3:D:842:ARG:NH2	3:D:1254:GLU:OE1	2.54	0.41
4:K:36:ASP:O	4:K:38:LEU:N	2.54	0.41
3:D:573:THR:O	3:D:577:ALA:N	2.43	0.41
3:D:513:MET:O	3:D:575:GLY:HA3	2.20	0.41
2:I:524:ILE:O	2:I:528:ARG:HG3	2.21	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.88	0.41
2:I:726:TYR:HB2	2:I:733:VAL:HB	2.02	0.41
3:J:267:ASP:O	3:J:271:ARG:HG3	2.21	0.41
5:F:344:LEU:HA	5:F:344:LEU:HD12	1.82	0.41
3:J:612:LEU:HA	3:J:612:LEU:HD12	1.96	0.41
2:I:848:GLU:OE2	2:I:888:THR:OG1	2.39	0.41
2:C:939:VAL:O	2:C:941:LYS:N	2.53	0.41
2:I:754:THR:N	2:I:767:GLN:OE1	2.45	0.41
2:I:870:ILE:HG21	2:I:944:ARG:CZ	2.51	0.41
2:C:548:ARG:NE	2:C:569:ILE:O	2.51	0.41
2:I:678:ARG:HD2	2:I:678:ARG:HA	1.86	0.41
5:F:608:ARG:C	5:F:610:PHE:H	2.23	0.41
5:F:590:ILE:HG22	5:F:593:LYS:HE2	2.03	0.40
2:I:404:LYS:HE2	2:I:586:PHE:CZ	2.55	0.40
2:I:666:SER:HA	2:I:1186:VAL:HG21	2.03	0.40
2:C:1020:GLU:O	2:C:1024:GLU:HG2	2.21	0.40
3:D:233:LYS:HA	3:D:234:PRO:HD3	1.89	0.40
2:C:623:LEU:HD12	2:C:629:PHE:HA	2.03	0.40
2:C:27:LEU:HD23	2:C:27:LEU:HA	1.86	0.40
3:D:452:LEU:HG	3:D:625:MET:CE	2.48	0.40
1:H:102:LEU:O	1:H:141:SER:HA	2.21	0.40
3:D:686:TRP:CE3	3:D:758:PRO:HG3	2.56	0.40
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.03	0.40
5:L:277:MET:HE1	5:L:359:LYS:HG2	2.04	0.40
3:J:1225:GLY:O	3:J:1229:VAL:HG23	2.20	0.40
3:D:514:THR:O	3:D:595:ALA:HA	2.21	0.40
3:D:899:TYR:O	3:D:1251:LYS:HD3	2.21	0.40
2:C:1199:LEU:O	2:C:1203:ASP:N	2.54	0.40
1:B:125:LYS:HA	1:B:126:PRO:HD2	1.94	0.40
2:C:1328:LYS:HA	2:C:1328:LYS:HD3	1.86	0.40
1:H:47:LEU:HA	1:H:51:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.83	0.40
5:F:251:LYS:O	5:F:255:VAL:HG23	2.20	0.40
2:I:1030:GLU:O	2:I:1034:ARG:HG3	2.21	0.40
1:G:22:THR:HB	1:G:207:THR:O	2.21	0.40
3:J:232:ASN:ND2	3:J:1337:VAL:O	2.55	0.40
2:C:151:ARG:HB3	2:C:151:ARG:HE	1.81	0.40
5:L:415:ALA:HB2	5:L:434:TRP:HB2	2.03	0.40
2:C:233:ARG:O	2:C:236:LYS:HG2	2.22	0.40
3:D:114:ILE:HD11	3:D:311:ARG:HB3	2.02	0.40
1:A:32:GLU:HB2	1:A:35:PHE:CD2	2.56	0.40
3:J:242:LEU:HA	3:J:243:PRO:HD3	1.92	0.40
2:C:905:ILE:HD11	5:F:598:LEU:HD13	2.04	0.40
2:C:920:VAL:HA	2:C:921:PRO:HD3	1.90	0.40
5:L:509:THR:HA	5:L:510:PRO:HD3	1.90	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	292/335 (87%)	268 (92%)	14 (5%)	10 (3%)	5 43
1	B	281/335 (84%)	257 (92%)	12 (4%)	12 (4%)	3 35
1	G	212/335 (63%)	193 (91%)	14 (7%)	5 (2%)	7 50
1	H	211/335 (63%)	195 (92%)	12 (6%)	4 (2%)	10 54
2	C	1338/1342 (100%)	1259 (94%)	60 (4%)	19 (1%)	14 59
2	I	1338/1342 (100%)	1257 (94%)	65 (5%)	16 (1%)	16 62
3	D	1141/1407 (81%)	1030 (90%)	75 (7%)	36 (3%)	5 44
3	J	1134/1407 (81%)	1026 (90%)	71 (6%)	37 (3%)	5 43
4	E	87/91 (96%)	72 (83%)	6 (7%)	9 (10%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	K	73/91 (80%)	61 (84%)	5 (7%)	7 (10%)	1 14
5	F	456/613 (74%)	437 (96%)	14 (3%)	5 (1%)	17 63
5	L	456/613 (74%)	436 (96%)	14 (3%)	6 (1%)	15 60
All	All	7019/8246 (85%)	6491 (92%)	362 (5%)	166 (2%)	7 50

