Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 12:37 PM JST

PDB ID	:	5X50
Title	:	RNA Polymerase II from Komagataella Pastoris (Type-2 crystal)
Authors	:	Ehara, H.; Umehara, T.; Sekine, S.; Yokoyama, S.
Deposited on	:	2017-02-14
Resolution	:	4.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

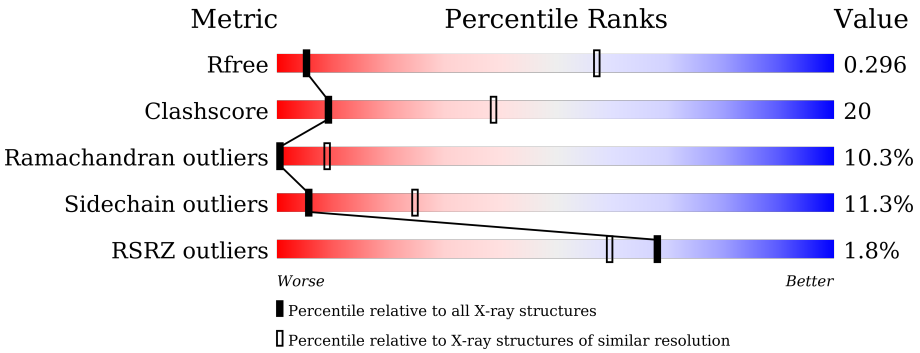
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1743	2% 44% 30% 6% • 19%
2	B	1227	2% 46% 34% 8% 12%
3	C	304	48% 32% 6% 13%
4	D	186	% 46% 24% 6% • 23%
5	E	214	60% 34% 5% •
6	F	155	% 26% 25% • 46%

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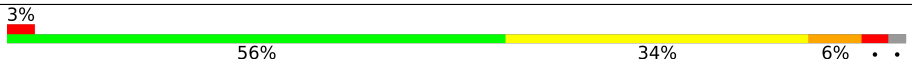
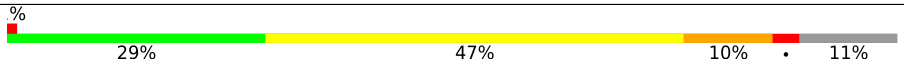
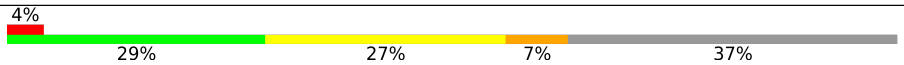
Mol	Chain	Length	Quality of chain
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	73	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 28437 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1409	10410	6594	1819	1943	54	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1079	8241	5236	1442	1517	46	0	0	0

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	263	1852	1181	308	355	8	0	0	0

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	143	1004	647	170	185	2	0	0	0

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	214	1638	1045	288	297	8	0	0	0

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			637	406	109	119	3			

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1187	775	192	217	3			

- Molecule 8 is a protein called RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	131	Total	C	N	O	S	0	0	0
			965	616	155	191	3			

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	113	Total	C	N	O	S	0	0	0
			856	537	150	158	11			

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	64	Total	C	N	O	S	0	0	0
			500	327	87	80	6			

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	112	Total	C	N	O	S	0	0	0
			820	535	137	146	2			

- Molecule 12 is a protein called RNA polymerase subunit, found in RNA polymerase complexes I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			319	196	64	55	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

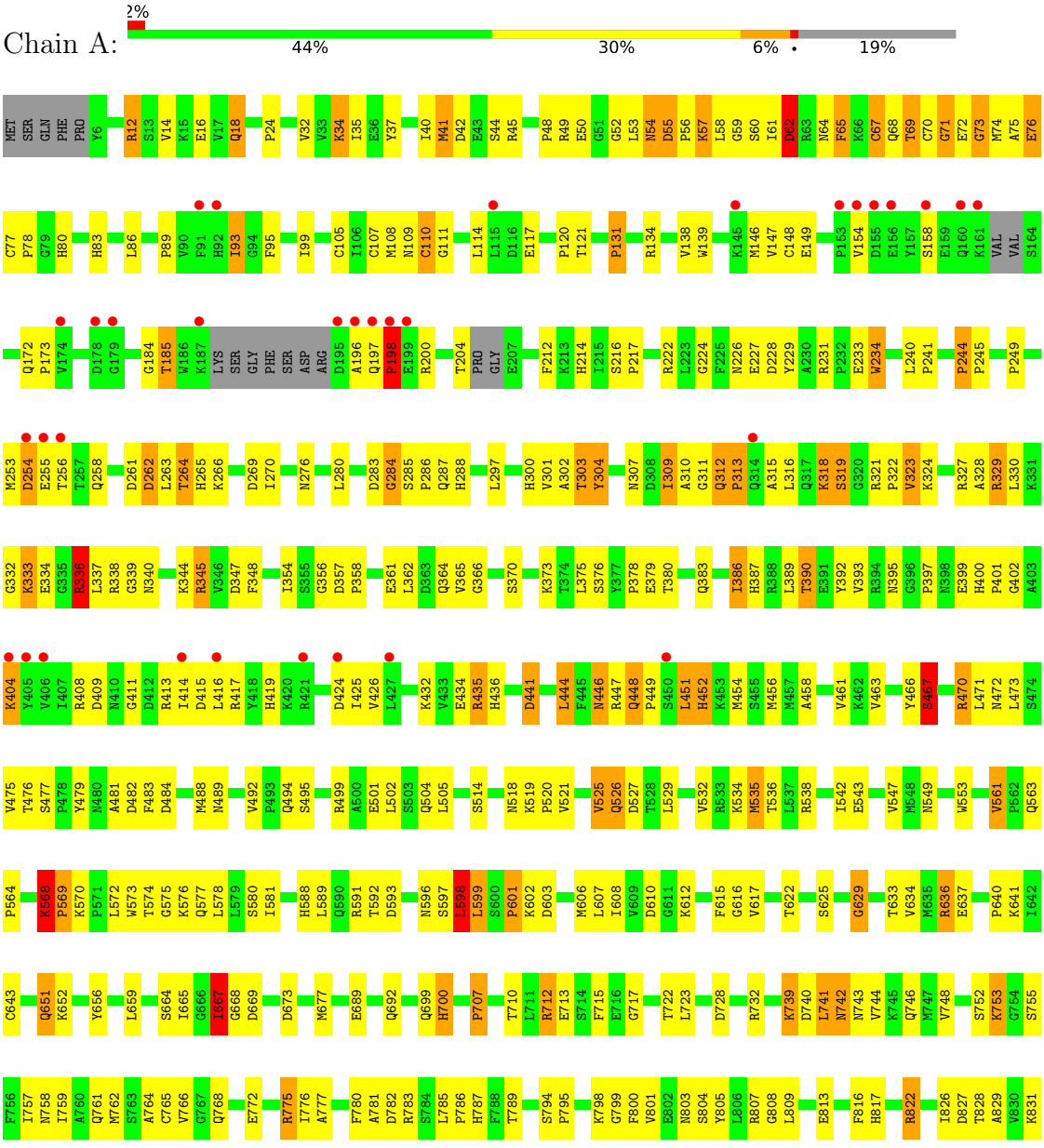
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	2	Total Zn 2 2	0	0
13	B	1	Total Zn 1 1	0	0
13	C	1	Total Zn 1 1	0	0
13	I	2	Total Zn 2 2	0	0
13	J	1	Total Zn 1 1	0	0
13	L	1	Total Zn 1 1	0	0

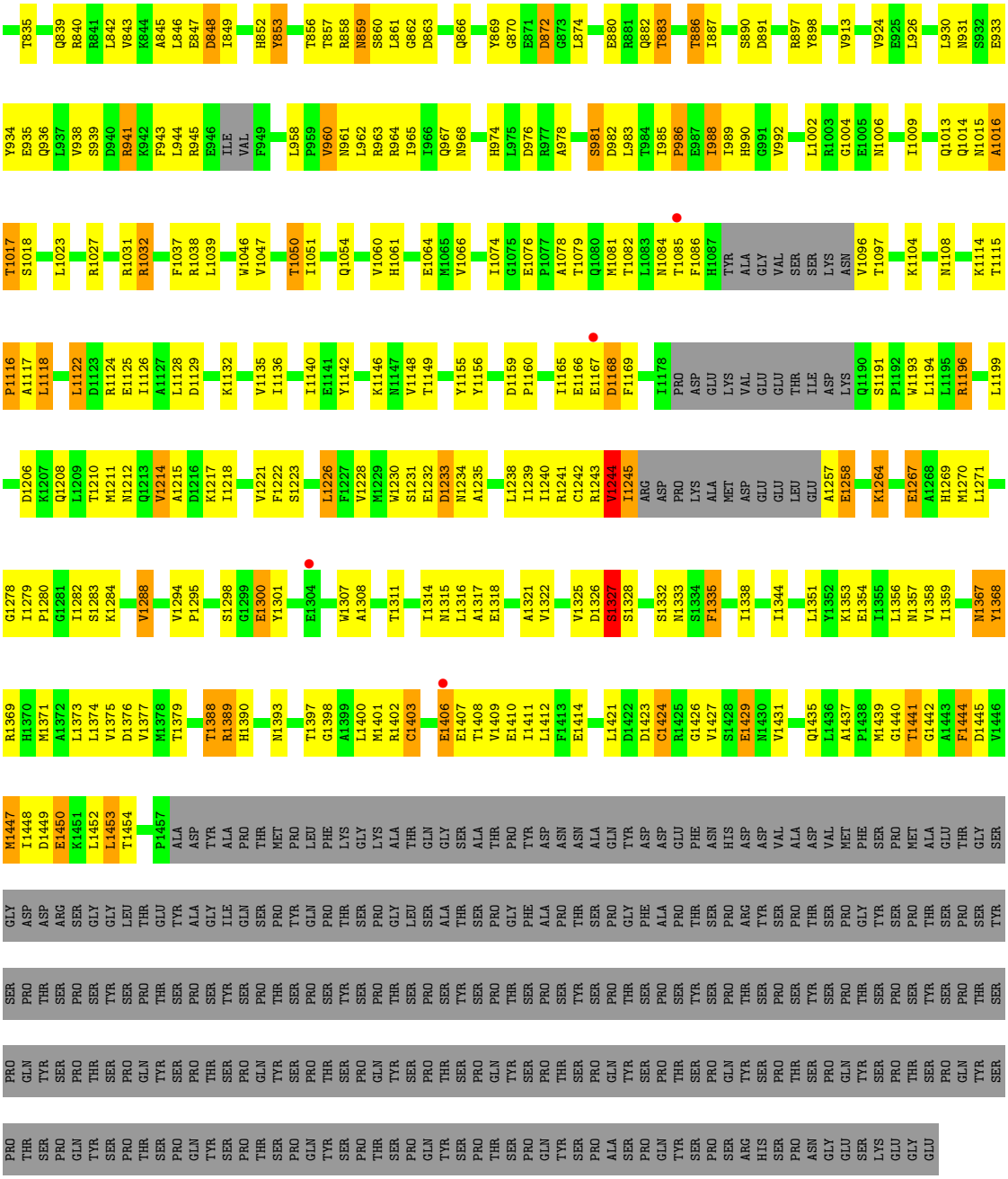
3 Residue-property plots (i)

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

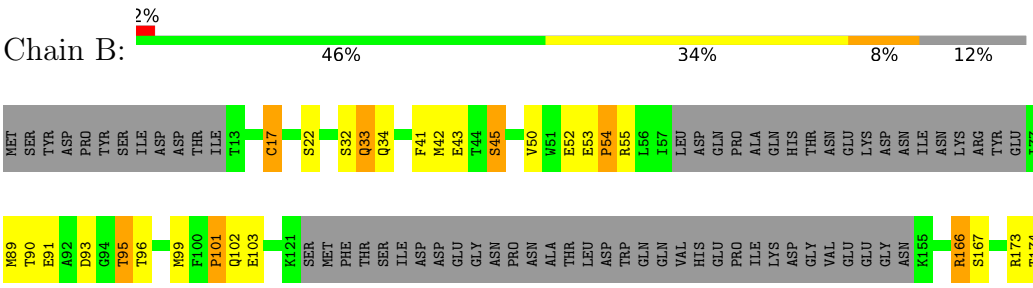
• Molecule 1: DNA-directed RNA polymerase subunit

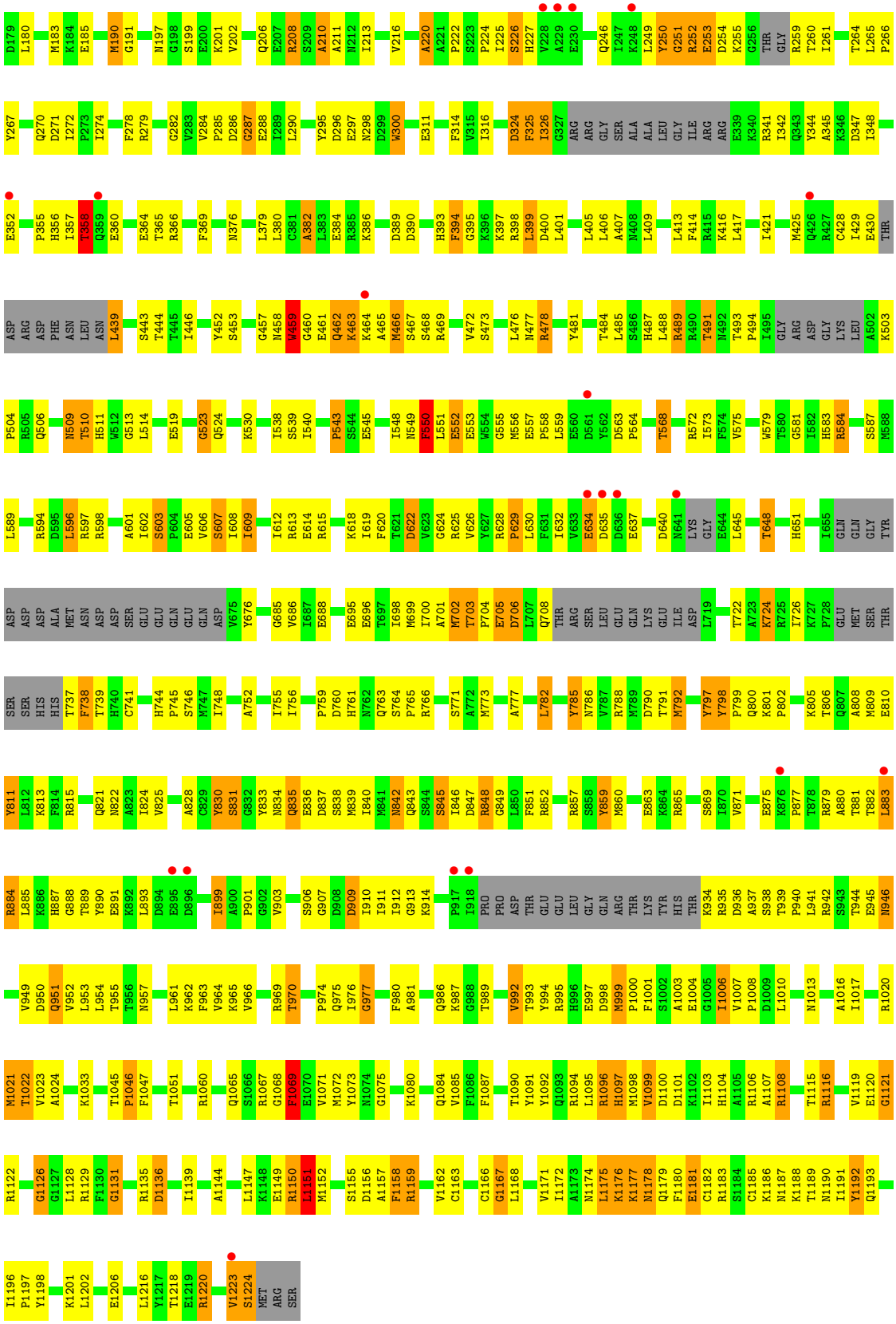
Chain A:





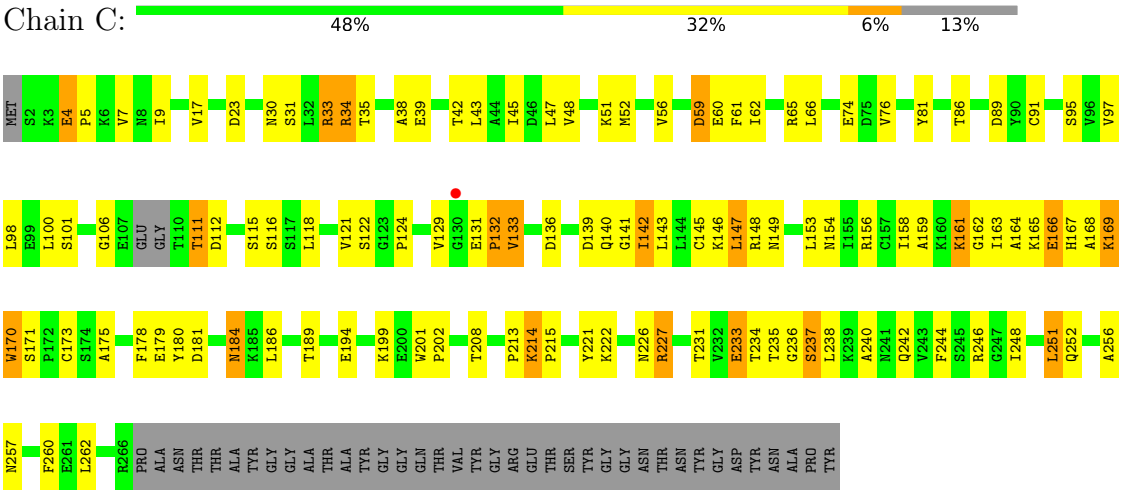
• Molecule 2: DNA-directed RNA polymerase subunit beta





