Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:23 am BST

PDB ID	:	5U5Q
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 ⓘ symbol.

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

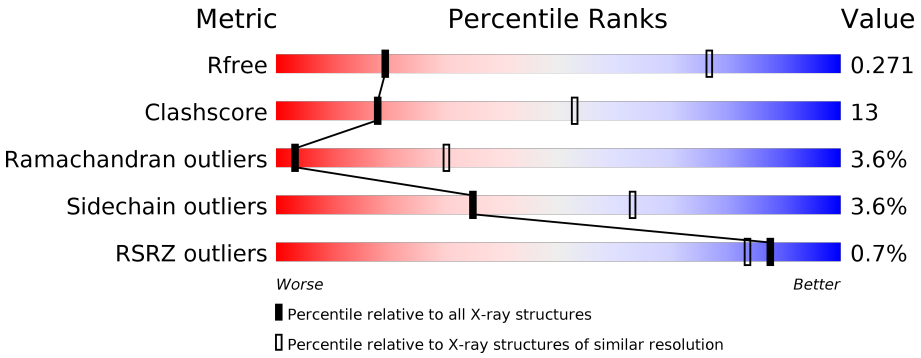
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	53% 27% • 17%
2	B	1224	% 59% 31% • 6%
3	C	318	53% 28% • 16%
4	D	221	52% 31% • 17%
5	E	215	72% 27%
6	F	155	35% 20% • 44%

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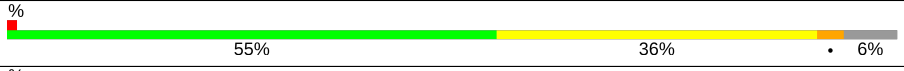
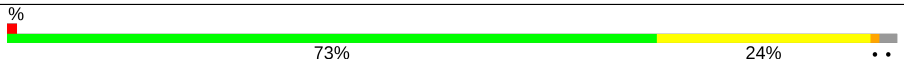
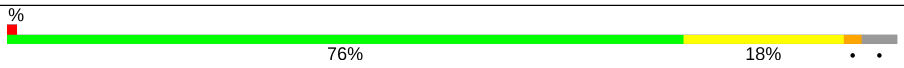
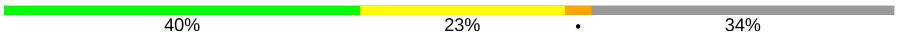
Mol	Chain	Length	Quality of chain
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

2 Entry composition

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
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