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	188	GLU
1	A	229	GLU
1	A	319	GLU
1	A	320	ASN
1	B	93	GLN
1	B	188	GLU
1	B	192	VAL
1	B	195	ARG
1	B	319	GLU
1	B	320	ASN
2	C	110	PRO
2	C	214	ASN
2	C	346	TYR
2	C	748	ILE
2	C	1040	ASP
3	D	151	MET
3	D	407	VAL
3	D	539	SER
3	D	588	PRO
3	D	833	GLU
3	D	851	PRO
3	D	859	PRO
3	D	880	VAL
3	D	1153	PRO
3	D	1168	GLU
3	D	1169	THR
3	D	1185	PRO
3	D	1190	ILE
3	D	1191	PRO
3	D	1214	PRO
4	E	16	ARG
4	E	36	ASP

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Mol	Chain	Res	Type
4	E	37	PRO
4	E	40	PRO
4	E	80	LEU
5	F	488	LEU
5	F	490	PRO
1	G	93	GLN
1	G	188	GLU
1	G	231	PHE
1	H	93	GLN
1	H	188	GLU
2	I	9	LYS
2	I	110	PRO
2	I	214	ASN
2	I	346	TYR
2	I	748	ILE
3	J	151	MET
3	J	407	VAL
3	J	528	THR
3	J	539	SER
3	J	587	LEU
3	J	588	PRO
3	J	833	GLU
3	J	851	PRO
3	J	859	PRO
3	J	880	VAL
3	J	1153	PRO
3	J	1168	GLU
3	J	1185	PRO
3	J	1190	ILE
3	J	1191	PRO
3	J	1214	PRO
4	K	36	ASP
4	K	37	PRO
4	K	40	PRO
5	L	488	LEU
5	L	490	PRO
1	A	191	ARG
1	A	323	PRO
1	B	7	GLU
1	B	191	ARG
2	C	909	LYS
2	C	940	GLU

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Mol	Chain	Res	Type
2	C	1154	ASP
2	C	1155	VAL
3	D	555	TYR
3	D	825	VAL
3	D	906	GLY
3	D	1155	ILE
2	I	114	VAL
3	J	420	PRO
3	J	557	LYS
3	J	596	LEU
3	J	906	GLY
3	J	1149	ARG
3	J	1160	SER
3	J	1161	GLY
3	J	1169	THR
3	J	1176	VAL
3	J	1209	VAL
1	A	192	VAL
1	B	13	LEU
1	B	157	THR
2	C	114	VAL
2	C	746	ALA
3	D	420	PRO
3	D	462	ASP
3	D	1150	PRO
4	E	45	LYS
4	E	60	ASN
4	E	79	GLU
5	F	307	THR
2	I	169	LYS
2	I	746	ALA
2	I	941	LYS
3	J	522	GLY
3	J	560	ASN
3	J	1215	GLU
4	K	45	LYS
4	K	60	ASN
5	L	307	THR
1	A	30	PRO
1	B	30	PRO
2	C	40	GLU
2	C	892	GLU

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Mol	Chain	Res	Type
3	D	179	LYS
3	D	564	VAL
3	D	595	ALA
3	D	858	VAL
3	D	1160	SER
3	D	1176	VAL
3	D	1177	ILE
3	D	1208	ASP
2	I	40	GLU
2	I	891	GLY
3	J	462	ASP
3	J	1150	PRO
4	K	15	ASN
4	K	59	ILE
5	L	212	ILE
1	A	230	ALA
1	B	193	GLU
2	C	49	LEU
2	C	61	SER
2	C	741	MET
2	C	1204	LEU
3	D	148	GLU
3	D	834	PRO
3	D	1149	ARG
1	G	29	GLU
1	H	29	GLU
2	I	1203	ASP
2	I	1204	LEU
3	J	593	ASN
3	J	718	SER
2	C	9	LYS
3	D	718	SER
1	H	30	PRO
2	I	741	MET
3	J	1177	ILE
2	C	1181	PRO
3	D	582	ILE
5	F	606	VAL
1	G	30	PRO
3	J	564	VAL
3	J	582	ILE
3	D	828	GLY

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Mol	Chain	Res	Type
5	F	500	ILE
4	E	59	ILE
2	I	1155	VAL
2	I	1181	PRO
3	J	834	PRO
5	L	500	ILE
5	L	606	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/292 (82%)	220 (92%)	19 (8%)	15	54
1	B	233/292 (80%)	215 (92%)	18 (8%)	16	55
1	G	173/292 (59%)	163 (94%)	10 (6%)	25	64
1	H	171/292 (59%)	159 (93%)	12 (7%)	19	58
2	C	822/1157 (71%)	763 (93%)	59 (7%)	18	57
2	I	828/1157 (72%)	770 (93%)	58 (7%)	19	58
3	D	517/1168 (44%)	451 (87%)	66 (13%)	5	31
3	J	515/1168 (44%)	447 (87%)	68 (13%)	5	30
4	E	10/75 (13%)	8 (80%)	2 (20%)	1	13
4	K	9/75 (12%)	8 (89%)	1 (11%)	8	38
5	F	348/540 (64%)	312 (90%)	36 (10%)	9	41
5	L	348/540 (64%)	317 (91%)	31 (9%)	12	48
All	All	4213/7048 (60%)	3833 (91%)	380 (9%)	12	47

