Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:58 AM GMT

PDB ID	:	3CQZ
Title	:	Crystal structure of 10 subunit RNA polymerase II in complex with the inhibitor alpha-amanitin
Authors	:	Kaplan, C.D.; Larsson, K.-M.; Kornberg, R.D.
Deposited on	:	2008-04-03
Resolution	:	2.80 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:

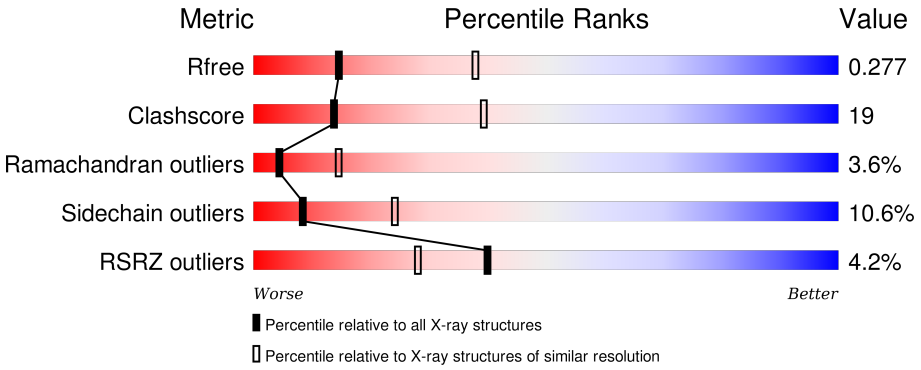
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	1733	3% 50% 22% 22%
2	B	1224	4% 57% 24% 13%
3	C	318	2% 57% 23% 17%
4	E	215	3% 60% 27% 10%
5	F	155	% 40% 12% 46%

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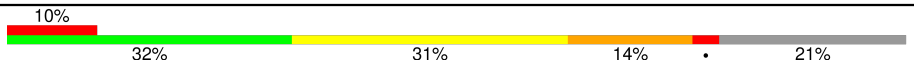
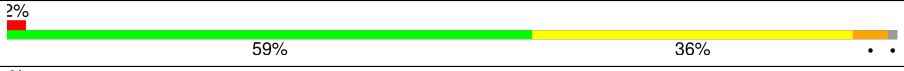
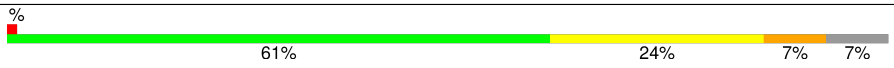
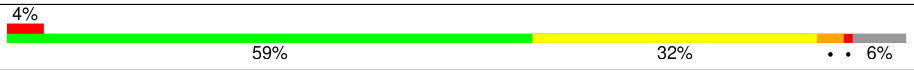
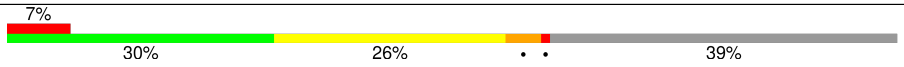
Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	M	8	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27340 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 II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1349	Total	C	N	O	S	0	0	0
			10616	6710	1838	2009	59			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1061	Total	C	N	O	S	0	0	0
			8419	5340	1465	1563	51			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2087	1313	347	414	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	116	Total	C	N	O	S	0	0	0
			932	589	154	185	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			989	608	181	190	10			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	113	Total	C	N	O	S	0	0	0
			911	585	155	170	1			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	43	Total	C	N	O	S	0	0	0
			342	211	68	59	4			

- Molecule 11 is a protein called ALPHA-AMANITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	I	2	Total Zn 2 2	0	0
12	C	1	Total Zn 1 1	0	0
12	A	2	Total Zn 2 2	0	0
12	L	1	Total Zn 1 1	0	0

- Molecule 13 is water.

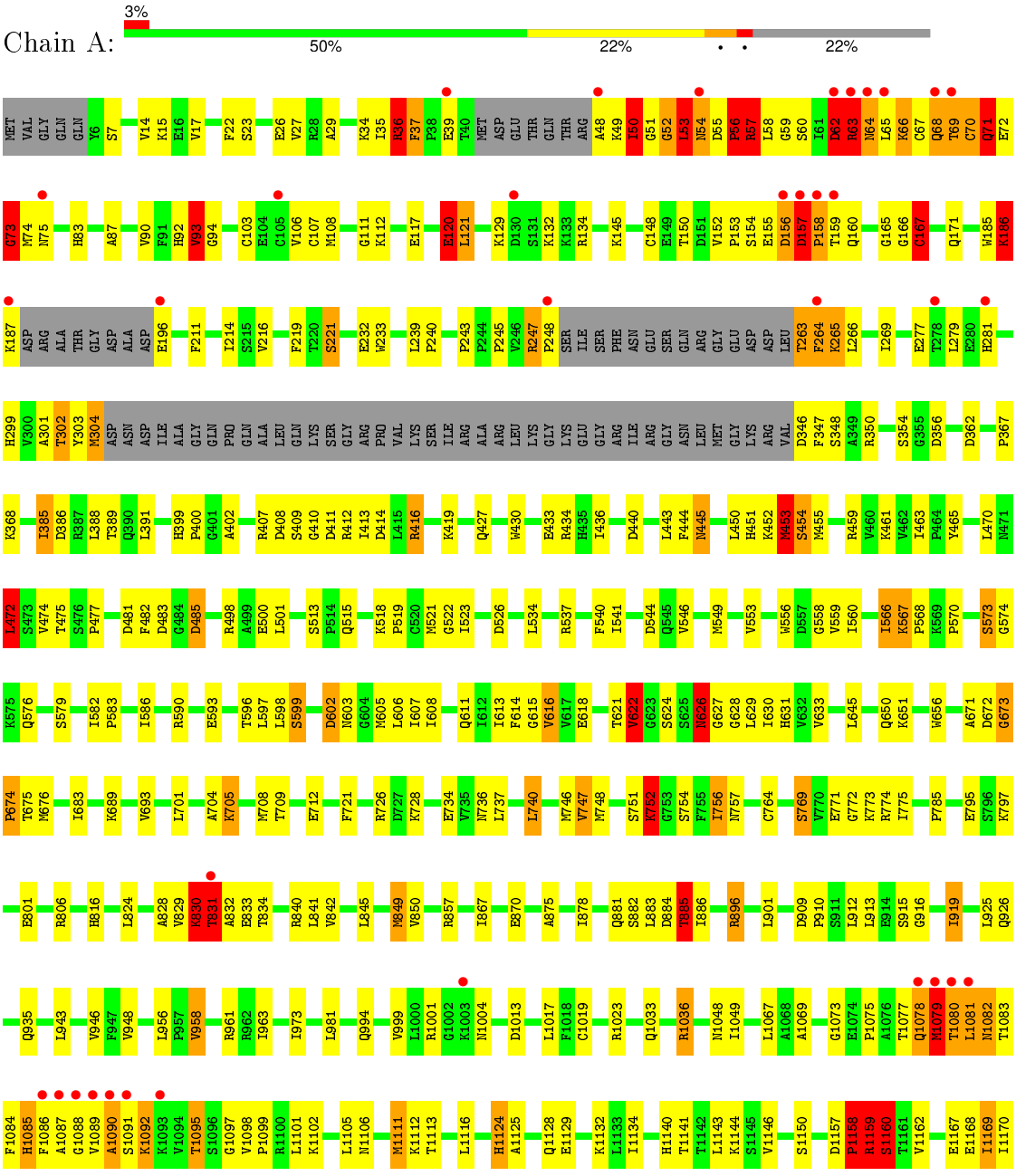
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	11	Total O 11 11	0	0
13	B	4	Total O 4 4	0	0
13	E	1	Total O 1 1	0	0
13	F	1	Total O 1 1	0	0

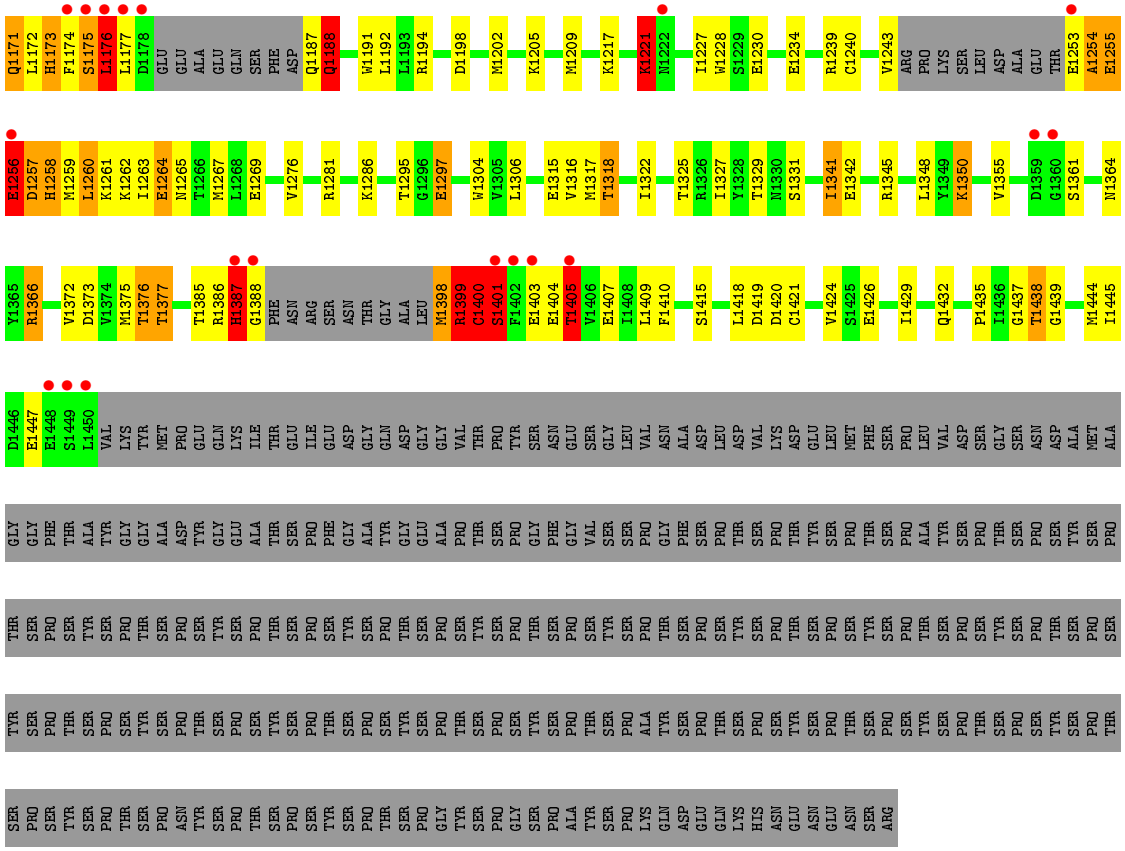
3 Residue-property plots (i)

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 II SUBUNIT RPB1

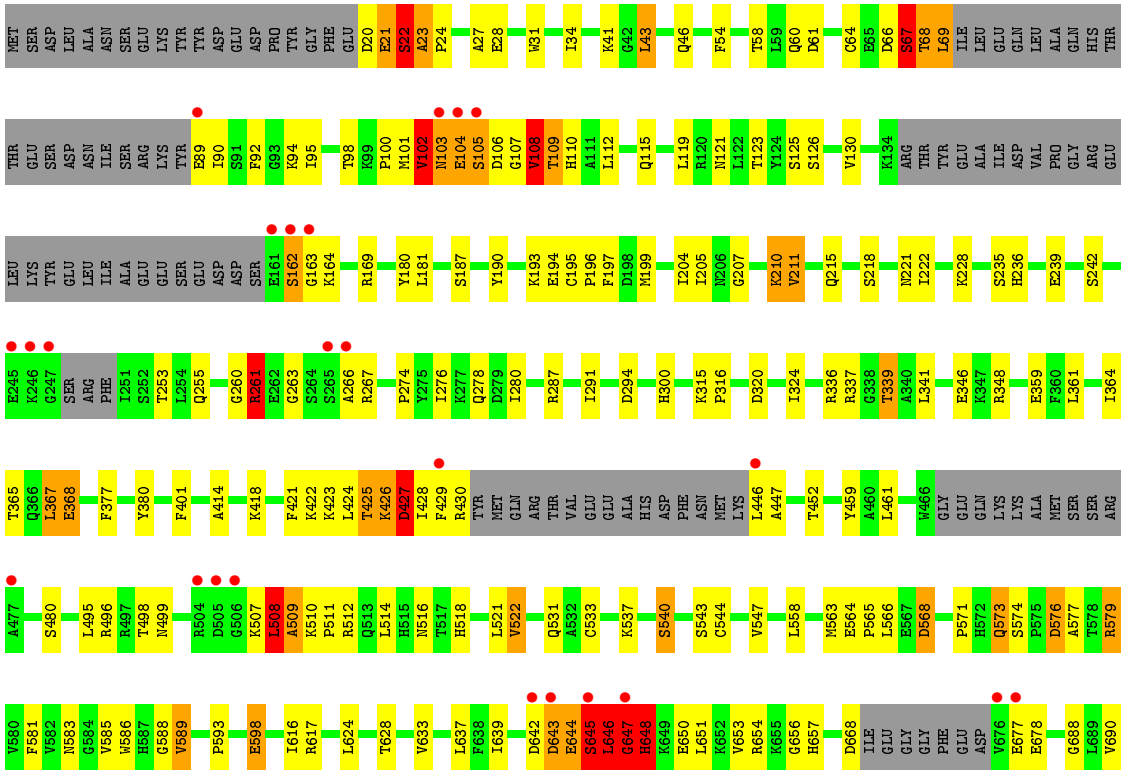
Chain A:

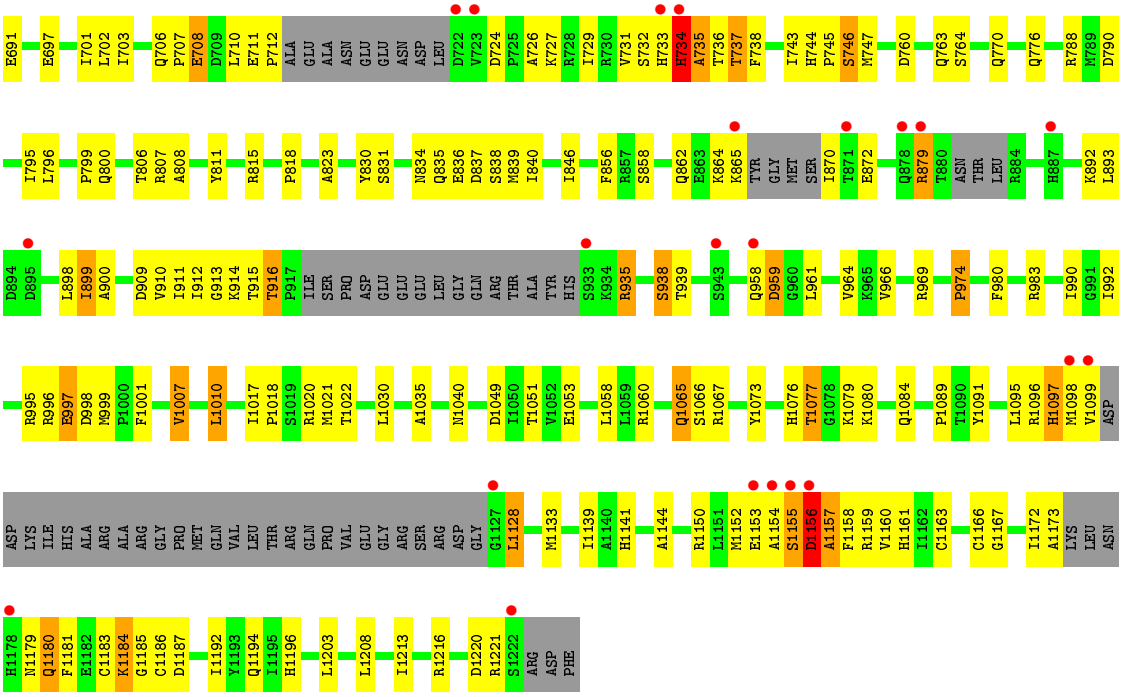




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

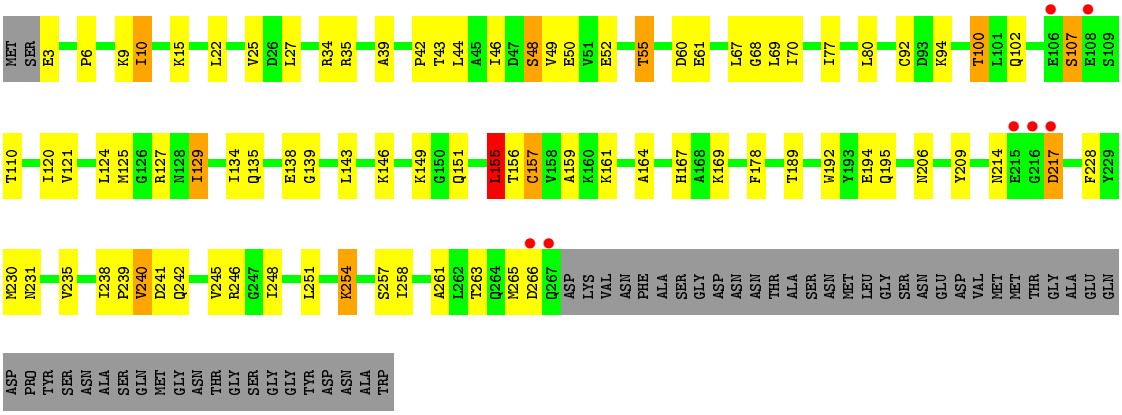
Chain B:





