Full wwPDB X-ray Structure Validation Report (i)

Mar 17, 2026 – 08:52 PM UTC

PDB ID	:	5U5Q / pdb_00005u5q
Title	:	12 Subunit RNA Polymerase II at Room Temperature collected using SFX
Authors	:	Bushnell, D.A.; Oberthur, D.; Mariani, V.; Yefanov, O.; Tolstikova, A.; Barty, A.
Deposited on	:	2016-12-07
Resolution	:	3.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

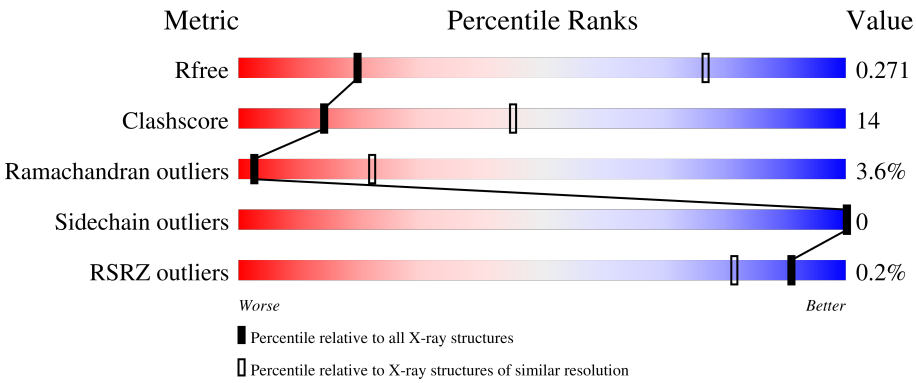
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1733	54% 27% • 17%
2	B	1224	59% 34% • 6%
3	C	318	53% 29% • 16%
4	D	221	52% 31% 17%
5	E	215	73% 27%

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Mol	Chain	Length	Quality of chain
6	F	155	37% 19% 44%
7	G	171	68% 32%
8	H	146	% 53% 38% 6%
9	I	122	74% 23%
10	J	70	46% 44% 7%
11	K	120	77% 19%
12	L	70	43% 20% 34%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 31634 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
			Total	C	N	O	S			
1	A	1434	11285	7106	1968	2149	62	38	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1150	9138	5778	1601	1703	56	50	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	184	1415	877	250	285	3	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	215	1760	1116	310	322	12	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	87	705	451	119	132	3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	171	1340	861	222	249	8	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	137	1101	692	185	220	4	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	119	971	596	179	186	10	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	115	920	590	157	171	2	0	0	1

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	363	224	72	63	4	0	0	0

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
13	A	2	2	2	0	0
13	B	1	1	1	0	0

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

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

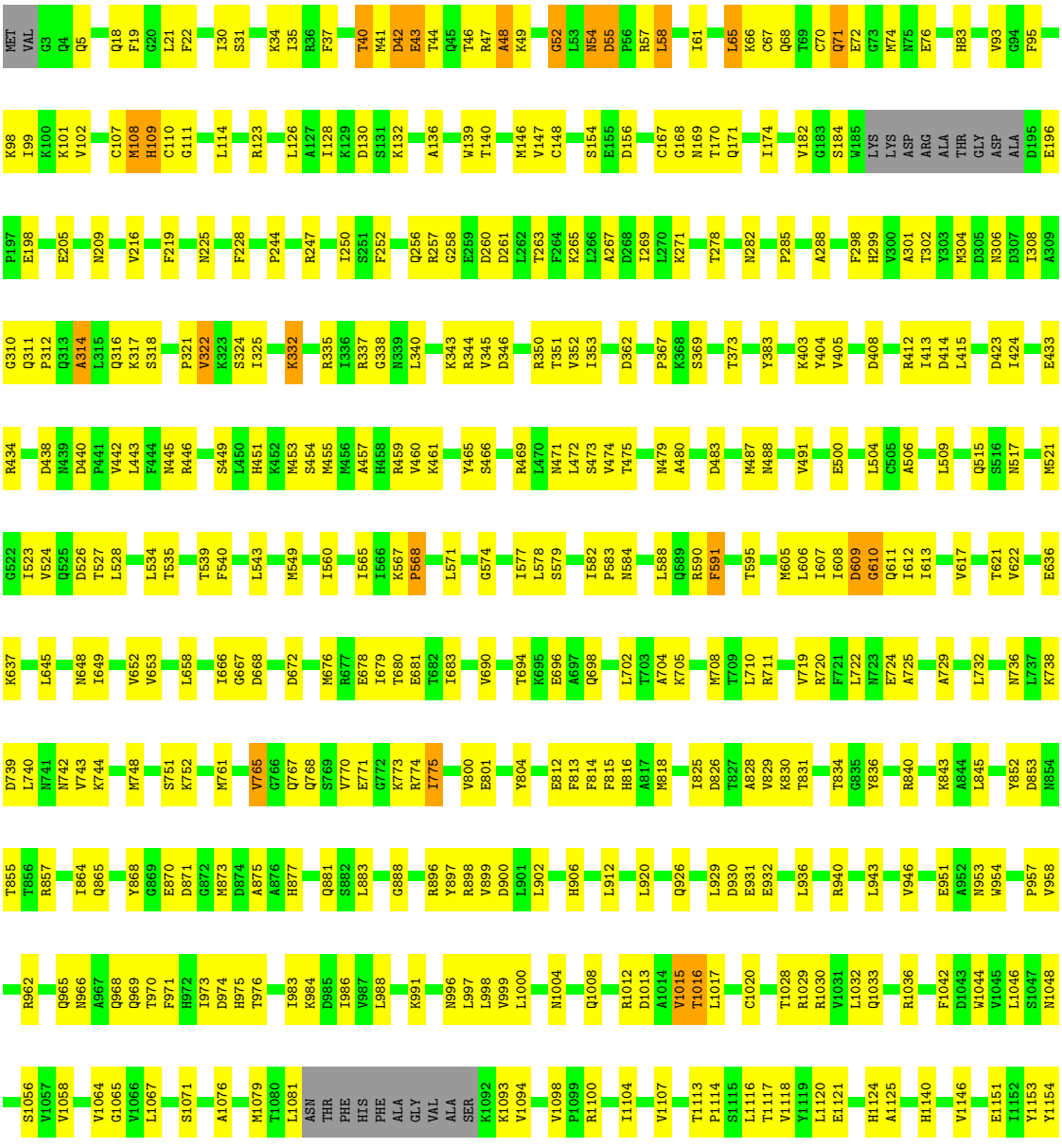
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
14	A	1	1	1	0	0

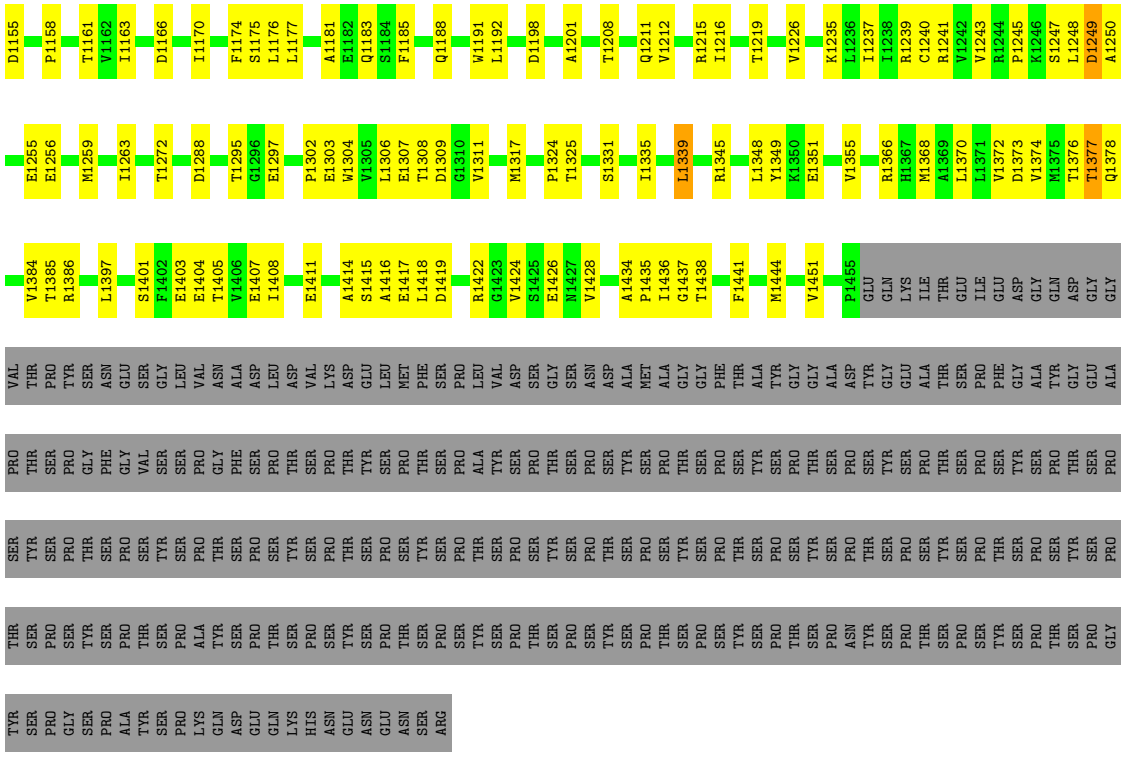
3 Residue-property plots (i)