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	14	VAL
1	A	29	GLU

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Mol	Chain	Res	Type
1	A	67	GLU
1	A	88	LEU
1	A	95	LYS
1	A	102	LEU
1	A	117	HIS
1	A	131	CYS
1	A	140	ILE
1	A	143	ARG
1	A	171	LEU
1	A	173	VAL
1	A	178	SER
1	A	210	THR
1	A	254	LEU
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP
1	B	12	ARG
1	B	29	GLU
1	B	88	LEU
1	B	95	LYS
1	B	102	LEU
1	B	117	HIS
1	B	131	CYS
1	B	140	ILE
1	B	143	ARG
1	B	171	LEU
1	B	173	VAL
1	B	178	SER
1	B	196	THR
1	B	205	MET
1	B	254	LEU
1	B	318	LEU
1	B	319	GLU
1	B	321	TRP
2	C	15	PHE
2	C	24	VAL
2	C	71	VAL
2	C	90	VAL
2	C	117	ILE
2	C	135	THR
2	C	150	HIS
2	C	151	ARG

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Mol	Chain	Res	Type
2	C	378	ARG
2	C	451	ARG
2	C	478	ARG
2	C	486	THR
2	C	525	THR
2	C	529	ARG
2	C	538	LEU
2	C	542	ARG
2	C	547	VAL
2	C	554	HIS
2	C	574	SER
2	C	581	THR
2	C	595	THR
2	C	600	THR
2	C	602	GLU
2	C	610	GLU
2	C	634	VAL
2	C	635	THR
2	C	657	THR
2	C	666	SER
2	C	678	ARG
2	C	692	THR
2	C	694	ARG
2	C	731	ARG
2	C	754	THR
2	C	761	GLN
2	C	776	PRO
2	C	818	VAL
2	C	823	VAL
2	C	830	THR
2	C	878	THR
2	C	896	THR
2	C	902	LEU
2	C	917	SER
2	C	936	ARG
2	C	1029	LEU
2	C	1042	LEU
2	C	1056	VAL
2	C	1057	LYS
2	C	1075	VAL
2	C	1186	VAL
2	C	1191	LYS

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Mol	Chain	Res	Type
2	C	1197	GLU
2	C	1216	ARG
2	C	1226	THR
2	C	1239	VAL
2	C	1250	SER
2	C	1293	VAL
2	C	1298	VAL
2	C	1302	THR
2	C	1341	ASP
3	D	42	GLU
3	D	58	CYS
3	D	92	VAL
3	D	93	THR
3	D	118	LYS
3	D	167	ASP
3	D	191	SER
3	D	193	ASP
3	D	208	THR
3	D	218	THR
3	D	232	ASN
3	D	240	THR
3	D	250	ARG
3	D	254	PRO
3	D	272	VAL
3	D	301	GLU
3	D	311	ARG
3	D	312	ARG
3	D	352	ARG
3	D	374	LEU
3	D	392	THR
3	D	401	VAL
3	D	419	HIS
3	D	420	PRO
3	D	430	HIS
3	D	491	LEU
3	D	505	ASP
3	D	514	THR
3	D	607	THR
3	D	612	LEU
3	D	616	PRO
3	D	635	SER
3	D	638	SER

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Mol	Chain	Res	Type
3	D	646	ILE
3	D	661	VAL
3	D	674	THR
3	D	690	ASN
3	D	721	SER
3	D	738	ARG
3	D	739	GLN
3	D	743	MET
3	D	753	SER
3	D	764	ARG
3	D	767	LEU
3	D	769	VAL
3	D	781	LYS
3	D	783	LEU
3	D	785	ASP
3	D	786	THR
3	D	790	THR
3	D	810	THR
3	D	816	THR
3	D	842	ARG
3	D	844	THR
3	D	862	THR
3	D	869	CYS
3	D	877	VAL
3	D	880	VAL
3	D	886	VAL
3	D	894	VAL
3	D	913	GLU
3	D	1226	VAL
3	D	1265	THR
3	D	1282	TYR
3	D	1316	THR
3	D	1355	ARG
4	E	4	VAL
4	E	10	VAL
5	F	107	THR
5	F	137	TYR
5	F	154	GLU
5	F	158	LEU
5	F	159	SER
5	F	218	ARG
5	F	235	ILE