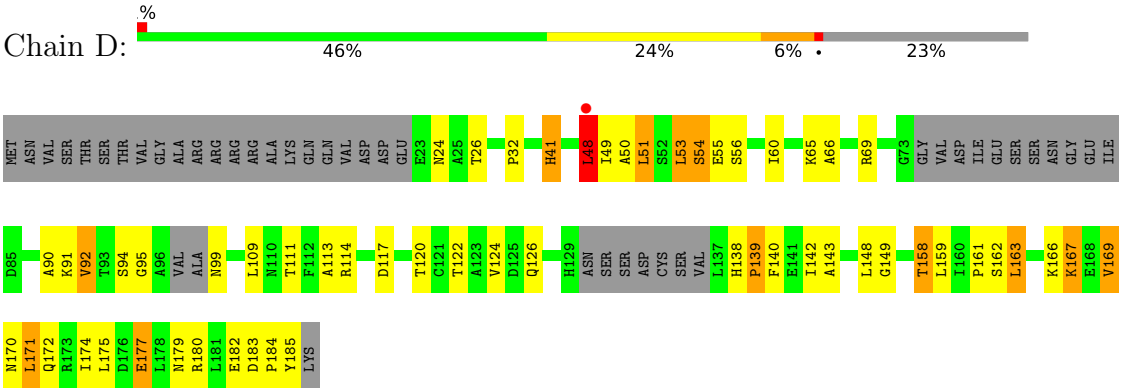
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:



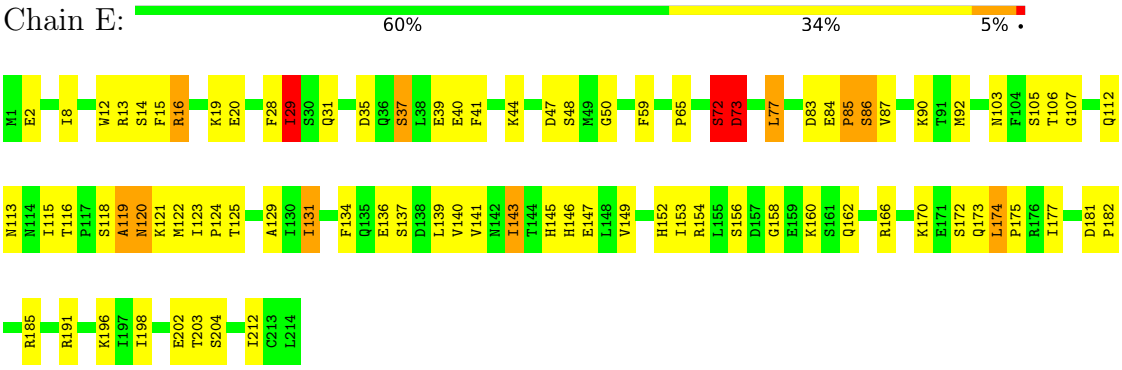
• Molecule 4: RNA polymerase II subunit B32

Chain D:



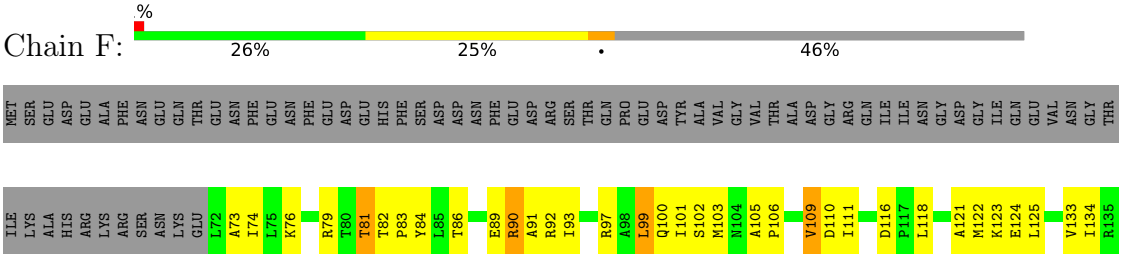
• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

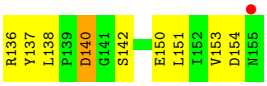
Chain E:



• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

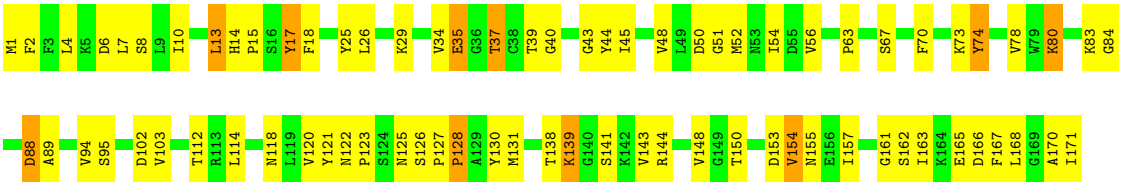
Chain F:





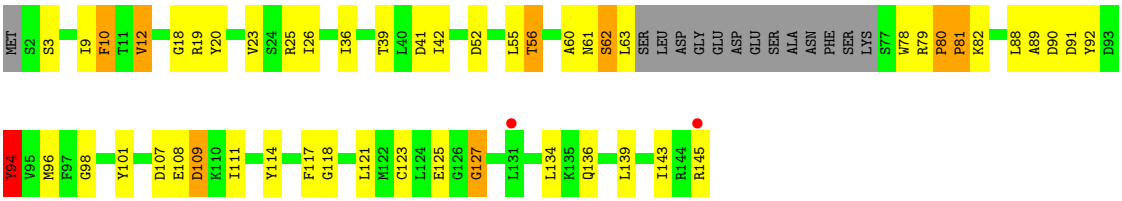
• Molecule 7: RNA polymerase II subunit

Chain G:



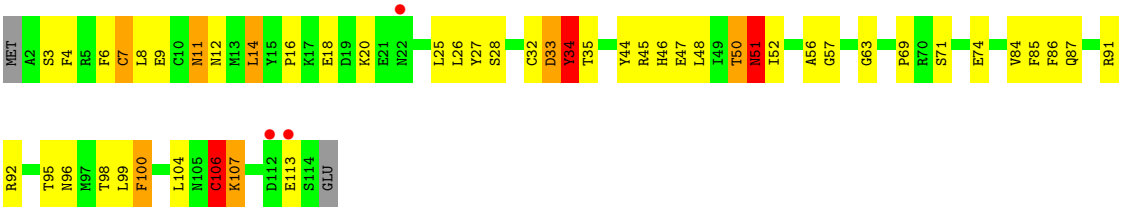
• Molecule 8: RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III

Chain H:



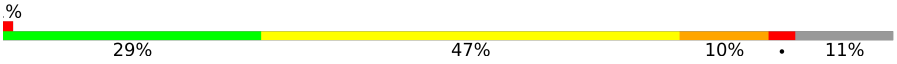
• Molecule 9: DNA-directed RNA polymerase subunit

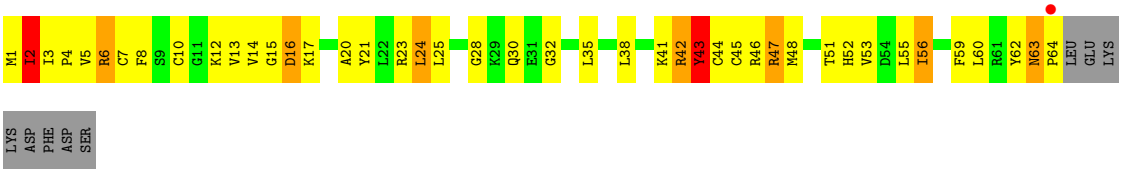
Chain I:



• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

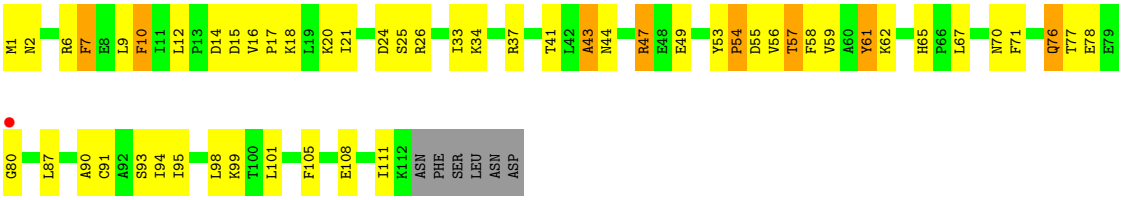
Chain J:





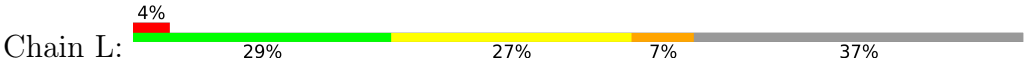
• Molecule 11: RNA polymerase II subunit B12.5

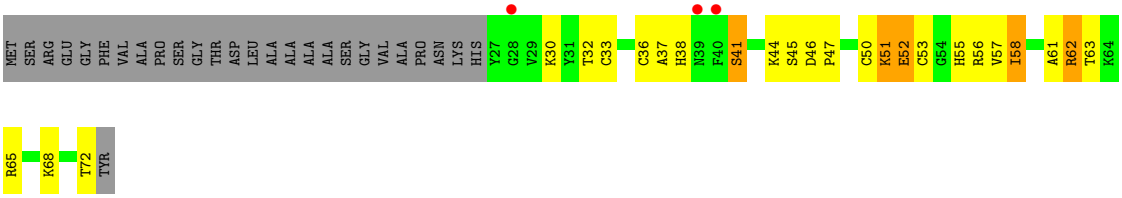
Chain K:



• Molecule 12: RNA polymerase subunit, found in RNA polymerase complexes I, II, and III

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	211.75Å 211.75Å 132.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.70 – 4.29 49.15 – 4.29	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.70-4.29) 99.6 (49.15-4.29)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.235 , 0.296 0.235 , 0.296	Depositor DCC
R_{free} test set	1992 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å^2)	191.6	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 174.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.124 for -h,-k,l 0.128 for h,-h-k,-l 0.125 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	28437	wwPDB-VP
Average B, all atoms (Å^2)	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.27	0/10569	0.71	3/14276 (0.0%)
2	B	0.28	0/8386	0.69	3/11301 (0.0%)
3	C	0.28	0/1877	0.74	2/2543 (0.1%)
4	D	0.25	0/1010	0.69	0/1357
5	E	0.27	0/1668	0.66	0/2245
6	F	0.27	0/646	0.73	1/873 (0.1%)
7	G	0.26	0/1207	0.71	0/1629
8	H	0.28	0/980	0.67	0/1324
9	I	0.28	0/871	0.70	0/1175
10	J	0.33	0/509	0.77	0/684
11	K	0.25	0/836	0.63	0/1131
12	L	0.28	0/321	0.78	0/425
All	All	0.27	0/28880	0.70	9/38963 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1245	ILE	CG1-CB-CG2	-7.11	95.75	111.40
1	A	568	LYS	C-N-CD	6.23	141.49	128.40
2	B	399	LEU	CA-CB-CG	5.98	129.06	115.30
3	C	4	GLU	C-N-CD	5.74	140.45	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	251	LEU	CA-CB-CG	5.58	128.12	115.30
2	B	439	LEU	CA-CB-CG	5.30	127.48	115.30
6	F	99	LEU	CA-CB-CG	5.22	127.31	115.30
2	B	782	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	1453	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	30	GLN	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	10410	0	9856	448	0
2	B	8241	0	7943	372	0
3	C	1852	0	1639	79	0
4	D	1004	0	913	37	0
5	E	1638	0	1551	45	0
6	F	637	0	620	33	0
7	G	1187	0	1092	54	0
8	H	965	0	864	35	0
9	I	856	0	774	41	0
10	J	500	0	503	54	0
11	K	820	0	719	36	0
12	L	319	0	288	13	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28437	0	26762	1096	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 20.