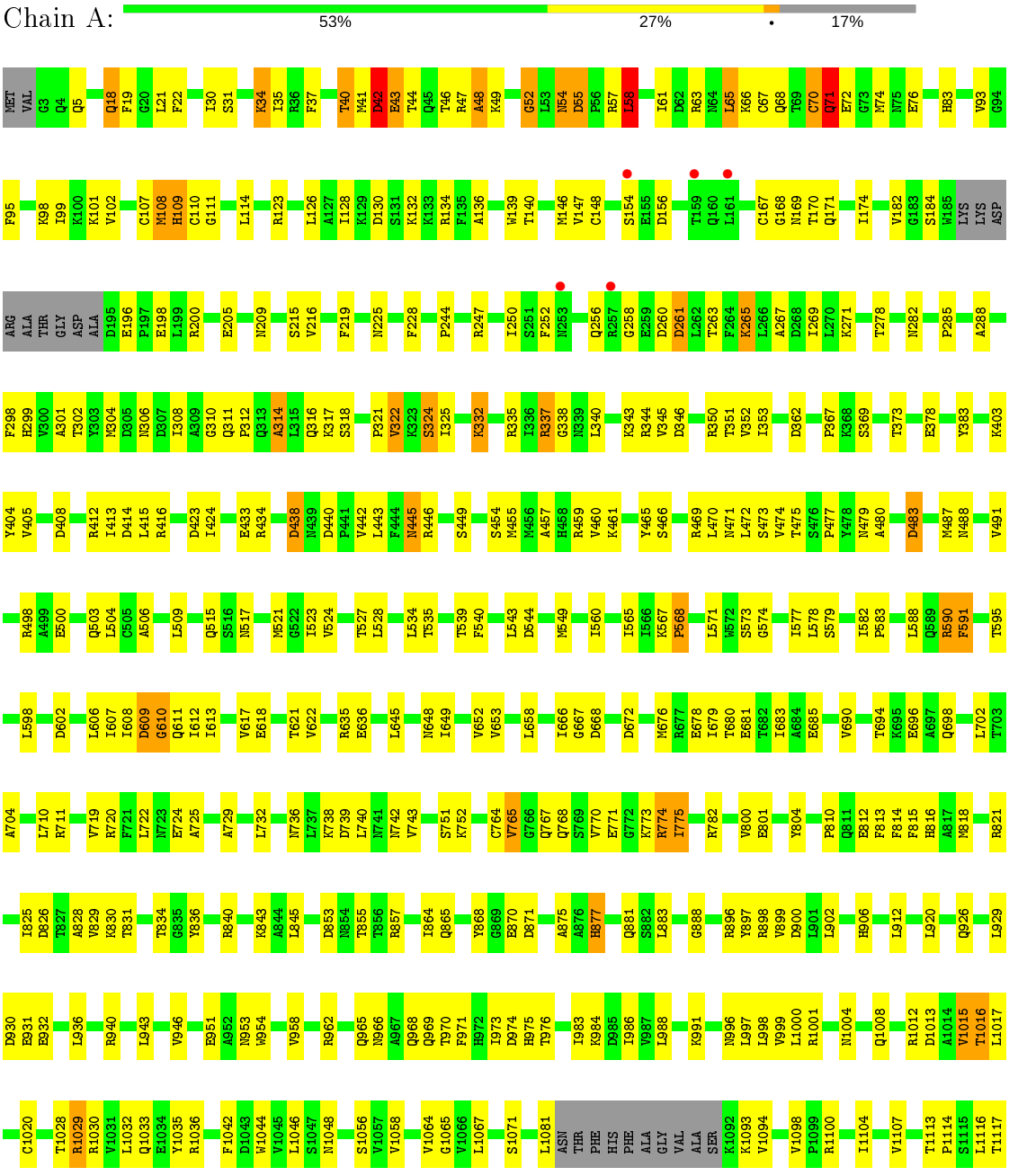
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0

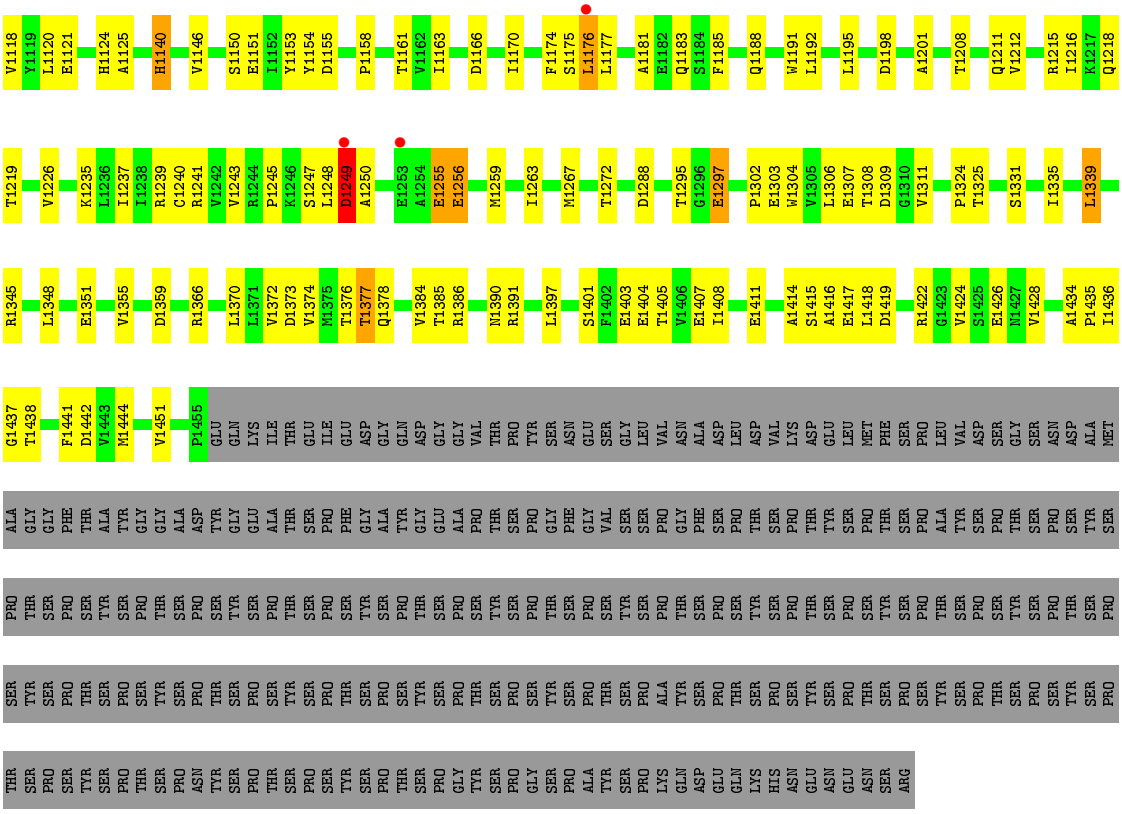
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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