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 II subunit RPB1

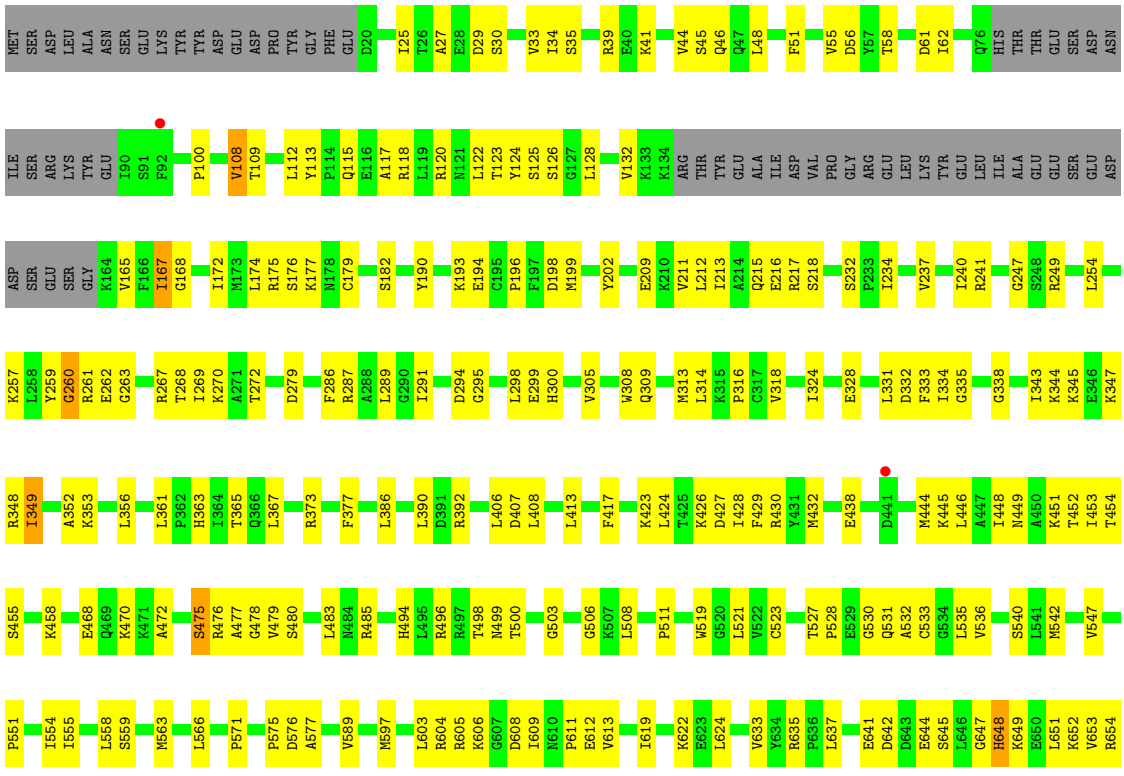
Chain A: 54% 27% • 17%

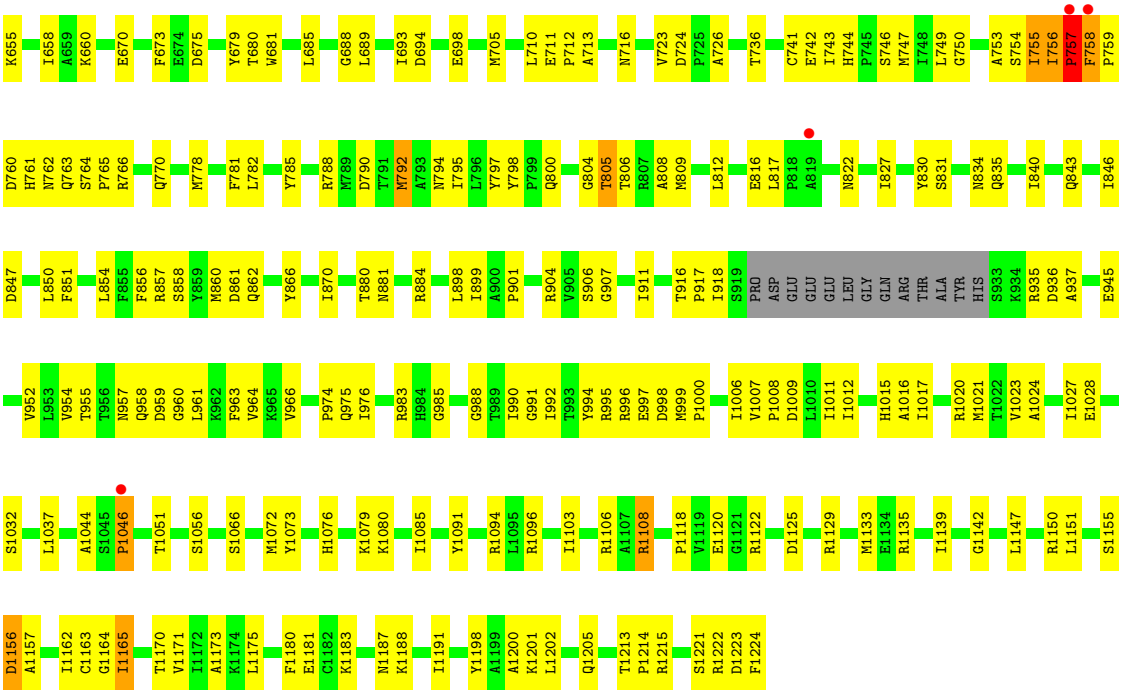




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

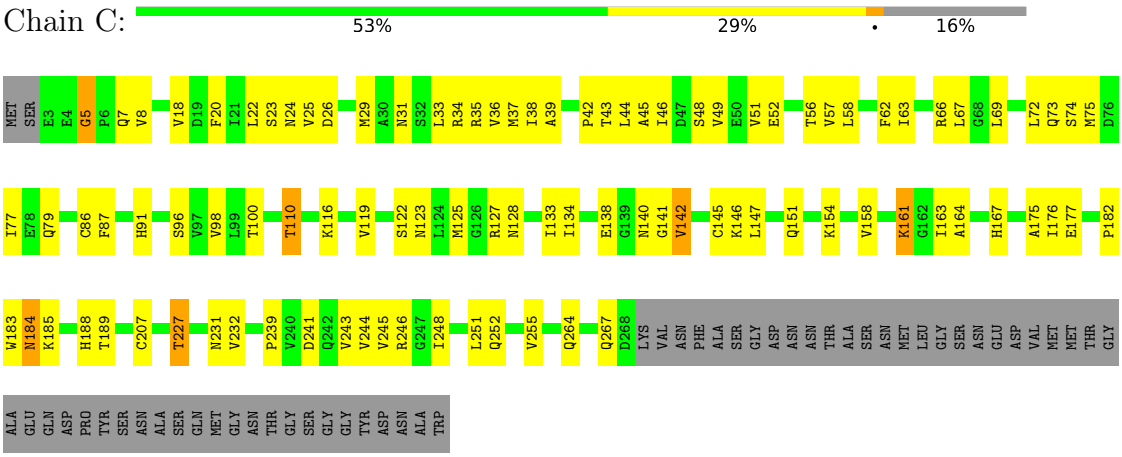
Chain B: 59% 34% • 6%





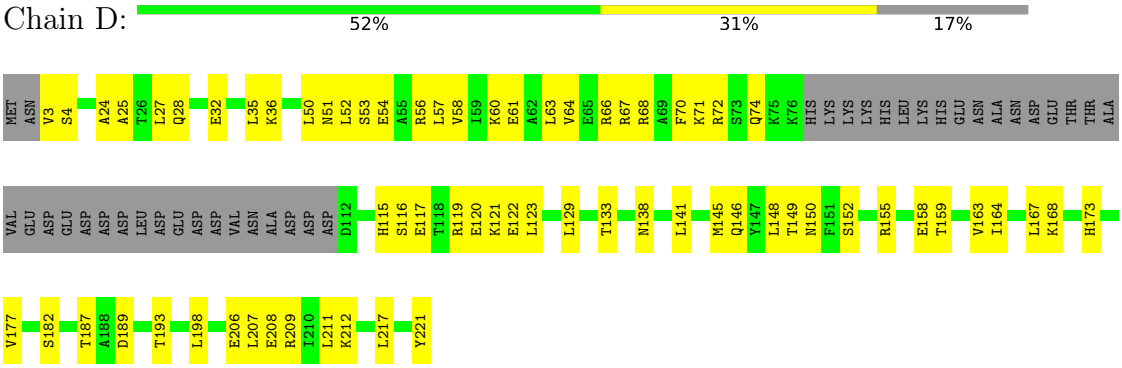
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



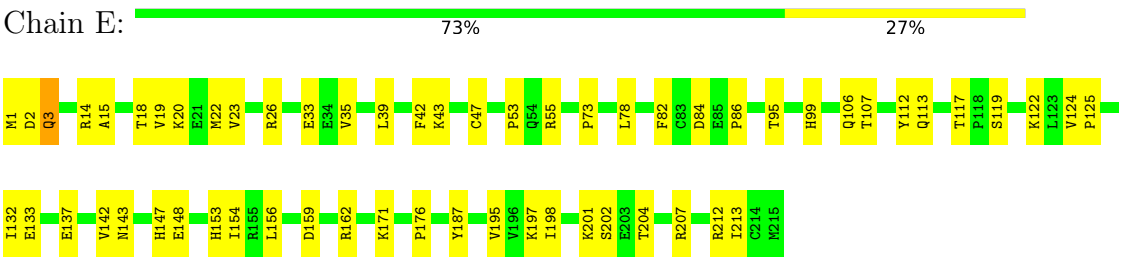
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



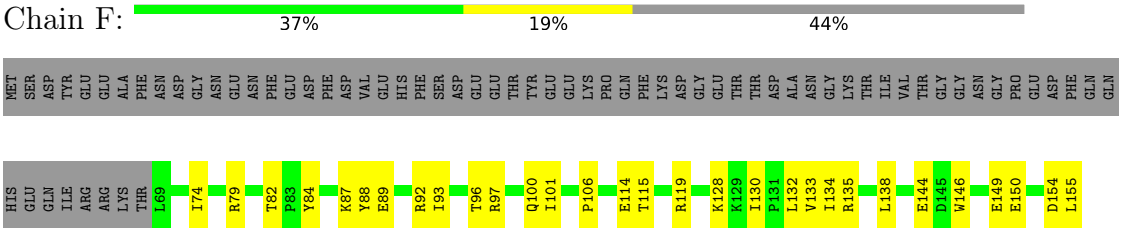
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



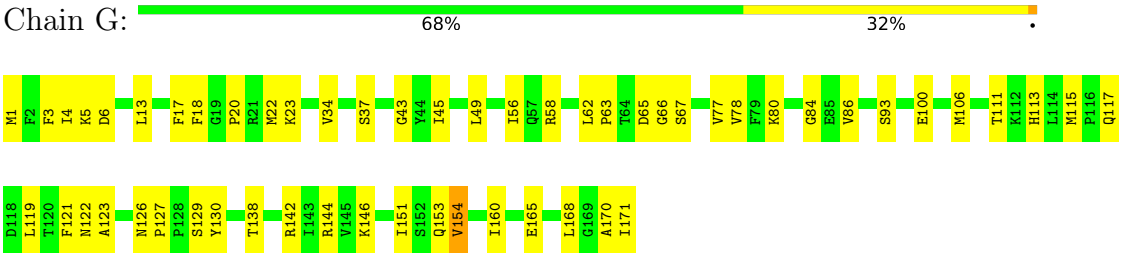
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



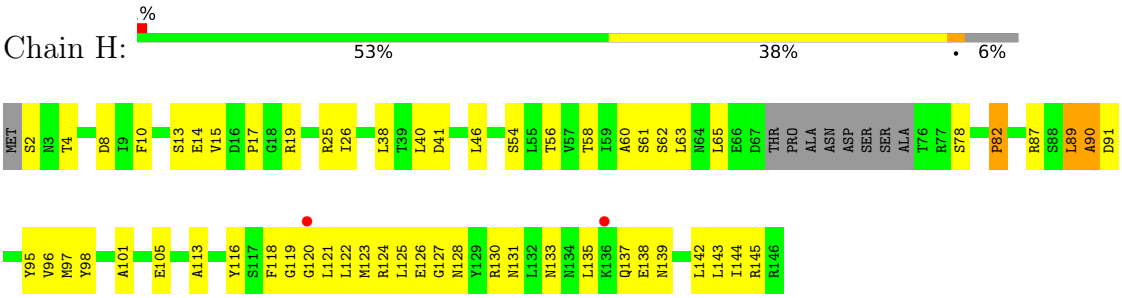
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



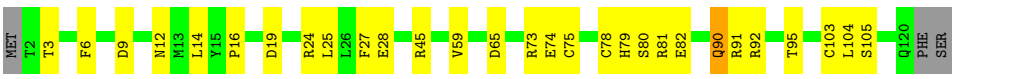
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



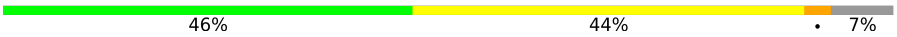
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

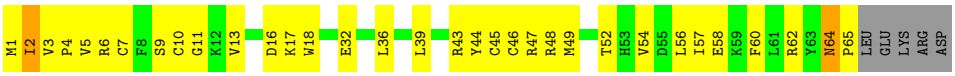
Chain I:



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



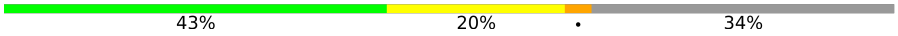


• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:

• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	223.40Å 396.80Å 287.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.61 – 3.80 40.61 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.61-3.80) 98.8 (40.61-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 3.76Å)	Xtriage
Refinement program	PHENIX (dev_2356: ???)	Depositor
R, R_{free}	0.218 , 0.271 0.220 , 0.271	Depositor DCC
R_{free} test set	2493 reflections (0.55%)	wwPDB-VP
Wilson B-factor (Å^2)	141.0	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 180.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.105 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.118 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31634	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.13	0/11488	0.37	0/15539
2	B	0.14	0/9317	0.39	0/12566
3	C	0.11	0/2133	0.31	0/2891
4	D	0.10	0/1426	0.31	0/1919
5	E	0.27	1/1796 (0.1%)	0.35	0/2416
6	F	0.12	0/717	0.34	0/967
7	G	0.12	0/1368	0.33	0/1844
8	H	0.13	0/1119	0.37	0/1515
9	I	0.12	0/989	0.40	0/1331
10	J	0.15	0/541	0.43	0/727
11	K	0.11	0/938	0.29	0/1267
12	L	0.13	0/365	0.38	0/485
All	All	0.14	1/32197 (0.0%)	0.37	0/43467

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	1
2	B	0	4
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	124	VAL	C-N	10.18	1.57	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ASP	Peptide
2	B	755	ILE	Peptide
2	B	756	ILE	Peptide
2	B	757	PRO	Peptide
2	B	758	PHE	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	11285	0	11338	352	0
2	B	9138	0	9158	299	0
3	C	2095	0	2052	72	0
4	D	1415	0	1368	44	0
5	E	1760	0	1788	38	0
6	F	705	0	731	24	0
7	G	1340	0	1357	35	0
8	H	1101	0	1067	40	0
9	I	971	0	929	20	0
10	J	532	0	544	37	0
11	K	920	0	929	17	0
12	L	363	0	386	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
14	A	1	0	0	0	0
All	All	31634	0	31647	902	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 14.