All (1096) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:PRO:HB2	9:I:11:ASN:HB3	1.30	1.13
1:A:256:THR:H	2:B:935:ARG:HH12	1.10	0.97
1:A:67:CYS:SG	1:A:80:HIS:NE2	2.41	0.93
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.56	0.87
1:A:226:ASN:HD22	1:A:229:TYR:H	1.23	0.86
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.59	0.84
3:C:165:LYS:O	11:K:6:ARG:NH1	2.11	0.84
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.41	0.84
4:D:50:ALA:HB1	4:D:143:ALA:HB2	1.60	0.83
6:F:109:VAL:HG12	6:F:110:ASP:H	1.42	0.83
3:C:65:ARG:NH2	10:J:3:ILE:O	2.13	0.81
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.63	0.80
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.64	0.80
1:A:60:SER:OG	1:A:64:ASN:O	1.99	0.80
3:C:171:SER:O	10:J:6:ARG:NH2	2.14	0.79
3:C:42:THR:HG22	3:C:43:LEU:H	1.45	0.79
2:B:848:ARG:NH1	10:J:8:PHE:O	2.16	0.79
2:B:1159:ARG:HH11	2:B:1159:ARG:HB3	1.48	0.78
1:A:446:ASN:HB2	1:A:456:MET:HG2	1.66	0.78
1:A:700:HIS:HA	9:I:113:GLU:HA	1.66	0.77
2:B:799:PRO:HG2	10:J:55:LEU:HD11	1.67	0.77
11:K:56:VAL:HA	11:K:77:THR:HG22	1.67	0.77
1:A:710:THR:HB	1:A:713:GLU:HG3	1.68	0.75
2:B:300:TRP:CZ3	9:I:45:ARG:HB3	2.20	0.74
1:A:780:PHE:HE1	1:A:786:PRO:HD3	1.53	0.74
2:B:270:GLN:HG2	2:B:271:ASP:H	1.52	0.73
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.36	0.73
3:C:74:GLU:O	3:C:246:ARG:NH2	2.17	0.73
2:B:509:ASN:N	2:B:509:ASN:HD22	1.87	0.73
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.71	0.73
6:F:82:THR:HG22	6:F:84:TYR:H	1.51	0.73
2:B:202:VAL:HG21	2:B:476:LEU:HD13	1.71	0.73
2:B:800:GLN:HG2	10:J:51:THR:HG22	1.70	0.73
2:B:52:GLU:HG3	2:B:53:GLU:H	1.53	0.72
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.71	0.72
1:A:739:LYS:H	1:A:739:LYS:HD2	1.55	0.71
1:A:1241:ARG:HH22	1:A:1243:ARG:HH22	1.36	0.71
3:C:175:ALA:HB3	10:J:42:ARG:HH22	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:HIS:CD2	2:B:700:ILE:HB	2.26	0.71
1:A:913:VAL:O	1:A:981:SER:N	2.24	0.71
2:B:22:SER:HA	2:B:811:TYR:HE2	1.56	0.71
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.73	0.70
2:B:225:ILE:HA	2:B:250:TYR:HA	1.73	0.70
1:A:1104:LYS:HG2	1:A:1108:ASN:HD21	1.56	0.70
5:E:83:ASP:O	5:E:85:PRO:HD3	1.91	0.70
1:A:447:ARG:HB2	1:A:488:MET:SD	2.31	0.70
1:A:1074:ILE:HD11	1:A:1371:MET:HA	1.73	0.70
2:B:882:THR:HG1	2:B:934:LYS:N	1.89	0.70
2:B:822:ASN:O	10:J:47:ARG:NH1	2.24	0.70
9:I:106:CYS:SG	9:I:107:LYS:N	2.64	0.70
1:A:333:LYS:H	1:A:338:ARG:HB3	1.57	0.70
2:B:942:ARG:HB2	2:B:945:GLU:HG3	1.73	0.70
1:A:538:ARG:HD2	8:H:20:TYR:HE1	1.56	0.69
2:B:806:THR:HG22	2:B:808:ALA:H	1.57	0.69
1:A:336:ARG:HA	1:A:340:ASN:HD22	1.57	0.69
1:A:710:THR:HG22	1:A:712:ARG:H	1.56	0.69
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.74	0.69
1:A:93:ILE:HG21	1:A:302:ALA:HA	1.74	0.69
1:A:1084:ASN:HB3	1:A:1086:PHE:HD1	1.57	0.69
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.74	0.69
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.74	0.69
10:J:1:MET:HB2	10:J:55:LEU:HD12	1.75	0.69
1:A:739:LYS:HB2	1:A:741:LEU:HD23	1.74	0.68
2:B:821:GLN:HE22	2:B:851:PHE:H	1.40	0.68
2:B:287:GLY:H	2:B:290:LEU:HD23	1.56	0.68
1:A:68:GLN:HE21	1:A:80:HIS:CE1	2.11	0.68
1:A:70:CYS:HB3	2:B:1172:ILE:HG23	1.73	0.68
1:A:780:PHE:CE1	1:A:786:PRO:HD3	2.28	0.68
2:B:503:LYS:HG2	2:B:504:PRO:HD3	1.75	0.68
3:C:233:GLU:OE1	10:J:12:LYS:HE2	1.94	0.68
9:I:34:TYR:HD2	9:I:35:THR:N	1.91	0.68
1:A:240:LEU:HD12	1:A:241:PRO:HD2	1.76	0.68
2:B:594:ARG:O	2:B:598:ARG:HG3	1.93	0.68
1:A:380:THR:HG22	1:A:432:LYS:HG2	1.76	0.68
1:A:1118:LEU:HB2	1:A:1332:SER:HA	1.76	0.68
1:A:451:LEU:HD22	1:A:1079:THR:HG21	1.76	0.67
1:A:1351:LEU:HG	1:A:1375:VAL:HG22	1.76	0.67
2:B:997:GLU:HB3	3:C:34:ARG:HB3	1.76	0.67
1:A:527:ASP:OD1	2:B:1013:ASN:ND2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ARG:HA	1:A:636:ARG:HH11	1.58	0.67
2:B:1181:GLU:HA	2:B:1188:LYS:HG2	1.76	0.67
1:A:781:ALA:N	2:B:696:GLU:OE1	2.24	0.67
4:D:90:ALA:O	4:D:92:VAL:N	2.25	0.67
4:D:24:ASN:O	7:G:83:LYS:HD2	1.94	0.67
2:B:1006:ILE:HG22	10:J:44:CYS:HB3	1.77	0.67
1:A:361:GLU:HB2	1:A:364:GLN:HG3	1.76	0.66
2:B:1099:VAL:O	2:B:1101:ASP:N	2.28	0.66
9:I:95:THR:HG22	9:I:96:ASN:H	1.60	0.66
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.78	0.66
4:D:53:LEU:O	4:D:55:GLU:N	2.27	0.66
12:L:36:CYS:O	12:L:38:HIS:N	2.29	0.65
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.79	0.65
3:C:142:ILE:HG22	10:J:15:GLY:HA3	1.78	0.65
10:J:42:ARG:H	10:J:42:ARG:HD3	1.60	0.65
5:E:134:PHE:HB3	5:E:139:LEU:HD11	1.78	0.65
3:C:116:SER:HB3	3:C:140:GLN:HB3	1.77	0.65
9:I:50:THR:HG22	9:I:51:ASN:H	1.61	0.65
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.11	0.65
1:A:347:ASP:HB3	2:B:1108:ARG:H	1.63	0.64
1:A:1447:MET:HE2	1:A:1447:MET:N	2.12	0.64
2:B:519:GLU:HB2	2:B:752:ALA:HB3	1.80	0.64
2:B:1004:GLU:HB2	2:B:1006:ILE:HG12	1.80	0.64
3:C:147:LEU:HA	10:J:60:LEU:HD21	1.78	0.64
9:I:50:THR:OG1	9:I:92:ARG:NH1	2.30	0.64
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.33	0.64
1:A:883:THR:O	1:A:1027:ARG:NH2	2.29	0.64
3:C:65:ARG:NH1	10:J:2:ILE:HG21	2.13	0.64
2:B:33:GLN:HG3	2:B:34:GLN:H	1.63	0.64
2:B:95:THR:OG1	2:B:96:THR:N	2.28	0.64
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.78	0.64
1:A:1129:ASP:HB3	1:A:1132:LYS:HB3	1.80	0.64
7:G:138:THR:HG22	7:G:139:LYS:H	1.62	0.63
2:B:954:LEU:HA	2:B:964:VAL:HG22	1.79	0.63
5:E:116:THR:HG22	5:E:118:SER:H	1.63	0.63
1:A:256:THR:OG1	2:B:935:ARG:NH1	2.31	0.63
2:B:801:LYS:O	10:J:51:THR:HG23	1.98	0.63
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.34	0.63
1:A:783:ARG:NH2	2:B:696:GLU:O	2.31	0.63
3:C:100:LEU:HD13	3:C:118:LEU:HD23	1.81	0.63
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:95:ILE:O	11:K:99:LYS:N	2.29	0.63
1:A:1397:THR:HG22	1:A:1398:GLY:H	1.64	0.62
1:A:16:GLU:HG2	1:A:1421:LEU:HD11	1.81	0.62
2:B:798:TYR:HD1	10:J:4:PRO:HG3	1.64	0.62
1:A:86:LEU:HD21	1:A:240:LEU:HB2	1.81	0.62
2:B:596:LEU:HB3	2:B:602:ILE:HD11	1.81	0.62
3:C:161:LYS:O	3:C:170:TRP:NE1	2.32	0.62
2:B:341:ARG:O	2:B:345:ALA:N	2.30	0.62
2:B:885:LEU:HA	2:B:936:ASP:HB3	1.80	0.62
1:A:1450:GLU:HA	1:A:1453:LEU:HB3	1.80	0.62
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.81	0.62
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.32	0.62
1:A:529:LEU:O	1:A:532:VAL:HG12	1.99	0.62
1:A:882:GLN:NE2	1:A:960:VAL:O	2.33	0.62
1:A:41:MET:HE3	1:A:41:MET:H	1.65	0.62
1:A:880:GLU:OE1	1:A:964:ARG:NH2	2.33	0.62
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.62
2:B:1223:VAL:O	2:B:1224:SER:HB2	1.98	0.62
1:A:41:MET:HB3	1:A:49:ARG:HA	1.81	0.62
1:A:266:LYS:H	1:A:266:LYS:HD2	1.65	0.62
1:A:454:MET:HE3	1:A:514:SER:HB2	1.82	0.62
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.00	0.62
1:A:1116:PRO:HB2	1:A:1314:ILE:HG23	1.80	0.61
1:A:357:ASP:OD2	11:K:65:HIS:HE1	1.82	0.61
1:A:380:THR:OG1	6:F:102:SER:HB2	2.00	0.61
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.33	0.61
2:B:1166:CYS:O	2:B:1168:LEU:N	2.32	0.61
1:A:354:ILE:HG21	1:A:488:MET:HG3	1.82	0.61
2:B:889:THR:HG22	2:B:891:GLU:H	1.65	0.61
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.40	0.61
2:B:41:PHE:HA	2:B:45:SER:HB2	1.81	0.61
1:A:37:TYR:HB2	1:A:52:GLY:HA3	1.82	0.61
1:A:568:LYS:HD2	1:A:569:PRO:HD2	1.83	0.61
1:A:598:LEU:O	1:A:599:LEU:HB2	2.01	0.61
1:A:891:ASP:OD1	1:A:941:ARG:NH1	2.32	0.61
5:E:174:LEU:HD23	5:E:175:PRO:HD2	1.82	0.61
3:C:30:ASN:O	3:C:33:ARG:HB3	2.00	0.60
10:J:1:MET:N	10:J:55:LEU:H	1.99	0.60
1:A:24:PRO:HD2	1:A:234:TRP:CD1	2.36	0.60
2:B:401:LEU:HD13	2:B:538:ILE:HD12	1.84	0.60
8:H:92:TYR:HB3	8:H:143:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1373:LEU:O	1:A:1377:VAL:HG23	2.00	0.60
2:B:357:ILE:O	2:B:358:THR:HB	2.01	0.60
2:B:513:GLY:HA2	2:B:748:ILE:HG22	1.84	0.60
3:C:146:LYS:HB2	10:J:60:LEU:HD11	1.83	0.60
5:E:47:ASP:CG	5:E:48:SER:H	2.04	0.60
2:B:910:ILE:HA	2:B:940:PRO:HA	1.83	0.60
3:C:56:VAL:HG11	10:J:59:PHE:HB3	1.82	0.60
9:I:16:PRO:HB2	9:I:25:LEU:HD11	1.83	0.60
3:C:175:ALA:CB	10:J:42:ARG:HH22	2.15	0.60
4:D:41:HIS:HB2	7:G:73:LYS:HE3	1.83	0.60
2:B:559:LEU:HB2	2:B:581:GLY:HA2	1.82	0.60
1:A:266:LYS:HD2	1:A:266:LYS:N	2.17	0.60
1:A:286:PRO:O	1:A:288:HIS:N	2.35	0.60
1:A:1217:LYS:O	1:A:1221:VAL:HG23	2.02	0.60
2:B:785:TYR:HE2	10:J:59:PHE:CE1	2.20	0.60
1:A:397:PRO:HG3	1:A:417:ARG:HB3	1.83	0.60
1:A:1132:LYS:O	1:A:1136:ILE:HG13	2.02	0.59
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.84	0.59
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	1.83	0.59
3:C:248:ILE:HG23	11:K:98:LEU:HD13	1.83	0.59
1:A:615:PHE:HB3	8:H:121:LEU:HD21	1.84	0.59
1:A:981:SER:OG	1:A:982:ASP:N	2.35	0.59
1:A:95:PHE:O	1:A:99:ILE:HG13	2.03	0.59
1:A:1326:ASP:O	1:A:1328:SER:N	2.33	0.59
3:C:34:ARG:HD3	11:K:41:THR:OG1	2.03	0.59
3:C:252:GLN:HE21	11:K:95:ILE:HG23	1.68	0.59
1:A:856:THR:HG21	1:A:858:ARG:HE	1.67	0.59
2:B:852:ARG:HH22	12:L:72:THR:HA	1.68	0.59
7:G:138:THR:HG22	7:G:139:LYS:N	2.17	0.59
1:A:1326:ASP:C	1:A:1328:SER:H	2.06	0.59
2:B:597:ARG:NH2	2:B:606:VAL:O	2.35	0.59
3:C:184:ASN:HD21	3:C:189:THR:HB	1.68	0.59
5:E:146:HIS:HB3	5:E:149:VAL:HG23	1.84	0.59
9:I:71:SER:HB3	9:I:85:PHE:CE2	2.37	0.59
1:A:303:THR:HG22	1:A:304:TYR:N	2.18	0.59
1:A:1136:ILE:HG22	1:A:1140:ILE:HD11	1.85	0.59
2:B:975:GLN:O	2:B:977:GLY:N	2.35	0.58
1:A:934:TYR:O	1:A:938:VAL:HG23	2.03	0.58
1:A:65:PHE:O	1:A:71:GLY:HA2	2.04	0.58
1:A:1407:GLU:HB2	1:A:1411:ILE:HG13	1.85	0.58
2:B:552:GLU:HA	2:B:556:MET:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.68	0.58
3:C:91:CYS:O	3:C:95:SER:N	2.35	0.58
1:A:1118:LEU:H	1:A:1311:THR:HG22	1.68	0.58
2:B:265:LEU:HD12	2:B:272:ILE:HD12	1.85	0.58
2:B:551:LEU:C	2:B:553:GLU:H	2.06	0.58
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.85	0.58
2:B:22:SER:HA	2:B:811:TYR:CE2	2.38	0.58
3:C:31:SER:O	3:C:35:THR:HG23	2.03	0.58
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.19	0.58
10:J:42:ARG:HD3	10:J:42:ARG:N	2.19	0.58
1:A:1047:VAL:O	1:A:1051:ILE:HG13	2.04	0.58
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.38	0.58
1:A:53:LEU:HD23	1:A:54:ASN:H	1.69	0.57
1:A:69:THR:C	1:A:71:GLY:H	2.07	0.57
1:A:870:GLY:O	5:E:203:THR:HG21	2.02	0.57
1:A:520:PRO:HG2	1:A:625:SER:HA	1.87	0.57
1:A:309:ILE:HG22	1:A:310:ALA:H	1.69	0.57
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.86	0.57
2:B:1129:ARG:HG2	2:B:1131:GLY:H	1.68	0.57
1:A:1199:LEU:HD11	1:A:1240:ILE:HD11	1.86	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.70	0.57
1:A:484:ASP:HB2	2:B:987:LYS:HG3	1.87	0.57
2:B:594:ARG:NH2	2:B:608:ILE:O	2.38	0.57
3:C:252:GLN:O	3:C:256:ALA:N	2.37	0.57
1:A:345:ARG:HA	2:B:1129:ARG:HA	1.87	0.57
2:B:352:GLU:O	2:B:355:PRO:HD3	2.05	0.57
2:B:509:ASN:HD22	2:B:509:ASN:H	1.53	0.57
4:D:49:ILE:HG21	7:G:4:LEU:HB2	1.86	0.57
1:A:339:GLY:HA2	2:B:1129:ARG:HH22	1.69	0.57
3:C:48:VAL:O	12:L:68:LYS:HA	2.05	0.57
9:I:44:TYR:OH	9:I:46:HIS:ND1	2.30	0.57
1:A:495:SER:HB2	2:B:1149:GLU:OE2	2.05	0.56
1:A:931:ASN:O	1:A:935:GLU:N	2.30	0.56
2:B:645:LEU:HG	2:B:708:GLN:HE22	1.69	0.56
11:K:20:LYS:HB3	11:K:34:LYS:HB2	1.87	0.56
10:J:35:LEU:HB3	10:J:46:ARG:HH12	1.70	0.56
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.87	0.56
1:A:134:ARG:O	1:A:138:VAL:HG23	2.05	0.56
1:A:775:ARG:NH2	1:A:798:LYS:HG3	2.20	0.56
1:A:1014:GLN:O	1:A:1017:THR:OG1	2.23	0.56
1:A:1066:VAL:HG12	1:A:1373:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:ALA:O	1:A:1439:MET:N	2.38	0.56
2:B:797:TYR:O	10:J:1:MET:HG2	2.05	0.56
2:B:882:THR:O	2:B:883:LEU:HB2	2.04	0.56
1:A:597:SER:O	1:A:599:LEU:N	2.38	0.56
1:A:829:ALA:HB1	2:B:523:GLY:HA2	1.88	0.56
3:C:97:VAL:N	3:C:122:SER:OG	2.36	0.56
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.86	0.56
1:A:1166:GLU:O	1:A:1168:ASP:N	2.35	0.56
1:A:1445:ASP:HB2	6:F:137:TYR:HE1	1.70	0.56
1:A:526:GLN:OE1	2:B:836:GLU:N	2.22	0.56
2:B:384:GLU:HB3	9:I:91:ARG:O	2.05	0.56
12:L:51:LYS:O	12:L:52:GLU:HB2	2.06	0.56
1:A:1376:ASP:HA	1:A:1379:THR:HG22	1.88	0.56
2:B:287:GLY:HA2	9:I:6:PHE:HE1	1.71	0.56
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.39	0.56
7:G:44:TYR:HE1	7:G:157:ILE:HB	1.71	0.56
2:B:540:ILE:N	2:B:605:GLU:OE2	2.39	0.56
6:F:97:ARG:HA	6:F:100:GLN:HG3	1.86	0.56
1:A:444:LEU:HD23	1:A:502:LEU:HD21	1.88	0.56
1:A:504:GLN:HE22	6:F:90:ARG:HH21	1.54	0.55
1:A:822:ARG:HH11	1:A:822:ARG:HB2	1.70	0.55
1:A:1449:ASP:HB2	6:F:133:VAL:HG21	1.87	0.55
2:B:379:LEU:HA	2:B:382:ALA:HB3	1.87	0.55
4:D:41:HIS:HB2	7:G:73:LYS:CE	2.35	0.55
4:D:51:LEU:HB2	7:G:2:PHE:O	2.06	0.55
9:I:16:PRO:HA	9:I:27:TYR:HA	1.87	0.55
10:J:63:ASN:HB3	10:J:64:PRO:CD	2.36	0.55
1:A:316:LEU:HB2	2:B:464:LYS:HB3	1.86	0.55
2:B:648:THR:H	2:B:651:HIS:HD2	1.52	0.55
8:H:88:LEU:O	8:H:90:ASP:N	2.39	0.55
11:K:10:PHE:HA	11:K:37:ARG:HB3	1.88	0.55
1:A:392:TYR:O	1:A:402:GLY:HA2	2.06	0.55
1:A:591:ARG:HD2	1:A:606:MET:HB3	1.86	0.55
1:A:817:HIS:CD2	2:B:764:SER:HB2	2.41	0.55
2:B:476:LEU:HA	2:B:487:HIS:ND1	2.21	0.55
2:B:612:ILE:C	2:B:614:GLU:H	2.10	0.55
6:F:82:THR:O	6:F:136:ARG:NH1	2.32	0.55
2:B:417:LEU:HD22	2:B:446:ILE:HD11	1.89	0.55
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	2.05	0.55
10:J:42:ARG:H	10:J:42:ARG:CD	2.19	0.55
2:B:356:HIS:O	2:B:357:ILE:HB	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:CYS:O	9:I:11:ASN:HA	2.07	0.55
1:A:348:PHE:H	2:B:1107:ALA:HA	1.72	0.55
2:B:398:ARG:O	2:B:399:LEU:HD23	2.07	0.55
2:B:773:MET:SD	2:B:987:LYS:HD3	2.47	0.55
8:H:88:LEU:C	8:H:90:ASP:H	2.10	0.55
2:B:325:PHE:O	2:B:326:ILE:HG13	2.06	0.55
5:E:107:GLY:HA3	5:E:131:ILE:HG23	1.89	0.55
11:K:65:HIS:CD2	11:K:67:LEU:H	2.25	0.55
1:A:822:ARG:O	1:A:826:ILE:HG13	2.07	0.54
2:B:199:SER:OG	2:B:201:LYS:NZ	2.39	0.54
1:A:943:PHE:HD2	1:A:944:LEU:HD23	1.72	0.54
3:C:133:VAL:HG21	3:C:237:SER:HA	1.89	0.54
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.88	0.54
1:A:146:MET:HA	1:A:172:GLN:HE21	1.72	0.54
1:A:400:HIS:HB3	1:A:401:PRO:HD3	1.90	0.54
2:B:1096:ARG:HD2	2:B:1097:HIS:ND1	2.22	0.54
2:B:995:ARG:O	2:B:999:MET:HB2	2.08	0.54
8:H:12:VAL:HB	8:H:52:ASP:H	1.73	0.54
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.71	0.54
1:A:263:LEU:C	1:A:265:HIS:H	2.11	0.54
1:A:835:THR:HG21	1:A:1079:THR:HG23	1.90	0.54
1:A:1165:ILE:HB	1:A:1168:ASP:HB2	1.89	0.54
2:B:249:LEU:HD13	2:B:261:ILE:HG12	1.90	0.54
2:B:366:ARG:HG2	2:B:559:LEU:HD23	1.90	0.54
2:B:912:ILE:O	2:B:938:SER:HB3	2.08	0.54
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.89	0.54
7:G:148:VAL:H	7:G:161:GLY:HA2	1.71	0.54
8:H:111:ILE:H	8:H:127:GLY:HA2	1.71	0.54
1:A:1232:GLU:O	1:A:1234:ASN:N	2.41	0.54
2:B:763:GLN:HG2	2:B:765:PRO:HG2	1.89	0.54
1:A:780:PHE:HE2	2:B:510:THR:HG22	1.71	0.54
1:A:843:VAL:HG11	2:B:1136:ASP:OD2	2.06	0.54
2:B:609:ILE:HB	2:B:618:LYS:HB2	1.89	0.54
2:B:1181:GLU:HG2	2:B:1188:LYS:HE2	1.90	0.54
1:A:53:LEU:HD23	1:A:54:ASN:N	2.23	0.54
1:A:858:ARG:HD3	1:A:862:GLY:O	2.08	0.54
1:A:1228:VAL:HG13	1:A:1242:CYS:HB3	1.90	0.54
2:B:266:PRO:HG2	2:B:352:GLU:HB3	1.90	0.54
7:G:88:ASP:OD2	7:G:88:ASP:N	2.39	0.54
1:A:249:PRO:O	1:A:261:ASP:HB2	2.08	0.54
1:A:408:ARG:HD2	1:A:414:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:ARG:NH2	1:A:1243:ARG:HH22	2.05	0.54
3:C:9:ILE:HD11	11:K:108:GLU:HB3	1.90	0.54
12:L:30:LYS:HG3	12:L:41:SER:HB2	1.89	0.54
1:A:452:HIS:CD2	1:A:1076:GLU:HG3	2.43	0.53
1:A:467:SER:HB3	2:B:1103:ILE:HD13	1.89	0.53
1:A:1136:ILE:O	1:A:1140:ILE:HG13	2.08	0.53
3:C:115:SER:OG	3:C:141:GLY:O	2.20	0.53
11:K:47:ARG:HH11	11:K:47:ARG:HB3	1.73	0.53
1:A:318:LYS:O	1:A:319:SER:HB3	2.07	0.53
1:A:321:ARG:HH22	1:A:324:LYS:HE3	1.73	0.53
1:A:926:LEU:HD13	1:A:985:ILE:HD12	1.90	0.53
1:A:941:ARG:O	1:A:945:ARG:HG3	2.08	0.53
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.73	0.53
2:B:890:TYR:CZ	2:B:910:ILE:HG21	2.43	0.53
3:C:52:MET:HB2	3:C:154:ASN:HB2	1.89	0.53
1:A:564:PRO:HG3	1:A:573:TRP:CZ2	2.43	0.53
1:A:1116:PRO:O	1:A:1333:ASN:ND2	2.40	0.53
2:B:285:PRO:CB	9:I:11:ASN:HB3	2.20	0.53
1:A:284:GLY:O	1:A:286:PRO:HD3	2.09	0.53
1:A:447:ARG:HD2	1:A:481:ALA:HB2	1.89	0.53
2:B:828:ALA:O	2:B:834:ASN:ND2	2.42	0.53
9:I:32:CYS:SG	9:I:33:ASP:N	2.80	0.53
1:A:316:LEU:HD12	2:B:464:LYS:O	2.09	0.53
1:A:472:ASN:OD1	1:A:473:LEU:N	2.42	0.53
2:B:286:ASP:O	2:B:288:GLU:N	2.41	0.53
9:I:63:GLY:HA3	9:I:104:LEU:HD11	1.89	0.53
1:A:333:LYS:O	1:A:334:GLU:HB2	2.09	0.53
1:A:786:PRO:HG3	2:B:695:GLU:OE2	2.09	0.53
2:B:572:ARG:NH1	2:B:615:ARG:O	2.41	0.53
2:B:609:ILE:O	2:B:618:LYS:N	2.34	0.53
1:A:857:THR:HB	1:A:866:GLN:HB2	1.91	0.53
2:B:805:LYS:HB2	2:B:809:MET:SD	2.49	0.53
4:D:51:LEU:HB3	7:G:2:PHE:HB2	1.90	0.53
4:D:66:ALA:HA	4:D:69:ARG:HD2	1.89	0.53
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.91	0.53
1:A:483:PHE:O	2:B:989:THR:HG23	2.09	0.53
1:A:1328:SER:O	5:E:147:GLU:HB2	2.08	0.53
1:A:1367:ASN:HD22	1:A:1368:TYR:N	2.06	0.53
10:J:35:LEU:HA	10:J:38:LEU:HD12	1.91	0.53
1:A:400:HIS:O	1:A:402:GLY:N	2.38	0.52