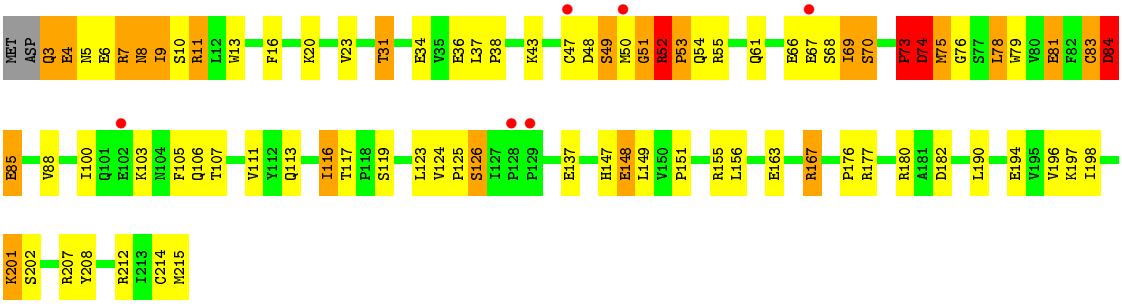
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



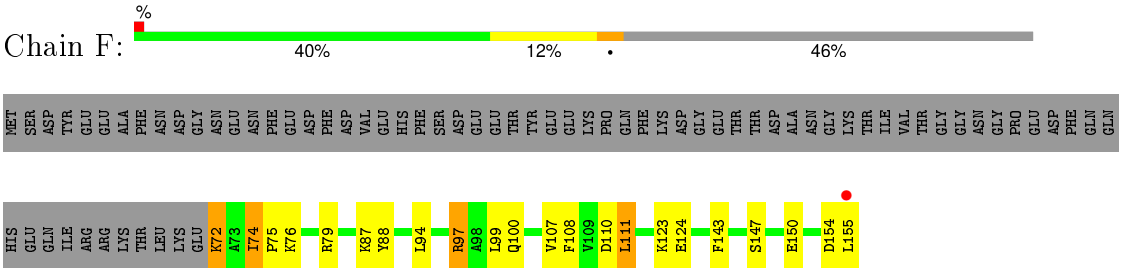
• Molecule 4: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E:



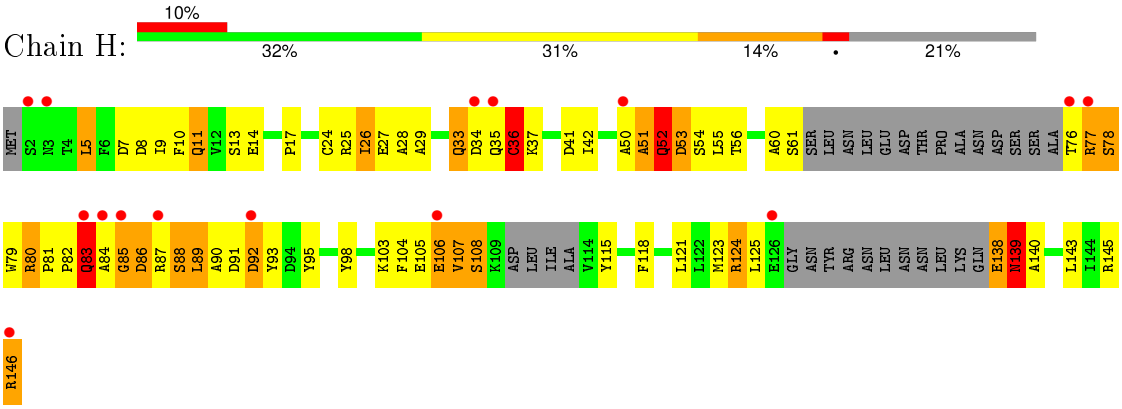
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F:



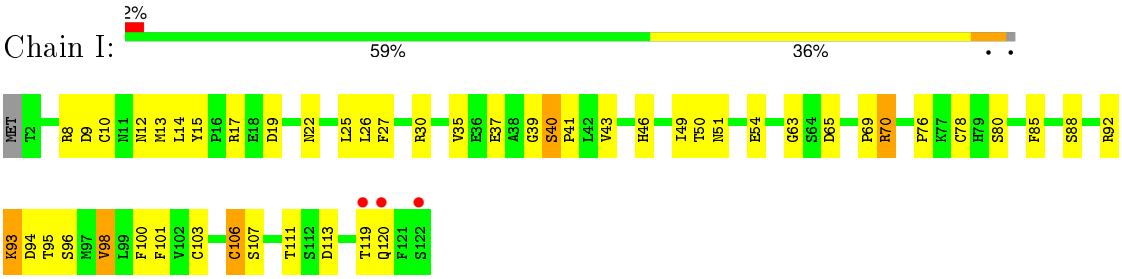
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

Chain H:



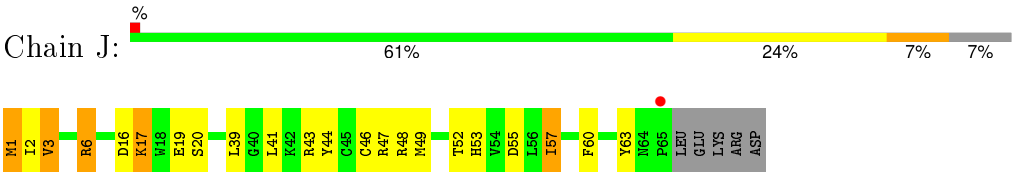
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



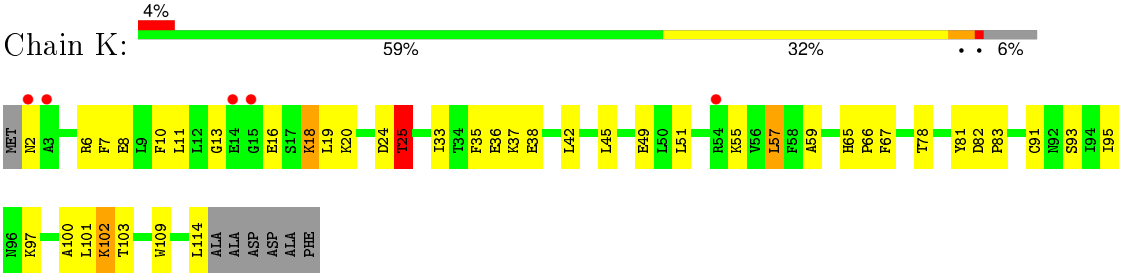
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5

Chain J:



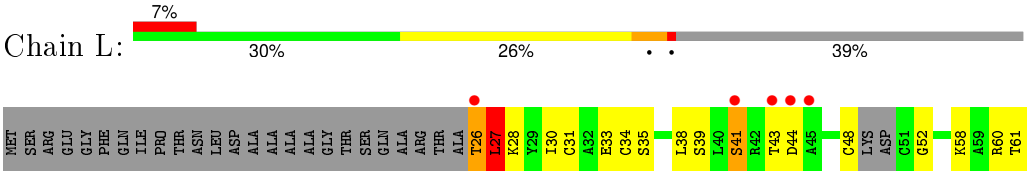
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:



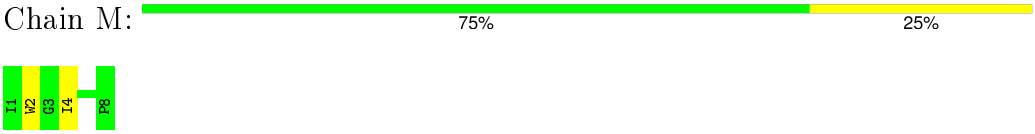
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

Chain L:



• Molecule 11: ALPHA-AMANITIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	122.51Å 222.48Å 374.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.80) 93.4 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.273 0.209 , 0.277	Depositor DCC
R_{free} test set	3507 reflections (3.10%)	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 125151 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: HYP, TRX, ZN, CSX, ILX

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	0.74	0/10809	0.91	20/14624 (0.1%)
2	B	0.73	0/8579	0.86	10/11565 (0.1%)
3	C	0.62	0/2125	0.74	1/2880 (0.0%)
4	E	0.71	0/1780	0.82	2/2395 (0.1%)
5	F	0.72	0/691	0.80	0/933
6	H	0.60	0/947	0.90	1/1279 (0.1%)
7	I	0.80	1/1008 (0.1%)	0.81	0/1355
8	J	0.68	0/541	0.90	0/727
9	K	0.63	0/929	0.74	0/1255
10	L	0.61	0/343	0.87	1/453 (0.2%)
11	M	1.99	1/22 (4.5%)	1.58	0/26
All	All	0.72	2/27774 (0.0%)	0.86	35/37492 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
2	B	0	12
4	E	0	2
8	J	0	1
All	All	0	31

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	4	ILE	C-O	7.28	1.37	1.23
7	I	103	CYS	CB-SG	5.83	1.92	1.82

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	LEU	CA-CB-CG	-8.37	96.05	115.30
3	C	155	LEU	CA-CB-CG	7.16	131.76	115.30
2	B	508	LEU	CA-CB-CG	6.93	131.24	115.30
4	E	74	ASP	N-CA-C	-6.77	92.72	111.00
2	B	1128	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	628	GLY	N-CA-C	-6.54	96.76	113.10
1	A	264	PHE	N-CA-C	6.51	128.59	111.00
2	B	648	HIS	N-CA-C	6.46	128.46	111.00
1	A	57	ARG	N-CA-C	6.40	128.28	111.00
1	A	73	GLY	N-CA-C	-6.37	97.19	113.10
1	A	1257	ASP	N-CA-C	6.18	127.69	111.00
6	H	5	LEU	CA-CB-CG	6.16	129.48	115.30
1	A	63	ARG	N-CA-C	-6.14	94.41	111.00
1	A	1160	SER	N-CA-C	6.11	127.50	111.00
10	L	27	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	157	ASP	C-N-CD	-5.89	107.63	120.60
2	B	43	LEU	CA-CB-CG	-5.75	102.08	115.30
1	A	263	THR	C-N-CA	5.67	135.88	121.70
1	A	1081	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	896	ARG	NE-CZ-NH2	-5.51	117.54	120.30
2	B	102	VAL	CB-CA-C	-5.50	100.94	111.40
1	A	56	PRO	C-N-CA	5.49	135.44	121.70
2	B	645	SER	CB-CA-C	5.45	120.46	110.10
1	A	485	ASP	CB-CG-OD1	-5.21	113.61	118.30
2	B	624	LEU	CA-CB-CG	5.21	127.28	115.30
2	B	22	SER	N-CA-C	5.18	124.98	111.00
1	A	156	ASP	C-N-CA	5.17	134.63	121.70
1	A	483	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	485	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	734	HIS	N-CA-C	-5.12	97.18	111.00
1	A	1418	LEU	CA-CB-CG	5.05	126.92	115.30
4	E	83	CYS	C-N-CA	5.02	134.25	121.70
1	A	1399	ARG	C-N-CA	5.01	134.24	121.70
2	B	1010	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	350	ARG	CG-CD-NE	-5.00	101.30	111.80

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1079	MET	Peptide

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Mol	Chain	Res	Type	Group
1	A	1082	ASN	Peptide
1	A	1085	HIS	Peptide
1	A	1097	GLY	Peptide
1	A	1158	PRO	Peptide
1	A	1159	ARG	Peptide
1	A	1256	GLU	Peptide
1	A	157	ASP	Peptide
1	A	158	PRO	Peptide
1	A	36	ARG	Peptide
1	A	602	ASP	Peptide
1	A	62	ASP	Peptide
1	A	624	SER	Peptide
1	A	673	GLY	Peptide
1	A	73	GLY	Peptide
1	A	830	LYS	Peptide
2	B	103	ASN	Peptide
2	B	105	SER	Peptide
2	B	1076	HIS	Peptide
2	B	21	GLU	Peptide
2	B	22	SER	Peptide
2	B	367	LEU	Peptide
2	B	507	LYS	Peptide
2	B	508	LEU	Peptide
2	B	645	SER	Peptide
2	B	647	GLY	Peptide
2	B	732	SER	Peptide
2	B	734	HIS	Peptide
4	E	4	GLU	Peptide
4	E	73	PRO	Peptide
8	J	63	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10616	0	10675	454	0
2	B	8419	0	8450	294	0
3	C	2087	0	2047	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1744	0	1772	87	0
5	F	679	0	701	18	0
6	H	932	0	899	75	0
7	I	989	0	942	34	0
8	J	532	0	542	18	0
9	K	911	0	917	35	0
10	L	342	0	363	16	0
11	M	64	0	51	1	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
13	A	11	0	0	2	0
13	B	4	0	0	1	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
All	All	27340	0	27359	1013	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 19.