All (902) 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)
4:D:66:ARG:O	4:D:70:PHE:HB2	1.52	1.10
2:B:475:SER:H	2:B:476:ARG:HA	1.35	0.91
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.62	0.82
3:C:66:ARG:NH2	10:J:3:VAL:O	2.13	0.81
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.63	0.80
6:F:82:THR:HG22	6:F:84:TYR:H	1.46	0.80
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.64	0.80
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.62	0.80
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.63	0.79
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.66	0.78
1:A:110:CYS:SG	1:A:111:GLY:N	2.58	0.77
1:A:332:LYS:H	1:A:337:ARG:HB3	1.48	0.77
1:A:469:ARG:NH2	2:B:991:GLY:O	2.18	0.77
1:A:174:ILE:HA	1:A:182:VAL:O	1.85	0.76
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.50	0.76
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.18	0.75
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.68	0.75
11:K:92:ASN:O	11:K:96:ASN:ND2	2.18	0.75
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.69	0.75
2:B:35:SER:HB3	2:B:39:ARG:HH21	1.52	0.75
3:C:123:ASN:ND2	3:C:125:MET:SD	2.60	0.75
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.69	0.74
1:A:1044:TRP:O	1:A:1048:ASN:ND2	2.20	0.74
8:H:2:SER:N	8:H:62:SER:HG	1.84	0.74
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.20	0.74
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.70	0.73
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.69	0.73
1:A:1151:GLU:OE2	9:I:45:ARG:NH1	2.22	0.73
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.70	0.73
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.71	0.73
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.69	0.72
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.55	0.72
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.22	0.72
2:B:260:GLY:O	2:B:267:ARG:NH1	2.23	0.72
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.25	0.71
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.23	0.71
3:C:142:VAL:H	10:J:16:ASP:HB3	1.55	0.71
1:A:966:ASN:O	1:A:970:THR:OG1	2.09	0.71
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.71	0.71
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.24	0.70
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.72	0.70
4:D:187:THR:HG22	4:D:189:ASP:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:CYS:HA	5:E:53:PRO:HA	1.74	0.69
3:C:145:CYS:SG	3:C:146:LYS:N	2.65	0.69
1:A:260:ASP:O	1:A:263:THR:OG1	2.10	0.69
5:E:143:ASN:ND2	5:E:187:TYR:OH	2.24	0.69
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.74	0.68
2:B:642:ASP:HA	2:B:649:LYS:HA	1.76	0.68
2:B:56:ASP:OD2	2:B:177:LYS:NZ	2.27	0.68
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.27	0.68
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.75	0.68
7:G:122:ASN:HB3	7:G:129:SER:O	1.94	0.68
1:A:278:THR:O	1:A:282:ASN:ND2	2.23	0.67
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.58	0.67
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.77	0.67
2:B:348:ARG:O	2:B:352:ALA:CB	2.43	0.67
4:D:50:LEU:HD11	7:G:4:ILE:HG13	1.74	0.67
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.77	0.67
1:A:946:VAL:HG13	5:E:201:LYS:HB3	1.75	0.67
3:C:100:THR:O	3:C:119:VAL:HB	1.95	0.67
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.28	0.67
2:B:995:ARG:HD3	11:K:6:ARG:HH12	1.59	0.67
3:C:44:LEU:HB3	3:C:74:SER:HB3	1.76	0.66
2:B:218:SER:OG	2:B:241:ARG:NH1	2.27	0.66
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.77	0.66
1:A:965:GLN:HA	1:A:968:GLN:HG3	1.77	0.66
2:B:215:GLN:O	2:B:406:LEU:HA	1.95	0.66
9:I:75:CYS:HB2	9:I:79:HIS:H	1.60	0.65
1:A:306:ASN:ND2	1:A:321:PRO:O	2.29	0.65
1:A:1170:ILE:HG22	1:A:1174:PHE:HE2	1.61	0.65
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.79	0.65
1:A:732:LEU:O	1:A:736:ASN:HB2	1.97	0.65
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.77	0.65
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.30	0.65
1:A:1013:ASP:OD1	5:E:207:ARG:NH1	2.29	0.65
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.78	0.65
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.61	0.65
11:K:88:LYS:O	11:K:92:ASN:ND2	2.27	0.65
1:A:30:ILE:O	2:B:1183:LYS:NZ	2.29	0.64
1:A:999:VAL:HG12	1:A:1000:LEU:HD12	1.80	0.64
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.79	0.64
1:A:1185:PHE:O	1:A:1188:GLN:NE2	2.18	0.64
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:ARG:O	1:A:1219:THR:OG1	2.15	0.64
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.80	0.64
1:A:767:GLN:HE21	1:A:774:ARG:HB2	1.62	0.63
1:A:836:TYR:OH	1:A:1403:GLU:OE2	2.17	0.63
1:A:840:ARG:NH2	1:A:1384:VAL:O	2.31	0.63
2:B:884:ARG:HD2	2:B:935:ARG:HD3	1.80	0.63
7:G:111:THR:HG22	7:G:113:HIS:H	1.62	0.63
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.31	0.63
8:H:61:SER:OG	8:H:62:SER:N	2.22	0.63
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.80	0.63
2:B:449:ASN:ND2	2:B:452:THR:OG1	2.32	0.63
2:B:957:ASN:OD1	2:B:958:GLN:N	2.31	0.63
4:D:24:ALA:HB3	4:D:28:GLN:HB2	1.81	0.63
1:A:43:GLU:HB2	1:A:46:THR:HB	1.81	0.63
1:A:225:ASN:OD1	1:A:228:PHE:N	2.24	0.63
2:B:680:THR:OG1	2:B:681:TRP:N	2.32	0.63
1:A:316:GLN:O	1:A:318:SER:N	2.32	0.62
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.31	0.62
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.17	0.62
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.82	0.62
2:B:287:ARG:NH1	2:B:324:ILE:O	2.32	0.62
2:B:642:ASP:HB3	2:B:649:LYS:HE3	1.80	0.62
1:A:528:LEU:HD23	1:A:751:SER:HA	1.81	0.62
2:B:530:GLY:O	2:B:532:ALA:N	2.33	0.62
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.80	0.62
2:B:822:ASN:O	10:J:48:ARG:NH1	2.33	0.62
1:A:761:MET:HE2	2:B:1021:MET:HG2	1.82	0.62
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.80	0.62
3:C:184:ASN:HD21	3:C:189:THR:H	1.45	0.62
1:A:351:THR:HB	2:B:1103:ILE:HG13	1.81	0.62
2:B:1156:ASP:OD1	2:B:1198:TYR:N	2.33	0.62
1:A:108:MET:O	1:A:110:CYS:N	2.33	0.61
1:A:108:MET:SD	1:A:108:MET:N	2.73	0.61
1:A:881:GLN:O	1:A:953:ASN:HA	2.00	0.61
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.83	0.61
1:A:1434:ALA:O	1:A:1436:ILE:N	2.33	0.61
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.82	0.61
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.72	0.61
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.33	0.61
4:D:164:ILE:O	4:D:168:LYS:HB2	2.01	0.61
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:HG22	2:B:983:ARG:HB3	1.83	0.61
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.83	0.61
5:E:202:SER:HB3	5:E:204:THR:HG22	1.81	0.61
7:G:117:GLN:N	7:G:117:GLN:OE1	2.33	0.61
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.81	0.61
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.83	0.61
1:A:1325:THR:HG22	5:E:148:GLU:HG3	1.83	0.61
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.82	0.60
2:B:343:ILE:HB	2:B:347:LYS:HB2	1.82	0.60
10:J:48:ARG:O	10:J:52:THR:OG1	2.15	0.60
7:G:142:ARG:HB3	7:G:171:ILE:HG13	1.82	0.60
2:B:444:MET:HB3	2:B:445:LYS:HA	1.84	0.60
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.84	0.60
1:A:855:THR:HG21	1:A:857:ARG:HE	1.65	0.60
1:A:350:ARG:HA	1:A:487:MET:O	2.00	0.60
1:A:433:GLU:OE1	2:B:1108:ARG:NH1	2.34	0.60
1:A:888:GLY:O	1:A:940:ARG:NH2	2.33	0.60
1:A:574:GLY:O	1:A:578:LEU:HB2	2.02	0.60
4:D:32:GLU:O	7:G:5:LYS:NZ	2.33	0.59
10:J:1:MET:N	10:J:54:VAL:O	2.35	0.59
2:B:175:ARG:NH1	2:B:198:ASP:O	2.35	0.59
2:B:604:ARG:NH2	2:B:613:VAL:O	2.35	0.59
2:B:806:THR:HG22	2:B:808:ALA:H	1.66	0.59
4:D:189:ASP:O	4:D:193:THR:OG1	2.15	0.59
2:B:705:MET:H	2:B:710:LEU:HD12	1.68	0.59
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.85	0.59
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.85	0.59
4:D:60:LYS:HD3	4:D:115:HIS:CE1	2.36	0.59
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.30	0.59
1:A:870:GLU:OE1	5:E:202:SER:OG	2.16	0.59
2:B:179:CYS:O	2:B:182:SER:OG	2.19	0.58
3:C:48:SER:HB3	3:C:158:VAL:HB	1.84	0.58
1:A:408:ASP:N	1:A:408:ASP:OD1	2.36	0.58
2:B:451:LYS:O	2:B:455:SER:OG	2.17	0.58
1:A:830:LYS:O	1:A:834:THR:OG1	2.21	0.58
1:A:1411:GLU:O	1:A:1415:SER:OG	2.22	0.58
2:B:858:SER:HA	2:B:966:VAL:O	2.03	0.58
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.83	0.58
2:B:750:GLY:O	2:B:754:SER:OG	2.21	0.58
2:B:770:GLN:O	2:B:770:GLN:NE2	2.36	0.58
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:GLU:HB2	1:A:1408:ILE:HD11	1.86	0.58
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.36	0.58
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.69	0.58
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.85	0.57
2:B:1222:ARG:O	2:B:1224:PHE:N	2.37	0.57
3:C:134:ILE:HD12	3:C:141:GLY:H	1.69	0.57
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.86	0.57
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.84	0.57
11:K:29:ASN:ND2	11:K:29:ASN:O	2.37	0.57
1:A:335:ARG:HH12	2:B:1202:LEU:HD13	1.70	0.57
1:A:403:LYS:HG3	1:A:404:TYR:HD2	1.69	0.57
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.87	0.57
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.87	0.57
8:H:113:ALA:HA	8:H:125:LEU:O	2.05	0.57
3:C:79:GLN:O	3:C:127:ARG:NH1	2.38	0.57
8:H:41:ASP:OD2	8:H:122:LEU:N	2.35	0.57
10:J:48:ARG:HE	10:J:49:MET:HE1	1.69	0.57
1:A:676:MET:O	1:A:680:THR:OG1	2.19	0.57
2:B:257:LYS:HB2	2:B:270:LYS:O	2.04	0.57
1:A:446:ARG:HB2	1:A:487:MET:SD	2.44	0.57
2:B:641:GLU:HG3	2:B:652:LYS:HE3	1.86	0.57
2:B:348:ARG:O	2:B:352:ALA:HB3	2.05	0.56
2:B:996:ARG:HB3	2:B:1007:VAL:HG21	1.87	0.56
1:A:645:LEU:O	1:A:649:ILE:HG13	2.06	0.56
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.40	0.56
1:A:943:LEU:HD11	1:A:1020:CYS:HB3	1.87	0.56
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.87	0.56
2:B:756:ILE:HD13	2:B:770:GLN:HE21	1.70	0.56
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.86	0.56
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.86	0.56
2:B:559:SER:HA	2:B:563:MET:HB3	1.87	0.56
6:F:130:ILE:HG22	6:F:132:LEU:H	1.71	0.56
9:I:75:CYS:SG	9:I:80:SER:OG	2.63	0.56
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.88	0.56
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.87	0.56
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.40	0.56
2:B:755:ILE:HG23	2:B:809:MET:HE3	1.88	0.56
5:E:1:MET:N	5:E:2:ASP:HA	2.19	0.56
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.87	0.56
2:B:1142:GLY:HA3	6:F:88:TYR:HE1	1.71	0.56
1:A:324:SER:OG	1:A:325:ILE:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG21	3:C:145:CYS:SG	2.47	0.55
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.86	0.55
1:A:609:ASP:OD1	1:A:969:GLN:NE2	2.32	0.55
2:B:916:THR:HB	2:B:935:ARG:HB2	1.87	0.55
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.89	0.55
1:A:107:CYS:H	1:A:114:LEU:HD21	1.72	0.55
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.72	0.55
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.71	0.55
8:H:65:LEU:H	8:H:65:LEU:HD23	1.71	0.55
1:A:58:LEU:HD12	1:A:244:PRO:HD3	1.86	0.55
1:A:1415:SER:O	1:A:1417:GLU:N	2.39	0.55
10:J:48:ARG:O	10:J:52:THR:CB	2.54	0.55
1:A:101:LYS:HB3	1:A:139:TRP:CD1	2.41	0.55
1:A:567:LYS:HB3	8:H:96:VAL:H	1.70	0.55
2:B:165:VAL:HG21	2:B:445:LYS:HE2	1.87	0.55
2:B:1163:CYS:SG	2:B:1164:GLY:N	2.80	0.55
2:B:115:GLN:NE2	2:B:193:LYS:O	2.36	0.55
1:A:474:VAL:HG23	1:A:521:MET:HE2	1.88	0.55
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.88	0.55
2:B:637:LEU:HB2	2:B:693:ILE:HD13	1.89	0.55
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.36	0.55
1:A:608:ILE:O	1:A:610:GLY:N	2.39	0.55
2:B:660:LYS:HB3	2:B:679:TYR:CD2	2.41	0.55
2:B:272:THR:OG1	2:B:279:ASP:OD1	2.26	0.55
2:B:348:ARG:O	2:B:352:ALA:HB2	2.07	0.55
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.88	0.55
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.89	0.55
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.89	0.54
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.42	0.54
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.88	0.54
1:A:40:THR:HG22	1:A:41:MET:HG3	1.89	0.54
3:C:183:TRP:O	3:C:185:LYS:N	2.40	0.54
2:B:132:VAL:HG11	2:B:445:LYS:HZ3	1.72	0.54
3:C:35:ARG:HA	3:C:38:ILE:HD12	1.89	0.54
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.90	0.54
1:A:54:ASN:ND2	1:A:54:ASN:O	2.41	0.54
1:A:67:CYS:O	1:A:70:CYS:HB3	2.07	0.54
1:A:362:ASP:OD1	1:A:362:ASP:N	2.40	0.54
1:A:1125:ALA:HB1	1:A:1303:GLU:HB2	1.87	0.54
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.30	0.54
1:A:298:PHE:HE1	1:A:312:PRO:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.88	0.54
3:C:43:THR:HG22	3:C:44:LEU:H	1.73	0.54
3:C:73:GLN:OE1	3:C:75:MET:N	2.41	0.54
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.90	0.54
1:A:672:ASP:HB3	1:A:736:ASN:HD21	1.73	0.54
1:A:42:ASP:O	1:A:44:THR:N	2.41	0.54
1:A:136:ALA:O	1:A:140:THR:OG1	2.23	0.54
1:A:1191:TRP:NE1	1:A:1256:GLU:OE1	2.41	0.54
2:B:1221:SER:O	2:B:1221:SER:OG	2.25	0.54
8:H:4:THR:HG23	8:H:60:ALA:HB2	1.88	0.54
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.88	0.54
1:A:668:ASP:OD1	1:A:742:ASN:N	2.37	0.54
2:B:58:THR:HG22	2:B:62:ILE:HD11	1.90	0.54
4:D:145:MET:O	4:D:149:THR:HG22	2.08	0.54
5:E:33:GLU:N	5:E:33:GLU:OE1	2.41	0.54
5:E:159:ASP:OD1	5:E:162:ARG:NH2	2.41	0.54
1:A:58:LEU:H	1:A:58:LEU:HD23	1.71	0.53
6:F:96:THR:O	6:F:100:GLN:HG3	2.08	0.53
2:B:123:THR:O	2:B:125:SER:N	2.41	0.53
9:I:16:PRO:HB3	9:I:25:LEU:HD11	1.90	0.53
1:A:369:SER:O	1:A:373:THR:OG1	2.22	0.53
1:A:996:ASN:O	1:A:998:LEU:N	2.42	0.53
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.89	0.53
2:B:1080:LYS:HB2	3:C:188:HIS:HB3	1.90	0.53
4:D:152:SER:OG	4:D:221:TYR:OH	2.22	0.53
6:F:97:ARG:O	6:F:101:ILE:HG13	2.09	0.53
1:A:1094:VAL:HG22	1:A:1113:THR:HG21	1.89	0.53
1:A:524:VAL:O	1:A:527:THR:OG1	2.24	0.53
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.89	0.53
1:A:826:ASP:O	1:A:830:LYS:HB2	2.07	0.53
1:A:974:ASP:OD2	1:A:976:THR:OG1	2.24	0.53
1:A:1345:ARG:NH1	1:A:1373:ASP:OD2	2.41	0.53
1:A:975:HIS:HA	1:A:1036:ARG:HG3	1.90	0.53
1:A:1117:THR:HG23	1:A:1307:GLU:HG2	1.89	0.53
3:C:18:VAL:O	3:C:231:ASN:HA	2.08	0.53
8:H:118:PHE:O	8:H:120:GLY:N	2.42	0.53
2:B:390:LEU:HB2	2:B:392:ARG:HG3	1.91	0.53
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.89	0.53
1:A:1067:LEU:O	1:A:1071:SER:OG	2.07	0.53
3:C:264:GLN:O	3:C:267:GLN:HG2	2.08	0.53
1:A:852:TYR:OH	6:F:89:GLU:OE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:957:ASN:HB3	2:B:961:LEU:H	1.74	0.53
7:G:115:MET:HB3	7:G:119:LEU:HD23	1.90	0.53
10:J:7:CYS:SG	10:J:9:SER:N	2.82	0.53
2:B:1009:ASP:OD2	10:J:48:ARG:NH2	2.42	0.53
1:A:898:ARG:NH1	1:A:899:VAL:O	2.42	0.52