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Mol	Chain	Res	Type
5	F	262	VAL
5	F	264	LYS
5	F	266	PHE
5	F	273	MET
5	F	309	ASN
5	F	333	VAL
5	F	336	GLU
5	F	354	THR
5	F	360	ASP
5	F	374	ARG
5	F	397	ARG
5	F	400	GLN
5	F	401	PHE
5	F	420	GLU
5	F	421	TYR
5	F	425	TYR
5	F	437	GLN
5	F	479	THR
5	F	480	PRO
5	F	513	ASP
5	F	526	THR
5	F	527	THR
5	F	537	THR
5	F	544	THR
5	F	551	LEU
5	F	552	THR
5	F	554	ARG
5	F	569	THR
5	F	584	ARG
1	G	14	VAL
1	G	88	LEU
1	G	95	LYS
1	G	102	LEU
1	G	117	HIS
1	G	131	CYS
1	G	140	ILE
1	G	171	LEU
1	G	173	VAL
1	G	182	ARG
1	H	14	VAL
1	H	88	LEU
1	H	95	LYS

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Mol	Chain	Res	Type
1	H	102	LEU
1	H	117	HIS
1	H	131	CYS
1	H	140	ILE
1	H	171	LEU
1	H	173	VAL
1	H	182	ARG
1	H	210	THR
1	H	211	ILE
2	I	15	PHE
2	I	24	VAL
2	I	79	VAL
2	I	150	HIS
2	I	151	ARG
2	I	378	ARG
2	I	451	ARG
2	I	456	VAL
2	I	478	ARG
2	I	529	ARG
2	I	530	ILE
2	I	538	LEU
2	I	542	ARG
2	I	547	VAL
2	I	554	HIS
2	I	574	SER
2	I	595	THR
2	I	600	THR
2	I	602	GLU
2	I	610	GLU
2	I	634	VAL
2	I	635	THR
2	I	657	THR
2	I	666	SER
2	I	678	ARG
2	I	692	THR
2	I	694	ARG
2	I	717	VAL
2	I	731	ARG
2	I	761	GLN
2	I	776	PRO
2	I	789	THR
2	I	818	VAL

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Mol	Chain	Res	Type
2	I	823	VAL
2	I	857	VAL
2	I	888	THR
2	I	893	THR
2	I	896	THR
2	I	902	LEU
2	I	903	ARG
2	I	914	LYS
2	I	917	SER
2	I	936	ARG
2	I	1029	LEU
2	I	1042	LEU
2	I	1075	VAL
2	I	1184	THR
2	I	1191	LYS
2	I	1197	GLU
2	I	1216	ARG
2	I	1226	THR
2	I	1239	VAL
2	I	1250	SER
2	I	1262	LYS
2	I	1293	VAL
2	I	1296	ASP
2	I	1298	VAL
2	I	1341	ASP
3	J	42	GLU
3	J	58	CYS
3	J	92	VAL
3	J	93	THR
3	J	114	ILE
3	J	118	LYS
3	J	167	ASP
3	J	191	SER
3	J	193	ASP
3	J	232	ASN
3	J	250	ARG
3	J	254	PRO
3	J	301	GLU
3	J	311	ARG
3	J	312	ARG
3	J	352	ARG
3	J	374	LEU

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Mol	Chain	Res	Type
3	J	419	HIS
3	J	430	HIS
3	J	491	LEU
3	J	501	VAL
3	J	505	ASP
3	J	514	THR
3	J	612	LEU
3	J	616	PRO
3	J	635	SER
3	J	638	SER
3	J	673	VAL
3	J	674	THR
3	J	690	ASN
3	J	721	SER
3	J	738	ARG
3	J	739	GLN
3	J	740	LEU
3	J	743	MET
3	J	753	SER
3	J	760	THR
3	J	764	ARG
3	J	767	LEU
3	J	769	VAL
3	J	776	THR
3	J	777	HIS
3	J	781	LYS
3	J	783	LEU
3	J	785	ASP
3	J	786	THR
3	J	790	THR
3	J	802	ASP
3	J	810	THR
3	J	816	THR
3	J	842	ARG
3	J	862	THR
3	J	864	LEU
3	J	868	TRP
3	J	869	CYS
3	J	877	VAL
3	J	880	VAL
3	J	885	VAL
3	J	894	VAL