All (1013) 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)
1:A:1399:ARG:HB3	1:A:1400:CYS:CB	1.60	1.30
4:E:53:PRO:HB2	4:E:54:GLN:CA	1.65	1.25
1:A:1399:ARG:CB	1:A:1400:CYS:HB3	1.68	1.24
4:E:53:PRO:CB	4:E:54:GLN:HA	1.64	1.22
1:A:1398:MET:HA	1:A:1399:ARG:HB2	1.24	1.17
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.11	1.15
1:A:1386:ARG:HA	1:A:1387:HIS:HB2	1.15	1.14
2:B:645:SER:HB3	2:B:646:LEU:HB2	1.22	1.14
1:A:834:THR:HB	1:A:1077:THR:HG22	1.28	1.13
1:A:57:ARG:HB3	1:A:68:GLN:CG	1.78	1.12
1:A:830:LYS:O	1:A:830:LYS:HG2	1.47	1.12
1:A:65:LEU:CB	1:A:66:LYS:HB2	1.81	1.10
6:H:52:GLN:H	6:H:53:ASP:HB2	0.98	1.10
1:A:57:ARG:CB	1:A:68:GLN:HG3	1.81	1.10
1:A:65:LEU:HB3	1:A:66:LYS:CB	1.81	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:107:VAL:HG12	6:H:108:SER:H	1.14	1.10
6:H:138:GLU:HA	6:H:139:ASN:HB2	1.23	1.10
2:B:1179:ASN:HA	2:B:1180:GLN:HB2	1.27	1.10
1:A:1187:GLN:HB3	1:A:1188:GLN:HB3	1.34	1.09
2:B:67:SER:HA	2:B:68:THR:HB	1.31	1.08
6:H:52:GLN:N	6:H:53:ASP:HB2	1.66	1.08
2:B:107:GLY:HA2	2:B:108:VAL:HB	1.36	1.07
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.31	1.07
2:B:68:THR:HG23	2:B:69:LEU:H	0.97	1.07
1:A:67:CYS:HB3	1:A:68:GLN:C	1.73	1.07
2:B:643:ASP:HA	2:B:644:GLU:HB2	1.34	1.06
2:B:107:GLY:CA	2:B:108:VAL:HB	1.85	1.06
2:B:1179:ASN:CA	2:B:1180:GLN:HB2	1.86	1.05
2:B:644:GLU:HB3	2:B:645:SER:HB2	1.09	1.04
1:A:626:ASN:HB3	1:A:627:GLY:HA2	1.35	1.04
2:B:1185:GLY:HA2	2:B:1186:CYS:HB2	1.39	1.04
6:H:76:THR:HA	6:H:77:ARG:CB	1.88	1.04
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.36	1.01
1:A:56:PRO:HB3	1:A:57:ARG:HG3	1.43	1.00
6:H:76:THR:CA	6:H:77:ARG:HB2	1.91	1.00
2:B:22:SER:N	2:B:23:ALA:HB3	1.76	1.00
1:A:626:ASN:HB3	1:A:627:GLY:CA	1.89	1.00
3:C:69:LEU:O	8:J:6:ARG:NH1	1.95	0.99
4:E:79:TRP:NE1	4:E:81:GLU:HG3	1.78	0.98
2:B:644:GLU:CB	2:B:645:SER:HB2	1.94	0.97
4:E:88:VAL:HB	4:E:116:ILE:HG23	1.47	0.97
1:A:1386:ARG:CA	1:A:1387:HIS:HB2	1.94	0.96
6:H:76:THR:HA	6:H:77:ARG:HB2	0.97	0.96
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.29	0.96
2:B:68:THR:CG2	2:B:69:LEU:H	1.79	0.95
1:A:598:LEU:HD11	6:H:124:ARG:HG2	1.50	0.93
2:B:643:ASP:HA	2:B:644:GLU:CB	1.95	0.93
6:H:11:GLN:H	6:H:54:SER:HA	1.33	0.93
6:H:138:GLU:HA	6:H:139:ASN:CB	1.99	0.93
2:B:278:GLN:NE2	2:B:337:ARG:HE	1.66	0.93
2:B:68:THR:HG23	2:B:69:LEU:N	1.79	0.92
1:A:57:ARG:HB3	1:A:68:GLN:HG3	0.93	0.91
1:A:1398:MET:HB2	1:A:1400:CYS:SG	2.10	0.91
1:A:834:THR:HB	1:A:1077:THR:CG2	2.00	0.91
1:A:566:ILE:O	1:A:567:LYS:HD3	1.70	0.90
1:A:157:ASP:HB3	1:A:160:GLN:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HB3	1:A:66:LYS:HB2	0.92	0.89
2:B:22:SER:H	2:B:23:ALA:HB3	1.38	0.89
9:K:65:HIS:HD2	9:K:67:PHE:H	1.20	0.89
6:H:82:PRO:HA	6:H:83:GLN:HB2	1.55	0.89
1:A:1078:GLN:N	1:A:1079:MET:HA	1.88	0.89
1:A:1087:ALA:H	1:A:1088:GLY:HA3	1.36	0.88
1:A:67:CYS:HB3	1:A:69:THR:N	1.88	0.88
2:B:106:ASP:HB3	2:B:107:GLY:HA3	1.53	0.88
1:A:1399:ARG:HG3	1:A:1419:ASP:OD2	1.74	0.88
4:E:7:ARG:HG3	4:E:7:ARG:O	1.74	0.88
4:E:74:ASP:O	4:E:75:MET:HB3	1.73	0.87
1:A:67:CYS:CB	1:A:68:GLN:C	2.43	0.87
1:A:1082:ASN:HB3	1:A:1083:THR:HB	1.57	0.87
1:A:1254:ALA:HB1	1:A:1255:GLU:C	1.95	0.87
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.57	0.87
1:A:1386:ARG:HA	1:A:1387:HIS:CB	2.03	0.86
1:A:673:GLY:HA2	1:A:674:PRO:C	1.95	0.86
1:A:1084:PHE:CE2	1:A:1087:ALA:HB2	2.10	0.86
1:A:1079:MET:HB2	1:A:1080:THR:O	1.76	0.86
1:A:673:GLY:HA2	1:A:676:MET:H	1.39	0.86
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.57	0.86
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.40	0.85
2:B:21:GLU:HB3	2:B:22:SER:HB2	1.59	0.85
8:J:2:ILE:HG22	8:J:3:VAL:HG23	1.59	0.85
1:A:673:GLY:CA	1:A:676:MET:H	1.90	0.85
2:B:644:GLU:HB3	2:B:645:SER:CB	2.02	0.85
6:H:107:VAL:HG12	6:H:108:SER:N	1.91	0.84
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.41	0.84
1:A:629:LEU:O	1:A:633:VAL:HG23	1.78	0.83
2:B:260:GLY:HA3	2:B:267:ARG:HD2	1.59	0.83
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.43	0.83
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.59	0.83
5:F:111:LEU:H	5:F:111:LEU:HD12	1.42	0.83
2:B:1185:GLY:CA	2:B:1187:ASP:H	1.92	0.82
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.62	0.82
2:B:1153:GLU:HG3	2:B:1155:SER:H	1.45	0.81
4:E:163:GLU:OE2	4:E:167:ARG:HD2	1.79	0.81
1:A:1086:PHE:N	1:A:1087:ALA:HA	1.95	0.81
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.15	0.81
6:H:84:ALA:HA	6:H:86:ASP:HB2	1.62	0.81
1:A:1258:HIS:HB2	1:A:1261:LYS:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:106:CYS:O	7:I:107:SER:HB2	1.80	0.81
1:A:72:GLU:HB3	1:A:73:GLY:HA2	1.63	0.81
1:A:1078:GLN:H	1:A:1079:MET:HA	1.44	0.81
1:A:50:ILE:HG23	1:A:51:GLY:CA	2.10	0.80
1:A:1158:PRO:HB2	1:A:1159:ARG:HG2	1.63	0.80
2:B:711:GLU:HB2	2:B:712:PRO:HD2	1.63	0.80
6:H:50:ALA:HB3	6:H:53:ASP:OD2	1.80	0.80
1:A:50:ILE:HG23	1:A:51:GLY:HA3	1.63	0.80
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.46	0.80
1:A:156:ASP:HB3	1:A:157:ASP:O	1.81	0.79
4:E:49:SER:HA	4:E:51:GLY:H	1.47	0.79
1:A:48:ALA:HA	1:A:49:LYS:HB2	1.63	0.79
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.63	0.79
2:B:645:SER:CB	2:B:646:LEU:HB2	2.08	0.79
2:B:278:GLN:HE21	2:B:337:ARG:HE	1.29	0.78
1:A:50:ILE:HG23	1:A:51:GLY:O	1.82	0.78
2:B:103:ASN:HB2	2:B:169:ARG:NH2	1.98	0.78
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.64	0.78
2:B:1179:ASN:N	2:B:1180:GLN:HB2	1.99	0.78
6:H:26:ILE:HD13	6:H:42:ILE:HD12	1.62	0.78
1:A:829:VAL:O	1:A:830:LYS:HB3	1.83	0.78
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.47	0.78
1:A:1090:ALA:H	1:A:1092:LYS:HG2	1.49	0.78
1:A:265:LYS:HE2	1:A:299:HIS:HD2	1.46	0.78
10:L:26:THR:N	10:L:62:LYS:HZ1	1.82	0.78
2:B:66:ASP:O	2:B:67:SER:HB3	1.84	0.78
1:A:1400:CYS:HA	1:A:1401:SER:HB2	1.66	0.77
5:F:97:ARG:HE	5:F:100:GLN:NE2	1.83	0.77
2:B:106:ASP:HB3	2:B:107:GLY:CA	2.14	0.76
2:B:1022:THR:HA	13:B:2004:HOH:O	1.83	0.76
2:B:1185:GLY:HA3	2:B:1187:ASP:H	1.50	0.76
1:A:1254:ALA:HB1	1:A:1255:GLU:O	1.86	0.76
2:B:67:SER:HA	2:B:68:THR:CB	2.13	0.76
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.16	0.76
2:B:734:HIS:H	2:B:734:HIS:CD2	2.04	0.76
1:A:303:TYR:CD2	1:A:304:MET:HG3	2.21	0.76
1:A:673:GLY:HA2	1:A:676:MET:N	1.99	0.76
1:A:537:ARG:NH2	1:A:602:ASP:HB2	2.00	0.75
7:I:8:ARG:HH11	7:I:8:ARG:HG2	1.52	0.75
6:H:35:GLN:O	6:H:36:CYS:HB3	1.85	0.74
1:A:49:LYS:HB3	1:A:50:ILE:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:LEU:O	1:A:886:ILE:HG22	1.87	0.74
4:E:7:ARG:O	4:E:8:ASN:HB2	1.86	0.74
4:E:52:ARG:HB3	4:E:53:PRO:CD	2.18	0.73
1:A:1173:HIS:HA	1:A:1174:PHE:HB2	1.69	0.73
2:B:583:ASN:HD21	2:B:628:THR:H	1.35	0.73
2:B:41:LYS:NZ	2:B:544:CYS:SG	2.59	0.73
2:B:1179:ASN:HA	2:B:1180:GLN:CB	2.13	0.73
3:C:167:HIS:HD2	3:C:169:LYS:H	1.34	0.73
1:A:1079:MET:HG2	1:A:1081:LEU:HB2	1.71	0.72
1:A:1410:PHE:HD2	2:B:1213:ILE:HD11	1.54	0.72
1:A:1400:CYS:O	1:A:1400:CYS:SG	2.47	0.72
1:A:56:PRO:HB3	1:A:57:ARG:CG	2.18	0.72
1:A:673:GLY:HA3	1:A:676:MET:HB2	1.70	0.72
1:A:1265:ASN:HD21	2:B:263:GLY:HA2	1.55	0.72
2:B:893:LEU:HD21	2:B:910:VAL:HG12	1.72	0.72
6:H:107:VAL:O	6:H:108:SER:HB2	1.90	0.72
1:A:445:ASN:CB	1:A:455:MET:HG2	2.19	0.71
2:B:21:GLU:CB	2:B:22:SER:HB2	2.21	0.71
4:E:75:MET:CE	4:E:155:ARG:HH22	2.03	0.71
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.89	0.71
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.72	0.71
1:A:67:CYS:HB3	1:A:68:GLN:CA	2.20	0.71
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.36	0.71
2:B:579:ARG:HG2	2:B:586:TRP:CE2	2.26	0.71
1:A:1398:MET:CA	1:A:1399:ARG:HB2	2.13	0.71
1:A:1257:ASP:O	1:A:1258:HIS:HB3	1.91	0.70
4:E:49:SER:HA	4:E:51:GLY:N	2.05	0.70
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.38	0.70
2:B:1051:THR:HG22	2:B:1053:GLU:N	2.06	0.70
6:H:10:PHE:O	6:H:55:LEU:N	2.22	0.70
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.25	0.70
2:B:423:LYS:O	2:B:424:LEU:HB3	1.90	0.70
6:H:84:ALA:CA	6:H:86:ASP:HB2	2.22	0.69
4:E:155:ARG:HD2	4:E:194:GLU:OE2	1.91	0.69
4:E:75:MET:HG2	4:E:76:GLY:H	1.57	0.69
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.72	0.69
1:A:1084:PHE:HE2	1:A:1087:ALA:HB2	1.54	0.69
7:I:8:ARG:NH1	7:I:9:ASP:OD1	2.26	0.69
1:A:754:SER:H	1:A:757:ASN:HD22	1.40	0.69
1:A:56:PRO:HB3	1:A:57:ARG:HE	1.55	0.69
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ILE:HD12	2:B:210:LYS:HG3	1.75	0.69
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.74	0.69
1:A:68:GLN:CB	1:A:69:THR:HA	2.22	0.69
7:I:63:GLY:O	7:I:70:ARG:NH1	2.25	0.69
1:A:1116:LEU:HD23	1:A:1329:THR:HB	1.74	0.69
2:B:294:ASP:H	7:I:12:ASN:ND2	1.92	0.68
1:A:1187:GLN:CB	1:A:1188:GLN:HB3	2.19	0.68
2:B:1173:ALA:HA	2:B:1181:PHE:HB3	1.75	0.68
1:A:526:ASP:HB2	2:B:835:GLN:OE1	1.93	0.68
2:B:107:GLY:CA	2:B:108:VAL:CB	2.67	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.75	0.67
4:E:74:ASP:O	4:E:75:MET:CB	2.42	0.67
1:A:795:GLU:HG2	2:B:731:VAL:HG11	1.76	0.67
8:J:1:MET:HG3	8:J:60:PHE:CE2	2.22	0.67
2:B:509:ALA:O	2:B:511:PRO:HD3	1.95	0.67
1:A:1401:SER:HB2	1:A:1429:ILE:HD11	1.77	0.67
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.07	0.67
2:B:734:HIS:CD2	2:B:734:HIS:N	2.62	0.67
1:A:67:CYS:CB	1:A:69:THR:N	2.57	0.67
1:A:606:LEU:HD21	1:A:608:ILE:CD1	2.25	0.67
1:A:579:SER:HB3	1:A:611:GLN:OE1	1.94	0.66
4:E:6:GLU:HA	4:E:9:ILE:HG12	1.78	0.66
4:E:83:CYS:HA	4:E:84:ASP:HB2	1.76	0.66
5:F:97:ARG:HE	5:F:100:GLN:HE21	1.44	0.66
1:A:265:LYS:NZ	1:A:302:THR:HB	2.10	0.66
1:A:534:LEU:O	1:A:574:GLY:HA3	1.95	0.66
10:L:26:THR:HG23	10:L:27:LEU:H	1.60	0.66
1:A:1078:GLN:N	1:A:1079:MET:CA	2.59	0.65
6:H:11:GLN:H	6:H:54:SER:CA	2.07	0.65
1:A:56:PRO:HB3	1:A:57:ARG:NE	2.11	0.65
1:A:829:VAL:HG12	1:A:829:VAL:O	1.95	0.65
5:F:79:ARG:HH22	5:F:150:GLU:CD	1.99	0.65
6:H:37:LYS:O	6:H:125:LEU:HD23	1.97	0.65
1:A:50:ILE:HG23	1:A:51:GLY:C	2.16	0.65
1:A:606:LEU:HD21	1:A:608:ILE:HD12	1.79	0.65
1:A:1082:ASN:HB3	1:A:1083:THR:CB	2.25	0.65
2:B:1185:GLY:HA2	2:B:1186:CYS:CB	2.14	0.65
3:C:9:LYS:O	3:C:10:ILE:HG13	1.98	0.65
2:B:278:GLN:HE21	2:B:337:ARG:NE	1.94	0.64
1:A:549:MET:CE	1:A:656:TRP:HD1	2.10	0.64
2:B:647:GLY:HA2	2:B:648:HIS:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:THR:CB	1:A:1077:THR:HG22	2.18	0.64
1:A:166:GLY:CA	1:A:167:CYS:HB3	2.27	0.64
1:A:452:LYS:HG3	2:B:1141:HIS:CE1	2.32	0.64
3:C:67:LEU:HD11	3:C:155:LEU:HD11	1.79	0.64
1:A:606:LEU:HD22	1:A:613:ILE:HB	1.80	0.64
2:B:509:ALA:C	2:B:511:PRO:HD3	2.18	0.64
8:J:2:ILE:HG22	8:J:3:VAL:N	2.13	0.64
2:B:558:LEU:HB3	2:B:563:MET:HE2	1.80	0.64
2:B:107:GLY:HA3	2:B:108:VAL:HB	1.79	0.64
4:E:5:ASN:O	4:E:8:ASN:HB3	1.98	0.63
1:A:771:GLU:HG2	1:A:1086:PHE:CE1	2.32	0.63
6:H:138:GLU:CA	6:H:139:ASN:CB	2.75	0.63
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.80	0.63
3:C:239:PRO:O	3:C:242:GLN:HB2	1.98	0.63
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.81	0.63
6:H:61:SER:C	6:H:89:LEU:HD11	2.19	0.63
1:A:1079:MET:HB2	1:A:1080:THR:C	2.18	0.62
6:H:11:GLN:N	6:H:54:SER:HA	2.11	0.62
6:H:82:PRO:HA	6:H:83:GLN:CB	2.28	0.62
2:B:770:GLN:OE1	2:B:770:GLN:HA	1.99	0.62
2:B:654:ARG:H	2:B:657:HIS:HD2	1.45	0.62
1:A:773:LYS:HZ2	1:A:1089:VAL:H	1.46	0.62
1:A:1111:MET:HE1	1:A:1331:SER:CB	2.28	0.62
4:E:190:LEU:HD23	4:E:214:CYS:HB2	1.79	0.62
1:A:56:PRO:CB	1:A:57:ARG:HE	2.12	0.62
1:A:775:ILE:O	1:A:797:LYS:HE3	1.99	0.62
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.34	0.62
1:A:1254:ALA:CB	1:A:1255:GLU:HA	2.29	0.62
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.96	0.62
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.81	0.62
1:A:69:THR:H	1:A:70:CYS:HB3	1.63	0.62
2:B:899:ILE:N	2:B:899:ILE:HD13	2.15	0.62
6:H:50:ALA:O	6:H:51:ALA:HB2	1.99	0.62
1:A:23:SER:O	1:A:27:VAL:HG23	2.00	0.62
8:J:48:ARG:CZ	8:J:49:MET:HE1	2.29	0.62
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.63	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.81	0.61
2:B:734:HIS:H	2:B:734:HIS:HD2	1.49	0.61
5:F:147:SER:OG	5:F:150:GLU:HB2	2.00	0.61
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.81	0.61
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.99	0.61
2:B:294:ASP:H	7:I:12:ASN:HD22	1.48	0.61
1:A:885:THR:CG2	1:A:943:LEU:HD12	2.31	0.61
2:B:1185:GLY:CA	2:B:1186:CYS:HB2	2.24	0.61
2:B:260:GLY:CA	2:B:267:ARG:HD2	2.27	0.61
9:K:57:LEU:HD21	9:K:78:THR:CG2	2.31	0.61
1:A:54:ASN:HB2	1:A:55:ASP:OD1	1.99	0.61
1:A:1254:ALA:HB1	1:A:1255:GLU:CA	2.31	0.61
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.15	0.61
1:A:830:LYS:H	1:A:831:THR:C	2.04	0.61
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.81	0.61
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.28	0.61
2:B:898:LEU:HB2	10:L:58:LYS:HE3	1.83	0.61
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.60
1:A:673:GLY:HA2	1:A:675:THR:N	2.16	0.60
1:A:1091:SER:N	1:A:1092:LYS:HA	2.16	0.60
1:A:1410:PHE:CD2	2:B:1213:ILE:HD11	2.36	0.60
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.83	0.60
1:A:746:MET:HE3	2:B:1018:PRO:HG3	1.82	0.60
1:A:53:LEU:HD12	1:A:53:LEU:N	2.15	0.60
1:A:156:ASP:CB	1:A:157:ASP:O	2.49	0.60
1:A:773:LYS:NZ	1:A:1089:VAL:HG22	2.16	0.60
6:H:84:ALA:HA	6:H:86:ASP:N	2.16	0.60
1:A:303:TYR:HD2	1:A:304:MET:HG3	1.66	0.60
1:A:913:LEU:HD11	1:A:981:LEU:O	2.01	0.60
1:A:1398:MET:HA	1:A:1399:ARG:CB	2.12	0.60
1:A:1085:HIS:N	1:A:1086:PHE:HB3	2.17	0.60
4:E:53:PRO:HB3	4:E:55:ARG:HH11	1.64	0.60
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.83	0.60
2:B:67:SER:CA	2:B:68:THR:HB	2.20	0.60
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.32	0.60
2:B:706:GLN:HB3	2:B:708:GLU:HG2	1.84	0.60
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.83	0.60
1:A:367:PRO:HB3	9:K:2:ASN:HD21	1.66	0.60
9:K:7:PHE:HB2	9:K:11:LEU:HD12	1.83	0.60
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.67	0.60
2:B:864:LYS:H	2:B:872:GLU:HB2	1.67	0.59
1:A:453:MET:H	1:A:453:MET:CE	2.14	0.59
2:B:54:PHE:HA	2:B:58:THR:HB	1.83	0.59
4:E:84:ASP:H	4:E:113:GLN:HE21	1.49	0.59
2:B:68:THR:CG2	2:B:90:ILE:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:26:THR:HG23	10:L:27:LEU:N	2.18	0.59
1:A:754:SER:OG	1:A:756:ILE:HG22	2.03	0.59
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.84	0.59
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.50	0.59
1:A:68:GLN:HB2	1:A:69:THR:HA	1.85	0.59
9:K:65:HIS:CD2	9:K:67:PHE:H	2.11	0.59
1:A:1004:ASN:ND2	4:E:167:ARG:HD3	2.18	0.59
1:A:472:LEU:O	1:A:475:THR:HB	2.03	0.59
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.18	0.59
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.02	0.59
2:B:422:LYS:O	2:B:426:LYS:HB2	2.03	0.59
1:A:1004:ASN:CG	4:E:167:ARG:HD3	2.23	0.59
5:F:76:LYS:HA	5:F:79:ARG:HD2	1.83	0.59
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.02	0.59
1:A:1106:ASN:OD1	1:A:1385:THR:CG2	2.51	0.59
6:H:138:GLU:CA	6:H:139:ASN:HB2	2.15	0.58
2:B:864:LYS:HG3	2:B:870:ILE:O	2.03	0.58
1:A:1098:VAL:H	1:A:1099:PRO:HD2	1.68	0.58
1:A:946:VAL:HG22	4:E:201:LYS:HB2	1.84	0.58
1:A:596:THR:HG22	1:A:597:LEU:H	1.68	0.58
4:E:7:ARG:CG	4:E:7:ARG:O	2.49	0.58
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.84	0.58
1:A:596:THR:HG22	1:A:597:LEU:N	2.19	0.58
2:B:68:THR:CG2	2:B:69:LEU:N	2.50	0.58
2:B:899:ILE:N	2:B:899:ILE:CD1	2.66	0.58
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.85	0.58
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.85	0.58
2:B:21:GLU:O	2:B:656:GLY:N	2.36	0.58
2:B:98:THR:O	2:B:126:SER:HB3	2.02	0.58
2:B:558:LEU:HB3	2:B:563:MET:CE	2.33	0.58
1:A:540:PHE:C	1:A:541:ILE:HD12	2.24	0.58
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.85	0.58
2:B:260:GLY:CA	2:B:267:ARG:CD	2.82	0.58
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.39	0.58
6:H:107:VAL:CG1	6:H:108:SER:N	2.62	0.58
2:B:558:LEU:HD13	2:B:563:MET:CE	2.33	0.58
2:B:498:THR:OG1	2:B:537:LYS:HB2	2.03	0.58
2:B:106:ASP:CB	2:B:107:GLY:HA3	2.28	0.58
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.37	0.58