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.09	0.52
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.90	0.52
1:A:690:VAL:O	1:A:694:THR:OG1	2.26	0.52
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.42	0.52
4:D:51:ASN:HB2	4:D:182:SER:HB3	1.90	0.52
2:B:445:LYS:HG3	2:B:446:LEU:HA	1.91	0.52
2:B:746:SER:HB3	2:B:1046:PRO:HG2	1.90	0.52
1:A:443:LEU:HD11	1:A:455:MET:HB3	1.91	0.52
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.09	0.52
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.91	0.52
5:E:39:LEU:HA	5:E:42:PHE:HB3	1.91	0.52
8:H:10:PHE:O	8:H:54:SER:HA	2.09	0.52
1:A:1198:ASP:OD2	1:A:1201:ALA:N	2.43	0.52
2:B:757:PRO:HB2	2:B:759:PRO:HA	1.91	0.52
2:B:805:THR:HA	2:B:809:MET:SD	2.50	0.52
3:C:63:ILE:O	3:C:67:LEU:HG	2.09	0.52
12:L:68:GLU:OE1	12:L:68:GLU:N	2.33	0.52
1:A:506:ALA:HB3	1:A:509:LEU:HG	1.92	0.52
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.44	0.52
1:A:1441:PHE:HE1	6:F:92:ARG:HD3	1.74	0.52
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.92	0.52
8:H:56:THR:HB	8:H:145:ARG:HG2	1.92	0.52
1:A:739:ASP:OD1	8:H:19:ARG:NH1	2.38	0.52
1:A:1348:LEU:HD23	1:A:1372:VAL:HG23	1.90	0.52
2:B:1106:ARG:NH1	2:B:1125:ASP:O	2.41	0.52
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.91	0.52
1:A:932:GLU:OE1	1:A:1028:THR:OG1	2.26	0.52
2:B:51:PHE:O	2:B:55:VAL:HG23	2.10	0.52
2:B:168:GLY:H	2:B:453:ILE:HD12	1.75	0.52
2:B:427:ASP:OD1	2:B:430:ARG:NH1	2.43	0.52
11:K:91:CYS:O	11:K:95:ILE:HG13	2.10	0.52
1:A:666:ILE:HD12	1:A:667:GLY:N	2.25	0.51
3:C:134:ILE:HD12	3:C:141:GLY:N	2.25	0.51
8:H:135:LEU:HB3	8:H:137:GLN:HG3	1.92	0.51
1:A:610:GLY:O	1:A:611:GLN:NE2	2.43	0.51
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.51
8:H:56:THR:O	8:H:144:ILE:HA	2.10	0.51
2:B:1028:GLU:O	2:B:1032:SER:OG	2.26	0.51
2:B:1056:SER:OG	2:B:1066:SER:O	2.25	0.51
2:B:851:PHE:CD1	2:B:1094:ARG:HB2	2.45	0.51
2:B:898:LEU:HB2	12:L:58:LYS:NZ	2.25	0.51
3:C:69:LEU:O	10:J:6:ARG:NH1	2.39	0.51
4:D:27:LEU:HD13	4:D:173:HIS:CE1	2.46	0.51
8:H:82:PRO:O	8:H:87:ARG:NH2	2.43	0.51
1:A:367:PRO:HB3	1:A:465:TYR:O	2.10	0.51
1:A:1376:THR:O	1:A:1378:GLN:N	2.36	0.51
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.92	0.51
1:A:285:PRO:HD2	1:A:288:ALA:HB3	1.92	0.51
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.92	0.51
2:B:41:LYS:HE2	2:B:45:SER:HB2	1.93	0.51
1:A:123:ARG:HA	1:A:126:LEU:HD12	1.92	0.51
1:A:1121:GLU:HB3	1:A:1124:HIS:ND1	2.26	0.51
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.10	0.51
2:B:475:SER:H	2:B:476:ARG:CA	2.17	0.51
4:D:52:LEU:HG	4:D:182:SER:HB2	1.93	0.51
1:A:128:ILE:HG22	1:A:130:ASP:H	1.76	0.51
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.93	0.51
1:A:560:ILE:HB	8:H:78:SER:HB2	1.93	0.50
7:G:146:LYS:NZ	7:G:165:GLU:OE2	2.42	0.50
10:J:9:SER:OG	10:J:45:CYS:HB2	2.11	0.50
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.92	0.50
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.76	0.50
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.11	0.50
1:A:19:PHE:HZ	1:A:1397:LEU:HD21	1.77	0.50
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.76	0.50
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.11	0.50
1:A:986:ILE:HD11	1:A:1032:LEU:HD21	1.94	0.50
2:B:349:ILE:O	2:B:353:LYS:HG3	2.12	0.50
2:B:954:VAL:HA	2:B:963:PHE:O	2.11	0.50
3:C:241:ASP:OD1	3:C:241:ASP:N	2.45	0.50
1:A:65:LEU:HB3	1:A:71:GLN:HB3	1.93	0.50
2:B:530:GLY:O	2:B:533:CYS:N	2.44	0.50
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.47	0.50
1:A:414:ASP:OD1	1:A:415:LEU:N	2.45	0.50
1:A:1015:VAL:O	1:A:1017:LEU:N	2.45	0.50
1:A:1372:VAL:O	1:A:1376:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1419:ASP:OD1	1:A:1426:GLU:OE1	2.29	0.50
2:B:286:PHE:HA	2:B:289:LEU:HD12	1.94	0.50
4:D:120:GLU:HA	4:D:123:LEU:HG	1.92	0.50
1:A:896:ARG:HH21	1:A:1030:ARG:HH21	1.59	0.50
1:A:1407:GLU:OE2	1:A:1407:GLU:N	2.39	0.50
1:A:1386:ARG:HG2	1:A:1403:GLU:OE1	2.12	0.50
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.93	0.50
2:B:314:LEU:O	2:B:318:VAL:HG23	2.11	0.50
1:A:725:ALA:O	1:A:729:ALA:CB	2.60	0.49
2:B:477:ALA:O	2:B:479:VAL:N	2.45	0.49
2:B:753:ALA:O	2:B:757:PRO:HD3	2.12	0.49
3:C:45:ALA:HA	3:C:72:LEU:HD13	1.94	0.49
1:A:260:ASP:OD1	1:A:261:ASP:N	2.44	0.49
2:B:352:ALA:O	2:B:356:LEU:HG	2.12	0.49
1:A:67:CYS:HB2	1:A:71:GLN:H	1.76	0.49
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.93	0.49
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.93	0.49
2:B:291:ILE:HG12	2:B:300:HIS:NE2	2.26	0.49
3:C:7:GLN:O	3:C:23:SER:OG	2.30	0.49
5:E:39:LEU:O	5:E:43:LYS:HG3	2.13	0.49
1:A:351:THR:OG1	1:A:352:VAL:N	2.44	0.49
1:A:679:ILE:O	1:A:683:ILE:HG13	2.13	0.49
2:B:649:LYS:NZ	2:B:736:THR:O	2.43	0.49
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.95	0.49
2:B:128:LEU:HB2	2:B:167:ILE:HD11	1.94	0.49
2:B:261:ARG:O	2:B:263:GLY:N	2.45	0.49
2:B:1037:LEU:O	10:J:47:ARG:NH1	2.45	0.49
2:B:860:MET:HA	2:B:964:VAL:O	2.13	0.49
3:C:8:VAL:HG22	3:C:22:LEU:HA	1.94	0.49
1:A:590:ARG:HH11	1:A:590:ARG:HB2	1.78	0.49
1:A:617:VAL:HG13	1:A:621:THR:HB	1.95	0.49
1:A:813:PHE:HE1	2:B:759:PRO:HB2	1.77	0.49
1:A:971:PHE:HB2	1:A:973:ILE:HD11	1.95	0.49
2:B:426:LYS:O	2:B:430:ARG:HG3	2.12	0.49
1:A:828:ALA:O	1:A:831:THR:HG22	2.13	0.49
1:A:1004:ASN:O	1:A:1008:GLN:HG2	2.12	0.49
2:B:295:GLY:H	2:B:298:LEU:HD23	1.78	0.49
3:C:75:MET:O	3:C:246:ARG:NH2	2.42	0.49
7:G:3:PHE:HB2	7:G:78:VAL:HG23	1.94	0.49
8:H:15:VAL:HG13	8:H:26:ILE:HD11	1.95	0.49
2:B:851:PHE:CE1	2:B:1094:ARG:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:PHE:CE2	7:G:123:ALA:HB2	2.48	0.49
1:A:472:LEU:O	1:A:474:VAL:N	2.44	0.48
1:A:775:ILE:HG21	1:A:815:PHE:CD1	2.47	0.48
3:C:24:ASN:O	3:C:24:ASN:ND2	2.46	0.48
10:J:32:GLU:O	10:J:36:LEU:HG	2.13	0.48
1:A:184:SER:HA	1:A:198:GLU:O	2.14	0.48
1:A:579:SER:HA	1:A:582:ILE:HG13	1.94	0.48
6:F:79:ARG:HH21	6:F:146:TRP:HA	1.77	0.48
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.48	0.48
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.48
2:B:611:PRO:HG2	2:B:685:LEU:HD21	1.95	0.48
1:A:711:ARG:NH1	9:I:95:THR:OG1	2.47	0.48
2:B:232:SER:OG	2:B:234:ILE:O	2.28	0.48
1:A:966:ASN:O	1:A:970:THR:CB	2.62	0.48
2:B:785:TYR:HE1	10:J:60:PHE:CE1	2.31	0.48
1:A:267:ALA:O	1:A:271:LYS:HG3	2.13	0.48
2:B:778:MET:SD	2:B:794:ASN:HB3	2.54	0.48
1:A:304:MET:O	1:A:324:SER:OG	2.32	0.48
1:A:804:TYR:O	2:B:761:HIS:ND1	2.46	0.48
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.44	0.48
8:H:105:GLU:OE1	8:H:124:ARG:NH2	2.47	0.48
1:A:95:PHE:O	1:A:99:ILE:HG13	2.14	0.48
1:A:475:THR:O	1:A:479:ASN:N	2.47	0.48
1:A:984:LYS:O	1:A:988:LEU:HB2	2.13	0.48
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.13	0.48
3:C:57:VAL:HG23	3:C:58:LEU:HD22	1.96	0.48
5:E:1:MET:H3	5:E:2:ASP:HA	1.78	0.48
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.96	0.48
2:B:723:VAL:HA	2:B:724:ASP:HB3	1.94	0.48
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.49	0.48
7:G:34:VAL:O	7:G:37:SER:OG	2.22	0.48
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.95	0.48
1:A:591:PHE:HA	1:A:595:THR:HG21	1.95	0.48
1:A:813:PHE:CE1	2:B:759:PRO:HB2	2.49	0.48
1:A:853:ASP:OD1	1:A:853:ASP:N	2.47	0.48
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.95	0.48
11:K:90:ALA:O	11:K:94:ILE:HG13	2.13	0.48
1:A:54:ASN:HB3	1:A:247:ARG:NH1	2.26	0.47
1:A:732:LEU:O	1:A:736:ASN:CB	2.62	0.47
1:A:877:HIS:ND1	1:A:1056:SER:HA	2.29	0.47
2:B:804:GLY:O	2:B:805:THR:OG1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:HIS:HA	5:E:197:LYS:O	2.14	0.47
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.46	0.47
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.96	0.47
1:A:442:VAL:O	1:A:457:ALA:HA	2.14	0.47
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.96	0.47
2:B:597:MET:SD	2:B:624:LEU:HD11	2.54	0.47
6:F:74:ILE:HG21	6:F:144:GLU:HG2	1.96	0.47
1:A:265:LYS:O	1:A:269:ILE:HG13	2.14	0.47
5:E:15:ALA:O	5:E:19:VAL:HG23	2.14	0.47
7:G:142:ARG:O	7:G:170:ALA:HA	2.15	0.47
8:H:15:VAL:HA	8:H:26:ILE:HG13	1.97	0.47
1:A:588:LEU:O	1:A:606:LEU:HA	2.15	0.47
2:B:547:VAL:H	2:B:612:GLU:CD	2.23	0.47
4:D:57:LEU:O	4:D:61:GLU:HG3	2.15	0.47
1:A:108:MET:HE1	1:A:171:GLN:HB3	1.95	0.47
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.96	0.47
2:B:781:PHE:HD1	2:B:782:LEU:HG	1.79	0.47
4:D:52:LEU:O	4:D:54:GLU:N	2.39	0.47
10:J:16:ASP:OD1	10:J:16:ASP:N	2.48	0.47
1:A:41:MET:HB3	1:A:48:ALA:O	2.15	0.47
1:A:98:LYS:O	1:A:102:VAL:HG23	2.15	0.47
1:A:252:PHE:O	1:A:256:GLN:HB2	2.15	0.47
1:A:694:THR:O	1:A:698:GLN:HG3	2.15	0.47
1:A:843:LYS:NZ	1:A:1401:SER:OG	2.47	0.47
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.95	0.47
2:B:445:LYS:H	2:B:446:LEU:HA	1.78	0.47
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.95	0.47
4:D:25:ALA:HB2	7:G:84:GLY:HA3	1.96	0.47
6:F:87:LYS:HA	6:F:155:LEU:HD11	1.96	0.47
8:H:113:ALA:HB2	8:H:126:GLU:HG2	1.96	0.47
8:H:130:ARG:HB2	8:H:133:ASN:HB2	1.97	0.47
10:J:1:MET:H2	10:J:56:LEU:H	1.62	0.47
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.96	0.47
2:B:904:ARG:NH1	12:L:66:GLN:O	2.48	0.47
1:A:648:ASN:O	1:A:652:VAL:HG23	2.14	0.47
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.80	0.47
2:B:606:LYS:NZ	2:B:608:ASP:OD2	2.42	0.47
8:H:58:THR:HB	8:H:143:LEU:HB2	1.97	0.47
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.97	0.47
2:B:1006:ILE:HG23	10:J:45:CYS:HB3	1.97	0.47
4:D:187:THR:HG22	4:D:189:ASP:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:84:ASP:HA	5:E:113:GLN:HE21	1.80	0.47
1:A:515:GLN:HB2	1:A:1071:SER:HB3	1.98	0.46
1:A:1248:LEU:HD12	1:A:1249:ASP:N	2.30	0.46
2:B:46:GLN:HG2	2:B:408:LEU:HD21	1.96	0.46
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.98	0.46
2:B:174:LEU:HD22	2:B:202:TYR:CE2	2.50	0.46
6:F:128:LYS:HD3	6:F:149:GLU:HA	1.97	0.46
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.31	0.46
1:A:1451:VAL:HG22	7:G:20:PRO:HA	1.96	0.46
2:B:34:ILE:HD11	2:B:743:ILE:HG22	1.97	0.46
3:C:138:GLU:OE1	3:C:138:GLU:N	2.43	0.46
1:A:311:GLN:N	1:A:312:PRO:HD2	2.30	0.46
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.48	0.46
3:C:176:ILE:HG23	3:C:232:VAL:HA	1.97	0.46
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.96	0.46
2:B:834:ASN:OD1	2:B:834:ASN:N	2.46	0.46
10:J:10:CYS:SG	10:J:11:GLY:N	2.88	0.46
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.98	0.46
1:A:1166:ASP:O	1:A:1170:ILE:HG13	2.15	0.46
2:B:429:PHE:HA	2:B:432:MET:HE3	1.96	0.46
2:B:475:SER:OG	2:B:476:ARG:O	2.24	0.46
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.15	0.46
3:C:91:HIS:HB2	3:C:96:SER:OG	2.16	0.46
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.97	0.46
1:A:298:PHE:O	1:A:302:THR:HG22	2.16	0.46
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.46	0.46
2:B:199:MET:SD	2:B:199:MET:N	2.77	0.46
2:B:954:VAL:HG22	2:B:964:VAL:HG13	1.98	0.46
5:E:117:THR:HG22	5:E:119:SER:H	1.80	0.46
7:G:93:SER:OG	7:G:100:GLU:OE1	2.33	0.46
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.16	0.46
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.81	0.46
3:C:34:ARG:HA	3:C:37:MET:HE3	1.98	0.46
4:D:68:ARG:O	4:D:72:ARG:HG3	2.16	0.46
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.96	0.46
1:A:565:ILE:HD11	1:A:567:LYS:HE2	1.96	0.46
1:A:1436:ILE:O	1:A:1438:THR:N	2.49	0.46
2:B:332:ASP:O	2:B:348:ARG:HD3	2.16	0.46
2:B:554:ILE:O	2:B:558:LEU:HG	2.16	0.46
4:D:208:GLU:O	4:D:212:LYS:HG3	2.16	0.46
5:E:153:HIS:C	5:E:154:ILE:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:13:SER:OG	8:H:14:GLU:N	2.49	0.46
1:A:1226:VAL:HG13	1:A:1240:CYS:SG	2.55	0.46
2:B:651:LEU:H	2:B:651:LEU:HD12	1.79	0.46
3:C:239:PRO:O	3:C:243:VAL:HG23	2.16	0.46
6:F:87:LYS:HB3	6:F:155:LEU:HD21	1.98	0.46
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.98	0.46
1:A:438:ASP:OD1	1:A:438:ASP:N	2.48	0.46
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.97	0.46
1:A:1441:PHE:CE2	6:F:89:GLU:HG3	2.52	0.46
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.97	0.46
1:A:216:VAL:HA	1:A:219:PHE:CD2	2.51	0.45
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.97	0.45
2:B:1155:SER:OG	2:B:1156:ASP:N	2.48	0.45
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.81	0.45
3:C:26:ASP:HB2	3:C:29:MET:HB2	1.98	0.45
3:C:167:HIS:CD2	12:L:70:ARG:HG3	2.51	0.45
11:K:61:TYR:HB3	11:K:73:LEU:HD13	1.97	0.45
2:B:212:LEU:HD23	2:B:480:SER:H	1.81	0.45
8:H:96:VAL:HA	8:H:142:LEU:O	2.16	0.45
10:J:1:MET:O	10:J:2:ILE:HG22	2.16	0.45
1:A:46:THR:O	1:A:48:ALA:N	2.49	0.45
1:A:250:ILE:HD12	1:A:250:ILE:H	1.81	0.45
1:A:451:HIS:NE2	1:A:453:MET:HE2	2.31	0.45
2:B:655:LYS:HA	2:B:658:ILE:HD12	1.99	0.45
3:C:22:LEU:O	3:C:227:THR:HA	2.16	0.45
2:B:328:GLU:HA	2:B:331:LEU:HD12	1.99	0.45
2:B:770:GLN:HB2	2:B:985:GLY:H	1.81	0.45
4:D:146:GLN:O	4:D:150:ASN:ND2	2.28	0.45
11:K:7:PHE:C	11:K:9:LEU:H	2.24	0.45
1:A:500:GLU:O	1:A:504:LEU:HB2	2.17	0.45
1:A:534:LEU:HA	1:A:539:THR:HG21	1.98	0.45
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.98	0.45
2:B:496:ARG:NH1	2:B:540:SER:O	2.50	0.45
2:B:619:ILE:HD12	9:I:65:ASP:HB2	1.98	0.45
4:D:158:GLU:H	4:D:158:GLU:CD	2.24	0.45
4:D:159:THR:O	4:D:163:VAL:HG23	2.17	0.45
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.98	0.45
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.50	0.45
1:A:449:SER:HB2	2:B:1133:MET:HB3	1.99	0.45
1:A:466:SER:HB3	2:B:1103:ILE:HD12	1.99	0.45
1:A:855:THR:CG2	1:A:857:ARG:HE	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.97	0.45
5:E:1:MET:HB2	5:E:3:GLN:N	2.32	0.45
5:E:19:VAL:O	5:E:23:VAL:HG23	2.16	0.45
1:A:607:ILE:HG13	1:A:612:ILE:HA	1.98	0.45
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.98	0.45
1:A:1418:LEU:HD12	1:A:1419:ASP:H	1.82	0.45
2:B:343:ILE:O	2:B:345:LYS:N	2.49	0.45
2:B:726:ALA:HB1	2:B:1051:THR:HB	1.98	0.45
2:B:1180:PHE:H	2:B:1188:LYS:HE3	1.80	0.45
7:G:62:LEU:HA	7:G:63:PRO:HD3	1.82	0.45
1:A:720:ARG:O	1:A:724:GLU:HG3	2.17	0.45
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.99	0.45
1:A:814:PHE:O	1:A:818:MET:HG3	2.17	0.45
1:A:1308:THR:OG1	1:A:1309:ASP:N	2.49	0.45
2:B:338:GLY:HA3	2:B:347:LYS:HD3	1.99	0.45
2:B:523:CYS:HB2	2:B:750:GLY:HA3	1.98	0.45
2:B:788:ARG:NH1	2:B:790:ASP:OD2	2.50	0.45
2:B:806:THR:HB	2:B:809:MET:HG3	1.99	0.45
2:B:827:ILE:HG23	2:B:1012:ILE:HG13	1.99	0.45
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.99	0.45
10:J:17:LYS:HB3	10:J:39:LEU:HD22	1.99	0.45
10:J:46:CYS:HA	10:J:49:MET:HE2	1.99	0.45
12:L:55:ILE:HG13	12:L:56:LEU:H	1.82	0.45
1:A:926:GLN:NE2	1:A:930:ASP:OD1	2.49	0.45
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.99	0.45
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.99	0.45