1:A:568:LYS:HB2	1:A:569:PRO:CD	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:ARG:NH1	2:B:632:ILE:HD13	2.24	0.52
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.74	0.52
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.44	0.52
12:L:33:CYS:HB2	12:L:50:CYS:SG	2.49	0.52
1:A:761:GLN:HG2	1:A:766:VAL:O	2.09	0.52
2:B:1174:ASN:O	2:B:1176:LYS:N	2.43	0.52
1:A:827:ASP:O	1:A:831:LYS:HG2	2.09	0.52
5:E:152:HIS:O	5:E:153:ILE:HG13	2.09	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.24	0.52
1:A:114:LEU:HD13	1:A:172:GLN:HE22	1.75	0.52
1:A:664:SER:OG	1:A:665:ILE:N	2.43	0.52
1:A:333:LYS:N	1:A:338:ARG:HD2	2.25	0.52
1:A:890:SER:HB3	1:A:1300:GLU:HG3	1.91	0.52
2:B:226:SER:HB2	2:B:252:ARG:HA	1.92	0.52
4:D:94:SER:HB3	4:D:99:ASN:HB3	1.90	0.52
10:J:35:LEU:CB	10:J:46:ARG:HH12	2.22	0.52
1:A:310:ALA:O	1:A:312:GLN:N	2.43	0.52
1:A:1156:TYR:OH	9:I:18:GLU:OE2	2.25	0.52
1:A:1423:ASP:O	1:A:1424:CYS:HB2	2.09	0.52
2:B:369:PHE:HB3	2:B:579:TRP:CZ3	2.45	0.52
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.43	0.52
1:A:553:TRP:CD1	11:K:62:LYS:HB2	2.44	0.52
8:H:134:LEU:HD13	8:H:136:GLN:NE2	2.25	0.52
10:J:42:ARG:HG2	10:J:44:CYS:SG	2.49	0.52
1:A:61:ILE:HG22	1:A:62:ASP:H	1.75	0.52
1:A:534:LYS:HE3	1:A:746:GLN:HE22	1.73	0.52
2:B:279:ARG:HG2	2:B:284:VAL:HA	1.92	0.52
2:B:992:VAL:HG22	2:B:993:THR:H	1.74	0.52
2:B:1003:ALA:HA	3:C:178:PHE:O	2.10	0.52
2:B:452:TYR:CG	2:B:462:GLN:HG2	2.45	0.52
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.10	0.52
2:B:180:LEU:O	2:B:183:MET:N	2.40	0.51
10:J:23:ARG:C	10:J:25:LEU:H	2.14	0.51
1:A:859:ASN:HD22	1:A:859:ASN:C	2.13	0.51
2:B:880:ALA:O	2:B:882:THR:N	2.40	0.51
2:B:1065:GLN:N	3:C:202:PRO:HG2	2.24	0.51
3:C:112:ASP:HB3	3:C:143:LEU:HD11	1.92	0.51
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.75	0.51
1:A:1166:GLU:C	1:A:1168:ASP:H	2.12	0.51
1:A:1388:THR:HG23	1:A:1390:HIS:H	1.76	0.51
2:B:210:ALA:HB2	2:B:398:ARG:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.92	0.51
1:A:173:PRO:HB2	1:A:184:GLY:HA3	1.93	0.51
1:A:848:ASP:OD2	1:A:860:SER:OG	2.18	0.51
1:A:1191:SER:O	1:A:1243:ARG:HD3	2.10	0.51
3:C:244:PHE:O	3:C:248:ILE:HG13	2.10	0.51
1:A:799:GLY:HA2	1:A:816:PHE:CD1	2.45	0.51
2:B:605:GLU:O	2:B:625:ARG:NH2	2.37	0.51
3:C:62:ILE:HA	3:C:65:ARG:HG3	1.92	0.51
1:A:527:ASP:HB2	2:B:835:GLN:OE1	2.11	0.51
1:A:589:LEU:HB3	1:A:608:ILE:HB	1.93	0.51
2:B:695:GLU:O	2:B:698:ILE:HG12	2.10	0.51
7:G:13:LEU:HD21	7:G:17:TYR:HB2	1.92	0.51
1:A:489:ASN:ND2	2:B:1128:LEU:HD22	2.26	0.51
1:A:1393:ASN:HD21	1:A:1411:ILE:HD11	1.75	0.51
2:B:413:LEU:O	2:B:416:LYS:N	2.42	0.51
1:A:542:ILE:HG22	1:A:547:VAL:HG23	1.92	0.51
1:A:1450:GLU:O	1:A:1454:THR:HG23	2.11	0.51
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.44	0.51
5:E:16:ARG:O	5:E:20:GLU:HG3	2.11	0.51
1:A:339:GLY:O	2:B:1129:ARG:NH1	2.40	0.51
1:A:525:VAL:HG12	1:A:526:GLN:H	1.75	0.51
1:A:1118:LEU:N	1:A:1311:THR:HG22	2.25	0.51
1:A:1211:MET:HG2	1:A:1233:ASP:OD1	2.11	0.51
3:C:65:ARG:NH1	10:J:2:ILE:CG2	2.73	0.51
1:A:327:ARG:HB2	1:A:1409:VAL:HG21	1.93	0.50
2:B:286:ASP:C	2:B:288:GLU:H	2.14	0.50
11:K:12:LEU:HD11	11:K:18:LYS:HE2	1.93	0.50
1:A:822:ARG:HB2	1:A:822:ARG:NH1	2.25	0.50
2:B:799:PRO:HG2	10:J:55:LEU:CD1	2.38	0.50
1:A:441:ASP:O	1:A:461:VAL:HG23	2.11	0.50
1:A:606:MET:HE2	1:A:607:LEU:H	1.76	0.50
1:A:640:PRO:HG2	1:A:641:LYS:H	1.76	0.50
1:A:1353:LYS:O	1:A:1357:ASN:ND2	2.45	0.50
2:B:224:PRO:O	2:B:251:GLY:N	2.43	0.50
2:B:545:GLU:HA	2:B:548:ILE:HB	1.93	0.50
6:F:92:ARG:NH2	7:G:63:PRO:HG3	2.27	0.50
1:A:1037:PHE:O	1:A:1039:LEU:N	2.44	0.50
5:E:90:LYS:C	5:E:92:MET:H	2.15	0.50
10:J:46:ARG:HH11	10:J:46:ARG:HG2	1.76	0.50
1:A:1215:ALA:HA	1:A:1218:ILE:HD12	1.93	0.50
2:B:224:PRO:HG2	2:B:225:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:THR:CG2	7:G:139:LYS:H	2.24	0.50
12:L:32:THR:O	12:L:58:ILE:HA	2.12	0.50
1:A:322:PRO:O	1:A:323:VAL:HB	2.11	0.50
2:B:344:TYR:O	2:B:348:ILE:HG13	2.11	0.50
4:D:120:THR:O	4:D:124:VAL:HG23	2.12	0.50
8:H:134:LEU:HD13	8:H:136:GLN:HE21	1.77	0.50
11:K:87:LEU:O	11:K:91:CYS:HB2	2.11	0.50
1:A:547:VAL:HG21	1:A:573:TRP:CE3	2.46	0.50
1:A:637:GLU:OE1	1:A:968:ASN:ND2	2.45	0.50
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.76	0.50
2:B:857:ARG:HG2	2:B:859:TYR:CE1	2.46	0.50
4:D:41:HIS:HB2	7:G:73:LYS:HZ1	1.77	0.50
1:A:362:LEU:HA	1:A:472:ASN:HD22	1.77	0.50
8:H:109:ASP:N	8:H:109:ASP:OD1	2.45	0.50
10:J:63:ASN:HB3	10:J:64:PRO:HD3	1.93	0.50
1:A:70:CYS:O	1:A:72:GLU:HG2	2.12	0.50
1:A:669:ASP:HB3	1:A:744:VAL:HG23	1.92	0.50
1:A:1128:LEU:HA	1:A:1307:TRP:CD1	2.47	0.50
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.93	0.50
4:D:65:LYS:O	4:D:69:ARG:HG3	2.12	0.50
1:A:561:VAL:HG23	8:H:78:TRP:H	1.77	0.49
1:A:1244:VAL:HG12	1:A:1245:ILE:H	1.75	0.49
2:B:220:ALA:HB1	2:B:222:PRO:HD2	1.93	0.49
2:B:394:PHE:HA	2:B:397:LYS:HG3	1.94	0.49
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.12	0.49
1:A:375:LEU:HD13	1:A:492:VAL:HG21	1.93	0.49
1:A:853:TYR:CD1	6:F:136:ARG:HB3	2.47	0.49
2:B:376:ASN:O	2:B:380:LEU:HD13	2.12	0.49
8:H:36:ILE:HA	8:H:125:GLU:O	2.12	0.49
8:H:39:THR:HB	8:H:123:CYS:HB3	1.94	0.49
1:A:764:ALA:O	1:A:804:SER:HB3	2.12	0.49
2:B:539:SER:HG	2:B:624:GLY:H	1.59	0.49
10:J:56:ILE:HA	10:J:59:PHE:HD2	1.76	0.49
1:A:253:MET:O	1:A:254:ASP:HB2	2.11	0.49
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.43	0.49
7:G:26:LEU:HD12	7:G:56:VAL:HG11	1.95	0.49
1:A:266:LYS:HA	1:A:269:ASP:HB2	1.94	0.49
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.10	0.49
5:E:134:PHE:HD2	5:E:139:LEU:HD21	1.78	0.49
5:E:177:ILE:HG22	5:E:212:ILE:O	2.13	0.49
2:B:575:VAL:HA	2:B:619:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:PHE:CE2	6:F:89:GLU:HG2	2.48	0.49
2:B:208:ARG:HD2	2:B:208:ARG:O	2.13	0.49
2:B:311:GLU:O	2:B:314:PHE:HB3	2.12	0.49
2:B:489:ARG:HB3	2:B:489:ARG:HH11	1.78	0.49
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.11	0.49
7:G:34:VAL:O	7:G:37:THR:OG1	2.24	0.49
9:I:7:CYS:HB2	9:I:34:TYR:CE1	2.48	0.49
1:A:458:ALA:HB2	1:A:502:LEU:HD22	1.94	0.49
1:A:519:LYS:HE2	1:A:625:SER:O	2.11	0.49
1:A:606:MET:HE2	1:A:607:LEU:N	2.27	0.49
1:A:768:GLN:HA	1:A:800:PHE:HA	1.95	0.49
1:A:780:PHE:HE2	2:B:510:THR:CG2	2.25	0.49
2:B:399:LEU:HD12	2:B:538:ILE:HD11	1.95	0.49
1:A:283:ASP:O	1:A:285:SER:N	2.46	0.49
1:A:307:ASN:HD21	1:A:315:ALA:HB3	1.77	0.49
1:A:380:THR:HG1	6:F:102:SER:HB2	1.76	0.49
1:A:535:MET:O	1:A:575:GLY:HA3	2.13	0.49
2:B:86:ARG:HB3	2:B:87:PRO:HD2	1.94	0.49
2:B:540:ILE:H	2:B:605:GLU:CD	2.16	0.49
2:B:699:MET:O	2:B:739:THR:OG1	2.27	0.49
11:K:10:PHE:N	11:K:10:PHE:CD2	2.81	0.49
1:A:941:ARG:HH11	1:A:941:ARG:HG2	1.78	0.48
1:A:1321:ALA:HA	5:E:13:ARG:NH2	2.27	0.48
2:B:393:HIS:O	2:B:395:GLY:N	2.46	0.48
2:B:998:ASP:OD1	3:C:34:ARG:NH2	2.46	0.48
3:C:111:THR:O	3:C:147:LEU:HD23	2.13	0.48
1:A:1351:LEU:HD23	1:A:1375:VAL:HG13	1.95	0.48
2:B:190:MET:SD	2:B:190:MET:N	2.87	0.48
2:B:405:LEU:C	2:B:407:ALA:H	2.17	0.48
3:C:97:VAL:O	3:C:98:LEU:HD23	2.13	0.48
4:D:158:THR:HG22	4:D:159:LEU:HD23	1.94	0.48
8:H:98:GLY:HA3	8:H:117:PHE:HA	1.95	0.48
1:A:34:LYS:HD3	1:A:34:LYS:N	2.29	0.48
1:A:742:ASN:HD22	1:A:743:ASN:N	2.11	0.48
1:A:807:ARG:NH1	2:B:726:ILE:HG13	2.28	0.48
7:G:153:ASP:CG	7:G:154:VAL:H	2.17	0.48
1:A:828:THR:HA	1:A:831:LYS:HE2	1.94	0.48
2:B:503:LYS:HG2	2:B:504:PRO:CD	2.42	0.48
4:D:114:ARG:NH1	4:D:148:LEU:O	2.46	0.48
4:D:172:GLN:HA	4:D:175:LEU:HD12	1.96	0.48
5:E:112:GLN:HA	5:E:136:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:51:GLY:O	7:G:54:ILE:HG13	2.13	0.48
1:A:402:GLY:O	1:A:436:HIS:HD2	1.97	0.48
1:A:1241:ARG:HH12	1:A:1243:ARG:HH12	1.61	0.48
2:B:52:GLU:HG3	2:B:53:GLU:N	2.24	0.48
2:B:344:TYR:O	2:B:347:ASP:HB2	2.14	0.48
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.46	0.48
3:C:51:LYS:O	12:L:62:ARG:NE	2.46	0.48
10:J:46:ARG:HG2	10:J:46:ARG:NH1	2.28	0.48
2:B:208:ARG:NH1	2:B:400:ASP:OD2	2.47	0.48
2:B:551:LEU:HD23	2:B:589:LEU:HD11	1.96	0.48
2:B:1001:PHE:O	2:B:1072:MET:HA	2.14	0.48
2:B:1177:LYS:O	2:B:1179:GLN:N	2.44	0.48
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.96	0.48
9:I:69:PRO:O	9:I:84:VAL:HG23	2.14	0.48
1:A:794:SER:HB2	1:A:795:PRO:HD2	1.94	0.48
1:A:859:ASN:ND2	1:A:861:LEU:H	2.11	0.48
1:A:965:ILE:HA	1:A:968:ASN:HD22	1.79	0.48
2:B:800:GLN:CG	10:J:51:THR:HG22	2.39	0.48
3:C:236:GLY:O	3:C:238:LEU:N	2.47	0.48
9:I:50:THR:HG22	9:I:52:ILE:H	1.79	0.48
11:K:90:ALA:O	11:K:94:ILE:HG13	2.14	0.48
1:A:357:ASP:HB2	1:A:470:ARG:NH1	2.29	0.48
1:A:467:SER:CB	11:K:2:ASN:HD22	2.27	0.48
1:A:536:THR:HG21	1:A:617:VAL:HA	1.95	0.48
1:A:1128:LEU:HA	1:A:1307:TRP:HD1	1.78	0.48
1:A:1354:GLU:O	1:A:1358:VAL:HG23	2.13	0.48
9:I:14:LEU:HD13	9:I:28:SER:O	2.14	0.48
1:A:231:ARG:HG3	1:A:234:TRP:CH2	2.49	0.48
1:A:1397:THR:HG22	1:A:1398:GLY:N	2.27	0.48
1:A:452:HIS:NE2	1:A:1076:GLU:HG3	2.29	0.47
1:A:505:LEU:HD11	6:F:91:ALA:CB	2.44	0.47
1:A:1335:PHE:N	1:A:1335:PHE:HD2	2.12	0.47
1:A:1410:GLU:H	1:A:1410:GLU:CD	2.17	0.47
2:B:369:PHE:HB3	2:B:579:TRP:HZ3	1.79	0.47
5:E:123:ILE:CG1	5:E:124:PRO:HD3	2.44	0.47
2:B:519:GLU:HA	2:B:771:SER:HB3	1.97	0.47
2:B:882:THR:HG22	2:B:884:ARG:H	1.80	0.47
2:B:1099:VAL:C	2:B:1101:ASP:H	2.18	0.47
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.15	0.47
1:A:93:ILE:CG2	1:A:302:ALA:HA	2.41	0.47
1:A:389:LEU:O	1:A:393:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:LYS:O	1:A:1267:GLU:HB3	2.14	0.47
1:A:1335:PHE:N	1:A:1335:PHE:CD2	2.82	0.47
1:A:1389:ARG:HD2	1:A:1390:HIS:CE1	2.50	0.47
2:B:901:PRO:HA	2:B:949:VAL:HB	1.96	0.47
4:D:171:LEU:HA	4:D:174:ILE:HD12	1.95	0.47
1:A:276:ASN:O	1:A:280:LEU:HG	2.15	0.47
1:A:321:ARG:NH2	1:A:324:LYS:HE3	2.29	0.47
1:A:549:ASN:OD1	11:K:61:TYR:HD2	1.98	0.47
2:B:300:TRP:CH2	9:I:45:ARG:HB3	2.49	0.47
2:B:463:LYS:C	2:B:465:ALA:H	2.18	0.47
2:B:701:ALA:HB2	2:B:738:PHE:HD2	1.78	0.47
2:B:744:HIS:ND1	2:B:745:PRO:HD2	2.28	0.47
4:D:48:LEU:HD13	4:D:49:ILE:H	1.80	0.47
1:A:226:ASN:ND2	1:A:229:TYR:H	2.02	0.47
1:A:755:SER:H	1:A:758:ASN:HD22	1.62	0.47
1:A:831:LYS:HZ3	1:A:1082:THR:HG23	1.79	0.47
1:A:1444:PHE:HE1	6:F:92:ARG:HD3	1.80	0.47
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.49	0.47
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.15	0.47
5:E:143:ILE:O	5:E:149:VAL:HG21	2.15	0.47
6:F:118:LEU:O	6:F:122:MET:HG3	2.14	0.47
1:A:108:MET:C	1:A:110:CYS:H	2.18	0.47
1:A:395:ASN:O	1:A:399:GLU:HB2	2.14	0.47
1:A:606:MET:HG2	1:A:622:THR:HG21	1.96	0.47
1:A:1300:GLU:HG3	1:A:1300:GLU:H	1.40	0.47
2:B:825:VAL:HG21	2:B:1090:THR:HB	1.94	0.47
3:C:184:ASN:ND2	3:C:189:THR:HB	2.28	0.47
1:A:185:THR:HA	1:A:198:PRO:O	2.15	0.47
1:A:598:LEU:HD22	8:H:114:TYR:CE1	2.49	0.47
1:A:839:GLN:O	1:A:843:VAL:HG23	2.15	0.47
2:B:166:ARG:HG3	2:B:166:ARG:HH11	1.78	0.47
2:B:851:PHE:O	2:B:974:PRO:HD3	2.14	0.47
3:C:201:TRP:HE3	3:C:202:PRO:HD2	1.80	0.47
1:A:846:LEU:HB3	1:A:849:ILE:HD12	1.96	0.47
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.47
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.47	0.47
7:G:74:TYR:H	7:G:74:TYR:HD2	1.63	0.47
1:A:519:LYS:HB2	1:A:520:PRO:HD2	1.97	0.47
1:A:1210:THR:O	1:A:1214:VAL:HG23	2.15	0.47
1:A:1282:ILE:HD11	1:A:1315:ASN:HB3	1.97	0.47
1:A:1439:MET:O	2:B:1144:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:LEU:O	2:B:553:GLU:N	2.43	0.47
2:B:630:LEU:HD22	2:B:741:CYS:O	2.15	0.47
4:D:166:LYS:O	4:D:167:LYS:HB2	2.14	0.47
6:F:125:LEU:HG	6:F:153:VAL:HG11	1.97	0.47
7:G:39:THR:O	7:G:43:GLY:N	2.46	0.47
1:A:110:CYS:SG	1:A:111:GLY:N	2.87	0.47
1:A:962:LEU:HA	1:A:965:ILE:HG22	1.97	0.47
1:A:1400:LEU:HB2	1:A:1429:GLU:OE1	2.15	0.47
2:B:476:LEU:HD11	2:B:484:THR:HG23	1.97	0.47
2:B:550:PHE:HD2	2:B:550:PHE:O	1.98	0.47
2:B:835:GLN:O	2:B:838:SER:OG	2.24	0.47
4:D:177:GLU:HA	4:D:180:ARG:HB2	1.97	0.47
1:A:134:ARG:NH1	1:A:224:GLY:HA2	2.30	0.46
1:A:656:TYR:O	1:A:659:LEU:HB3	2.15	0.46
1:A:766:VAL:HG23	1:A:803:ASN:O	2.15	0.46
2:B:405:LEU:HB3	2:B:459:TRP:HZ2	1.80	0.46
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.97	0.46
3:C:47:LEU:HB3	3:C:158:ILE:CG1	2.45	0.46
7:G:95:SER:O	7:G:130:TYR:OH	2.22	0.46
10:J:20:ALA:O	10:J:24:LEU:HG	2.15	0.46
1:A:495:SER:O	1:A:499:ARG:HG3	2.16	0.46
1:A:988:ILE:O	1:A:992:VAL:HG23	2.15	0.46
7:G:120:VAL:O	7:G:131:MET:N	2.39	0.46
8:H:41:ASP:O	8:H:42:ILE:HG13	2.14	0.46
11:K:65:HIS:HD2	11:K:67:LEU:HB2	1.80	0.46
1:A:362:LEU:HA	1:A:472:ASN:ND2	2.31	0.46
1:A:415:ASP:OD1	1:A:417:ARG:HG2	2.16	0.46
1:A:752:SER:O	1:A:753:LYS:HG2	2.15	0.46
1:A:761:GLN:HA	1:A:766:VAL:HA	1.97	0.46
2:B:459:TRP:HA	2:B:459:TRP:CE3	2.50	0.46
2:B:865:ARG:CG	2:B:871:VAL:HG22	2.45	0.46
3:C:45:ILE:O	3:C:169:LYS:NZ	2.27	0.46
1:A:808:GLY:HA2	2:B:760:ASP:O	2.15	0.46
4:D:179:ASN:HA	4:D:182:GLU:HB2	1.97	0.46
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.30	0.46
2:B:266:PRO:O	2:B:267:TYR:HB2	2.16	0.46
3:C:167:HIS:HD2	3:C:168:ALA:H	1.64	0.46
5:E:84:GLU:O	5:E:86:SER:N	2.44	0.46
9:I:74:GLU:O	9:I:74:GLU:HG3	2.14	0.46
1:A:212:PHE:HB3	1:A:233:GLU:HB3	1.98	0.46
1:A:601:PRO:HA	8:H:25:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:GLN:O	1:A:939:SER:N	2.49	0.46
2:B:612:ILE:O	2:B:614:GLU:N	2.49	0.46
2:B:1167:GLY:O	2:B:1168:LEU:HD23	2.15	0.46
4:D:163:LEU:HA	4:D:166:LYS:HB2	1.97	0.46
1:A:570:LYS:O	1:A:572:LEU:HD12	2.16	0.46
2:B:572:ARG:HB2	2:B:579:TRP:HE1	1.80	0.46
2:B:766:ARG:HH22	2:B:1020:ARG:NH1	2.10	0.46
6:F:97:ARG:O	6:F:101:ILE:HG13	2.16	0.46
1:A:41:MET:HE3	1:A:41:MET:N	2.31	0.46
1:A:270:ILE:HG12	1:A:300:HIS:HB3	1.98	0.46
1:A:386:ILE:HG22	1:A:387:HIS:N	2.30	0.46
1:A:574:THR:O	1:A:577:GLN:HB2	2.15	0.46
1:A:853:TYR:HB3	6:F:81:THR:HG22	1.97	0.46
1:A:1449:ASP:HB3	1:A:1452:LEU:CG	2.46	0.46
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.98	0.46
1:A:80:HIS:O	1:A:244:PRO:HB3	2.15	0.46
1:A:447:ARG:HD3	1:A:479:TYR:HB3	1.97	0.46
1:A:504:GLN:NE2	6:F:90:ARG:HH21	2.14	0.46
1:A:1142:TYR:HA	1:A:1278:GLY:HA3	1.98	0.46
2:B:481:TYR:O	2:B:485:LEU:HG	2.16	0.46
2:B:609:ILE:N	2:B:609:ILE:HD12	2.30	0.46
2:B:955:THR:O	2:B:963:PHE:N	2.35	0.46
3:C:100:LEU:HD22	3:C:118:LEU:HD21	1.98	0.46
5:E:28:PHE:O	5:E:29:ILE:HG13	2.16	0.46
7:G:166:ASP:O	7:G:168:LEU:HG	2.15	0.46
1:A:358:PRO:HD2	2:B:833:TYR:CE1	2.51	0.45
2:B:409:LEU:HD12	2:B:459:TRP:CE2	2.51	0.45
2:B:607:SER:OG	2:B:620:PHE:HB2	2.16	0.45
7:G:122:ASN:OD1	7:G:125:ASN:HB3	2.15	0.45
1:A:762:MET:HA	1:A:805:TYR:HB2	1.98	0.45
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.97	0.45
1:A:1076:GLU:C	1:A:1078:ALA:H	2.19	0.45
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.57	0.45
8:H:90:ASP:O	8:H:92:TYR:N	2.42	0.45
1:A:842:LEU:O	1:A:846:LEU:HG	2.16	0.45
1:A:976:ASP:C	1:A:978:ALA:H	2.19	0.45
1:A:1322:VAL:O	1:A:1325:VAL:HG22	2.17	0.45
1:A:1447:MET:HE2	1:A:1447:MET:H	1.80	0.45
2:B:421:ILE:O	2:B:425:MET:HG3	2.17	0.45
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.81	0.45
2:B:843:GLN:N	2:B:994:TYR:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:945:GLU:O	2:B:946:ASN:HB3	2.17	0.45
2:B:955:THR:N	2:B:963:PHE:O	2.49	0.45
4:D:122:THR:O	4:D:126:GLN:HG3	2.17	0.45
8:H:12:VAL:HG13	8:H:26:ILE:HG23	1.97	0.45
11:K:43:ALA:HB1	11:K:61:TYR:CD1	2.51	0.45
1:A:501:GLU:OE2	1:A:1441:THR:HG21	2.16	0.45
1:A:576:LYS:HE2	1:A:616:GLY:O	2.16	0.45
2:B:326:ILE:HG22	2:B:326:ILE:O	2.15	0.45
3:C:257:ASN:HA	3:C:260:PHE:HB3	1.99	0.45
11:K:70:ASN:O	11:K:71:PHE:HB3	2.15	0.45
2:B:752:ALA:HB1	2:B:771:SER:HA	1.97	0.45
2:B:797:TYR:C	2:B:798:TYR:HD2	2.20	0.45
2:B:847:ASP:C	2:B:849:GLY:H	2.19	0.45
1:A:117:GLU:CD	1:A:117:GLU:H	2.20	0.45
1:A:712:ARG:O	1:A:715:PHE:HB3	2.17	0.45
2:B:477:ASN:O	2:B:478:ARG:HD2	2.17	0.45
2:B:596:LEU:HD13	2:B:601:ALA:HB3	1.98	0.45
2:B:913:GLY:HA2	2:B:938:SER:OG	2.17	0.45
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.65	0.45
4:D:48:LEU:CD1	4:D:49:ILE:H	2.29	0.45
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.98	0.45
1:A:467:SER:HB2	2:B:1099:VAL:HG11	1.97	0.45
1:A:869:TYR:CD2	1:A:1060:VAL:HG21	2.51	0.45
2:B:101:PRO:O	2:B:103:GLU:N	2.49	0.45
2:B:514:LEU:HB3	2:B:626:VAL:HG11	1.98	0.45
3:C:39:GLU:HG2	3:C:165:LYS:HE3	1.99	0.45
1:A:107:CYS:HA	1:A:172:GLN:OE1	2.17	0.45
1:A:762:MET:HG2	1:A:805:TYR:HD1	1.81	0.45
2:B:344:TYR:CE2	2:B:348:ILE:HD11	2.52	0.45
5:E:166:ARG:HA	5:E:166:ARG:HD3	1.85	0.45
6:F:109:VAL:HG12	6:F:110:ASP:N	2.21	0.45
1:A:40:ILE:HB	1:A:41:MET:HE2	1.99	0.45
1:A:634:VAL:HG12	1:A:643:CYS:HB2	1.98	0.45
1:A:744:VAL:O	1:A:748:VAL:HG23	2.17	0.45
1:A:1440:GLY:O	1:A:1442:GLY:N	2.50	0.45
1:A:1452:LEU:C	1:A:1454:THR:H	2.20	0.45
2:B:428:CYS:C	2:B:430:GLU:H	2.20	0.45
2:B:1201:LYS:HG2	2:B:1202:LEU:N	2.32	0.45
4:D:41:HIS:HB2	7:G:73:LYS:NZ	2.30	0.45
4:D:169:VAL:O	4:D:171:LEU:N	2.50	0.45
7:G:35:GLU:HG2	7:G:48:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:VAL:HA	7:G:170:ALA:HA	1.98	0.45
1:A:357:ASP:OD2	11:K:65:HIS:CE1	2.66	0.45
2:B:555:GLY:HA3	2:B:583:HIS:HE1	1.82	0.45