1:A:840:ARG:HB3	1:A:1385:THR:HA	1.86	0.58
7:I:95:THR:HG22	7:I:96:SER:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.84	0.58
1:A:1083:THR:CG2	1:A:1084:PHE:N	2.66	0.58
1:A:112:LYS:HE3	1:A:165:GLY:H	1.69	0.58
9:K:24:ASP:CG	9:K:25:THR:H	2.06	0.58
4:E:36:GLU:O	4:E:38:PRO:HD3	2.04	0.58
1:A:54:ASN:HA	1:A:56:PRO:HD3	1.86	0.57
6:H:103:LYS:HG3	6:H:105:GLU:HB3	1.85	0.57
1:A:53:LEU:HD12	1:A:53:LEU:H	1.70	0.57
1:A:155:GLU:HB2	1:A:156:ASP:CB	2.34	0.57
3:C:238:ILE:HG22	3:C:242:GLN:HB2	1.86	0.57
1:A:830:LYS:CG	1:A:830:LYS:O	2.34	0.57
1:A:626:ASN:CB	1:A:627:GLY:CA	2.66	0.57
3:C:52:GLU:HA	10:L:64:LEU:CD1	2.34	0.57
2:B:571:PRO:C	2:B:573:GLN:H	2.08	0.57
2:B:339:THR:HG21	2:B:348:ARG:HG2	1.85	0.57
2:B:43:LEU:HD11	2:B:811:TYR:O	2.04	0.57
2:B:645:SER:HB3	2:B:646:LEU:CB	2.15	0.57
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.40	0.57
1:A:1399:ARG:CB	1:A:1400:CYS:CB	2.51	0.57
7:I:49:ILE:HA	7:I:92:ARG:HH22	1.70	0.57
4:E:61:GLN:HG3	4:E:105:PHE:CZ	2.40	0.57
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.85	0.57
1:A:62:ASP:HA	1:A:63:ARG:HG2	1.85	0.57
1:A:453:MET:HE3	1:A:453:MET:H	1.68	0.57
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.39	0.57
4:E:79:TRP:HB3	4:E:100:ILE:HD11	1.85	0.57
3:C:155:LEU:HD21	3:C:157:CYS:SG	2.45	0.57
8:J:2:ILE:HG22	8:J:3:VAL:H	1.69	0.57
2:B:711:GLU:CB	2:B:712:PRO:HD2	2.34	0.57
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.40	0.57
4:E:52:ARG:HB3	4:E:53:PRO:HD2	1.85	0.57
3:C:120:ILE:HD13	3:C:124:LEU:HD11	1.86	0.57
6:H:9:ILE:HG12	6:H:56:THR:HG22	1.87	0.57
1:A:1404:GLU:O	1:A:1405:THR:C	2.43	0.57
1:A:452:LYS:C	1:A:454:SER:H	2.08	0.57
6:H:107:VAL:O	6:H:108:SER:CB	2.53	0.56
4:E:31:THR:O	4:E:34:GLU:HB2	2.05	0.56
1:A:56:PRO:CB	1:A:57:ARG:HG3	2.27	0.56
1:A:773:LYS:HZ1	1:A:1089:VAL:HG22	1.69	0.56
2:B:579:ARG:HG2	2:B:586:TRP:CZ2	2.41	0.56
1:A:751:SER:O	1:A:752:LYS:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.40	0.56
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.86	0.56
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.88	0.56
3:C:52:GLU:HA	10:L:64:LEU:HD11	1.86	0.56
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.41	0.56
2:B:651:LEU:HD23	2:B:710:LEU:CD1	2.36	0.56
1:A:602:ASP:O	1:A:615:GLY:HA2	2.06	0.56
1:A:1401:SER:HA	1:A:1404:GLU:OE2	2.05	0.56
1:A:54:ASN:N	1:A:54:ASN:OD1	2.39	0.56
2:B:21:GLU:CA	2:B:22:SER:HB2	2.36	0.56
1:A:450:LEU:HD23	2:B:1133:MET:CE	2.36	0.56
1:A:1399:ARG:HB3	1:A:1400:CYS:HB3	0.71	0.56
1:A:68:GLN:HB2	1:A:69:THR:CA	2.36	0.56
2:B:1185:GLY:CA	2:B:1187:ASP:N	2.67	0.55
4:E:43:LYS:O	4:E:47:CYS:HB2	2.06	0.55
5:F:72:LYS:HG2	5:F:72:LYS:O	2.06	0.55
2:B:646:LEU:H	2:B:647:GLY:HA3	1.71	0.55
3:C:100:THR:HG21	3:C:102:GLN:NE2	2.18	0.55
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.89	0.55
1:A:1325:THR:O	4:E:148:GLU:HB2	2.05	0.55
4:E:147:HIS:HD2	4:E:149:LEU:H	1.55	0.55
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.06	0.55
1:A:48:ALA:CA	1:A:49:LYS:HB2	2.35	0.55
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.88	0.55
2:B:421:PHE:O	2:B:425:THR:HB	2.07	0.55
2:B:806:THR:HG22	2:B:808:ALA:H	1.70	0.55
2:B:702:LEU:HD23	2:B:737:THR:HG22	1.88	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.88	0.55
1:A:1254:ALA:HB1	1:A:1255:GLU:HA	1.89	0.55
1:A:1087:ALA:N	1:A:1088:GLY:HA3	2.08	0.55
4:E:6:GLU:HA	4:E:9:ILE:CG1	2.37	0.55
2:B:735:ALA:CB	2:B:738:PHE:CE1	2.90	0.55
7:I:39:GLY:O	7:I:40:SER:CB	2.54	0.55
4:E:75:MET:CG	4:E:76:GLY:H	2.20	0.55
1:A:399:HIS:HE1	1:A:436:ILE:O	1.89	0.55
1:A:72:GLU:HB3	1:A:73:GLY:CA	2.36	0.55
2:B:27:ALA:HB2	2:B:708:GLU:OE2	2.07	0.55
2:B:637:LEU:HA	2:B:743:ILE:HD12	1.89	0.55
9:K:65:HIS:HD2	9:K:67:PHE:N	1.99	0.55
1:A:1175:SER:HB3	1:A:1177:LEU:HD12	1.89	0.55
1:A:64:ASN:HB2	1:A:65:LEU:HG	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG21	7:I:93:LYS:O	2.07	0.54
1:A:474:VAL:O	1:A:477:PRO:HD2	2.07	0.54
3:C:206:ASN:HA	3:C:209:TYR:CD1	2.42	0.54
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.30	0.54
1:A:67:CYS:SG	1:A:69:THR:HB	2.48	0.54
1:A:1187:GLN:HB3	1:A:1188:GLN:CB	2.22	0.54
2:B:68:THR:HG22	2:B:90:ILE:O	2.07	0.54
1:A:53:LEU:CD1	1:A:53:LEU:N	2.71	0.54
2:B:69:LEU:HB2	2:B:89:GLU:HG2	1.88	0.54
1:A:35:ILE:HG23	1:A:54:ASN:OD1	2.07	0.54
2:B:103:ASN:CB	2:B:169:ARG:HH22	2.17	0.54
3:C:214:ASN:O	3:C:217:ASP:HB2	2.07	0.54
4:E:3:GLN:C	4:E:3:GLN:HE21	2.11	0.54
6:H:77:ARG:O	6:H:78:SER:HB2	2.08	0.54
2:B:1067:ARG:NH1	3:C:194:GLU:OE1	2.37	0.54
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.55	0.54
2:B:744:HIS:CD2	2:B:746:SER:H	2.25	0.54
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.90	0.53
1:A:673:GLY:CA	1:A:674:PRO:C	2.71	0.53
6:H:35:GLN:O	6:H:36:CYS:CB	2.53	0.53
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.38	0.53
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.90	0.53
3:C:15:LYS:HZ1	3:C:135:GLN:HG2	1.74	0.53
1:A:1400:CYS:HA	1:A:1401:SER:CB	2.36	0.53
10:L:30:ILE:HG22	10:L:31:CYS:H	1.72	0.53
1:A:74:MET:O	1:A:75:ASN:HB2	2.09	0.53
1:A:704:ALA:O	1:A:705:LYS:HB2	2.08	0.53
9:K:100:ALA:O	9:K:103:THR:HG22	2.08	0.53
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.49	0.53
1:A:1387:HIS:H	1:A:1388:GLY:HA3	1.73	0.53
6:H:61:SER:O	6:H:89:LEU:HD11	2.08	0.53
4:E:147:HIS:CD2	4:E:149:LEU:H	2.26	0.53
4:E:84:ASP:H	4:E:113:GLN:NE2	2.06	0.53
1:A:53:LEU:HA	1:A:56:PRO:HD3	1.89	0.53
1:A:1084:PHE:C	1:A:1086:PHE:HB3	2.28	0.53
4:E:75:MET:HE1	4:E:155:ARG:HH22	1.70	0.53
2:B:581:PHE:HA	2:B:585:VAL:O	2.08	0.53
5:F:154:ASP:O	5:F:155:LEU:HD23	2.08	0.53
6:H:11:GLN:HB3	6:H:29:ALA:O	2.09	0.53
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.08	0.53
3:C:107:SER:O	3:C:149:LYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.08	0.53
2:B:1098:MET:HB3	2:B:1099:VAL:HA	1.91	0.53
3:C:254:LYS:HE2	9:K:38:GLU:OE1	2.09	0.53
9:K:57:LEU:HD21	9:K:78:THR:HG22	1.90	0.52
1:A:1372:VAL:O	1:A:1376:THR:HB	2.09	0.52
1:A:134:ARG:HD2	1:A:221:SER:O	2.09	0.52
1:A:50:ILE:CG2	1:A:51:GLY:HA3	2.37	0.52
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.55	0.52
1:A:885:THR:HG22	1:A:943:LEU:HD12	1.91	0.52
10:L:41:SER:C	10:L:43:THR:H	2.12	0.52
6:H:91:ASP:O	6:H:93:TYR:N	2.41	0.52
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.92	0.52
1:A:1158:PRO:N	1:A:1159:ARG:HB2	2.25	0.52
5:F:97:ARG:HH11	5:F:124:GLU:CD	2.13	0.52
1:A:751:SER:O	1:A:752:LYS:CB	2.56	0.52
4:E:83:CYS:SG	4:E:85:GLU:HG3	2.50	0.52
2:B:1154:ALA:C	2:B:1156:ASP:H	2.13	0.52
6:H:33:GLN:H	6:H:33:GLN:HE21	1.56	0.52
1:A:1398:MET:HG2	1:A:1398:MET:O	2.09	0.52
7:I:8:ARG:NH1	7:I:8:ARG:HG2	2.25	0.52
6:H:8:ASP:CG	6:H:9:ILE:H	2.14	0.52
2:B:121:ASN:HA	2:B:207:GLY:CA	2.40	0.52
1:A:412:ARG:NH1	1:A:433:GLU:OE1	2.43	0.51
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.91	0.51
1:A:385:ILE:HG23	1:A:386:ASP:N	2.25	0.51
1:A:597:LEU:HD21	6:H:103:LYS:HG2	1.90	0.51
1:A:602:ASP:CG	1:A:602:ASP:O	2.48	0.51
2:B:823:ALA:O	2:B:1089:PRO:HA	2.09	0.51
9:K:93:SER:O	9:K:97:LYS:HG3	2.11	0.51
3:C:124:LEU:O	3:C:127:ARG:HD3	2.10	0.51
1:A:726:ARG:HD2	11:M:2:TRX:CE3	2.40	0.51
1:A:391:LEU:CD2	1:A:400:PRO:HB2	2.40	0.51
2:B:864:LYS:O	2:B:865:LYS:HB2	2.09	0.51
7:I:78:CYS:SG	7:I:80:SER:HB3	2.50	0.51
6:H:87:ARG:O	6:H:88:SER:HB3	2.10	0.51
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.94	0.51
1:A:1191:TRP:CZ3	7:I:43:VAL:HG21	2.45	0.51
1:A:1083:THR:HG23	1:A:1084:PHE:H	1.76	0.51
2:B:735:ALA:O	2:B:737:THR:N	2.44	0.51
1:A:1254:ALA:CB	1:A:1255:GLU:CA	2.89	0.51
6:H:145:ARG:HB2	6:H:146:ARG:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:724:ASP:HB3	2:B:727:LYS:HD2	1.92	0.51
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.45	0.51
2:B:508:LEU:HD13	2:B:508:LEU:O	2.11	0.51
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.93	0.51
3:C:80:LEU:HD12	3:C:127:ARG:NH2	2.26	0.51
4:E:52:ARG:CB	4:E:53:PRO:CD	2.88	0.51
2:B:744:HIS:HD2	2:B:746:SER:H	1.57	0.51
2:B:583:ASN:ND2	2:B:628:THR:H	2.06	0.50
1:A:541:ILE:N	1:A:541:ILE:HD12	2.25	0.50
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.94	0.50
2:B:708:GLU:O	2:B:711:GLU:HG2	2.11	0.50
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.93	0.50
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.92	0.50
2:B:862:GLN:NE2	2:B:961:LEU:HD13	2.27	0.50
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.93	0.50
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.11	0.50
1:A:52:GLY:HA3	1:A:53:LEU:C	2.32	0.50
2:B:509:ALA:O	2:B:511:PRO:CD	2.58	0.50
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.50
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.76	0.50
2:B:836:GLU:O	2:B:837:ASP:HB2	2.12	0.50
1:A:132:LYS:HE2	1:A:1415:SER:OG	2.12	0.50
1:A:414:ASP:OD2	1:A:416:ARG:NH2	2.35	0.50
1:A:1258:HIS:HD2	1:A:1262:LYS:HE3	1.77	0.50
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.27	0.50
4:E:123:LEU:O	4:E:126:SER:HB3	2.12	0.50
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.94	0.50
3:C:231:ASN:C	3:C:231:ASN:OD1	2.50	0.50
6:H:106:GLU:O	6:H:107:VAL:HB	2.12	0.50
2:B:22:SER:N	2:B:23:ALA:CB	2.64	0.50
4:E:73:PRO:O	4:E:74:ASP:HB2	2.11	0.50
2:B:1067:ARG:HH11	2:B:1067:ARG:HG3	1.77	0.50
10:L:30:ILE:HG22	10:L:31:CYS:N	2.27	0.50
1:A:884:ASP:O	1:A:886:ILE:N	2.45	0.50
1:A:1129:GLU:HA	1:A:1132:LYS:HD2	1.93	0.50
1:A:54:ASN:CB	1:A:55:ASP:OD1	2.59	0.49
2:B:68:THR:HG21	2:B:90:ILE:O	2.12	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.94	0.49
5:F:99:LEU:HD12	5:F:99:LEU:O	2.11	0.49
1:A:1316:VAL:C	1:A:1318:THR:H	2.14	0.49
4:E:66:GLU:CD	4:E:66:GLU:N	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:79:TRP:HE1	4:E:81:GLU:CG	2.02	0.49
1:A:57:ARG:CA	1:A:68:GLN:HG3	2.39	0.49
1:A:537:ARG:CZ	1:A:602:ASP:HB2	2.42	0.49
4:E:61:GLN:HG3	4:E:105:PHE:HZ	1.78	0.49
1:A:1168:GLU:O	1:A:1171:GLN:HB2	2.12	0.49
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.11	0.49
2:B:654:ARG:N	2:B:657:HIS:HD2	2.10	0.49
4:E:117:THR:C	4:E:119:SER:H	2.15	0.49
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.95	0.49
1:A:1073:GLY:O	1:A:1077:THR:HG23	2.12	0.49
6:H:84:ALA:HA	6:H:85:GLY:C	2.33	0.49
2:B:727:LYS:HE2	2:B:1049:ASP:OD2	2.11	0.49
2:B:598:GLU:HA	2:B:598:GLU:OE2	2.08	0.49
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.78	0.49
1:A:1254:ALA:C	1:A:1256:GLU:HG2	2.32	0.49
1:A:1341:ILE:O	1:A:1345:ARG:N	2.37	0.49
4:E:16:PHE:CE2	4:E:20:LYS:NZ	2.79	0.49
2:B:21:GLU:O	2:B:656:GLY:HA3	2.13	0.49
2:B:428:ILE:C	2:B:430:ARG:H	2.15	0.49
7:I:15:TYR:CD1	7:I:30:ARG:HG3	2.47	0.49
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.22	0.49
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.94	0.49
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	2.28	0.49
1:A:994:GLN:NE2	1:A:1023:ARG:HE	2.09	0.49
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.10	0.49
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.94	0.49
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.20	0.48
2:B:899:ILE:H	2:B:899:ILE:CD1	2.26	0.48
2:B:508:LEU:N	2:B:509:ALA:CB	2.76	0.48
1:A:1098:VAL:O	1:A:1099:PRO:C	2.52	0.48
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.16	0.48
7:I:65:ASP:C	7:I:65:ASP:OD1	2.52	0.48
2:B:914:LYS:H	2:B:938:SER:HB3	1.78	0.48
4:E:79:TRP:HB3	4:E:100:ILE:CD1	2.43	0.48
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.48
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.94	0.48
4:E:176:PRO:O	4:E:212:ARG:HA	2.13	0.48
3:C:46:ILE:HA	3:C:159:ALA:HA	1.95	0.48
4:E:23:VAL:HG22	4:E:78:LEU:HD21	1.95	0.48
1:A:166:GLY:HA3	1:A:167:CYS:HB3	1.94	0.48
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:HB2	1:A:69:THR:OG1	2.14	0.48
1:A:166:GLY:CA	1:A:167:CYS:CB	2.90	0.48
2:B:959:ASP:OD2	2:B:959:ASP:N	2.46	0.48
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.78	0.48
1:A:1364:ASN:ND2	1:A:1366:ARG:H	2.11	0.48
1:A:1106:ASN:OD1	1:A:1385:THR:HG21	2.13	0.48
2:B:795:ILE:HG22	2:B:796:LEU:O	2.13	0.48
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.13	0.48
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.48	0.48
4:E:50:MET:HG2	4:E:50:MET:O	2.14	0.48
1:A:1075:PRO:HA	1:A:1078:GLN:HB3	1.95	0.48
1:A:772:GLY:HA3	1:A:1086:PHE:H	1.79	0.48
2:B:830:TYR:O	2:B:831:SER:CB	2.61	0.48
1:A:157:ASP:HB3	1:A:160:GLN:N	2.18	0.48
1:A:152:VAL:HG13	1:A:153:PRO:CD	2.40	0.48
6:H:17:PRO:HA	6:H:24:CYS:SG	2.54	0.48
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.28	0.48
1:A:1399:ARG:HB3	1:A:1400:CYS:SG	2.53	0.48
2:B:108:VAL:HG13	2:B:108:VAL:O	2.13	0.48
1:A:598:LEU:HG	6:H:115:TYR:CE2	2.49	0.48
1:A:1084:PHE:CG	1:A:1085:HIS:N	2.81	0.48
1:A:541:ILE:CG2	1:A:546:VAL:HG23	2.43	0.48
10:L:48:CYS:HB3	10:L:52:GLY:H	1.79	0.48
4:E:55:ARG:HD3	4:E:84:ASP:HA	1.96	0.48
2:B:1183:CYS:O	2:B:1184:LYS:HG2	2.14	0.48
2:B:1067:ARG:NH1	3:C:194:GLU:CD	2.67	0.48
1:A:1158:PRO:HB2	1:A:1159:ARG:CG	2.40	0.47
2:B:514:LEU:CD1	2:B:518:HIS:HD2	2.27	0.47
1:A:919:ILE:HD11	1:A:925:LEU:HD12	1.96	0.47
1:A:185:TRP:O	1:A:186:LYS:HB2	2.13	0.47
6:H:13:SER:N	6:H:27:GLU:O	2.41	0.47
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.53	0.47
1:A:1083:THR:CG2	1:A:1084:PHE:H	2.27	0.47
2:B:864:LYS:CG	2:B:865:LYS:H	2.26	0.47
2:B:427:ASP:O	2:B:430:ARG:HB3	2.14	0.47
1:A:93:VAL:HG21	1:A:304:MET:HB3	1.96	0.47
1:A:120:GLU:HB2	1:A:121:LEU:HG	1.96	0.47
1:A:885:THR:HG21	1:A:943:LEU:HD12	1.96	0.47
2:B:571:PRO:C	2:B:573:GLN:N	2.67	0.47
1:A:477:PRO:HG3	1:A:521:MET:HG2	1.95	0.47
2:B:992:ILE:HD11	9:K:66:PRO:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.95	0.47
7:I:17:ARG:O	7:I:25:LEU:HD12	2.14	0.47
7:I:51:ASN:O	7:I:54:GLU:HB2	2.14	0.47
5:F:97:ARG:NH1	5:F:124:GLU:OE2	2.48	0.47
2:B:651:LEU:CD2	2:B:710:LEU:CD1	2.92	0.47
1:A:15:LYS:HB2	2:B:1220:ASP:O	2.14	0.47
9:K:13:GLY:HA2	9:K:16:GLU:HB2	1.95	0.47
5:F:107:VAL:HG12	5:F:108:PHE:N	2.30	0.47
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.35	0.47
7:I:69:PRO:HB2	7:I:85:PHE:CZ	2.50	0.47
1:A:1124:HIS:O	1:A:1125:ALA:HB3	2.14	0.47
2:B:839:MET:HE2	2:B:1010:LEU:HD11	1.97	0.47
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.96	0.47
2:B:260:GLY:HA3	2:B:267:ARG:CD	2.34	0.47
8:J:48:ARG:CZ	8:J:49:MET:CE	2.93	0.47
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.14	0.47
2:B:1185:GLY:HA2	2:B:1187:ASP:H	1.73	0.47
1:A:567:LYS:NZ	1:A:570:PRO:HD3	2.30	0.47
2:B:1065:GLN:OE1	2:B:1067:ARG:HB2	2.15	0.47
1:A:774:ARG:HD2	13:A:2005:HOH:O	2.15	0.47
4:E:177:ARG:HD3	4:E:215:MET:SD	2.54	0.47
1:A:560:ILE:HB	6:H:79:TRP:HB3	1.97	0.47
2:B:190:TYR:CZ	2:B:196:PRO:HG2	2.50	0.47
4:E:13:TRP:NE1	4:E:37:LEU:O	2.43	0.47
3:C:265:MET:CE	9:K:19:LEU:HB2	2.45	0.47
4:E:55:ARG:HD3	4:E:84:ASP:N	2.30	0.46
1:A:65:LEU:CA	1:A:66:LYS:HB2	2.43	0.46
4:E:177:ARG:HB3	4:E:215:MET:HG2	1.96	0.46
2:B:21:GLU:O	2:B:656:GLY:CA	2.63	0.46
1:A:1090:ALA:H	1:A:1092:LYS:CG	2.25	0.46
1:A:605:MET:HE2	1:A:607:ILE:HD11	1.97	0.46
10:L:28:LYS:HD2	10:L:39:SER:OG	2.15	0.46
3:C:60:ASP:OD2	10:L:60:ARG:NH2	2.48	0.46
3:C:195:GLN:HB2	3:C:195:GLN:HE21	1.60	0.46
6:H:25:ARG:HG3	6:H:41:ASP:OD2	2.15	0.46
1:A:673:GLY:CA	1:A:676:MET:N	2.66	0.46
1:A:709:THR:HB	1:A:712:GLU:H	1.79	0.46
2:B:92:PHE:HB3	2:B:130:VAL:HG11	1.97	0.46
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.30	0.46
2:B:650:GLU:HB3	2:B:654:ARG:HH21	1.81	0.46
2:B:864:LYS:HG2	2:B:865:LYS:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.48	0.46
2:B:60:GLN:HA	2:B:95:ILE:CD1	2.45	0.46
6:H:139:ASN:C	6:H:139:ASN:HD22	2.18	0.46
1:A:673:GLY:HA3	1:A:676:MET:H	1.78	0.46
1:A:1258:HIS:HA	1:A:1260:LEU:N	2.30	0.46
1:A:1258:HIS:H	1:A:1260:LEU:HB3	1.80	0.46
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.98	0.46
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.98	0.46
2:B:291:ILE:HD13	2:B:300:HIS:CE1	2.50	0.46
4:E:180:ARG:HE	4:E:180:ARG:HB2	1.62	0.46
2:B:911:ILE:HD13	2:B:911:ILE:HA	1.84	0.46
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.97	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.51	0.46