2:B:1187:ASN:O	2:B:1191:ILE:HD11	2.17	0.45
1:A:1288:ASP:HA	1:A:1302:PRO:HA	1.99	0.44
2:B:27:ALA:O	2:B:30:SER:OG	2.36	0.44
4:D:67:ARG:HA	4:D:133:THR:HG21	1.99	0.44
8:H:127:GLY:HA3	8:H:130:ARG:NH1	2.32	0.44
1:A:67:CYS:HB2	1:A:71:GLN:N	2.32	0.44
1:A:773:LYS:H	1:A:773:LYS:HD2	1.82	0.44
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.14	0.44
1:A:1177:LEU:HB2	1:A:1181:ALA:HA	1.98	0.44
2:B:542:MET:HG3	2:B:747:MET:HB3	2.00	0.44
2:B:901:PRO:HD2	12:L:59:ALA:O	2.17	0.44
3:C:22:LEU:HB3	3:C:25:VAL:HG21	1.99	0.44
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.99	0.44
4:D:206:GLU:HG2	4:D:209:ARG:HD2	1.98	0.44
6:F:79:ARG:HH22	6:F:150:GLU:CD	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:129:SER:HB3	7:G:138:THR:HG23	1.98	0.44
1:A:31:SER:HB2	1:A:83:HIS:HB3	2.00	0.44
1:A:438:ASP:OD2	1:A:461:LYS:HD2	2.17	0.44
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.83	0.44
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.99	0.44
2:B:475:SER:N	2:B:476:ARG:HA	2.17	0.44
2:B:756:ILE:CG2	2:B:983:ARG:HB3	2.46	0.44
2:B:1171:VAL:HG11	2:B:1191:ILE:HG21	1.99	0.44
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.98	0.44
11:K:107:THR:O	11:K:111:LEU:HG	2.17	0.44
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.98	0.44
1:A:951:GLU:O	1:A:954:TRP:NE1	2.49	0.44
2:B:25:ILE:HG13	2:B:658:ILE:HD11	1.99	0.44
2:B:294:ASP:OD1	9:I:12:ASN:ND2	2.42	0.44
2:B:413:LEU:O	2:B:417:PHE:HB2	2.17	0.44
2:B:605:ARG:HB3	2:B:688:GLY:HA2	2.00	0.44
2:B:694:ASP:O	2:B:698:GLU:HB2	2.18	0.44
8:H:98:TYR:OH	8:H:138:GLU:OE1	2.35	0.44
9:I:90:GLN:C	9:I:92:ARG:H	2.25	0.44
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.47	0.44
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.00	0.44
1:A:549:MET:CE	1:A:577:ILE:HD13	2.48	0.44
1:A:584:ASN:O	1:A:637:LYS:NZ	2.41	0.44
1:A:1349:TYR:HE2	1:A:1368:MET:HE3	1.82	0.44
2:B:386:LEU:O	2:B:390:LEU:HG	2.17	0.44
2:B:494:HIS:O	2:B:494:HIS:ND1	2.51	0.44
2:B:870:ILE:HG22	2:B:917:PRO:HG2	2.00	0.44
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.43	0.44
1:A:1235:LYS:HD3	1:A:1237:ILE:HD11	2.00	0.44
2:B:445:LYS:H	2:B:446:LEU:CA	2.31	0.44
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.52	0.44
4:D:56:ARG:NH1	4:D:122:GLU:OE1	2.50	0.44
7:G:65:ASP:O	7:G:67:SER:N	2.51	0.44
2:B:216:GLU:OE1	2:B:500:THR:OG1	2.33	0.44
2:B:247:GLY:C	2:B:249:ARG:H	2.26	0.44
2:B:259:TYR:HB2	2:B:268:THR:HG23	2.00	0.44
2:B:506:GLY:C	2:B:508:LEU:H	2.26	0.44
7:G:151:ILE:HD11	7:G:160:ILE:HD11	2.00	0.44
1:A:752:LYS:HB2	2:B:1015:HIS:HD2	1.83	0.44
1:A:1158:PRO:HG3	1:A:1188:GLN:HE22	1.82	0.44
2:B:309:GLN:OE1	2:B:392:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:GLU:HB2	2:B:470:LYS:HG3	1.99	0.44
2:B:1079:LYS:HE3	3:C:188:HIS:NE2	2.32	0.44
3:C:86:CYS:SG	3:C:87:PHE:N	2.91	0.44
10:J:2:ILE:HD12	10:J:2:ILE:HA	1.85	0.44
1:A:825:ILE:O	1:A:829:VAL:HG23	2.18	0.44
1:A:1325:THR:HG23	5:E:147:HIS:HA	1.99	0.44
3:C:66:ARG:HH21	10:J:4:PRO:HA	1.82	0.44
9:I:6:PHE:HA	9:I:14:LEU:HG	1.99	0.44
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.48	0.43
2:B:809:MET:HA	2:B:812:LEU:HD12	2.00	0.43
2:B:1201:LYS:O	2:B:1205:GLN:HG3	2.18	0.43
4:D:63:LEU:HD13	4:D:66:ARG:HD2	2.00	0.43
1:A:18:GLN:O	2:B:1215:ARG:N	2.43	0.43
1:A:71:GLN:CD	1:A:72:GLU:H	2.22	0.43
1:A:308:ILE:HG22	1:A:310:GLY:H	1.83	0.43
1:A:696:GLU:HG2	1:A:702:LEU:HG	1.99	0.43
1:A:1248:LEU:HD12	1:A:1249:ASP:H	1.83	0.43
1:A:1422:ARG:NH2	2:B:1224:PHE:O	2.51	0.43
4:D:54:GLU:O	4:D:58:VAL:HG23	2.19	0.43
7:G:1:MET:HE1	7:G:80:LYS:H	1.82	0.43
1:A:676:MET:HE3	1:A:676:MET:HB3	1.93	0.43
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.52	0.43
2:B:112:LEU:HD12	2:B:113:TYR:H	1.84	0.43
2:B:480:SER:O	2:B:480:SER:OG	2.32	0.43
4:D:152:SER:HG	4:D:221:TYR:HH	1.56	0.43
5:E:22:MET:HE3	5:E:26:ARG:HE	1.82	0.43
7:G:23:LYS:HE3	7:G:56:ILE:HD13	2.01	0.43
1:A:306:ASN:ND2	1:A:322:VAL:HB	2.34	0.43
1:A:534:LEU:HD23	1:A:578:LEU:HD22	2.00	0.43
1:A:1175:SER:HA	1:A:1176:LEU:HA	1.49	0.43
2:B:756:ILE:HG21	2:B:770:GLN:CG	2.48	0.43
2:B:850:LEU:HG	2:B:851:PHE:HD2	1.83	0.43
3:C:73:GLN:OE1	3:C:74:SER:N	2.51	0.43
6:F:114:GLU:OE2	6:F:119:ARG:HD3	2.19	0.43
1:A:472:LEU:C	1:A:474:VAL:H	2.25	0.43
1:A:523:ILE:HG23	1:A:527:THR:HB	1.99	0.43
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.48	0.43
1:A:883:LEU:HD12	1:A:883:LEU:H	1.83	0.43
2:B:755:ILE:CD1	2:B:812:LEU:HD13	2.49	0.43
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.48	0.43
2:B:999:MET:HG3	2:B:1008:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASP:O	1:A:460:VAL:HG23	2.19	0.43
1:A:932:GLU:CD	1:A:1028:THR:HG1	2.24	0.43
2:B:744:HIS:CE1	2:B:746:SER:HG	2.33	0.43
3:C:244:VAL:O	3:C:248:ILE:HG13	2.19	0.43
1:A:931:GLU:OE2	1:A:991:LYS:NZ	2.49	0.43
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	2.01	0.43
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.01	0.43
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.43
2:B:936:ASP:OD2	2:B:937:ALA:N	2.52	0.43
4:D:60:LYS:O	4:D:64:VAL:HG23	2.18	0.43
5:E:125:PRO:HB3	5:E:132:ILE:HB	2.00	0.43
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.84	0.43
1:A:1140:HIS:CE1	1:A:1272:THR:HG23	2.54	0.43
2:B:794:ASN:C	2:B:795:ILE:HD12	2.44	0.43
2:B:918:ILE:HB	2:B:935:ARG:HG3	2.00	0.43
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.52	0.43
3:C:46:ILE:HD12	3:C:72:LEU:HD11	1.99	0.43
4:D:129:LEU:O	4:D:133:THR:OG1	2.37	0.43
2:B:333:PHE:O	2:B:335:GLY:N	2.49	0.43
2:B:363:HIS:O	2:B:365:THR:N	2.52	0.43
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.19	0.43
7:G:6:ASP:OD1	7:G:6:ASP:N	2.52	0.43
1:A:308:ILE:HD12	1:A:308:ILE:H	1.83	0.42
1:A:683:ILE:HG21	1:A:801:GLU:HG3	2.00	0.42
1:A:900:ASP:HB3	1:A:906:HIS:HB3	2.00	0.42
2:B:454:THR:O	2:B:458:LYS:HB2	2.19	0.42
2:B:551:PRO:O	2:B:555:ILE:HG13	2.19	0.42
2:B:861:ASP:OD1	2:B:862:GLN:N	2.52	0.42
3:C:18:VAL:HG12	3:C:20:PHE:CD1	2.55	0.42
3:C:42:PRO:HA	3:C:163:ILE:HG22	2.01	0.42
4:D:53:SER:O	4:D:57:LEU:HG	2.19	0.42
4:D:119:ARG:HD3	4:D:221:TYR:HD2	1.84	0.42
9:I:78:CYS:SG	9:I:80:SER:OG	2.77	0.42
9:I:103:CYS:SG	9:I:105:SER:N	2.85	0.42
1:A:605:MET:HE2	1:A:607:ILE:HD11	2.00	0.42
1:A:1188:GLN:HA	1:A:1243:VAL:HA	2.00	0.42
2:B:535:LEU:HD23	2:B:535:LEU:HA	1.87	0.42
2:B:645:SER:O	2:B:647:GLY:N	2.49	0.42
7:G:18:PHE:HA	7:G:22:MET:HE3	2.01	0.42
1:A:345:VAL:HA	2:B:1155:SER:HB2	2.00	0.42
1:A:445:ASN:HB2	1:A:454:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:816:GLU:HB3	2:B:817:LEU:HD12	2.00	0.42
3:C:51:VAL:HB	12:L:65:VAL:HG23	1.99	0.42
7:G:106:MET:HE2	7:G:106:MET:HB3	1.74	0.42
1:A:1076:ALA:HA	1:A:1079:MET:HE2	2.02	0.42
2:B:830:TYR:HB3	2:B:831:SER:H	1.55	0.42
2:B:1000:PRO:HB2	2:B:1072:MET:HE3	2.00	0.42
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.59	0.42
1:A:70:CYS:O	1:A:72:GLU:HG2	2.20	0.42
1:A:412:ARG:HH22	2:B:1108:ARG:NH1	2.17	0.42
1:A:719:VAL:HA	1:A:722:LEU:HD12	2.01	0.42
1:A:873:MET:HE3	1:A:957:PRO:HG3	2.01	0.42
3:C:33:LEU:HG	3:C:37:MET:HE2	2.01	0.42
3:C:56:THR:HG22	3:C:57:VAL:H	1.85	0.42
3:C:251:LEU:O	3:C:255:VAL:HG23	2.18	0.42
4:D:115:HIS:HB3	4:D:116:SER:H	1.55	0.42
5:E:14:ARG:O	5:E:18:THR:OG1	2.36	0.42
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.54	0.42
1:A:606:LEU:HG	1:A:613:ILE:HD13	2.02	0.42
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.83	0.42
1:A:1317:MET:HB2	1:A:1317:MET:HE3	1.77	0.42
2:B:637:LEU:HD12	2:B:693:ILE:HD13	2.00	0.42
2:B:644:GLU:HG2	2:B:654:ARG:HH22	1.83	0.42
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.20	0.42
5:E:55:ARG:O	5:E:82:PHE:HB2	2.19	0.42
8:H:8:ASP:HB3	8:H:10:PHE:HE1	1.83	0.42
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.45	0.42
1:A:34:LYS:HE2	1:A:34:LYS:HB2	1.83	0.42
1:A:74:MET:HB2	1:A:74:MET:HE3	1.71	0.42
1:A:132:LYS:NZ	1:A:1411:GLU:HB3	2.35	0.42
1:A:583:PRO:O	1:A:610:GLY:HA3	2.20	0.42
1:A:1036:ARG:H	1:A:1036:ARG:HG2	1.71	0.42
2:B:756:ILE:N	2:B:757:PRO:CD	2.83	0.42
2:B:760:ASP:OD1	2:B:760:ASP:N	2.53	0.42
3:C:34:ARG:O	3:C:38:ILE:HG13	2.19	0.42
5:E:20:LYS:HB3	5:E:35:VAL:HG22	2.01	0.42
6:F:138:LEU:HD23	6:F:138:LEU:HA	1.82	0.42
1:A:22:PHE:CD2	2:B:1213:THR:HG22	2.55	0.42
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.35	0.42
1:A:344:ARG:NE	2:B:1120:GLU:HB2	2.35	0.42
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.19	0.42
8:H:63:LEU:HB3	8:H:90:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:118:PHE:HB2	8:H:121:LEU:HB2	2.01	0.42
9:I:73:ARG:O	9:I:81:ARG:HA	2.20	0.42
1:A:565:ILE:HG22	1:A:571:LEU:H	1.85	0.42
1:A:658:LEU:HD12	2:B:830:TYR:O	2.19	0.42
1:A:873:MET:C	1:A:1058:VAL:HG13	2.44	0.42
2:B:61:ASP:OD1	2:B:61:ASP:N	2.53	0.42
2:B:193:LYS:NZ	12:L:32:ALA:O	2.37	0.42
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.55	0.42
3:C:56:THR:HA	3:C:151:GLN:NE2	2.35	0.42
3:C:110:THR:HA	3:C:147:LEU:O	2.20	0.42
8:H:89:LEU:C	8:H:91:ASP:H	2.24	0.42
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.54	0.42
1:A:146:MET:O	1:A:171:GLN:N	2.45	0.41
1:A:472:LEU:O	1:A:475:THR:HG22	2.19	0.41
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.35	0.41
3:C:62:PHE:CE1	3:C:66:ARG:HD2	2.54	0.41
4:D:207:LEU:O	4:D:211:LEU:HG	2.20	0.41
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.86	0.41
1:A:383:TYR:HB3	6:F:115:THR:HA	2.02	0.41
1:A:678:GLU:O	1:A:681:GLU:HG2	2.20	0.41
1:A:768:GLN:HG3	1:A:816:HIS:HA	2.02	0.41
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.49	0.41
2:B:797:TYR:CE1	2:B:854:LEU:HG	2.55	0.41
3:C:5:GLY:O	3:C:7:GLN:N	2.53	0.41
4:D:138:ASN:CG	4:D:141:LEU:HB2	2.44	0.41
10:J:32:GLU:H	10:J:32:GLU:CD	2.27	0.41
1:A:41:MET:HE1	1:A:257:ARG:HG2	2.02	0.41
1:A:540:PHE:HB3	1:A:571:LEU:HD23	2.01	0.41
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.21	0.41
2:B:424:LEU:O	2:B:428:ILE:HG13	2.19	0.41
2:B:1106:ARG:NH2	2:B:1118:PRO:HB3	2.36	0.41
3:C:98:VAL:HG23	3:C:122:SER:HB3	2.01	0.41
7:G:43:GLY:HA3	7:G:80:LYS:HB3	2.02	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.95	0.41
9:I:14:LEU:HA	9:I:28:GLU:O	2.20	0.41
9:I:74:GLU:HB2	9:I:79:HIS:HA	2.02	0.41
10:J:48:ARG:O	10:J:52:THR:HB	2.20	0.41
2:B:213:ILE:HD11	2:B:494:HIS:CE1	2.55	0.41
2:B:576:ASP:OD1	2:B:622:LYS:NZ	2.54	0.41
1:A:107:CYS:HB2	1:A:171:GLN:OE1	2.20	0.41
1:A:1444:MET:O	6:F:133:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:741:CYS:SG	2:B:742:GLU:N	2.94	0.41
2:B:959:ASP:OD1	2:B:959:ASP:N	2.54	0.41
5:E:95:THR:O	5:E:99:HIS:HB3	2.20	0.41
5:E:112:TYR:O	5:E:137:GLU:HB2	2.20	0.41
6:F:97:ARG:NH2	6:F:106:PRO:O	2.53	0.41
12:L:32:ALA:HB3	12:L:55:ILE:HD12	2.03	0.41
1:A:549:MET:HE3	1:A:577:ILE:HD13	2.01	0.41
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.20	0.41
4:D:52:LEU:C	4:D:53:SER:HG	2.25	0.41
1:A:1211:GLN:H	1:A:1211:GLN:HG3	1.59	0.41
2:B:648:HIS:CG	2:B:649:LYS:H	2.39	0.41
2:B:758:PHE:CZ	2:B:1044:ALA:HB1	2.56	0.41
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.50	0.41
10:J:5:VAL:HG12	10:J:6:ARG:HG3	2.01	0.41
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.21	0.41
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.56	0.41
1:A:107:CYS:N	1:A:114:LEU:HD21	2.34	0.41
1:A:306:ASN:HD22	1:A:322:VAL:HB	1.86	0.41
1:A:770:VAL:HG12	1:A:771:GLU:HG3	2.03	0.41
1:A:1015:VAL:HB	1:A:1016:THR:H	1.75	0.41
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	2.03	0.41
2:B:33:VAL:HG12	2:B:681:TRP:HZ3	1.86	0.41
2:B:44:VAL:HG23	2:B:48:LEU:HD11	2.03	0.41
2:B:308:TRP:CH2	9:I:45:ARG:HD3	2.55	0.41
2:B:498:THR:O	2:B:536:VAL:HA	2.21	0.41
2:B:499:ASN:OD1	2:B:500:THR:N	2.54	0.41
2:B:898:LEU:HB2	12:L:58:LYS:HZ2	1.83	0.41
2:B:906:SER:OG	2:B:907:GLY:N	2.54	0.41
2:B:975:GLN:O	2:B:990:ILE:HD12	2.21	0.41
2:B:1165:ILE:H	2:B:1165:ILE:HD12	1.85	0.41
4:D:3:VAL:HB	4:D:4:SER:H	1.66	0.41
8:H:89:LEU:O	8:H:91:ASP:N	2.45	0.41
10:J:45:CYS:SG	10:J:46:CYS:N	2.94	0.41
11:K:77:THR:OG1	11:K:81:TYR:O	2.32	0.41
11:K:94:ILE:O	11:K:98:LEU:HG	2.21	0.41
1:A:68:GLN:C	1:A:70:CYS:H	2.29	0.41
1:A:147:VAL:HG22	1:A:170:THR:HA	2.02	0.41
1:A:405:VAL:O	1:A:413:ILE:HB	2.21	0.41
1:A:517:ASN:O	1:A:517:ASN:ND2	2.53	0.41
1:A:1116:LEU:HG	1:A:1308:THR:CG2	2.51	0.41
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HB3	7:G:58:ARG:HB3	2.03	0.41
5:E:171:LYS:HA	5:E:171:LYS:HD3	1.90	0.41
1:A:471:ASN:OD1	1:A:472:LEU:N	2.54	0.40
1:A:649:ILE:O	1:A:653:VAL:HG23	2.21	0.40
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.21	0.40
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.86	0.40
8:H:25:ARG:C	8:H:26:ILE:HD12	2.46	0.40
1:A:205:GLU:O	1:A:209:ASN:HB2	2.21	0.40
1:A:855:THR:HG21	1:A:857:ARG:NE	2.33	0.40
2:B:446:LEU:HD12	2:B:448:ILE:HD13	2.04	0.40
4:D:67:ARG:O	4:D:71:LYS:HG3	2.21	0.40
6:F:89:GLU:HG2	6:F:134:ILE:HD13	2.02	0.40
1:A:443:LEU:CD1	1:A:455:MET:HE2	2.51	0.40
2:B:108:VAL:HB	2:B:109:THR:H	1.71	0.40
2:B:209:GLU:OE1	2:B:485:ARG:NH2	2.51	0.40
2:B:542:MET:CG	2:B:747:MET:HB3	2.50	0.40
2:B:854:LEU:HB3	2:B:856:PHE:CE1	2.57	0.40
2:B:1173:ALA:HB1	2:B:1175:LEU:HD21	2.04	0.40
5:E:78:LEU:HA	5:E:107:THR:HB	2.03	0.40
8:H:97:MET:HE3	8:H:142:LEU:HD23	2.03	0.40
11:K:29:ASN:ND2	11:K:77:THR:O	2.54	0.40
1:A:216:VAL:HA	1:A:219:PHE:HD2	1.85	0.40
1:A:765:VAL:HB	1:A:800:VAL:HB	2.02	0.40
1:A:1247:SER:H	1:A:1248:LEU:HA	1.86	0.40
2:B:299:GLU:OE2	2:B:571:PRO:HD2	2.22	0.40
2:B:313:MET:O	2:B:316:PRO:HD2	2.22	0.40
2:B:423:LYS:O	2:B:426:LYS:HG2	2.22	0.40
2:B:764:SER:N	2:B:765:PRO:HD2	2.37	0.40
2:B:866:TYR:HD2	2:B:870:ILE:HB	1.85	0.40
3:C:73:GLN:HA	3:C:133:ILE:HD11	2.03	0.40
3:C:146:LYS:HB2	10:J:57:ILE:HD11	2.02	0.40
1:A:70:CYS:C	1:A:71:GLN:HG3	2.46	0.40
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.57	0.40
1:A:109:HIS:CE1	1:A:169:ASN:HB2	2.56	0.40
1:A:1116:LEU:HD23	1:A:1311:VAL:HA	2.02	0.40
2:B:1147:LEU:HD23	2:B:1147:LEU:HA	1.80	0.40
3:C:49:VAL:HG21	3:C:67:LEU:HD12	2.04	0.40
4:D:121:LYS:H	4:D:121:LYS:HG2	1.67	0.40
4:D:148:LEU:O	4:D:152:SER:HB3	2.21	0.40
4:D:167:LEU:HB2	4:D:177:VAL:HG13	2.03	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	1428/1733 (82%)	1222 (86%)	149 (10%)	57 (4%)	2 20
2	B	1142/1224 (93%)	943 (83%)	155 (14%)	44 (4%)	2 20
3	C	264/318 (83%)	221 (84%)	35 (13%)	8 (3%)	3 25
4	D	180/221 (81%)	155 (86%)	19 (11%)	6 (3%)	3 24
5	E	213/215 (99%)	188 (88%)	21 (10%)	4 (2%)	6 32
6	F	85/155 (55%)	77 (91%)	7 (8%)	1 (1%)	10 40
7	G	169/171 (99%)	156 (92%)	11 (6%)	2 (1%)	10 40
8	H	133/146 (91%)	103 (77%)	22 (16%)	8 (6%)	1 14
9	I	117/122 (96%)	98 (84%)	15 (13%)	4 (3%)	3 23
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2 17
11	K	113/120 (94%)	105 (93%)	8 (7%)	0	100 100
12	L	44/70 (63%)	25 (57%)	14 (32%)	5 (11%)	0 5
All	All	3951/4565 (86%)	3344 (85%)	465 (12%)	142 (4%)	2 22