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.52	0.45
3:C:167:HIS:CD2	3:C:168:ALA:H	2.35	0.45
4:D:51:LEU:O	7:G:2:PHE:HB2	2.17	0.45
5:E:170:LYS:O	5:E:172:SER:N	2.48	0.45
7:G:40:GLY:HA2	7:G:157:ILE:HD11	1.99	0.45
1:A:105:CYS:SG	1:A:139:TRP:HA	2.57	0.44
1:A:354:ILE:CG2	1:A:488:MET:HG3	2.46	0.44
1:A:1295:PRO:HG3	1:A:1301:TYR:CZ	2.52	0.44
1:A:1403:CYS:HB2	1:A:1412:LEU:HD21	2.00	0.44
2:B:509:ASN:N	2:B:509:ASN:ND2	2.59	0.44
2:B:550:PHE:CE1	2:B:596:LEU:HG	2.51	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.17	0.44
3:C:81:TYR:HE2	3:C:162:GLY:H	1.64	0.44
5:E:123:ILE:C	5:E:125:THR:H	2.21	0.44
5:E:196:LYS:HE2	5:E:198:ILE:HD11	1.99	0.44
11:K:53:TYR:C	11:K:55:ASP:H	2.19	0.44
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.98	0.44
1:A:1085:THR:O	1:A:1085:THR:HG22	2.16	0.44
1:A:1326:ASP:OD1	1:A:1328:SER:HB2	2.17	0.44
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.17	0.44
5:E:39:GLU:C	5:E:41:PHE:H	2.19	0.44
9:I:100:PHE:N	9:I:100:PHE:CD1	2.85	0.44
1:A:67:CYS:O	1:A:70:CYS:SG	2.76	0.44
1:A:72:GLU:OE2	2:B:1175:LEU:HB2	2.18	0.44
1:A:356:GLY:HA2	1:A:471:LEU:O	2.17	0.44
1:A:629:GLY:O	1:A:633:THR:HG23	2.17	0.44
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.00	0.44
2:B:890:TYR:O	2:B:893:LEU:HB2	2.17	0.44
5:E:160:LYS:C	5:E:162:GLN:H	2.19	0.44
1:A:447:ARG:CD	1:A:481:ALA:HB2	2.48	0.44
1:A:786:PRO:HG2	1:A:787:HIS:CD2	2.53	0.44
2:B:992:VAL:HG22	2:B:993:THR:N	2.33	0.44
3:C:42:THR:HG22	3:C:43:LEU:N	2.24	0.44
3:C:147:LEU:HA	10:J:60:LEU:CD2	2.46	0.44
5:E:31:GLN:HE21	5:E:35:ASP:CG	2.21	0.44
1:A:340:ASN:O	1:A:344:LYS:HB3	2.17	0.44
1:A:1214:VAL:O	1:A:1218:ILE:HG13	2.18	0.44
2:B:1151:LEU:HD13	2:B:1151:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:GLU:HB3	3:C:170:TRP:CZ3	2.52	0.44
5:E:156:SER:C	5:E:158:GLY:H	2.21	0.44
8:H:61:ASN:O	8:H:62:SER:HB2	2.18	0.44
1:A:269:ASP:HB3	1:A:300:HIS:CE1	2.53	0.44
1:A:386:ILE:O	1:A:390:THR:OG1	2.34	0.44
1:A:601:PRO:HG2	1:A:602:LYS:H	1.83	0.44
2:B:414:PHE:HA	2:B:417:LEU:HB3	1.99	0.44
2:B:596:LEU:HD22	2:B:596:LEU:HA	1.86	0.44
2:B:632:ILE:HG22	2:B:634:GLU:HG2	2.00	0.44
2:B:883:LEU:O	2:B:885:LEU:N	2.51	0.44
1:A:1222:PHE:CG	1:A:1226:LEU:HD23	2.52	0.44
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.83	0.44
3:C:5:PRO:HA	3:C:23:ASP:HB3	2.00	0.44
7:G:127:PRO:HG2	7:G:138:THR:HG21	2.00	0.44
1:A:1367:ASN:HD22	1:A:1368:TYR:H	1.66	0.44
5:E:14:SER:HA	5:E:140:VAL:HA	1.98	0.44
6:F:76:LYS:O	6:F:79:ARG:HD3	2.18	0.44
10:J:59:PHE:HA	10:J:62:TYR:HD1	1.83	0.44
1:A:14:VAL:HG21	2:B:1216:LEU:HD12	1.99	0.44
1:A:89:PRO:C	1:A:204:THR:HG21	2.37	0.44
1:A:262:ASP:OD1	1:A:323:VAL:HA	2.18	0.44
1:A:328:ALA:C	1:A:330:LEU:H	2.21	0.44
1:A:886:THR:HG22	1:A:941:ARG:HD2	2.00	0.44
1:A:1444:PHE:CE2	6:F:89:GLU:HA	2.53	0.44
5:E:77:LEU:HA	5:E:106:THR:HB	2.00	0.44
7:G:121:TYR:HA	7:G:130:TYR:HA	1.98	0.44
1:A:669:ASP:CG	1:A:743:ASN:HD22	2.22	0.43
2:B:549:ASN:O	2:B:551:LEU:N	2.51	0.43
2:B:698:ILE:HD11	2:B:700:ILE:HD11	2.00	0.43
2:B:950:ASP:O	2:B:951:GLN:HB2	2.18	0.43
2:B:1080:LYS:HG3	3:C:180:TYR:CE2	2.53	0.43
3:C:213:PRO:O	3:C:214:LYS:HB2	2.18	0.43
5:E:90:LYS:C	5:E:92:MET:N	2.71	0.43
6:F:89:GLU:O	6:F:93:ILE:HG13	2.18	0.43
1:A:297:LEU:O	1:A:301:VAL:HG23	2.18	0.43
1:A:379:GLU:OE1	1:A:435:ARG:HD3	2.18	0.43
1:A:667:ILE:HD12	1:A:668:GLY:H	1.83	0.43
1:A:827:ASP:O	1:A:831:LYS:N	2.43	0.43
1:A:1032:ARG:HH11	1:A:1032:ARG:HB3	1.83	0.43
1:A:1096:VAL:HA	1:A:1115:THR:HG21	2.00	0.43
2:B:914:LYS:HG2	2:B:937:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1060:ARG:NH2	3:C:199:LYS:O	2.42	0.43
2:B:1073:TYR:OH	3:C:179:GLU:HA	2.18	0.43
2:B:1157:ALA:O	2:B:1158:PHE:HB2	2.18	0.43
5:E:115:ILE:HG22	5:E:119:ALA:HB3	2.00	0.43
1:A:12:ARG:HE	2:B:1192:TYR:HE2	1.65	0.43
1:A:73:GLY:O	1:A:75:ALA:N	2.51	0.43
1:A:897:ARG:HD3	1:A:898:TYR:CE1	2.52	0.43
1:A:1149:THR:O	9:I:48:LEU:HB2	2.18	0.43
2:B:1162:VAL:HG12	2:B:1163:CYS:N	2.32	0.43
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.78	0.43
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.53	0.43
7:G:114:LEU:HB3	7:G:162:SER:HB3	2.00	0.43
1:A:568:LYS:HD3	8:H:94:TYR:HA	1.99	0.43
1:A:859:ASN:HD22	1:A:861:LEU:H	1.66	0.43
1:A:1288:VAL:O	1:A:1308:ALA:N	2.46	0.43
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.53	0.43
4:D:53:LEU:C	4:D:54:SER:HG	2.22	0.43
7:G:154:VAL:HB	7:G:155:ASN:H	1.57	0.43
1:A:264:THR:HG22	1:A:264:THR:O	2.19	0.43
1:A:336:ARG:CA	1:A:340:ASN:HD22	2.28	0.43
1:A:580:SER:HB3	1:A:612:LYS:HA	2.01	0.43
1:A:1426:GLY:O	1:A:1429:GLU:HG2	2.18	0.43
2:B:211:ALA:O	2:B:213:ILE:HG13	2.17	0.43
2:B:572:ARG:HG2	2:B:572:ARG:HH11	1.83	0.43
1:A:226:ASN:HD21	1:A:228:ASP:HB3	1.83	0.43
1:A:768:GLN:NE2	1:A:798:LYS:O	2.45	0.43
1:A:856:THR:HG21	1:A:858:ARG:NE	2.32	0.43
1:A:986:PRO:O	1:A:990:HIS:HB2	2.18	0.43
1:A:1097:THR:HG21	1:A:1114:LYS:HB2	2.01	0.43
10:J:52:HIS:CD2	10:J:53:VAL:N	2.87	0.43
1:A:588:HIS:CD2	1:A:967:GLN:HB3	2.54	0.43
1:A:723:LEU:HB3	1:A:800:PHE:CE1	2.54	0.43
1:A:831:LYS:NZ	1:A:1082:THR:HA	2.34	0.43
1:A:872:ASP:OD2	1:A:874:LEU:HB2	2.18	0.43
1:A:988:ILE:HG22	1:A:989:ILE:N	2.34	0.43
2:B:724:LYS:HG2	2:B:1051:THR:HG21	2.00	0.43
1:A:347:ASP:OD1	2:B:1106:ARG:NE	2.44	0.43
1:A:561:VAL:CG2	8:H:78:TRP:H	2.32	0.43
2:B:785:TYR:CE2	10:J:59:PHE:CE1	3.03	0.43
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.33	0.43
5:E:15:PHE:CZ	5:E:19:LYS:HE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:43:GLY:HA3	7:G:80:LYS:HB3	2.00	0.43
8:H:90:ASP:C	8:H:92:TYR:H	2.21	0.43
1:A:1427:VAL:O	1:A:1431:VAL:HG23	2.19	0.43
1:A:933:GLU:OE1	1:A:989:ILE:HG22	2.19	0.43
2:B:484:THR:O	2:B:488:LEU:HD12	2.19	0.43
4:D:56:SER:O	4:D:60:ILE:HG13	2.19	0.43
8:H:9:ILE:HG12	8:H:56:THR:HG23	2.01	0.43
9:I:33:ASP:O	9:I:35:THR:HG23	2.19	0.43
1:A:32:VAL:HG11	1:A:68:GLN:OE1	2.19	0.42
1:A:107:CYS:SG	1:A:108:MET:N	2.92	0.42
1:A:373:LYS:HA	1:A:436:HIS:CE1	2.54	0.42
1:A:553:TRP:CD1	11:K:62:LYS:CB	3.01	0.42
1:A:1328:SER:HA	5:E:146:HIS:HA	2.01	0.42
1:A:1393:ASN:HA	1:A:1402:ARG:HG2	2.01	0.42
2:B:342:ILE:O	2:B:345:ALA:HB3	2.19	0.42
2:B:478:ARG:NH2	2:B:782:LEU:HD11	2.33	0.42
2:B:1220:ARG:HB3	2:B:1220:ARG:NH1	2.33	0.42
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.54	0.42
1:A:454:MET:N	1:A:454:MET:SD	2.93	0.42
1:A:1193:TRP:O	1:A:1243:ARG:HG2	2.19	0.42
2:B:166:ARG:HB2	2:B:191:GLY:HA3	2.01	0.42
2:B:632:ILE:HD12	2:B:685:GLY:O	2.19	0.42
3:C:252:GLN:NE2	11:K:95:ILE:HG23	2.34	0.42
11:K:65:HIS:CD2	11:K:67:LEU:HB2	2.55	0.42
1:A:964:ARG:O	1:A:967:GLN:N	2.52	0.42
1:A:1061:HIS:ND1	6:F:86:THR:HA	2.33	0.42
1:A:1149:THR:HB	9:I:48:LEU:HD12	2.02	0.42
1:A:1211:MET:HB3	1:A:1230:TRP:CD1	2.54	0.42
2:B:458:ASN:HD22	2:B:458:ASN:N	2.17	0.42
2:B:702:MET:HB3	2:B:703:THR:H	1.56	0.42
2:B:986:GLN:NE2	2:B:1016:ALA:O	2.52	0.42
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.34	0.42
4:D:54:SER:HB3	4:D:113:ALA:HB1	2.00	0.42
6:F:81:THR:HB	6:F:136:ARG:HH11	1.85	0.42
1:A:262:ASP:OD2	1:A:321:ARG:NE	2.48	0.42
1:A:1327:SER:HB2	5:E:141:VAL:HG11	2.00	0.42
2:B:252:ARG:NH1	2:B:252:ARG:HB3	2.34	0.42
2:B:401:LEU:O	2:B:405:LEU:HG	2.18	0.42
2:B:785:TYR:HA	2:B:788:ARG:HG3	2.01	0.42
2:B:1177:LYS:C	2:B:1179:GLN:H	2.23	0.42
10:J:3:ILE:HA	10:J:4:PRO:HD3	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:GLN:HA	1:A:449:PRO:C	2.40	0.42
1:A:1294:VAL:HA	1:A:1295:PRO:HD3	1.82	0.42
2:B:91:GLU:OE1	12:L:56:ARG:NH2	2.52	0.42
5:E:12:TRP:O	5:E:15:PHE:HB3	2.19	0.42
12:L:62:ARG:HG2	12:L:63:THR:H	1.84	0.42
1:A:72:GLU:HB3	1:A:76:GLU:HB3	2.01	0.42
1:A:475:VAL:HG22	1:A:475:VAL:O	2.20	0.42
2:B:202:VAL:HG11	2:B:488:LEU:HA	2.01	0.42
2:B:416:LYS:HB2	2:B:416:LYS:NZ	2.34	0.42
2:B:755:ILE:HA	2:B:809:MET:HE2	2.01	0.42
2:B:1176:LYS:C	2:B:1178:ASN:H	2.23	0.42
7:G:80:LYS:HE2	7:G:80:LYS:N	2.34	0.42
1:A:55:ASP:N	1:A:56:PRO:CD	2.83	0.42
1:A:329:ARG:O	1:A:336:ARG:HB2	2.19	0.42
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.85	0.42
2:B:704:PRO:HG2	2:B:705:GLU:H	1.84	0.42
2:B:1162:VAL:O	2:B:1191:ILE:HG23	2.19	0.42
5:E:14:SER:HA	5:E:139:LEU:O	2.20	0.42
5:E:119:ALA:O	5:E:121:LYS:N	2.52	0.42
6:F:123:LYS:HE3	6:F:123:LYS:HB2	1.79	0.42
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.55	0.42
8:H:94:TYR:HE2	8:H:96:MET:HG3	1.85	0.42
9:I:50:THR:HG22	9:I:51:ASN:N	2.30	0.42
1:A:59:GLY:HA2	1:A:67:CYS:HA	2.01	0.42
1:A:147:VAL:O	1:A:149:GLU:N	2.52	0.42
1:A:576:LYS:NZ	1:A:616:GLY:H	2.18	0.42
1:A:689:GLU:HA	1:A:692:GLN:HB3	2.01	0.42
2:B:279:ARG:NH1	2:B:316:ILE:O	2.52	0.42
2:B:324:ASP:OD1	2:B:341:ARG:NE	2.51	0.42
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.87	0.42
2:B:842:ASN:ND2	2:B:845:SER:OG	2.53	0.42
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.40	0.42
8:H:12:VAL:HG13	8:H:26:ILE:CG2	2.50	0.42
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.55	0.42
1:A:18:GLN:HG2	1:A:1421:LEU:HD13	2.01	0.42
1:A:316:LEU:HD22	1:A:322:PRO:HA	2.01	0.42
2:B:298:ASN:ND2	9:I:3:SER:OG	2.53	0.42
2:B:598:ARG:NH2	2:B:688:GLU:OE1	2.53	0.42
7:G:138:THR:O	7:G:141:SER:OG	2.37	0.42
10:J:3:ILE:HG22	10:J:52:HIS:CE1	2.54	0.42
12:L:30:LYS:HG3	12:L:41:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:C	1:A:52:GLY:H	2.24	0.42
1:A:578:LEU:O	1:A:581:ILE:HG23	2.19	0.42
1:A:615:PHE:CB	8:H:121:LEU:HD21	2.49	0.42
1:A:856:THR:CG2	1:A:858:ARG:HE	2.33	0.42
1:A:1016:ALA:HA	5:E:204:SER:HB2	2.01	0.42
2:B:390:ASP:HB3	2:B:393:HIS:HB2	2.02	0.42
2:B:491:THR:HG22	2:B:530:LYS:HB2	2.02	0.42
2:B:849:GLY:HA2	2:B:852:ARG:HD2	2.02	0.42
2:B:1021:MET:O	2:B:1023:VAL:HG23	2.19	0.42
2:B:1152:MET:HE3	2:B:1157:ALA:HA	2.02	0.42
7:G:10:ILE:HA	7:G:70:PHE:O	2.20	0.42
1:A:146:MET:HA	1:A:172:GLN:NE2	2.34	0.41
1:A:601:PRO:HA	8:H:25:ARG:HH12	1.84	0.41
1:A:782:ASP:CG	9:I:91:ARG:HH22	2.23	0.41
1:A:1316:LEU:O	1:A:1318:GLU:N	2.53	0.41
2:B:405:LEU:HB3	2:B:459:TRP:CZ2	2.55	0.41
3:C:42:THR:HB	3:C:170:TRP:HD1	1.85	0.41
4:D:41:HIS:CD2	7:G:73:LYS:HG2	2.54	0.41
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.35	0.41
9:I:34:TYR:CD2	9:I:35:THR:N	2.81	0.41
1:A:601:PRO:C	1:A:603:ASP:H	2.23	0.41
1:A:699:GLN:HE21	9:I:99:LEU:HD21	1.84	0.41
1:A:699:GLN:HB3	9:I:99:LEU:HG	2.02	0.41
1:A:983:LEU:HD13	1:A:988:ILE:HD11	2.02	0.41
2:B:227:HIS:O	2:B:249:LEU:HB3	2.20	0.41
2:B:266:PRO:CG	2:B:352:GLU:HB3	2.49	0.41
2:B:572:ARG:HG2	2:B:572:ARG:H	1.70	0.41
4:D:26:THR:CB	7:G:84:GLY:HA3	2.51	0.41
5:E:72:SER:HB2	5:E:73:ASP:H	1.67	0.41
5:E:120:ASN:C	5:E:122:MET:H	2.23	0.41
9:I:26:LEU:HD23	9:I:26:LEU:HA	1.92	0.41
1:A:845:ALA:O	1:A:846:LEU:HD23	2.20	0.41
1:A:1298:SER:O	1:A:1298:SER:OG	2.35	0.41
2:B:252:ARG:HB3	2:B:252:ARG:HH11	1.86	0.41
2:B:458:ASN:N	2:B:458:ASN:ND2	2.68	0.41
2:B:563:ASP:HA	2:B:564:PRO:HD2	1.91	0.41
2:B:629:PRO:O	2:B:630:LEU:HD23	2.21	0.41
8:H:79:ARG:HA	8:H:80:PRO:HD3	1.88	0.41
11:K:90:ALA:HA	11:K:93:SER:HB3	2.02	0.41
1:A:593:ASP:H	1:A:596:ASN:CG	2.24	0.41
2:B:246:GLN:O	2:B:264:THR:N	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:GLN:CG	2:B:271:ASP:H	2.27	0.41
2:B:557:GLU:HA	2:B:558:PRO:HD2	1.84	0.41
2:B:792:MET:H	2:B:857:ARG:HA	1.86	0.41
2:B:822:ASN:HA	2:B:1091:TYR:HA	2.03	0.41
7:G:138:THR:CG2	7:G:139:LYS:N	2.81	0.41
8:H:88:LEU:C	8:H:90:ASP:N	2.74	0.41
1:A:316:LEU:CD2	1:A:322:PRO:HA	2.51	0.41
1:A:563:GLN:HA	1:A:564:PRO:HD3	1.88	0.41
2:B:519:GLU:OE2	2:B:752:ALA:HB2	2.21	0.41
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	2.02	0.41
7:G:25:TYR:CE2	7:G:29:LYS:HD2	2.55	0.41
10:J:23:ARG:C	10:J:25:LEU:N	2.73	0.41
10:J:47:ARG:HE	10:J:48:MET:CE	2.32	0.41
1:A:108:MET:O	1:A:110:CYS:N	2.53	0.41
1:A:1082:THR:HG21	1:A:1084:ASN:HD22	1.85	0.41
1:A:1230:TRP:HD1	1:A:1231:SER:O	2.03	0.41
2:B:550:PHE:HE1	2:B:596:LEU:HG	1.85	0.41
2:B:744:HIS:HD2	2:B:746:SER:OG	2.03	0.41
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.56	0.41
2:B:969:ARG:HG2	2:B:970:THR:N	2.36	0.41
2:B:997:GLU:CD	2:B:997:GLU:H	2.22	0.41
3:C:168:ALA:C	3:C:170:TRP:H	2.24	0.41
3:C:242:GLN:C	3:C:244:PHE:H	2.23	0.41
4:D:138:HIS:O	4:D:140:PHE:N	2.53	0.41
4:D:162:SER:O	4:D:166:LYS:HD2	2.21	0.41
5:E:134:PHE:CZ	5:E:185:ARG:HB3	2.55	0.41
6:F:140:ASP:OD1	6:F:142:SER:OG	2.38	0.41
11:K:6:ARG:O	11:K:9:LEU:HG	2.21	0.41
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.56	0.41
1:A:376:SER:OG	1:A:434:GLU:HB3	2.21	0.41
2:B:89:MET:HB2	2:B:99:MET:HB2	2.03	0.41
2:B:287:GLY:CA	9:I:6:PHE:CE1	3.03	0.41
2:B:572:ARG:HB2	2:B:579:TRP:NE1	2.36	0.41
2:B:830:TYR:HB3	2:B:831:SER:H	1.68	0.41
2:B:1073:TYR:CD1	2:B:1073:TYR:N	2.89	0.41
3:C:161:LYS:HB3	3:C:162:GLY:H	1.58	0.41
6:F:121:ALA:HA	6:F:124:GLU:HB2	2.03	0.41
8:H:20:TYR:HD1	8:H:23:VAL:HB	1.85	0.41
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.36	0.41
1:A:146:MET:HB3	1:A:172:GLN:HB2	2.03	0.41
1:A:404:LYS:O	1:A:404:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:VAL:HG11	11:K:105:PHE:HD1	1.85	0.41
7:G:126:SER:HA	7:G:127:PRO:HA	1.84	0.41
1:A:55:ASP:C	1:A:57:LYS:H	2.23	0.41
1:A:476:THR:HG23	1:A:477:SER:N	2.35	0.41
1:A:831:LYS:HD2	1:A:1081:MET:O	2.21	0.41
1:A:863:ASP:HA	5:E:173:GLN:HA	2.01	0.41
1:A:1196:ARG:HG3	1:A:1239:ILE:HG23	2.01	0.41
2:B:416:LYS:NZ	2:B:461:GLU:OE1	2.54	0.41
2:B:811:TYR:CD1	2:B:811:TYR:N	2.88	0.41
2:B:906:SER:O	2:B:941:LEU:HD23	2.21	0.41
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.33	0.41
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.20	0.41
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	2.03	0.41
3:C:226:ASN:O	3:C:227:ARG:HB2	2.21	0.41
10:J:59:PHE:O	10:J:62:TYR:HB2	2.21	0.41
1:A:114:LEU:CD1	1:A:172:GLN:HE22	2.33	0.41
1:A:332:GLY:O	1:A:333:LYS:HB3	2.21	0.41
1:A:333:LYS:H	1:A:338:ARG:HD2	1.86	0.41
1:A:961:ASN:OD1	1:A:963:ARG:HB3	2.21	0.41
1:A:1444:PHE:C	1:A:1444:PHE:CD1	2.94	0.41
2:B:493:THR:HA	2:B:494:PRO:HD2	1.76	0.41
2:B:828:ALA:HB2	2:B:1085:VAL:HG13	2.03	0.41
11:K:57:THR:H	11:K:77:THR:HA	1.86	0.41
1:A:392:TYR:HA	1:A:401:PRO:O	2.21	0.40
1:A:444:LEU:HD22	1:A:444:LEU:HA	1.91	0.40
1:A:1146:LYS:HB2	1:A:1271:LEU:O	2.20	0.40
1:A:1159:ASP:HA	1:A:1160:PRO:HD2	1.89	0.40
1:A:1279:ILE:CG1	1:A:1282:ILE:HD12	2.51	0.40
2:B:287:GLY:N	2:B:290:LEU:HD23	2.29	0.40
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.40
3:C:33:ARG:HG2	3:C:34:ARG:N	2.36	0.40
5:E:153:ILE:HG22	5:E:154:ARG:O	2.21	0.40
9:I:14:LEU:HD12	9:I:27:TYR:HB3	2.02	0.40
9:I:71:SER:HB3	9:I:85:PHE:HE2	1.83	0.40
11:K:24:ASP:OD1	11:K:26:ARG:HB2	2.21	0.40
1:A:785:LEU:HB3	1:A:786:PRO:HD2	2.02	0.40
1:A:1046:TRP:O	1:A:1050:THR:OG1	2.39	0.40
1:A:1155:TYR:HB2	1:A:1194:LEU:HD23	2.02	0.40
2:B:324:ASP:O	2:B:326:ILE:N	2.54	0.40
2:B:573:ILE:O	2:B:579:TRP:HD1	2.05	0.40
2:B:1006:ILE:HG22	10:J:44:CYS:CB	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1096:ARG:HD2	2:B:1097:HIS:CE1	2.57	0.40
2:B:1187:ASN:ND2	2:B:1190:ASN:O	2.53	0.40
3:C:131:GLU:HA	3:C:132:PRO:HD3	1.75	0.40
4:D:114:ARG:CZ	4:D:149:GLY:HA2	2.50	0.40
6:F:82:THR:HA	6:F:83:PRO:HD3	1.92	0.40
8:H:19:ARG:C	8:H:20:TYR:HD2	2.24	0.40
1:A:366:GLY:HA3	1:A:470:ARG:HB2	2.04	0.40
1:A:768:GLN:HB2	1:A:800:PHE:HD1	1.86	0.40
2:B:466:MET:O	2:B:468:SER:N	2.43	0.40
2:B:705:GLU:HG3	2:B:706:ASP:H	1.86	0.40
7:G:88:ASP:HB3	7:G:144:ARG:HA	2.04	0.40
7:G:89:ALA:HB1	7:G:102:ASP:O	2.21	0.40
8:H:55:LEU:HD23	8:H:145:ARG:OXT	2.21	0.40
12:L:33:CYS:HB3	12:L:36:CYS:O	2.21	0.40
12:L:52:GLU:HB3	12:L:53:CYS:H	1.63	0.40
1:A:134:ARG:HD3	1:A:222:ARG:O	2.22	0.40
1:A:227:GLU:HA	1:A:231:ARG:HG2	2.03	0.40
1:A:598:LEU:N	1:A:598:LEU:HD12	2.36	0.40
1:A:699:GLN:NE2	9:I:99:LEU:HD11	2.37	0.40
1:A:852:HIS:HB2	1:A:856:THR:CG2	2.51	0.40
1:A:1257:ALA:O	1:A:1258:GLU:HB2	2.22	0.40
1:A:1356:LEU:HA	1:A:1359:ILE:HD12	2.03	0.40
2:B:206:GLN:OE1	2:B:472:VAL:HG22	2.21	0.40
2:B:253:GLU:HG2	2:B:253:GLU:O	2.21	0.40
3:C:45:ILE:HA	3:C:159:ALA:HA	2.03	0.40
4:D:169:VAL:C	4:D:171:LEU:N	2.74	0.40
8:H:10:PHE:CD1	8:H:10:PHE:N	2.88	0.40
8:H:80:PRO:CB	8:H:81:PRO:HD2	2.52	0.40
1:A:759:ILE:H	1:A:759:ILE:HG13	1.60	0.40
1:A:775:ARG:HB2	1:A:798:LYS:HD2	2.04	0.40
1:A:1002:LEU:HD13	1:A:1009:ILE:HG23	2.03	0.40
1:A:1393:ASN:HD21	1:A:1411:ILE:CD1	2.34	0.40
5:E:181:ASP:HA	5:E:182:PRO:HD3	1.99	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	1393/1743 (80%)	972 (70%)	291 (21%)	130 (9%)	0 12
2	B	1055/1227 (86%)	723 (68%)	214 (20%)	118 (11%)	0 7
3	C	259/304 (85%)	186 (72%)	50 (19%)	23 (9%)	1 12
4	D	135/186 (73%)	98 (73%)	23 (17%)	14 (10%)	0 9
5	E	212/214 (99%)	150 (71%)	44 (21%)	18 (8%)	1 13
6	F	82/155 (53%)	58 (71%)	14 (17%)	10 (12%)	0 5
7	G	169/171 (99%)	129 (76%)	27 (16%)	13 (8%)	1 15
8	H	127/145 (88%)	95 (75%)	17 (13%)	15 (12%)	0 6
9	I	111/115 (96%)	71 (64%)	26 (23%)	14 (13%)	0 5
10	J	62/72 (86%)	37 (60%)	15 (24%)	10 (16%)	0 3
11	K	110/118 (93%)	83 (76%)	16 (14%)	11 (10%)	0 10
12	L	44/73 (60%)	20 (46%)	11 (25%)	13 (30%)	0 0
All	All	3759/4523 (83%)	2622 (70%)	748 (20%)	389 (10%)	0 9