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Mol	Chain	Res	Type
3	J	903	LEU
3	J	913	GLU
3	J	1226	VAL
3	J	1265	THR
3	J	1280	VAL
3	J	1282	TYR
3	J	1316	THR
3	J	1353	VAL
3	J	1355	ARG
4	K	4	VAL
5	L	107	THR
5	L	137	TYR
5	L	154	GLU
5	L	158	LEU
5	L	159	SER
5	L	218	ARG
5	L	264	LYS
5	L	266	PHE
5	L	273	MET
5	L	309	ASN
5	L	333	VAL
5	L	336	GLU
5	L	354	THR
5	L	360	ASP
5	L	374	ARG
5	L	397	ARG
5	L	401	PHE
5	L	420	GLU
5	L	421	TYR
5	L	425	TYR
5	L	437	GLN
5	L	446	GLN
5	L	479	THR
5	L	480	PRO
5	L	497	VAL
5	L	513	ASP
5	L	552	THR
5	L	554	ARG
5	L	569	THR
5	L	584	ARG
5	L	586	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	41	ASN
1	A	75	GLN
1	A	128	HIS
1	A	147	GLN
1	A	283	GLN
1	A	320	ASN
1	B	37	HIS
1	B	41	ASN
1	B	66	HIS
1	B	128	HIS
1	B	147	GLN
1	B	227	GLN
1	B	283	GLN
1	B	320	ASN
2	C	150	HIS
2	C	437	ASN
2	C	832	HIS
2	C	955	GLN
2	C	1013	GLN
2	C	1023	HIS
2	C	1257	GLN
3	D	113	HIS
3	D	294	ASN
3	D	424	ASN
3	D	690	ASN
3	D	777	HIS
3	D	1218	HIS
3	D	1326	GLN
5	F	128	ASN
5	F	129	GLN
5	F	131	GLN
5	F	309	ASN
5	F	357	GLN
5	F	383	ASN
5	F	437	GLN
5	F	472	GLN
1	G	37	HIS
1	G	41	ASN
1	G	128	HIS
1	G	147	GLN
1	G	227	GLN

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Mol	Chain	Res	Type
1	H	37	HIS
1	H	41	ASN
1	H	66	HIS
1	H	128	HIS
1	H	147	GLN
2	I	150	HIS
2	I	437	ASN
2	I	955	GLN
2	I	1013	GLN
2	I	1023	HIS
2	I	1061	GLN
3	J	274	ASN
3	J	477	GLN
3	J	690	ASN
3	J	777	HIS
3	J	897	HIS
3	J	1326	GLN
5	L	128	ASN
5	L	129	GLN
5	L	131	GLN
5	L	309	ASN
5	L	357	GLN
5	L	437	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	298/335 (88%)	0.26	23 (7%) 16 11	27, 114, 296, 459	0
1	B	287/335 (85%)	0.66	40 (13%) 4 4	36, 191, 420, 550	0
1	G	216/335 (64%)	0.33	10 (4%) 36 26	33, 168, 289, 370	0
1	H	215/335 (64%)	0.65	33 (15%) 3 3	68, 188, 341, 524	0
2	C	1340/1342 (99%)	0.16	88 (6%) 22 14	2, 102, 402, 550	1 (0%)
2	I	1340/1342 (99%)	0.40	146 (10%) 7 6	3, 144, 388, 550	1 (0%)
3	D	1147/1407 (81%)	-0.18	21 (1%) 71 61	3, 72, 236, 550	0
3	J	1140/1407 (81%)	-0.09	33 (2%) 55 42	3, 96, 268, 550	0
4	E	89/91 (97%)	-0.66	0 100 100	6, 76, 206, 285	0
4	K	75/91 (82%)	0.07	1 (1%) 79 70	47, 171, 393, 535	0
5	F	464/613 (75%)	0.35	46 (9%) 9 7	21, 149, 369, 550	0
5	L	464/613 (75%)	0.35	41 (8%) 12 9	31, 169, 397, 550	0
All	All	7075/8246 (85%)	0.17	482 (6%) 20 13	2, 121, 352, 550	2 (0%)