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	54	ASN
1	A	1114	PRO
1	A	1416	ALA
1	A	1437	GLY
2	B	124	TYR
2	B	367	LEU
2	B	531	GLN
2	B	670	GLU
2	B	712	PRO
2	B	1046	PRO
3	C	161	LYS

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Mol	Chain	Res	Type
4	D	117	GLU
8	H	17	PRO
8	H	82	PRO
9	I	3	THR
10	J	2	ILE
1	A	40	THR
1	A	43	GLU
1	A	58	LEU
1	A	109	HIS
1	A	156	ASP
1	A	317	LYS
1	A	543	LEU
1	A	775	ILE
1	A	997	LEU
1	A	1016	THR
1	A	1245	PRO
1	A	1339	LEU
2	B	176	SER
2	B	260	GLY
2	B	438	GLU
2	B	478	GLY
2	B	648	HIS
2	B	716	ASN
2	B	805	THR
2	B	1156	ASP
4	D	35	LEU
4	D	155	ARG
4	D	217	LEU
5	E	122	LYS
8	H	89	LEU
8	H	119	GLY
8	H	131	ASN
8	H	139	ASN
1	A	5	GLN
1	A	48	ALA
1	A	66	LYS
1	A	154	SER
1	A	167	CYS
1	A	196	GLU
1	A	314	ALA
1	A	332	LYS
1	A	423	ASP