1:A:157:ASP:HB2	1:A:160:GLN:HG3	1.97	0.46
2:B:162:SER:HA	2:B:163:GLY:HA2	1.70	0.46
4:E:69:ILE:HG12	4:E:69:ILE:H	1.65	0.46
1:A:626:ASN:CB	1:A:627:GLY:HA2	2.25	0.46
1:A:915:SER:O	1:A:919:ILE:HB	2.15	0.46
1:A:63:ARG:NH1	1:A:75:ASN:HD22	2.14	0.46
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.51	0.46
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.30	0.46
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.98	0.46
1:A:67:CYS:HB2	1:A:68:GLN:C	2.34	0.46
1:A:673:GLY:HA3	1:A:676:MET:CB	2.43	0.46
1:A:1258:HIS:CD2	1:A:1262:LYS:HE3	2.51	0.46
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.99	0.46
8:J:17:LYS:HG2	8:J:39:LEU:HD13	1.97	0.46
2:B:879:ARG:HB3	2:B:879:ARG:HE	1.65	0.46
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.97	0.45
1:A:63:ARG:HD3	1:A:74:MET:CB	2.47	0.45
7:I:69:PRO:HG2	7:I:85:PHE:O	2.16	0.45
9:K:8:GLU:O	9:K:37:LYS:HD2	2.15	0.45
2:B:899:ILE:HD12	2:B:911:ILE:O	2.17	0.45
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.98	0.45
1:A:881:GLN:NE2	1:A:958:VAL:O	2.48	0.45
2:B:28:GLU:OE2	2:B:807:ARG:NH2	2.49	0.45
1:A:1095:THR:HG22	1:A:1113:THR:OG1	2.17	0.45
6:H:50:ALA:O	6:H:51:ALA:CB	2.63	0.45
3:C:48:SER:O	3:C:157:CYS:HA	2.16	0.45
2:B:565:PRO:O	2:B:568:ASP:HB2	2.16	0.45
2:B:294:ASP:CG	7:I:12:ASN:HD22	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:143:PHE:CD1	5:F:143:PHE:C	2.89	0.45
1:A:829:VAL:O	1:A:830:LYS:CB	2.62	0.45
9:K:57:LEU:HD21	9:K:78:THR:HG23	1.99	0.45
1:A:1160:SER:H	1:A:1170:ILE:HG21	1.82	0.45
2:B:564:GLU:HB2	2:B:589:VAL:HG12	1.99	0.45
1:A:92:HIS:HD2	1:A:94:GLY:H	1.65	0.45
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.99	0.45
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.52	0.45
2:B:566:LEU:HD11	2:B:586:TRP:CE2	2.52	0.45
1:A:824:LEU:HA	1:A:824:LEU:HD23	1.82	0.45
1:A:567:LYS:HD2	1:A:568:PRO:C	2.38	0.45
4:E:75:MET:HE1	4:E:155:ARG:NH2	2.32	0.45
2:B:34:ILE:HD11	2:B:743:ILE:HG22	1.98	0.45
2:B:1067:ARG:HH11	2:B:1067:ARG:CG	2.30	0.45
2:B:577:ALA:HB1	2:B:589:VAL:HG22	1.99	0.45
2:B:235:SER:HB2	2:B:236:HIS:CD2	2.52	0.45
2:B:892:LYS:HE3	2:B:909:ASP:OD2	2.17	0.45
1:A:87:ALA:HB2	1:A:277:GLU:HG3	1.98	0.45
1:A:58:LEU:N	1:A:59:GLY:CA	2.80	0.45
1:A:408:ASP:O	1:A:410:GLY:N	2.50	0.45
1:A:830:LYS:N	1:A:831:THR:C	2.70	0.44
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.83	0.44
1:A:63:ARG:HD3	1:A:74:MET:HB3	1.98	0.44
1:A:69:THR:H	1:A:70:CYS:CB	2.30	0.44
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.99	0.44
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.99	0.44
2:B:800:GLN:HB3	8:J:52:THR:OG1	2.17	0.44
1:A:1083:THR:HG22	1:A:1084:PHE:N	2.31	0.44
6:H:42:ILE:HG23	6:H:95:TYR:CZ	2.52	0.44
3:C:68:GLY:O	3:C:169:LYS:HB2	2.17	0.44
2:B:315:LYS:N	2:B:316:PRO:HD2	2.32	0.44
1:A:346:ASP:O	1:A:347:PHE:HB2	2.18	0.44
2:B:1030:LEU:HA	2:B:1030:LEU:HD12	1.87	0.44
2:B:31:TRP:CH2	2:B:807:ARG:HB2	2.53	0.44
1:A:522:GLY:HA2	1:A:630:ILE:HD13	2.00	0.44
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.53	0.44
2:B:1153:GLU:HG2	2:B:1155:SER:HB2	1.98	0.44
2:B:205:ILE:CD1	2:B:210:LYS:HG3	2.45	0.44
1:A:606:LEU:HD23	1:A:606:LEU:C	2.38	0.44
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.53	0.44
4:E:66:GLU:H	4:E:66:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:CD2	1:A:94:GLY:H	2.35	0.44
1:A:1286:LYS:HE3	1:A:1304:TRP:CE2	2.52	0.44
1:A:117:GLU:H	1:A:117:GLU:CD	2.21	0.44
2:B:422:LYS:HA	2:B:425:THR:HG22	2.00	0.44
6:H:105:GLU:HB2	6:H:106:GLU:H	1.66	0.44
6:H:10:PHE:N	6:H:10:PHE:CD1	2.86	0.44
4:E:7:ARG:O	4:E:8:ASN:CB	2.60	0.44
4:E:5:ASN:O	4:E:9:ILE:HG12	2.17	0.44
2:B:426:LYS:HB3	2:B:427:ASP:H	1.63	0.44
5:F:72:LYS:N	5:F:72:LYS:HD3	2.33	0.44
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.99	0.44
2:B:644:GLU:CB	2:B:645:SER:CB	2.79	0.44
6:H:11:GLN:H	6:H:54:SER:CB	2.31	0.44
1:A:265:LYS:HE2	1:A:299:HIS:CD2	2.38	0.44
3:C:9:LYS:HB3	3:C:10:ILE:H	1.56	0.44
1:A:103:CYS:HA	1:A:106:VAL:HG12	2.00	0.44
1:A:155:GLU:HB2	1:A:156:ASP:HB2	2.00	0.44
1:A:579:SER:HA	1:A:582:ILE:HD12	2.00	0.44
1:A:1316:VAL:C	1:A:1318:THR:N	2.70	0.44
1:A:391:LEU:HD21	1:A:400:PRO:HB2	2.00	0.44
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.53	0.44
1:A:1169:ILE:O	1:A:1172:LEU:O	2.36	0.44
2:B:446:LEU:HA	2:B:447:ALA:HA	1.64	0.44
1:A:402:ALA:HA	1:A:434:ARG:HA	1.99	0.44
1:A:740:LEU:CD2	1:A:740:LEU:C	2.86	0.44
2:B:496:ARG:HG2	2:B:496:ARG:HH11	1.81	0.44
1:A:829:VAL:CG1	1:A:829:VAL:O	2.64	0.43
1:A:689:LYS:O	1:A:693:VAL:HG23	2.18	0.43
1:A:1134:ILE:HG22	1:A:1306:LEU:CD1	2.48	0.43
6:H:60:ALA:O	6:H:140:ALA:HB1	2.17	0.43
2:B:1067:ARG:NH1	3:C:194:GLU:OE2	2.51	0.43
1:A:1424:VAL:HG21	2:B:1139:ILE:HD11	2.00	0.43
5:F:74:ILE:HA	5:F:75:PRO:HD3	1.71	0.43
1:A:1350:LYS:HE3	1:A:1350:LYS:HB3	1.51	0.43
2:B:341:LEU:O	2:B:341:LEU:HD12	2.18	0.43
2:B:770:GLN:HG2	2:B:983:ARG:O	2.18	0.43
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.99	0.43
9:K:10:PHE:CD1	9:K:11:LEU:HG	2.53	0.43
2:B:865:LYS:NZ	2:B:961:LEU:HD11	2.33	0.43
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.17	0.43
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:83:GLN:HA	6:H:83:GLN:NE2	2.33	0.43
1:A:515:GLN:HE22	1:A:1075:PRO:HD3	1.83	0.43
4:E:4:GLU:HA	4:E:6:GLU:H	1.82	0.43
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.47	0.43
1:A:1342:GLU:HG2	4:E:151:PRO:HG2	1.99	0.43
1:A:909:ASP:HA	1:A:910:PRO:HD2	1.82	0.43
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.18	0.43
3:C:248:ILE:HD13	9:K:102:LYS:HA	1.99	0.43
2:B:760:ASP:OD1	2:B:760:ASP:N	2.51	0.43
1:A:67:CYS:C	1:A:68:GLN:HG2	2.36	0.43
1:A:1111:MET:HE3	1:A:1111:MET:HB3	1.86	0.43
2:B:316:PRO:O	2:B:320:ASP:HB2	2.18	0.43
3:C:22:LEU:HD21	9:K:101:LEU:HD13	1.99	0.43
1:A:785:PRO:HG2	2:B:703:ILE:HD12	2.00	0.43
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.99	0.43
3:C:258:ILE:HG12	9:K:35:PHE:HE2	1.84	0.43
1:A:155:GLU:HB2	1:A:156:ASP:CG	2.38	0.43
4:E:75:MET:CE	4:E:155:ARG:NH2	2.79	0.43
1:A:1157:ASP:O	1:A:1159:ARG:N	2.51	0.43
2:B:846:ILE:HG12	2:B:974:PRO:HB2	2.01	0.43
10:L:33:GLU:C	10:L:35:SER:H	2.22	0.43
3:C:134:ILE:HG21	3:C:139:GLY:HA2	2.01	0.43
1:A:368:LYS:HB2	1:A:368:LYS:HE3	1.83	0.43
9:K:20:LYS:O	9:K:33:ILE:HA	2.18	0.43
1:A:1403:GLU:OE2	1:A:1403:GLU:HA	2.19	0.43
1:A:56:PRO:HB3	1:A:57:ARG:CD	2.48	0.43
2:B:639:ILE:HD12	2:B:688:GLY:O	2.18	0.43
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.49	0.43
2:B:916:THR:HB	2:B:935:ARG:HG3	2.00	0.43
6:H:10:PHE:HA	6:H:29:ALA:O	2.17	0.43
10:L:61:THR:HB	10:L:63:ARG:H	1.83	0.43
2:B:1157:ALA:HB1	2:B:1196:HIS:HB3	1.99	0.43
1:A:92:HIS:C	1:A:92:HIS:CD2	2.91	0.43
2:B:211:VAL:O	2:B:480:SER:HA	2.18	0.43
1:A:747:VAL:HG12	1:A:748:MET:N	2.33	0.43
4:E:55:ARG:HD3	4:E:84:ASP:H	1.84	0.43
1:A:36:ARG:O	1:A:37:PHE:CD1	2.72	0.43
1:A:831:THR:HA	1:A:832:ALA:HA	1.78	0.43
1:A:919:ILE:HD12	1:A:919:ILE:HA	1.73	0.43
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.59	0.43
1:A:62:ASP:HA	1:A:63:ARG:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HA	1:A:83:HIS:CE1	2.54	0.43
1:A:849:MET:HG3	1:A:850:VAL:N	2.34	0.43
1:A:1078:GLN:O	1:A:1078:GLN:HG3	2.18	0.43
4:E:117:THR:C	4:E:119:SER:N	2.72	0.43
1:A:583:PRO:O	1:A:586:ILE:HG12	2.19	0.43
1:A:963:ILE:HD12	1:A:1049:ILE:HG13	1.99	0.43
1:A:106:VAL:HG23	1:A:111:GLY:O	2.19	0.42
2:B:228:LYS:O	2:B:261:ARG:NH1	2.51	0.42
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.54	0.42
2:B:1203:LEU:HA	2:B:1203:LEU:HD23	1.88	0.42
2:B:64:CYS:C	2:B:66:ASP:H	2.22	0.42
1:A:671:ALA:HB3	1:A:676:MET:CE	2.48	0.42
1:A:901:LEU:N	1:A:926:GLN:OE1	2.51	0.42
1:A:17:VAL:HA	2:B:1216:ARG:O	2.19	0.42
2:B:181:LEU:HD13	2:B:194:GLU:HG2	2.02	0.42
1:A:1209:MET:HB3	1:A:1228:TRP:CD1	2.54	0.42
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.19	0.42
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.03	0.42
1:A:602:ASP:O	1:A:616:VAL:HG23	2.18	0.42
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.42
2:B:651:LEU:HD23	2:B:710:LEU:HD11	2.01	0.42
1:A:70:CYS:H	2:B:1172:ILE:HG23	1.84	0.42
6:H:145:ARG:HB2	6:H:146:ARG:O	2.18	0.42
1:A:1341:ILE:HG13	4:E:182:ASP:OD2	2.19	0.42
1:A:416:ARG:HE	1:A:416:ARG:HB2	1.45	0.42
1:A:26:GLU:HA	1:A:29:ALA:HB3	2.01	0.42
2:B:1163:CYS:O	2:B:1167:GLY:HA2	2.19	0.42
1:A:1399:ARG:CB	1:A:1400:CYS:SG	3.06	0.42
2:B:276:ILE:CG2	2:B:280:ILE:HD11	2.23	0.42
9:K:7:PHE:CD1	9:K:7:PHE:C	2.93	0.42
2:B:872:GLU:OE1	2:B:914:LYS:HE2	2.19	0.42
9:K:91:CYS:O	9:K:95:ILE:HG12	2.19	0.42
1:A:1067:LEU:HD12	1:A:1067:LEU:HA	1.80	0.42
1:A:239:LEU:HD23	1:A:240:PRO:HD2	2.02	0.42
1:A:806:ARG:NH1	2:B:729:ILE:HD11	2.34	0.42
1:A:841:LEU:O	1:A:842:VAL:C	2.57	0.42
4:E:156:LEU:HD21	4:E:197:LYS:HB2	2.00	0.42
1:A:1128:GLN:HG2	1:A:1128:GLN:O	2.19	0.42
1:A:701:LEU:HD23	1:A:701:LEU:HA	1.88	0.42
1:A:559:VAL:HG13	6:H:78:SER:HA	2.02	0.42
2:B:508:LEU:N	2:B:509:ALA:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:VAL:C	3:C:242:GLN:N	2.71	0.42
1:A:63:ARG:HH12	1:A:75:ASN:HD22	1.67	0.42
2:B:414:ALA:O	2:B:418:LYS:HB2	2.19	0.42
2:B:377:PHE:O	2:B:380:TYR:HB3	2.19	0.42
1:A:35:ILE:O	1:A:36:ARG:HB2	2.19	0.42
1:A:1253:GLU:O	1:A:1254:ALA:HB3	2.20	0.42
8:J:2:ILE:HD11	8:J:57:ILE:HD13	2.01	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.54	0.42
4:E:124:VAL:O	4:E:126:SER:N	2.53	0.42
9:K:51:LEU:HD13	9:K:59:ALA:HB3	2.01	0.42
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.85	0.42
2:B:123:THR:HA	2:B:204:ILE:O	2.20	0.42
2:B:1058:LEU:HD23	2:B:1058:LEU:HA	1.92	0.42
6:H:52:GLN:HG3	6:H:52:GLN:O	2.20	0.42
1:A:674:PRO:O	1:A:675:THR:C	2.57	0.42
1:A:613:ILE:HG22	1:A:614:PHE:CD2	2.55	0.42
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.00	0.42
7:I:98:VAL:HG21	7:I:113:ASP:CB	2.50	0.42
4:E:198:ILE:HD11	4:E:212:ARG:HG3	2.02	0.42
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.68	0.42
1:A:247:ARG:N	1:A:248:PRO:HD3	2.35	0.42
2:B:221:ASN:OD1	2:B:242:SER:HA	2.20	0.42
1:A:166:GLY:HA2	1:A:167:CYS:CB	2.49	0.42
1:A:1175:SER:HA	1:A:1176:LEU:O	2.19	0.42
2:B:1067:ARG:HD3	2:B:1067:ARG:HA	1.47	0.42
5:F:143:PHE:CD1	5:F:143:PHE:O	2.73	0.42
3:C:245:VAL:HA	3:C:248:ILE:HD12	2.02	0.42
4:E:111:VAL:HG12	4:E:137:GLU:HG3	2.02	0.42
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.89	0.42
9:K:18:LYS:CE	9:K:36:GLU:O	2.67	0.42
1:A:56:PRO:CG	1:A:57:ARG:HE	2.32	0.41
1:A:1088:GLY:HA2	1:A:1089:VAL:HA	1.86	0.41
1:A:1255:GLU:N	1:A:1256:GLU:HB3	2.35	0.41
1:A:265:LYS:HZ3	1:A:302:THR:HB	1.81	0.41
1:A:840:ARG:HD3	1:A:840:ARG:HA	1.73	0.41
2:B:735:ALA:HB1	2:B:738:PHE:CE1	2.53	0.41
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.55	0.41
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.02	0.41
2:B:776:GLN:O	2:B:1095:LEU:HA	2.19	0.41
9:K:42:LEU:HA	9:K:42:LEU:HD23	1.86	0.41
1:A:70:CYS:SG	1:A:71:GLN:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1184:LYS:HA	2:B:1185:GLY:HA3	1.60	0.41
2:B:22:SER:CA	2:B:23:ALA:HB3	2.49	0.41
6:H:98:TYR:O	6:H:118:PHE:HD2	2.03	0.41
1:A:49:LYS:HA	1:A:50:ILE:HB	2.02	0.41
1:A:1124:HIS:ND1	1:A:1124:HIS:N	2.67	0.41
3:C:261:ALA:O	3:C:265:MET:HG2	2.20	0.41
1:A:1013:ASP:HB3	4:E:207:ARG:O	2.20	0.41
1:A:650:GLN:O	1:A:651:LYS:C	2.59	0.41
2:B:115:GLN:HE21	2:B:119:LEU:HG	1.85	0.41
2:B:858:SER:HA	2:B:966:VAL:O	2.21	0.41
6:H:52:GLN:N	6:H:53:ASP:CB	2.58	0.41
7:I:63:GLY:C	7:I:65:ASP:H	2.23	0.41
2:B:1156:ASP:O	2:B:1157:ALA:C	2.57	0.41
1:A:440:ASP:OD1	1:A:498:ARG:NH1	2.53	0.41
8:J:43:ARG:HH11	8:J:43:ARG:HD3	1.71	0.41
4:E:52:ARG:HG3	4:E:53:PRO:HD3	2.02	0.41
6:H:50:ALA:HB3	6:H:53:ASP:CG	2.41	0.41
1:A:566:ILE:HD11	6:H:98:TYR:HB2	2.03	0.41
1:A:301:ALA:C	1:A:303:TYR:H	2.24	0.41
8:J:48:ARG:NE	8:J:49:MET:HE2	2.34	0.41
1:A:867:ILE:HD11	1:A:999:VAL:CG1	2.50	0.41
7:I:13:MET:CE	7:I:15:TYR:CE2	3.03	0.41
3:C:265:MET:CE	9:K:19:LEU:HD12	2.50	0.41
1:A:443:LEU:HD13	1:A:501:LEU:HD13	2.01	0.41
1:A:481:ASP:O	1:A:485:ASP:HB2	2.20	0.41
1:A:828:ALA:O	1:A:831:THR:O	2.38	0.41
6:H:118:PHE:O	6:H:121:LEU:HD12	2.19	0.41
1:A:1256:GLU:O	1:A:1256:GLU:HG3	2.20	0.41
10:L:38:LEU:HD23	10:L:39:SER:N	2.36	0.41
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.20	0.41
1:A:108:MET:HG2	1:A:171:GLN:HE22	1.86	0.41
1:A:573:SER:HB3	1:A:576:GLN:H	1.84	0.41
2:B:576:ASP:N	2:B:576:ASP:OD1	2.53	0.41
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.84	0.41
7:I:50:THR:H	7:I:92:ARG:NH2	2.19	0.41
2:B:512:ARG:HG2	2:B:533:CYS:O	2.20	0.41
2:B:1159:ARG:HD3	2:B:1194:GLN:HG3	2.02	0.41
2:B:361:LEU:HB3	2:B:364:ILE:HD12	2.02	0.41
1:A:1102:LYS:HB2	1:A:1102:LYS:HE3	1.76	0.41
1:A:1403:GLU:HB3	1:A:1405:THR:H	1.85	0.41
6:H:52:GLN:HB2	6:H:52:GLN:HE21	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ALA:HA	2:B:24:PRO:HD2	1.86	0.41
4:E:6:GLU:HG3	4:E:9:ILE:HG13	2.02	0.41
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.60	0.41
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.53	0.41
1:A:53:LEU:HA	1:A:54:ASN:HA	1.87	0.41
1:A:1259:MET:O	1:A:1260:LEU:HB2	2.20	0.41
1:A:1316:VAL:O	1:A:1318:THR:N	2.54	0.41
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.54	0.41
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.61	0.41
4:E:67:GLU:HA	4:E:70:SER:HB2	2.02	0.41
1:A:769:SER:HB2	13:A:2006:HOH:O	2.20	0.41
7:I:88:SER:HB2	7:I:100:PHE:HE1	1.85	0.41
8:J:41:LEU:HD22	8:J:46:CYS:HB3	2.03	0.41
2:B:646:LEU:HD12	2:B:646:LEU:O	2.21	0.41
1:A:884:ASP:C	1:A:886:ILE:H	2.24	0.41
1:A:943:LEU:HA	1:A:943:LEU:HD23	1.93	0.41
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.34	0.41
1:A:1106:ASN:OD1	1:A:1385:THR:HG23	2.20	0.41
9:K:24:ASP:OD1	9:K:25:THR:N	2.29	0.41
1:A:1342:GLU:CG	4:E:151:PRO:HG2	2.51	0.41
2:B:745:PRO:O	2:B:747:MET:N	2.54	0.41
1:A:1101:LEU:O	1:A:1105:LEU:HG	2.21	0.41
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.56	0.41
2:B:516:ASN:HD22	2:B:516:ASN:H	1.69	0.41
6:H:33:GLN:HE21	6:H:33:GLN:N	2.18	0.41
2:B:745:PRO:C	2:B:747:MET:N	2.74	0.41
3:C:22:LEU:HD12	3:C:230:MET:CE	2.52	0.41
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.35	0.41
6:H:85:GLY:HA3	6:H:86:ASP:HA	1.80	0.40
3:C:238:ILE:CG2	3:C:242:GLN:CB	2.99	0.40
3:C:55:THR:HG22	3:C:151:GLN:HA	2.02	0.40
1:A:54:ASN:HA	1:A:56:PRO:CD	2.50	0.40
6:H:81:PRO:O	6:H:83:GLN:HG2	2.22	0.40
3:C:49:VAL:HG13	3:C:155:LEU:HG	2.02	0.40
1:A:58:LEU:H	1:A:59:GLY:CA	2.34	0.40
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.03	0.40
1:A:348:SER:OG	2:B:1128:LEU:HD23	2.21	0.40
4:E:53:PRO:HB3	4:E:55:ARG:NH1	2.34	0.40
1:A:746:MET:HB3	1:A:752:LYS:O	2.21	0.40
1:A:1341:ILE:HD12	1:A:1342:GLU:H	1.86	0.40
3:C:6:PRO:HB2	9:K:101:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH1	2:B:324:ILE:O	2.54	0.40
1:A:1373:ASP:O	1:A:1377:THR:HB	2.21	0.40
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.56	0.40
1:A:771:GLU:HA	1:A:1086:PHE:CZ	2.56	0.40
6:H:56:THR:N	6:H:145:ARG:O	2.55	0.40
7:I:39:GLY:O	7:I:40:SER:HB2	2.21	0.40
2:B:496:ARG:NH2	2:B:540:SER:O	2.55	0.40
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.56	0.40
1:A:50:ILE:CG2	1:A:51:GLY:O	2.62	0.40
8:J:16:ASP:OD1	8:J:17:LYS:HE3	2.21	0.40
2:B:701:ILE:HD11	2:B:703:ILE:HD11	2.02	0.40
1:A:211:PHE:HA	1:A:214:ILE:HD12	2.02	0.40
1:A:1409:LEU:HD13	2:B:1208:LEU:HD21	2.04	0.40
2:B:459:TYR:C	2:B:459:TYR:CD2	2.95	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	1333/1733 (77%)	1168 (88%)	110 (8%)	55 (4%)	3 11
2	B	1035/1224 (85%)	920 (89%)	79 (8%)	36 (4%)	4 15
3	C	263/318 (83%)	243 (92%)	19 (7%)	1 (0%)	39 74
4	E	211/215 (98%)	189 (90%)	12 (6%)	10 (5%)	3 9
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100 100
6	H	108/146 (74%)	76 (70%)	17 (16%)	15 (14%)	0 1
7	I	119/122 (98%)	106 (89%)	11 (9%)	2 (2%)	11 36
8	J	63/70 (90%)	62 (98%)	1 (2%)	0	100 100
9	K	111/120 (92%)	99 (89%)	10 (9%)	2 (2%)	11 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	L	39/70 (56%)	29 (74%)	9 (23%)	1 (3%)	7 22
11	M	4/8 (50%)	3 (75%)	1 (25%)	0	100 100
All	All	3368/4181 (81%)	2973 (88%)	273 (8%)	122 (4%)	4 14