All (389) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	48	PRO
1	A	54	ASN
1	A	57	LYS
1	A	67	CYS
1	A	73	GLY
1	A	74	MET
1	A	93	ILE
1	A	198	PRO
1	A	254	ASP
1	A	258	GLN
1	A	284	GLY

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Mol	Chain	Res	Type
1	A	287	GLN
1	A	303	THR
1	A	304	TYR
1	A	312	GLN
1	A	313	PRO
1	A	336	ARG
1	A	365	VAL
1	A	383	GLN
1	A	411	GLY
1	A	425	ILE
1	A	466	TYR
1	A	526	GLN
1	A	568	LYS
1	A	598	LEU
1	A	599	LEU
1	A	776	ILE
1	A	809	LEU
1	A	1015	ASN
1	A	1018	SER
1	A	1038	ARG
1	A	1117	ALA
1	A	1125	GLU
1	A	1126	ILE
1	A	1167	GLU
1	A	1208	GLN
1	A	1233	ASP
1	A	1235	ALA
1	A	1258	GLU
1	A	1284	LYS
1	A	1327	SER
1	A	1344	ILE
1	A	1408	THR
1	A	1441	THR
2	B	45	SER
2	B	54	PRO
2	B	93	ASP
2	B	95	THR
2	B	197	ASN
2	B	220	ALA
2	B	274	ILE
2	B	325	PHE
2	B	326	ILE