All (482) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1000	LEU	17.4
5	L	315	TRP	15.7
2	C	311	CYS	15.4
2	C	305	SER	12.6
2	I	999	GLU	12.2
2	I	1001	GLY	12.2
2	C	288	PRO	10.9
2	C	287	VAL	9.4
2	I	998	LEU	9.2
2	C	291	TYR	8.9
2	I	981	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	318	LEU	8.3
5	L	316	PHE	8.2
5	F	315	TRP	8.0
1	H	193	GLU	7.7
2	I	985	GLU	7.6
5	F	319	ALA	7.6
2	C	252	SER	7.5
2	I	982	GLY	7.5
2	I	234	ASP	7.2
2	I	1005	GLU	7.1
2	C	318	SER	7.0
5	L	337	VAL	6.5
2	C	65	ASN	6.4
2	I	979	LEU	6.3
5	F	316	PHE	6.3
2	I	334	GLU	6.2
2	C	332	ARG	6.1
2	C	265	LYS	6.0
1	H	55	ALA	5.9
5	L	305	LEU	5.9
5	F	317	ASN	5.9
2	I	203	LYS	5.8
2	C	304	GLU	5.7
2	C	331	LYS	5.7
5	F	336	GLU	5.7
2	C	322	LEU	5.7
1	H	146	VAL	5.6
1	B	260	LEU	5.6
1	A	262	LEU	5.6
2	C	230	PHE	5.5
5	L	336	GLU	5.5
5	F	305	LEU	5.5
2	C	333	ILE	5.5
2	C	253	PHE	5.5
2	C	270	THR	5.5
2	I	333	ILE	5.4
5	L	490	PRO	5.4
2	I	108	GLU	5.3
2	C	325	LEU	5.3
2	I	771	VAL	5.2
2	I	1021	LEU	5.2
5	L	306	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	5.2
2	I	263	VAL	5.2
1	H	172	LEU	5.2
2	I	494	ASN	5.1
3	D	1173	ARG	5.1
1	B	262	LEU	5.1
2	I	262	TYR	5.0
3	J	1203	ARG	5.0
2	C	166	SER	5.0
5	F	355	ILE	4.9
2	C	264	GLU	4.9
5	F	318	ALA	4.8
2	C	330	HIS	4.8
2	C	292	ILE	4.8
2	C	336	LEU	4.8
2	C	298	ALA	4.8
2	I	1004	ASP	4.7
2	I	389	PHE	4.7
1	A	269	CYS	4.7
5	L	340	ALA	4.7
2	I	231	GLU	4.6
5	L	487	MET	4.6
2	I	1006	GLU	4.6
2	I	980	VAL	4.6
2	C	205	PRO	4.6
1	B	55	ALA	4.6
2	C	286	GLU	4.6
3	D	69	GLU	4.4
2	I	252	SER	4.4
1	B	317	ARG	4.4
2	I	232	ILE	4.4
1	B	259	ASP	4.4
1	H	194	GLN	4.3
2	C	251	ALA	4.3
1	H	100	LEU	4.3
2	I	305	SER	4.3
5	F	337	VAL	4.3
2	C	257	ALA	4.3
1	B	283	GLN	4.3
5	L	307	THR	4.2
5	F	155	GLU	4.2
2	I	1017	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	I	974	ARG	4.2
2	I	116	ASP	4.2
2	C	321	LEU	4.2
5	L	234	THR	4.2
2	I	1020	GLU	4.2
2	I	204	LEU	4.2
2	C	285	ILE	4.1
5	F	323	ASN	4.1
5	F	158	LEU	4.1
2	I	489	PRO	4.1
1	B	98	VAL	4.1
2	I	450	ASN	4.1
2	C	290	GLU	4.1
1	G	90	VAL	4.1
2	I	235	ASN	4.1
1	B	295	LEU	4.1
5	F	423	ARG	4.1
2	C	113	THR	4.0
2	I	976	ARG	4.0
1	H	90	VAL	4.0
2	I	243	PRO	4.0
2	I	983	GLY	4.0
2	I	915	ASP	4.0
1	B	146	VAL	3.9
3	J	1161	GLY	3.9
1	B	69	SER	3.9
5	L	318	ALA	3.9
2	C	338	THR	3.9
1	H	92	VAL	3.9
2	C	235	ASN	3.9
2	I	151	ARG	3.9
2	I	978	VAL	3.8
2	I	254	ASP	3.8
2	C	207	THR	3.8
1	G	91	ARG	3.8
2	I	482	GLY	3.8
5	F	331	HIS	3.8
2	C	232	ILE	3.8
2	C	239	MET	3.8
2	C	314	ASN	3.8
2	I	246	LEU	3.8
2	I	265	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	303	ILE	3.8
5	L	489	MET	3.7
2	I	205	PRO	3.7
5	F	478	PRO	3.7
2	I	1007	LYS	3.7
3	J	69	GLU	3.7
2	C	269	ILE	3.7
3	D	562	GLU	3.7
2	C	165	HIS	3.7
5	L	341	LEU	3.6
2	C	301	TYR	3.6
1	A	29	GLU	3.6
2	C	350	THR	3.6
2	I	493	ILE	3.6
2	I	937	ASP	3.6
1	B	281	LEU	3.6
1	H	56	VAL	3.6
1	A	266	SER	3.6
1	B	296	GLY	3.6
5	L	330	LEU	3.5
2	I	987	GLU	3.5
2	I	994	ARG	3.5
1	H	176	CYS	3.5
2	C	256	GLU	3.5
2	C	259	GLY	3.4
2	I	301	TYR	3.4
5	L	420	GLU	3.4
5	L	304	THR	3.4
5	L	310	GLU	3.4