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	56	PRO
1	A	63	ARG
1	A	70	CYS
1	A	157	ASP
1	A	167	CYS
1	A	186	LYS
1	A	603	ASN
1	A	674	PRO
1	A	752	LYS
1	A	830	LYS
1	A	885	THR
1	A	1160	SER
1	A	1175	SER
1	A	1188	GLN
1	A	1221	LYS
1	A	1256	GLU
1	A	1260	LEU
1	A	1387	HIS
1	A	1399	ARG
1	A	1400	CYS
1	A	1401	SER
2	B	68	THR
2	B	104	GLU
2	B	105	SER
2	B	108	VAL
2	B	427	ASP
2	B	645	SER
2	B	648	HIS
2	B	1155	SER
2	B	1156	ASP
2	B	1180	GLN
3	C	10	ILE
4	E	49	SER

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Mol	Chain	Res	Type
4	E	52	ARG
4	E	74	ASP
4	E	148	GLU
6	H	36	CYS
6	H	51	ALA
6	H	77	ARG
6	H	78	SER
6	H	85	GLY
6	H	92	ASP
6	H	106	GLU
6	H	107	VAL
6	H	108	SER
6	H	139	ASN
7	I	40	SER
1	A	52	GLY
1	A	53	LEU
1	A	62	ASP
1	A	120	GLU
1	A	279	LEU
1	A	409	SER
1	A	419	LYS
1	A	626	ASN
1	A	831	THR
1	A	1080	THR
1	A	1176	LEU
1	A	1405	THR
2	B	22	SER
2	B	67	SER
2	B	266	ALA
2	B	368	GLU
2	B	426	LYS
2	B	429	PHE
2	B	735	ALA
2	B	736	THR
2	B	1097	HIS
2	B	1157	ALA
4	E	8	ASN
4	E	53	PRO
4	E	84	ASP
6	H	83	GLN
6	H	90	ALA
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	66	LYS
1	A	71	GLN
1	A	158	PRO
1	A	465	TYR
1	A	705	LYS
1	A	747	VAL
1	A	764	CYS
1	A	833	GLU
1	A	1158	PRO
1	A	1159	ARG
2	B	644	GLU
2	B	1066	SER
2	B	1184	LYS
6	H	52	GLN
6	H	88	SER
1	A	154	SER
1	A	599	SER
2	B	109	THR
2	B	509	ALA
2	B	510	LYS
2	B	746	SER
4	E	75	MET
9	K	25	THR
10	L	64	LEU
1	A	453	MET
1	A	958	VAL
1	A	1090	ALA
1	A	1254	ALA
2	B	1152	MET
6	H	11	GLN
9	K	45	LEU
1	A	221	SER
2	B	23	ALA
2	B	261	ARG
2	B	574	SER
2	B	646	LEU
2	B	1166	CYS
4	E	73	PRO
1	A	93	VAL
4	E	51	GLY
7	I	76	PRO
1	A	622	VAL