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Mol	Chain	Res	Type
1	A	568	PRO
1	A	765	VAL
1	A	920	LEU
1	A	1249	ASP
1	A	1250	ALA
1	A	1331	SER
1	A	1377	THR
1	A	1405	THR
2	B	262	GLU
2	B	344	LYS
2	B	675	ASP
2	B	711	GLU
2	B	881	ASN
2	B	1165	ILE
2	B	1223	ASP
3	C	5	GLY
3	C	128	ASN
3	C	175	ALA
3	C	184	ASN
7	G	66	GLY
7	G	154	VAL
8	H	128	ASN
9	I	9	ASP
10	J	64	ASN
12	L	55	ILE
1	A	42	ASP
1	A	52	GLY
1	A	76	GLU
1	A	258	GLY
1	A	473	SER
1	A	591	PHE
1	A	609	ASP
1	A	1255	GLU
2	B	334	ILE
2	B	475	SER
2	B	673	PHE
2	B	749	LEU
2	B	757	PRO
2	B	792	MET
2	B	880	THR
2	B	1096	ARG
3	C	110	THR

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Mol	Chain	Res	Type
4	D	198	LEU
9	I	90	GLN
12	L	50	ASP
1	A	35	ILE
1	A	57	ARG
1	A	65	LEU
1	A	71	GLN
1	A	108	MET
1	A	322	VAL
1	A	424	ILE
1	A	871	ASP
1	A	958	VAL
1	A	1093	LYS
1	A	1183	GLN
2	B	108	VAL
2	B	305	VAL
2	B	713	ALA
2	B	1017	ILE
2	B	1108	ARG
2	B	1157	ALA
2	B	1181	GLU
3	C	227	THR
4	D	36	LYS
5	E	73	PRO
5	E	106	GLN
8	H	90	ALA
9	I	91	ARG
10	J	62	ARG
12	L	53	HIS
1	A	1435	PRO
2	B	472	ALA
2	B	960	GLY
5	E	3	GLN
6	F	154	ASP
12	L	56	LEU
2	B	511	PRO
2	B	575	PRO
3	C	142	VAL
1	A	610	GLY
2	B	167	ILE
12	L	52	GLY
2	B	349	ILE