2	I	995	ASP	3.4
5	L	321	ALA	3.4
1	B	144	ILE	3.4
2	I	442	VAL	3.4
1	B	314	LEU	3.4
2	C	317	LEU	3.4
2	I	15	PHE	3.4
1	H	121	VAL	3.4
2	I	882	ILE	3.4
1	B	78	ILE	3.3
2	I	647	ARG	3.3
5	L	322	MET	3.3
5	F	314	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	95	LYS	3.3
2	C	337	PHE	3.3
3	J	1195	GLN	3.3
2	C	258	ASN	3.3
2	I	166	SER	3.3
2	I	1009	ASN	3.2
2	I	269	ILE	3.2
1	A	281	LEU	3.2
2	I	390	PHE	3.2
1	B	313	SER	3.2
1	B	201	LEU	3.2
2	I	1012	GLU	3.2
1	B	172	LEU	3.2
2	C	985	GLU	3.2
1	B	131	CYS	3.2
1	H	123	ILE	3.2
5	F	287	ILE	3.2
2	I	492	MET	3.1
2	I	1025	PHE	3.1
2	C	1000	LEU	3.1
2	C	208	ILE	3.1
2	I	944	ARG	3.1
2	I	59	ILE	3.1
2	C	246	LEU	3.1
3	J	543	SER	3.1
1	A	204	GLU	3.1
2	C	196	VAL	3.1
5	F	487	MET	3.1
2	I	227	LYS	3.1
2	I	975	ILE	3.1
2	I	111	GLU	3.1
3	D	1204	VAL	3.1
3	J	1162	ILE	3.0
2	I	115	LYS	3.0
5	L	325	PRO	3.0
1	A	271	LYS	3.0
1	G	54	CYS	3.0
2	C	1002	LEU	3.0
2	I	420	LEU	3.0
1	H	98	VAL	3.0
3	J	1204	VAL	3.0
2	I	1018	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	148	ARG	3.0
1	B	309	SER	3.0
2	C	263	VAL	3.0
2	C	56	VAL	3.0
5	L	344	LEU	3.0
5	F	280	VAL	3.0
5	F	234	THR	2.9
2	C	289	VAL	2.9
2	I	225	PHE	2.9
2	I	388	LEU	2.9
5	F	344	LEU	2.9
2	I	1008	GLN	2.9
2	C	224	PHE	2.9
3	J	670	SER	2.9
3	J	659	ALA	2.9
5	F	259	PHE	2.9
2	I	268	ARG	2.9
2	I	311	CYS	2.9
5	F	320	ILE	2.9
2	I	988	LYS	2.9
1	A	275	ILE	2.9
2	C	594	VAL	2.9
1	H	96	ASP	2.9
1	A	272	ALA	2.9
2	I	984	VAL	2.9
2	C	255	ILE	2.9
2	I	443	ASP	2.9
2	I	986	ALA	2.8
3	J	1214	PRO	2.8
2	I	276	GLN	2.8
5	F	261	LEU	2.8
1	B	319	GLU	2.8
2	I	1003	THR	2.8
2	I	233	ARG	2.8
2	I	251	ALA	2.8
1	A	205	MET	2.8
2	I	336	LEU	2.8
3	J	529	GLY	2.8
1	B	302	GLU	2.8
3	D	1174	ARG	2.8
2	I	239	MET	2.8
2	I	198	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
5	F	284	GLU	2.8
5	F	310	GLU	2.8
2	C	172	TYR	2.8
3	J	68	TYR	2.8
2	C	299	LYS	2.8
1	B	266	SER	2.8
2	I	274	ILE	2.8
2	I	972	PHE	2.8
5	F	301	ASN	2.8
5	F	326	TRP	2.8
2	C	1001	GLY	2.8
2	C	373	GLY	2.7
5	F	293	GLU	2.7
5	L	425	TYR	2.7
1	G	19	VAL	2.7
2	I	862	LEU	2.7
1	H	67	GLU	2.7
3	J	91	GLU	2.7
2	I	304	GLU	2.7
2	I	787	PRO	2.7
2	C	206	ALA	2.7
2	C	634	VAL	2.7
3	D	62	PHE	2.7
2	C	234	ASP	2.7
2	I	102	LEU	2.7
2	C	273	HIS	2.7
5	F	313	ASP	2.7
2	C	306	THR	2.6
1	B	97	GLU	2.6
3	D	1299	GLY	2.6
1	H	13	LEU	2.6
3	D	1175	LEU	2.6
3	J	528	THR	2.6
3	D	312	ARG	2.6
5	L	319	ALA	2.6
3	D	204	GLU	2.6
2	I	58	PRO	2.6
5	L	284	GLU	2.6
5	F	321	ALA	2.6
5	L	331	HIS	2.5
1	G	121	VAL	2.5
2	I	1016	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	567	THR	2.5
3	J	1212	ASP	2.5
2	C	326	SER	2.5
2	C	310	ILE	2.5
2	I	273	HIS	2.5
3	J	512	TYR	2.5
2	C	194	LEU	2.5
5	F	325	PRO	2.5
1	H	54	CYS	2.5
2	I	374	GLU	2.5
2	C	353	VAL	2.5
3	J	217	LEU	2.5
2	C	153	PRO	2.5
5	F	153	ALA	2.5
1	H	205	MET	2.5
2	I	230	PHE	2.5
5	L	416	VAL	2.5
5	L	338	HIS	2.5
1	A	253	LEU	2.5
1	H	149	GLY	2.5
2	I	255	ILE	2.5
2	I	1190	ALA	2.5
2	C	979	LEU	2.5
1	H	91	ARG	2.5
3	J	220	ARG	2.5
1	B	171	LEU	2.5
2	I	241	LEU	2.5
5	L	314	THR	2.5
1	A	300	LEU	2.5
2	C	376	PRO	2.5
2	I	597	GLY	2.5