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Mol	Chain	Res	Type
2	B	647	GLY
2	B	974	PRO
2	B	1017	ILE
1	A	1437	GLY

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	1182/1520 (78%)	1049 (89%)	133 (11%)	7 22
2	B	919/1061 (87%)	841 (92%)	78 (8%)	13 36
3	C	233/274 (85%)	207 (89%)	26 (11%)	7 22
4	E	195/197 (99%)	170 (87%)	25 (13%)	5 16
5	F	74/137 (54%)	67 (90%)	7 (10%)	11 30
6	H	102/128 (80%)	81 (79%)	21 (21%)	1 4
7	I	115/116 (99%)	105 (91%)	10 (9%)	13 35
8	J	60/65 (92%)	53 (88%)	7 (12%)	7 20
9	K	98/102 (96%)	91 (93%)	7 (7%)	18 46
10	L	38/57 (67%)	32 (84%)	6 (16%)	3 9
11	M	2/2 (100%)	2 (100%)	0	100 100
All	All	3018/3659 (82%)	2698 (89%)	320 (11%)	8 24

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	36	ARG
1	A	37	PHE
1	A	39	GLU
1	A	50	ILE
1	A	53	LEU
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	56	PRO
1	A	57	ARG
1	A	60	SER
1	A	63	ARG
1	A	64	ASN
1	A	68	GLN
1	A	69	THR
1	A	71	GLN
1	A	90	VAL
1	A	93	VAL
1	A	120	GLU
1	A	121	LEU
1	A	129	LYS
1	A	145	LYS
1	A	150	THR
1	A	159	THR
1	A	167	CYS
1	A	186	LYS
1	A	187	LYS
1	A	196	GLU
1	A	247	ARG
1	A	263	THR
1	A	264	PHE
1	A	265	LYS
1	A	266	LEU
1	A	281	HIS
1	A	302	THR
1	A	304	MET
1	A	354	SER
1	A	385	ILE
1	A	389	THR
1	A	411	ASP
1	A	416	ARG
1	A	445	ASN
1	A	451	HIS
1	A	453	MET
1	A	454	SER
1	A	461	LYS
1	A	463	ILE
1	A	472	LEU
1	A	513	SER
1	A	518	LYS

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Mol	Chain	Res	Type
1	A	544	ASP
1	A	553	VAL
1	A	566	ILE
1	A	567	LYS
1	A	573	SER
1	A	593	GLU
1	A	616	VAL
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	708	MET
1	A	728	LYS
1	A	734	GLU
1	A	737	LEU
1	A	740	LEU
1	A	752	LYS
1	A	756	ILE
1	A	769	SER
1	A	830	LYS
1	A	831	THR
1	A	849	MET
1	A	857	ARG
1	A	878	ILE
1	A	882	SER
1	A	885	THR
1	A	896	ARG
1	A	919	ILE
1	A	935	GLN
1	A	948	VAL
1	A	961	ARG
1	A	973	ILE
1	A	1001	ARG
1	A	1036	ARG
1	A	1048	ASN
1	A	1078	GLN
1	A	1079	MET
1	A	1092	LYS
1	A	1095	THR
1	A	1111	MET
1	A	1112	LYS
1	A	1124	HIS
1	A	1143	LEU