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Mol	Chain	Res	Type
2	B	358	THR
2	B	360	GLU
2	B	394	PHE
2	B	463	LYS
2	B	613	ARG
2	B	622	ASP
2	B	634	GLU
2	B	640	ASP
2	B	705	GLU
2	B	869	SER
2	B	879	ARG
2	B	881	THR
2	B	884	ARG
2	B	907	GLY
2	B	976	ILE
2	B	1046	PRO
2	B	1097	HIS
2	B	1100	ASP
2	B	1131	GLY
2	B	1155	SER
2	B	1156	ASP
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1182	CYS
2	B	1223	VAL
3	C	4	GLU
3	C	139	ASP
3	C	161	LYS
3	C	237	SER
4	D	48	LEU
4	D	91	LYS
4	D	139	PRO
4	D	167	LYS
5	E	73	ASP
5	E	86	SER
5	E	87	VAL
5	E	105	SER
6	F	73	ALA
6	F	74	ILE
7	G	52	MET
7	G	118	ASN

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Mol	Chain	Res	Type
7	G	123	PRO
7	G	154	VAL
8	H	60	ALA
8	H	82	LYS
8	H	107	ASP
8	H	139	LEU
9	I	20	LYS
9	I	50	THR
9	I	51	ASN
9	I	56	ALA
9	I	107	LYS
10	J	2	ILE
10	J	41	LYS
10	J	63	ASN
11	K	43	ALA
12	L	37	ALA
12	L	41	SER
12	L	46	ASP
12	L	47	PRO
12	L	52	GLU
12	L	61	ALA
12	L	62	ARG
1	A	35	ILE
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP
1	A	69	THR
1	A	71	GLY
1	A	76	GLU
1	A	319	SER
1	A	416	LEU
1	A	424	ASP
1	A	467	SER
1	A	518	ASN
1	A	629	GLY
1	A	673	ASP
1	A	700	HIS
1	A	717	GLY
1	A	847	GLU
1	A	853	TYR
1	A	974	HIS
1	A	1004	GLY

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Mol	Chain	Res	Type
1	A	1006	ASN
1	A	1016	ALA
1	A	1124	ARG
1	A	1214	VAL
1	A	1223	SER
1	A	1264	LYS
1	A	1317	ALA
1	A	1424	CYS
2	B	55	ARG
2	B	102	GLN
2	B	167	SER
2	B	177	GLU
2	B	210	ALA
2	B	250	TYR
2	B	251	GLY
2	B	255	LYS
2	B	287	GLY
2	B	297	GLU
2	B	406	LEU
2	B	459	TRP
2	B	460	GLY
2	B	510	THR
2	B	523	GLY
2	B	550	PHE
2	B	552	GLU
2	B	702	MET
2	B	706	ASP
2	B	792	MET
2	B	813	LYS
2	B	888	GLY
2	B	946	ASN
2	B	1006	ILE
2	B	1069	PHE
2	B	1075	GLY
2	B	1099	VAL
2	B	1126	GLY
2	B	1151	LEU
2	B	1176	LYS
2	B	1186	LYS
3	C	17	VAL
3	C	133	VAL
3	C	149	ASN

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Mol	Chain	Res	Type
3	C	156	ARG
3	C	173	CYS
3	C	184	ASN
4	D	53	LEU
4	D	92	VAL
4	D	163	LEU
4	D	170	ASN
5	E	29	ILE
5	E	44	LYS
5	E	119	ALA
5	E	120	ASN
5	E	129	ALA
5	E	137	SER
6	F	154	ASP
7	G	50	ASP
7	G	139	LYS
8	H	18	GLY
8	H	62	SER
8	H	81	PRO
8	H	89	ALA
9	I	11	ASN
9	I	57	GLY
9	I	106	CYS
10	J	6	ARG
10	J	14	VAL
11	K	7	PHE
11	K	14	ASP
11	K	15	ASP
11	K	44	ASN
11	K	49	GLU
11	K	59	VAL
11	K	80	GLY
12	L	44	LYS
12	L	55	HIS
12	L	57	VAL
12	L	58	ILE
1	A	65	PHE
1	A	109	ASN
1	A	131	PRO
1	A	154	VAL
1	A	197	GLN
1	A	264	THR