2	I	1072	ASN	2.4
3	D	220	ARG	2.4
2	I	722	GLY	2.4
2	I	332	ARG	2.4
2	I	989	LEU	2.4
2	I	224	PHE	2.4
2	I	867	GLU	2.4
3	J	1208	ASP	2.4
1	A	295	LEU	2.4
2	C	645	PHE	2.4
2	C	324	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	59	VAL	2.4
2	I	441	GLU	2.4
1	A	267	ALA	2.4
3	J	82	GLY	2.4
2	I	206	ALA	2.4
1	G	193	GLU	2.4
2	I	282	VAL	2.4
5	F	277	MET	2.4
1	H	209	GLY	2.4
2	I	1024	GLU	2.4
2	I	153	PRO	2.4
3	J	520	ALA	2.4
2	C	260	LYS	2.4
1	H	94	GLY	2.4
1	B	100	LEU	2.4
2	I	14	ASP	2.4
3	D	75	TYR	2.4
5	F	322	MET	2.3
1	A	273	GLU	2.3
2	I	734	ILE	2.3
5	F	330	LEU	2.3
2	C	164	THR	2.3
2	I	373	GLY	2.3
2	C	312	ALA	2.3
1	H	144	ILE	2.3
1	G	192	VAL	2.3
1	A	294	ASN	2.3
2	C	354	ASP	2.3
2	I	340	ASP	2.3
2	I	721	GLY	2.3
2	I	302	ILE	2.3
1	B	280	ASP	2.3
2	I	725	GLN	2.3
5	F	340	ALA	2.3
5	L	237	ALA	2.3
2	C	236	LYS	2.3
1	G	17	GLU	2.3
3	D	1157	ALA	2.3
1	B	68	TYR	2.3
1	A	278	ILE	2.3
5	F	235	ILE	2.3
1	H	52	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	1171	GLY	2.3
5	F	306	PHE	2.3
5	L	333	VAL	2.3
2	I	68	LEU	2.3
2	C	355	PRO	2.3
5	F	466	ILE	2.3
1	B	293	PRO	2.2
2	I	451	ARG	2.3
3	D	1225	GLY	2.3
1	A	54	CYS	2.2
2	I	883	LEU	2.2
2	I	892	GLU	2.2
1	A	9	LEU	2.2
3	J	319	SER	2.2
5	F	283	GLN	2.2
1	A	268	ASN	2.2
5	L	580	PHE	2.2
3	D	90	VAL	2.2
3	D	825	VAL	2.2
3	D	1169	THR	2.2
2	I	641	GLU	2.2
1	B	312	LEU	2.2
2	I	971	LEU	2.2
3	J	678	ARG	2.2
5	F	416	VAL	2.2
5	L	309	ASN	2.2
1	B	263	THR	2.2
2	I	1010	GLN	2.2
4	K	37	PRO	2.2
1	B	316	MET	2.2
5	L	312	SER	2.2
2	I	1067	ALA	2.2
1	H	171	LEU	2.2
3	D	68	TYR	2.2
2	I	264	GLU	2.2
1	H	88	LEU	2.2
1	H	208	ASN	2.2
5	L	311	THR	2.2
3	J	645	VAL	2.2
1	H	57	THR	2.2
2	I	555	TYR	2.2
1	B	147	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	J	218	THR	2.2
2	I	21	VAL	2.2
2	I	46	GLN	2.1
1	B	66	HIS	2.1
2	I	428	VAL	2.1
3	J	320	ASN	2.1
1	B	58	GLU	2.1
2	C	249	GLU	2.1
1	G	211	ILE	2.1
2	C	650	VAL	2.1
3	J	673	VAL	2.1
2	C	997	TRP	2.1
2	I	183	TRP	2.1
1	A	260	LEU	2.1
2	C	347	ILE	2.1
2	I	190	PRO	2.1
2	I	291	TYR	2.1
3	J	227	PHE	2.1
1	B	310	ARG	2.1
5	F	154	GLU	2.1
5	F	328	GLU	2.1
1	B	52	PRO	2.1
1	H	147	GLN	2.1
2	I	172	TYR	2.1
5	L	423	ARG	2.1
3	J	76	LYS	2.1
3	D	210	SER	2.1
2	I	107	ARG	2.1
5	L	235	ILE	2.1
1	H	210	THR	2.1
2	I	973	SER	2.1
2	I	977	ALA	2.1
5	L	317	ASN	2.1
1	A	289	LEU	2.1
1	H	122	GLU	2.1
2	C	313	ALA	2.1
3	J	1152	GLU	2.1
5	L	421	TYR	2.0
2	I	733	VAL	2.0
3	J	518	VAL	2.0
2	I	997	TRP	2.0
3	J	663	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
5	F	421	TYR	2.0
3	J	481	ARG	2.0
5	L	409	ASN	2.0
2	I	850	ILE	2.0
2	I	1002	LEU	2.0
2	I	1029	LEU	2.0
5	L	165	PHE	2.0
1	H	97	GLU	2.0
5	F	137	TYR	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
7	ZN	D	2002	1/1	0.99	0.20	-0.72	68,68,68,68	0
7	ZN	J	2002	1/1	1.00	0.19	-1.09	63,63,63,63	0
7	ZN	J	2001	1/1	0.99	0.09	-1.57	104,104,104,104	0
7	ZN	D	2001	1/1	0.99	0.07	-2.75	83,83,83,83	0
6	MG	D	2000	1/1	0.75	0.35	-	320,320,320,320	0
6	MG	J	2000	1/1	0.39	0.36	-	396,396,396,396	0

6.5 Other polymers (i)

There are no such residues in this entry.