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Mol	Chain	Res	Type
2	B	503	GLY
1	A	1015	VAL
1	A	1107	VAL
2	B	1214	PRO

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	1255/1520 (83%)	1255 (100%)	0	100	100
2	B	995/1061 (94%)	995 (100%)	0	100	100
3	C	234/274 (85%)	234 (100%)	0	100	100
4	D	147/200 (74%)	147 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	121/128 (94%)	121 (100%)	0	100	100
9	I	113/116 (97%)	113 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3490/4009 (87%)	3490 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	458	HIS
1	A	545	GLN
1	A	548	ASN

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Mol	Chain	Res	Type
1	A	736	ASN
1	A	975	HIS
1	A	1008	GLN
1	A	1009	ASN
1	A	1110	ASN
1	A	1140	HIS
1	A	1312	ASN
2	B	121	ASN
2	B	449	ASN
2	B	686	ASN
2	B	734	HIS
2	B	770	GLN
2	B	794	ASN
2	B	958	GLN
3	C	17	ASN
3	C	31	ASN
3	C	79	GLN
3	C	151	GLN
4	D	41	GLN
4	D	115	HIS
4	D	165	GLN
5	E	54	GLN
5	E	114	ASN
5	E	115	ASN
8	H	83	GLN
9	I	12	ASN
9	I	89	GLN
11	K	44	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1429/1733 (82%)	-0.58	0 100 100	57, 151, 244, 348	0
2	B	1144/1224 (93%)	-0.45	6 (0%) 87 71	78, 157, 266, 369	0
3	C	266/318 (83%)	-0.70	0 100 100	83, 158, 209, 278	0
4	D	184/221 (83%)	-0.54	0 100 100	135, 220, 290, 320	0
5	E	215/215 (100%)	-0.67	0 100 100	102, 201, 277, 336	0
6	F	87/155 (56%)	-0.71	0 100 100	71, 124, 184, 213	0
7	G	171/171 (100%)	-0.63	0 100 100	121, 185, 244, 270	0
8	H	137/146 (93%)	-0.51	2 (1%) 72 50	140, 201, 276, 327	0
9	I	119/122 (97%)	-0.65	0 100 100	121, 172, 245, 277	0
10	J	65/70 (92%)	-0.65	0 100 100	110, 154, 200, 238	0
11	K	115/120 (95%)	-0.75	0 100 100	85, 141, 206, 267	0
12	L	46/70 (65%)	-0.27	0 100 100	123, 198, 252, 288	0
All	All	3978/4565 (87%)	-0.56	8 (0%) 91 81	57, 161, 260, 369	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	758	PHE	3.4
2	B	757	PRO	3.2
2	B	819	ALA	2.9
2	B	441	ASP	2.9
8	H	120	GLY	2.7
2	B	1046	PRO	2.5
8	H	136	LYS	2.1
2	B	92	PHE	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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	ZN	A	1801	1/1	0.98	0.02	233,233,233,233	0
14	MG	A	1803	1/1	0.98	0.07	67,67,67,67	0
13	ZN	L	101	1/1	0.99	0.03	135,135,135,135	0
13	ZN	I	202	1/1	0.99	0.03	193,193,193,193	0
13	ZN	I	201	1/1	1.00	0.01	100,100,100,100	0
13	ZN	A	1802	1/1	1.00	0.02	107,107,107,107	0
13	ZN	J	101	1/1	1.00	0.03	131,131,131,131	0
13	ZN	B	1301	1/1	1.00	0.02	122,122,122,122	0
13	ZN	C	401	1/1	1.00	0.08	171,171,171,171	0

6.5 Other polymers (i)

There are no such residues in this entry.