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Mol	Chain	Res	Type
1	A	329	ARG
1	A	337	LEU
1	A	419	HIS
1	A	592	THR
1	A	610	ASP
1	A	772	GLU
1	A	777	ALA
1	A	872	ASP
1	A	886	THR
1	A	988	ILE
1	A	1122	LEU
1	A	1226	LEU
1	A	1269	HIS
1	A	1283	SER
1	A	1368	TYR
1	A	1389	ARG
2	B	17	CYS
2	B	42	MET
2	B	173	ARG
2	B	253	GLU
2	B	300	TRP
2	B	324	ASP
2	B	443	SER
2	B	453	SER
2	B	467	SER
2	B	524	GLN
2	B	584	ARG
2	B	635	ASP
2	B	848	ARG
2	B	883	LEU
2	B	909	ASP
2	B	951	GLN
2	B	1022	THR
2	B	1108	ARG
2	B	1121	GLY
2	B	1150	ARG
2	B	1158	PHE
2	B	1178	ASN
2	B	1181	GLU
3	C	89	ASP
3	C	132	PRO
3	C	148	ARG

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Mol	Chain	Res	Type
4	D	54	SER
4	D	95	GLY
4	D	177	GLU
5	E	2	GLU
5	E	40	GLU
5	E	50	GLY
5	E	72	SER
6	F	81	THR
6	F	150	GLU
7	G	35	GLU
7	G	94	VAL
7	G	165	GLU
7	G	167	PHE
8	H	80	PRO
8	H	108	GLU
9	I	47	GLU
10	J	24	LEU
12	L	45	SER
12	L	51	LYS
1	A	44	SER
1	A	45	ARG
1	A	196	ALA
1	A	318	LYS
1	A	323	VAL
1	A	535	MET
1	A	569	PRO
1	A	601	PRO
1	A	667	ILE
1	A	848	ASP
1	A	1116	PRO
1	A	1169	PHE
1	A	1338	ILE
1	A	1369	ARG
1	A	1406	GLU
2	B	33	GLN
2	B	43	GLU
2	B	101	PRO
2	B	382	ALA
2	B	568	THR
2	B	603	SER
2	B	724	LYS
2	B	842	ASN

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Mol	Chain	Res	Type
2	B	1116	ARG
2	B	1136	ASP
3	C	106	GLY
3	C	153	LEU
3	C	169	LYS
4	D	142	ILE
5	E	191	ARG
7	G	67	SER
8	H	127	GLY
9	I	8	LEU
9	I	9	GLU
9	I	34	TYR
9	I	86	PHE
11	K	54	PRO
11	K	78	GLU
11	K	111	ILE
1	A	234	TRP
1	A	311	GLY
1	A	651	GLN
1	A	707	PRO
1	A	753	LYS
1	A	960	VAL
1	A	981	SER
1	A	1013	GLN
1	A	1064	GLU
1	A	1206	ASP
1	A	1414	GLU
2	B	32	SER
2	B	175	LEU
2	B	254	ASP
2	B	296	ASP
2	B	429	ILE
2	B	462	GLN
2	B	587	SER
2	B	738	PHE
2	B	785	TYR
2	B	1177	LYS
2	B	1183	ARG
3	C	33	ARG
3	C	214	LYS
3	C	227	ARG
3	C	240	ALA

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Mol	Chain	Res	Type
5	E	37	SER
5	E	85	PRO
5	E	202	GLU
6	F	106	PRO
6	F	151	LEU
7	G	17	TYR
8	H	12	VAL
8	H	91	ASP
8	H	118	GLY
10	J	43	TYR
1	A	255	GLU
1	A	333	LYS
1	A	652	LYS
1	A	1017	THR
1	A	1401	MET
2	B	473	SER
2	B	1017	ILE
3	C	59	ASP
3	C	129	VAL
3	C	142	ILE
4	D	183	ASP
7	G	128	PRO
8	H	94	TYR
9	I	33	ASP
10	J	32	GLY
6	F	111	ILE
10	J	28	GLY
2	B	282	GLY
6	F	109	VAL
10	J	56	ILE
1	A	757	ILE
1	A	1244	VAL
2	B	457	GLY
4	D	161	PRO
1	A	245	PRO
1	A	378	PRO
2	B	543	PRO
2	B	977	GLY
2	B	992	VAL
2	B	629	PRO
6	F	105	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	988/1528 (65%)	885 (90%)	103 (10%)	7 27
2	B	822/1077 (76%)	731 (89%)	91 (11%)	6 25
3	C	155/264 (59%)	130 (84%)	25 (16%)	2 15
4	D	78/160 (49%)	65 (83%)	13 (17%)	2 14
5	E	155/197 (79%)	140 (90%)	15 (10%)	8 29
6	F	60/137 (44%)	54 (90%)	6 (10%)	7 28
7	G	102/148 (69%)	91 (89%)	11 (11%)	6 26
8	H	91/130 (70%)	84 (92%)	7 (8%)	13 39
9	I	82/109 (75%)	72 (88%)	10 (12%)	5 23
10	J	48/66 (73%)	40 (83%)	8 (17%)	2 14
11	K	67/109 (62%)	56 (84%)	11 (16%)	2 14
12	L	26/58 (45%)	25 (96%)	1 (4%)	33 58
All	All	2674/3983 (67%)	2373 (89%)	301 (11%)	6 25

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	62	ASP
1	A	77	CYS
1	A	83	HIS
1	A	110	CYS
1	A	120	PRO
1	A	121	THR
1	A	131	PRO
1	A	158	SER
1	A	185	THR
1	A	198	PRO

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Mol	Chain	Res	Type
1	A	200	ARG
1	A	214	HIS
1	A	216	SER
1	A	217	PRO
1	A	244	PRO
1	A	262	ASP
1	A	309	ILE
1	A	313	PRO
1	A	336	ARG
1	A	345	ARG
1	A	370	SER
1	A	386	ILE
1	A	390	THR
1	A	404	LYS
1	A	409	ASP
1	A	413	ARG
1	A	426	VAL
1	A	435	ARG
1	A	441	ASP
1	A	444	LEU
1	A	446	ASN
1	A	448	GLN
1	A	451	LEU
1	A	452	HIS
1	A	463	VAL
1	A	467	SER
1	A	470	ARG
1	A	482	ASP
1	A	494	GLN
1	A	521	VAL
1	A	525	VAL
1	A	543	GLU
1	A	561	VAL
1	A	598	LEU
1	A	636	ARG
1	A	651	GLN
1	A	667	ILE
1	A	677	MET
1	A	707	PRO
1	A	712	ARG
1	A	722	THR
1	A	728	ASP

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Mol	Chain	Res	Type
1	A	732	ARG
1	A	739	LYS
1	A	740	ASP
1	A	741	LEU
1	A	742	ASN
1	A	765	CYS
1	A	775	ARG
1	A	789	THR
1	A	822	ARG
1	A	840	ARG
1	A	859	ASN
1	A	883	THR
1	A	887	ILE
1	A	924	VAL
1	A	930	LEU
1	A	941	ARG
1	A	986	PRO
1	A	1031	ARG
1	A	1032	ARG
1	A	1050	THR
1	A	1054	GLN
1	A	1118	LEU
1	A	1122	LEU
1	A	1135	VAL
1	A	1148	VAL
1	A	1168	ASP
1	A	1196	ARG
1	A	1238	LEU
1	A	1244	VAL
1	A	1267	GLU
1	A	1270	MET
1	A	1280	PRO
1	A	1288	VAL
1	A	1300	GLU
1	A	1327	SER
1	A	1335	PHE
1	A	1367	ASN
1	A	1374	LEU
1	A	1388	THR
1	A	1403	CYS
1	A	1406	GLU
1	A	1429	GLU

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Mol	Chain	Res	Type
1	A	1435	GLN
1	A	1444	PHE
1	A	1447	MET
1	A	1448	ILE
1	A	1450	GLU
2	B	17	CYS
2	B	50	VAL
2	B	54	PRO
2	B	88	THR
2	B	90	THR
2	B	166	ARG
2	B	174	THR
2	B	178	VAL
2	B	185	GLU
2	B	190	MET
2	B	208	ARG
2	B	216	VAL
2	B	226	SER
2	B	252	ARG
2	B	259	ARG
2	B	260	THR
2	B	278	PHE
2	B	295	TYR
2	B	358	THR
2	B	364	GLU
2	B	365	THR
2	B	386	LYS
2	B	389	ASP
2	B	439	LEU
2	B	444	THR
2	B	459	TRP
2	B	466	MET
2	B	469	ARG
2	B	478	ARG
2	B	489	ARG
2	B	491	THR
2	B	506	GLN
2	B	509	ASN
2	B	511	HIS
2	B	543	PRO
2	B	550	PHE
2	B	568	THR

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Mol	Chain	Res	Type
2	B	584	ARG
2	B	596	LEU
2	B	603	SER
2	B	607	SER
2	B	609	ILE
2	B	622	ASP
2	B	628	ARG
2	B	637	GLU
2	B	648	THR
2	B	676	TYR
2	B	686	VAL
2	B	703	THR
2	B	722	THR
2	B	737	THR
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	797	TYR
2	B	798	TYR
2	B	811	TYR
2	B	830	TYR
2	B	831	SER
2	B	835	GLN
2	B	845	SER
2	B	859	TYR
2	B	887	HIS
2	B	899	ILE
2	B	909	ASP
2	B	939	THR
2	B	944	THR
2	B	953	LEU
2	B	970	THR
2	B	999	MET
2	B	1021	MET
2	B	1022	THR
2	B	1045	THR
2	B	1046	PRO
2	B	1047	PHE
2	B	1069	PHE
2	B	1071	VAL
2	B	1084	GLN
2	B	1092	TYR

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Mol	Chain	Res	Type
2	B	1096	ARG
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1185	CYS
2	B	1189	THR
2	B	1192	TYR
2	B	1198	TYR
2	B	1218	THR
2	B	1220	ARG
2	B	1224	SER
3	C	34	ARG
3	C	59	ASP
3	C	61	PHE
3	C	66	LEU
3	C	76	VAL
3	C	86	THR
3	C	101	SER
3	C	111	THR
3	C	121	VAL
3	C	124	PRO
3	C	136	ASP
3	C	145	CYS
3	C	147	LEU
3	C	163	ILE
3	C	166	GLU
3	C	170	TRP
3	C	194	GLU
3	C	208	THR
3	C	215	PRO
3	C	231	THR
3	C	233	GLU
3	C	234	THR
3	C	235	THR
3	C	251	LEU
3	C	262	LEU
4	D	32	PRO
4	D	41	HIS
4	D	48	LEU
4	D	51	LEU
4	D	109	LEU

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Mol	Chain	Res	Type
4	D	111	THR
4	D	117	ASP
4	D	139	PRO
4	D	158	THR
4	D	169	VAL
4	D	171	LEU
4	D	184	PRO
4	D	185	TYR
5	E	8	ILE
5	E	16	ARG
5	E	29	ILE
5	E	37	SER
5	E	59	PHE
5	E	65	PRO
5	E	72	SER
5	E	73	ASP
5	E	77	LEU
5	E	103	ASN
5	E	113	ASN
5	E	131	ILE
5	E	143	ILE
5	E	145	HIS
5	E	174	LEU
6	F	90	ARG
6	F	99	LEU
6	F	103	MET
6	F	116	ASP
6	F	138	LEU
6	F	140	ASP
7	G	1	MET
7	G	13	LEU
7	G	37	THR
7	G	74	TYR
7	G	80	LYS
7	G	88	ASP
7	G	112	THR
7	G	128	PRO
7	G	150	THR
7	G	163	ILE
7	G	171	ILE
8	H	3	SER
8	H	10	PHE

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Mol	Chain	Res	Type
8	H	56	THR
8	H	63	LEU
8	H	94	TYR
8	H	101	TYR
8	H	109	ASP
9	I	4	PHE
9	I	7	CYS
9	I	12	ASN
9	I	14	LEU
9	I	34	TYR
9	I	51	ASN
9	I	87	GLN
9	I	98	THR
9	I	100	PHE
9	I	106	CYS
10	J	2	ILE
10	J	7	CYS
10	J	13	VAL
10	J	16	ASP
10	J	42	ARG
10	J	43	TYR
10	J	45	CYS
10	J	47	ARG
11	K	1	MET
11	K	10	PHE
11	K	16	VAL
11	K	17	PRO
11	K	25	SER
11	K	47	ARG
11	K	54	PRO
11	K	57	THR
11	K	61	TYR
11	K	76	GLN
11	K	101	LEU
12	L	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	68	GLN
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	172	GLN
1	A	226	ASN
1	A	300	HIS
1	A	340	ASN
1	A	494	GLN
1	A	504	GLN
1	A	699	GLN
1	A	737	ASN
1	A	742	ASN
1	A	758	ASN
1	A	787	HIS
1	A	859	ASN
1	A	882	GLN
1	A	968	ASN
1	A	1084	ASN
1	A	1367	ASN
1	A	1390	HIS
1	A	1393	ASN
2	B	108	ASN
2	B	206	GLN
2	B	227	HIS
2	B	356	HIS
2	B	359	GLN
2	B	458	ASN
2	B	508	HIS
2	B	509	ASN
2	B	651	HIS
2	B	708	GLN
2	B	744	HIS
2	B	821	GLN
2	B	822	ASN
2	B	835	GLN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	167	HIS
3	C	252	GLN
5	E	31	GLN

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Mol	Chain	Res	Type
5	E	100	GLN
5	E	103	ASN
5	E	113	ASN
5	E	146	HIS
7	G	53	ASN
8	H	136	GLN
9	I	51	ASN
10	J	52	HIS
11	K	2	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1409/1743 (80%)	-0.18	37 (2%) 56 46	110, 206, 318, 455	0
2	B	1079/1227 (87%)	-0.19	20 (1%) 66 58	115, 226, 316, 418	0
3	C	263/304 (86%)	-0.36	1 (0%) 92 87	148, 216, 311, 349	0
4	D	143/186 (76%)	-0.11	1 (0%) 87 82	167, 263, 321, 343	0
5	E	214/214 (100%)	-0.46	0 100 100	122, 197, 260, 300	0
6	F	84/155 (54%)	-0.46	1 (1%) 79 70	160, 222, 270, 312	0
7	G	171/171 (100%)	-0.35	0 100 100	156, 213, 267, 311	0
8	H	131/145 (90%)	-0.04	2 (1%) 73 64	161, 214, 298, 344	0
9	I	113/115 (98%)	0.02	3 (2%) 54 44	211, 276, 343, 386	0
10	J	64/72 (88%)	-0.43	1 (1%) 72 62	154, 214, 272, 288	0
11	K	112/118 (94%)	-0.43	1 (0%) 84 77	149, 202, 274, 293	0
12	L	46/73 (63%)	0.09	3 (6%) 18 15	223, 275, 329, 350	0
All	All	3829/4523 (84%)	-0.22	70 (1%) 68 60	110, 219, 314, 455	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	ASP	5.3
1	A	155	ASP	5.3
1	A	156	GLU	5.2
1	A	195	ASP	4.6
9	I	113	GLU	4.6
9	I	112	ASP	4.5
1	A	115	LEU	4.1
3	C	130	GLY	4.0
1	A	255	GLU	3.9
1	A	199	GLU	3.8
1	A	158	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	228	VAL	3.6
1	A	1304	GLU	3.5
1	A	256	THR	3.5
2	B	229	ALA	3.3
2	B	635	ASP	3.3
1	A	421	ARG	3.2
1	A	404	LYS	3.2
12	L	39	ASN	3.1
2	B	248	LYS	3.1
2	B	352	GLU	3.1
1	A	196	ALA	3.0
1	A	314	GLN	3.0
2	B	359	GLN	2.9
1	A	154	VAL	2.9
12	L	28	GLY	2.9
2	B	641	ASN	2.9
2	B	883	LEU	2.8
1	A	197	GLN	2.8
1	A	414	ILE	2.8
1	A	427	LEU	2.8
1	A	424	ASP	2.8
2	B	230	GLU	2.7
2	B	634	GLU	2.7
1	A	198	PRO	2.7
1	A	153	PRO	2.6
2	B	464	LYS	2.6
2	B	918	ILE	2.6
1	A	161	LYS	2.6
6	F	155	ASN	2.5
2	B	636	ASP	2.5
1	A	179	GLY	2.5
1	A	406	VAL	2.4
4	D	48	LEU	2.4
1	A	187	LYS	2.4
2	B	895	GLU	2.4
1	A	178	ASP	2.3
2	B	1223	VAL	2.3
8	H	131	LEU	2.3
8	H	145	ARG	2.3
2	B	426	GLN	2.3
9	I	22	ASN	2.2
11	K	80	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
10	J	64	PRO	2.2
1	A	416	LEU	2.2
1	A	1085	THR	2.2
2	B	896	ASP	2.2
2	B	876	LYS	2.2
1	A	145	LYS	2.2
2	B	561	ASP	2.2
1	A	1406	GLU	2.1
1	A	450	SER	2.1
1	A	1167	GLU	2.1
1	A	405	TYR	2.1
1	A	92	HIS	2.1
12	L	40	PHE	2.0
1	A	91	PHE	2.0
2	B	917	PRO	2.0
1	A	174	VAL	2.0
1	A	160	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
13	ZN	A	1801	1/1	0.82	0.14	299,299,299,299	0
13	ZN	I	201	1/1	0.88	0.08	239,239,239,239	0
13	ZN	C	401	1/1	0.89	0.05	283,283,283,283	0
13	ZN	L	101	1/1	0.89	0.07	318,318,318,318	0
13	ZN	I	202	1/1	0.91	0.07	242,242,242,242	0
13	ZN	J	101	1/1	0.94	0.24	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	ZN	A	1802	1/1	0.98	0.13	270,270,270,270	0
13	ZN	B	1301	1/1	0.99	0.12	248,248,248,248	0

6.5 Other polymers (i)

There are no such residues in this entry.