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Mol	Chain	Res	Type
1	A	1144	LYS
1	A	1146	VAL
1	A	1159	ARG
1	A	1160	SER
1	A	1167	GLU
1	A	1169	ILE
1	A	1171	GLN
1	A	1173	HIS
1	A	1176	LEU
1	A	1188	GLN
1	A	1194	ARG
1	A	1221	LYS
1	A	1227	ILE
1	A	1230	GLU
1	A	1234	GLU
1	A	1240	CYS
1	A	1243	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1264	GLU
1	A	1269	GLU
1	A	1281	ARG
1	A	1297	GLU
1	A	1318	THR
1	A	1341	ILE
1	A	1350	LYS
1	A	1361	SER
1	A	1366	ARG
1	A	1376	THR
1	A	1377	THR
1	A	1387	HIS
1	A	1398	MET
1	A	1399	ARG
1	A	1400	CYS
1	A	1401	SER
1	A	1405	THR
1	A	1407	GLU
1	A	1420	ASP
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
1	A	1447	GLU

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Mol	Chain	Res	Type
2	B	22	SER
2	B	46	GLN
2	B	61	ASP
2	B	67	SER
2	B	69	LEU
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	104	GLU
2	B	108	VAL
2	B	109	THR
2	B	110	HIS
2	B	125	SER
2	B	162	SER
2	B	164	LYS
2	B	187	SER
2	B	199	MET
2	B	210	LYS
2	B	211	VAL
2	B	218	SER
2	B	222	ILE
2	B	253	THR
2	B	261	ARG
2	B	339	THR
2	B	346	GLU
2	B	365	THR
2	B	367	LEU
2	B	368	GLU
2	B	401	PHE
2	B	425	THR
2	B	427	ASP
2	B	452	THR
2	B	522	VAL
2	B	531	GLN
2	B	540	SER
2	B	543	SER
2	B	547	VAL
2	B	568	ASP
2	B	573	GLN
2	B	576	ASP
2	B	579	ARG
2	B	589	VAL

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Mol	Chain	Res	Type
2	B	598	GLU
2	B	642	ASP
2	B	643	ASP
2	B	646	LEU
2	B	648	HIS
2	B	653	VAL
2	B	668	ASP
2	B	677	GLU
2	B	678	GLU
2	B	690	VAL
2	B	708	GLU
2	B	733	HIS
2	B	734	HIS
2	B	737	THR
2	B	815	ARG
2	B	838	SER
2	B	879	ARG
2	B	899	ILE
2	B	915	THR
2	B	916	THR
2	B	935	ARG
2	B	938	SER
2	B	939	THR
2	B	958	GLN
2	B	959	ASP
2	B	964	VAL
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1060	ARG
2	B	1065	GLN
2	B	1077	THR
2	B	1150	ARG
2	B	1156	ASP
2	B	1192	ILE
2	B	1221	ARG
3	C	3	GLU
3	C	25	VAL
3	C	34	ARG
3	C	43	THR
3	C	48	SER
3	C	50	GLU

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Mol	Chain	Res	Type
3	C	55	THR
3	C	100	THR
3	C	107	SER
3	C	110	THR
3	C	121	VAL
3	C	125	MET
3	C	129	ILE
3	C	138	GLU
3	C	155	LEU
3	C	156	THR
3	C	157	CYS
3	C	189	THR
3	C	217	ASP
3	C	235	VAL
3	C	240	VAL
3	C	251	LEU
3	C	254	LYS
3	C	257	SER
3	C	263	THR
3	C	266	ASP
4	E	3	GLN
4	E	7	ARG
4	E	9	ILE
4	E	10	SER
4	E	11	ARG
4	E	31	THR
4	E	48	ASP
4	E	52	ARG
4	E	68	SER
4	E	69	ILE
4	E	70	SER
4	E	74	ASP
4	E	78	LEU
4	E	81	GLU
4	E	84	ASP
4	E	85	GLU
4	E	103	LYS
4	E	106	GLN
4	E	107	THR
4	E	116	ILE
4	E	126	SER
4	E	167	ARG

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Mol	Chain	Res	Type
4	E	196	VAL
4	E	201	LYS
4	E	202	SER
5	F	72	LYS
5	F	74	ILE
5	F	87	LYS
5	F	97	ARG
5	F	110	ASP
5	F	111	LEU
5	F	123	LYS
6	H	5	LEU
6	H	7	ASP
6	H	14	GLU
6	H	26	ILE
6	H	33	GLN
6	H	34	ASP
6	H	36	CYS
6	H	52	GLN
6	H	53	ASP
6	H	80	ARG
6	H	83	GLN
6	H	86	ASP
6	H	89	LEU
6	H	92	ASP
6	H	104	PHE
6	H	123	MET
6	H	124	ARG
6	H	138	GLU
6	H	139	ASN
6	H	143	LEU
6	H	146	ARG
7	I	10	CYS
7	I	35	VAL
7	I	70	ARG
7	I	93	LYS
7	I	94	ASP
7	I	98	VAL
7	I	106	CYS
7	I	111	THR
7	I	119	THR
7	I	120	GLN
8	J	1	MET

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Mol	Chain	Res	Type
8	J	3	VAL
8	J	6	ARG
8	J	17	LYS
8	J	19	GLU
8	J	20	SER
8	J	57	ILE
9	K	6	ARG
9	K	18	LYS
9	K	25	THR
9	K	49	GLU
9	K	57	LEU
9	K	102	LYS
9	K	114	LEU
10	L	26	THR
10	L	27	LEU
10	L	34	CYS
10	L	41	SER
10	L	44	ASP
10	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	HIS
1	A	119	ASN
1	A	299	HIS
1	A	358	ASN
1	A	394	ASN
1	A	399	HIS
1	A	451	HIS
1	A	479	ASN
1	A	517	ASN
1	A	626	ASN
1	A	659	HIS
1	A	736	ASN
1	A	742	ASN
1	A	854	ASN
1	A	994	GLN
1	A	1048	ASN
1	A	1171	GLN
1	A	1173	HIS

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Mol	Chain	Res	Type
1	A	1188	GLN
1	A	1258	HIS
1	A	1265	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	115	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	255	GLN
2	B	278	GLN
2	B	516	ASN
2	B	518	HIS
2	B	572	HIS
2	B	583	ASN
2	B	648	HIS
2	B	657	HIS
2	B	667	GLN
2	B	734	HIS
2	B	744	HIS
2	B	862	GLN
2	B	957	ASN
2	B	958	GLN
2	B	1025	HIS
2	B	1084	GLN
2	B	1161	HIS
2	B	1180	GLN
3	C	24	ASN
3	C	102	GLN
3	C	112	ASN
3	C	135	GLN
3	C	167	HIS
3	C	195	GLN
3	C	203	GLN
3	C	242	GLN
3	C	252	GLN
3	C	267	GLN
4	E	3	GLN
4	E	5	ASN
4	E	32	GLN
4	E	101	GLN

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Mol	Chain	Res	Type
4	E	113	GLN
4	E	146	HIS
4	E	147	HIS
5	F	100	GLN
6	H	33	GLN
6	H	52	GLN
6	H	83	GLN
7	I	12	ASN
7	I	51	ASN
8	J	53	HIS
9	K	2	ASN
9	K	65	HIS
11	M	7	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
11	ILX	M	1	11	7,9,10	0.88	0	7,11,13	2.16	3 (42%)
11	TRX	M	2	11	14,16,17	3.74	3 (21%)	10,22,24	5.18	4 (40%)
11	CSX	M	6	11	3,6,7	2.43	2 (66%)	3,6,8	1.89	1 (33%)
11	HYP	M	8	11	7,8,9	0.82	0	5,10,12	1.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ILX	M	1	11	-	0/10/12/14	0/0/0/0
11	TRX	M	2	11	-	0/3/6/8	0/2/2/2
11	CSX	M	6	11	-	0/1/5/7	0/0/0/0
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	2	TRX	CE3-CZ3	2.03	1.40	1.36
11	M	6	CSX	CB-CA	2.16	1.59	1.53
11	M	6	CSX	O-C	3.56	1.36	1.19
11	M	2	TRX	CZ2-CE2	8.66	1.54	1.41
11	M	2	TRX	CZ2-CH2	10.04	1.56	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	2	TRX	CH2-CZ2-CE2	-15.43	109.12	119.19
11	M	1	ILX	O-C-CA	-3.08	117.30	125.44
11	M	6	CSX	O-C-CA	-2.99	117.71	125.49
11	M	2	TRX	CB-CG-CD1	-2.47	124.92	127.97
11	M	2	TRX	CZ2-CE2-NE1	-2.03	125.14	130.77
11	M	1	ILX	CG2-CB-CG1	2.63	115.36	111.22
11	M	1	ILX	C-CA-N	3.00	116.10	109.83
11	M	2	TRX	CZ2-CE2-CD2	3.30	125.35	121.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	2	TRX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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	1349/1733 (77%)	-0.20	54 (4%) 42 30	2, 30, 63, 104	0
2	B	1061/1224 (86%)	-0.24	46 (4%) 39 27	6, 29, 63, 77	0
3	C	265/318 (83%)	-0.27	7 (2%) 59 47	16, 26, 43, 59	0
4	E	213/215 (99%)	-0.14	6 (2%) 56 44	13, 35, 60, 70	0
5	F	84/155 (54%)	-0.36	1 (1%) 81 73	10, 23, 41, 49	0
6	H	116/146 (79%)	0.53	15 (12%) 5 2	35, 48, 71, 72	0
7	I	121/122 (99%)	-0.20	3 (2%) 61 48	6, 24, 52, 65	0
8	J	65/70 (92%)	-0.46	1 (1%) 76 68	17, 26, 45, 46	0
9	K	113/120 (94%)	-0.25	5 (4%) 38 26	17, 32, 54, 57	0
10	L	43/70 (61%)	0.45	5 (11%) 6 3	34, 57, 72, 76	0
11	M	4/8 (50%)	0.49	0 100 100	44, 45, 48, 48	0
All	All	3434/4181 (82%)	-0.19	143 (4%) 40 28	2, 30, 62, 104	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	GLY	8.7
1	A	1089	VAL	6.9
1	A	62	ASP	6.2
2	B	265	SER	5.7
1	A	1087	ALA	5.7
1	A	1387	HIS	5.5
1	A	64	ASN	5.3
1	A	1088	GLY	5.3
7	I	122	SER	5.2
1	A	1090	ALA	5.0
2	B	1155	SER	4.8
1	A	1176	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
4	E	50	MET	4.7
2	B	505	ASP	4.7
1	A	1178	ASP	4.6
1	A	248	PRO	4.4
2	B	162	SER	4.3
1	A	1402	PHE	4.2
1	A	1177	LEU	4.2
2	B	161	GLU	4.2
1	A	1448	GLU	4.1
1	A	1449	SER	4.1
2	B	504	ARG	4.1
6	H	87	ARG	4.1
2	B	733	HIS	4.0
2	B	104	GLU	3.9
1	A	159	THR	3.8
1	A	1450	LEU	3.8
2	B	1154	ALA	3.8
3	C	267	GLN	3.7
6	H	85	GLY	3.7
2	B	103	ASN	3.7
2	B	677	GLU	3.6
1	A	63	ARG	3.6
5	F	155	LEU	3.5
6	H	2	SER	3.5
1	A	1175	SER	3.5
1	A	75	ASN	3.5
2	B	506	GLY	3.4
1	A	1078	GLN	3.4
2	B	89	GLU	3.4
4	E	129	PRO	3.4
1	A	281	HIS	3.3
2	B	871	THR	3.3
2	B	722	ASP	3.3
6	H	35	GLN	3.3
2	B	1127	GLY	3.3
7	I	119	THR	3.3
1	A	54	ASN	3.2
1	A	1091	SER	3.2
6	H	106	GLU	3.1
2	B	1099	VAL	3.1
1	A	187	LYS	3.1
2	B	647	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	163	GLY	3.0
2	B	1153	GLU	3.0
6	H	84	ALA	3.0
1	A	1401	SER	3.0
1	A	196	GLU	3.0
1	A	69	THR	2.9
2	B	895	ASP	2.9
9	K	15	GLY	2.9
2	B	429	PHE	2.9
2	B	1222	SER	2.9
1	A	1403	GLU	2.9
1	A	1086	PHE	2.9
2	B	865	LYS	2.8
2	B	676	VAL	2.8
1	A	68	GLN	2.8
2	B	933	SER	2.7
10	L	43	THR	2.7
2	B	105	SER	2.7
2	B	1156	ASP	2.7
6	H	126	GLU	2.7
2	B	266	ALA	2.7
6	H	3	ASN	2.6
1	A	1222	ASN	2.6
1	A	1079	MET	2.6
1	A	1388	GLY	2.6
2	B	477	ALA	2.6
2	B	878	GLN	2.6
3	C	216	GLY	2.6
1	A	278	THR	2.6
2	B	879	ARG	2.6
2	B	723	VAL	2.6
6	H	76	THR	2.6
2	B	887	HIS	2.5
2	B	1098	MET	2.5
1	A	1093	LYS	2.5
3	C	217	ASP	2.5
1	A	158	PRO	2.5
3	C	215	GLU	2.5
9	K	54	ARG	2.5
1	A	1003	LYS	2.5
1	A	1256	GLU	2.5
9	K	14	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	645	SER	2.4
2	B	1178	HIS	2.4
1	A	48	ALA	2.4
1	A	1174	PHE	2.4
2	B	734	HIS	2.4
2	B	446	LEU	2.4
6	H	146	ARG	2.4
2	B	643	ASP	2.4
9	K	3	ALA	2.3
10	L	44	ASP	2.3
4	E	128	PRO	2.3
6	H	77	ARG	2.3
7	I	120	GLN	2.3
1	A	130	ASP	2.2
6	H	83	GLN	2.2
1	A	1080	THR	2.2
10	L	26	THR	2.2
2	B	246	LYS	2.2
4	E	47	CYS	2.2
1	A	157	ASP	2.2
6	H	34	ASP	2.2
1	A	1405	THR	2.2
1	A	1253	GLU	2.2
2	B	245	GLU	2.2
4	E	102	GLU	2.2
1	A	39	GLU	2.2
1	A	1081	LEU	2.2
1	A	264	PHE	2.1
10	L	41	SER	2.1
1	A	1360	GLY	2.1
1	A	105	CYS	2.1
1	A	65	LEU	2.1
9	K	2	ASN	2.1
10	L	45	ALA	2.1
3	C	106	GLU	2.1
2	B	642	ASP	2.1
3	C	266	ASP	2.1
6	H	92	ASP	2.1
4	E	67	GLU	2.1
2	B	958	GLN	2.1
1	A	831	THR	2.0
1	A	156	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	943	SER	2.0
6	H	50	ALA	2.0
1	A	1359	ASP	2.0
8	J	65	PRO	2.0
3	C	108	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
11	TRX	M	2	15/16	0.94	0.20	-	44,50,51,51	0
11	HYP	M	8	8/9	0.95	0.18	-	42,47,48,48	0
11	ILX	M	1	10/11	0.94	0.21	-	37,40,44,44	0
11	CSX	M	6	7/8	0.95	0.26	-	48,50,52,54	0

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	ZN	I	3003	1/1	0.98	0.04	-1.56	33,33,33,33	0
12	ZN	I	3004	1/1	0.98	0.05	-1.68	46,46,46,46	0
12	ZN	C	3002	1/1	0.97	0.04	-2.13	39,39,39,39	0
12	ZN	A	3008	1/1	0.94	0.04	-2.20	77,77,77,77	0
12	ZN	L	3005	1/1	0.96	0.04	-2.48	73,73,73,73	0
12	ZN	A	3006	1/1	0.99	0.02	-3.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	ZN	J	3001	1/1	0.99	0.03	-3.12	34,34,34,34	0
12	ZN	B	3007	1/1	0.99	0.02	-3.24	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.