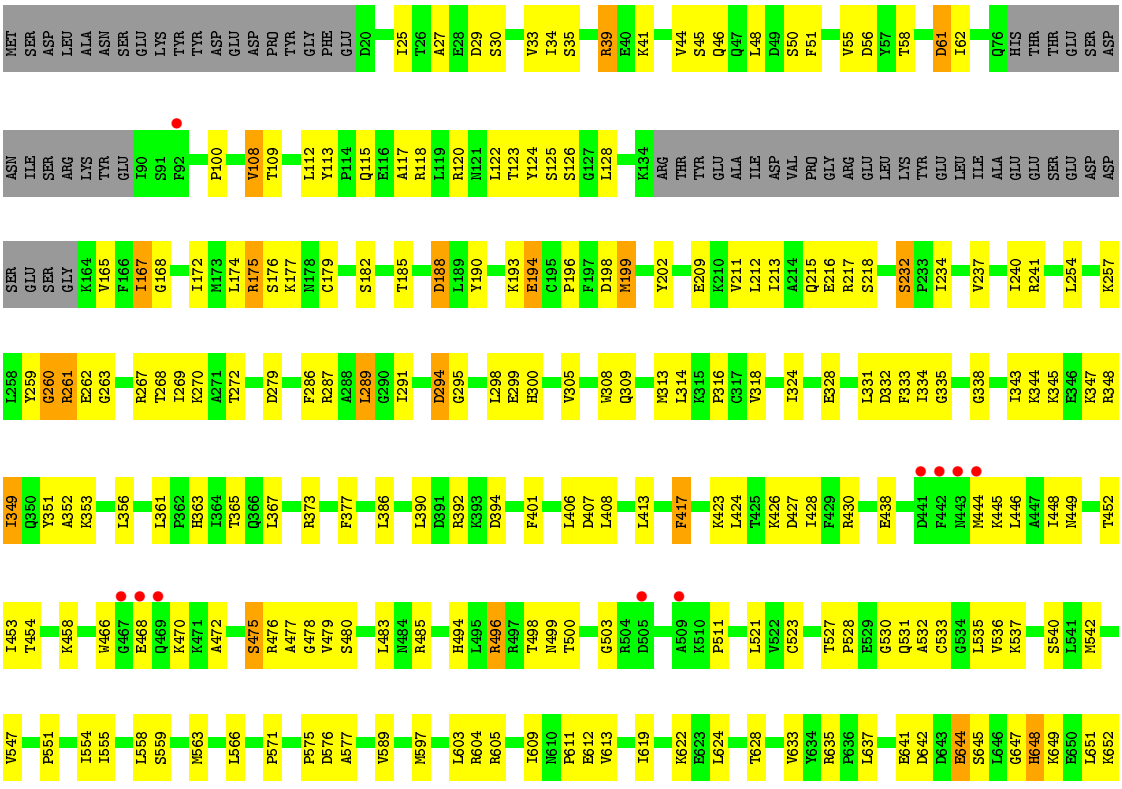
Chain A:

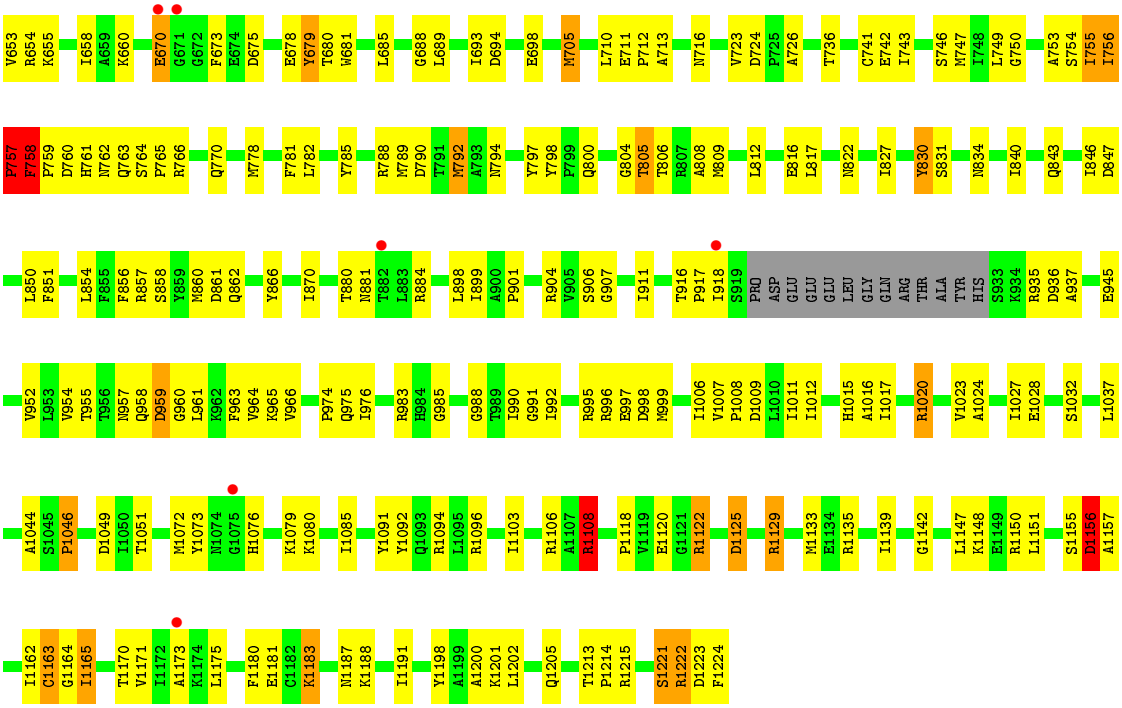




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

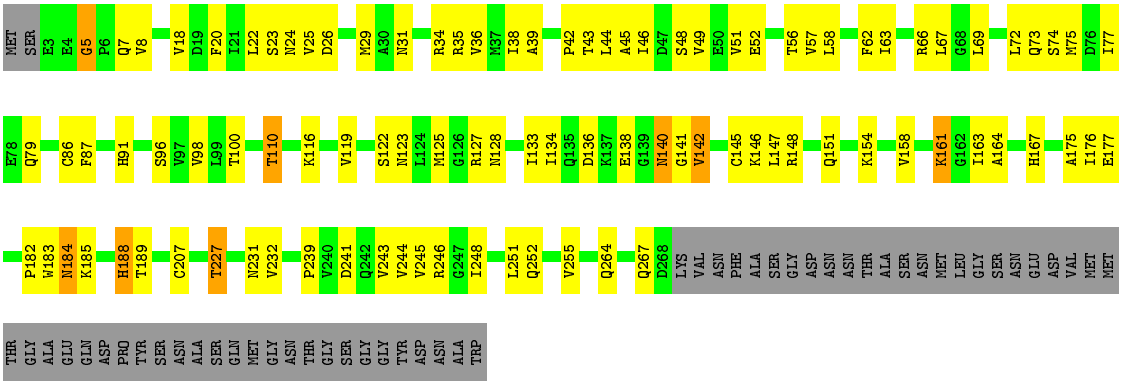
Chain B:





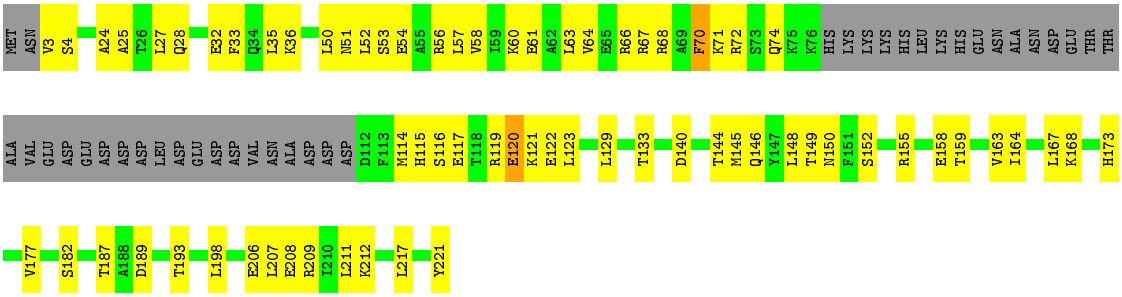
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



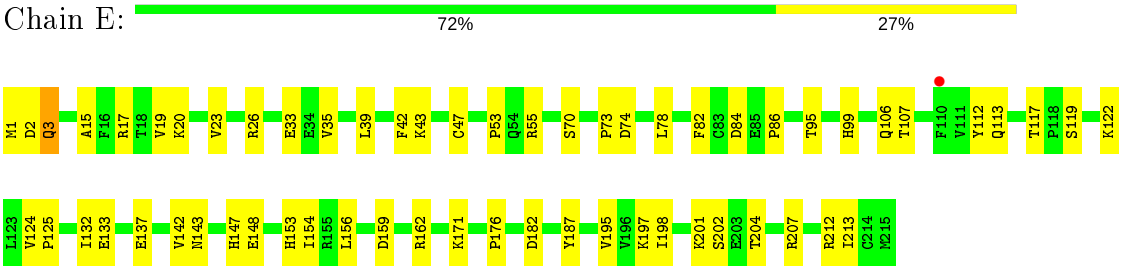
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



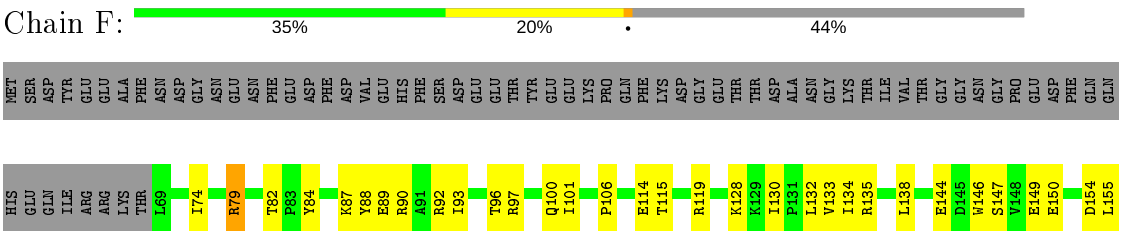
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



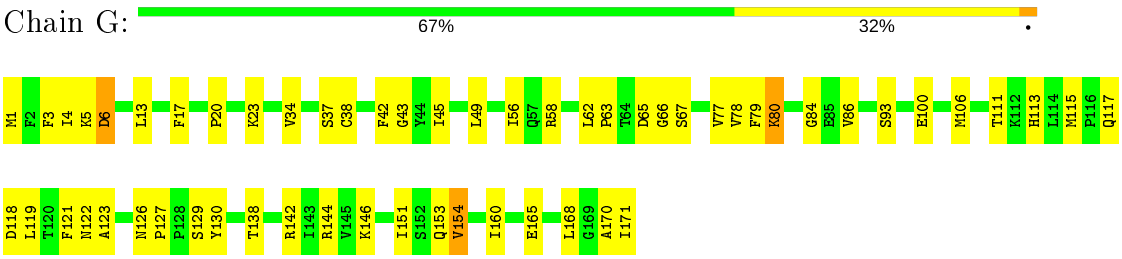
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



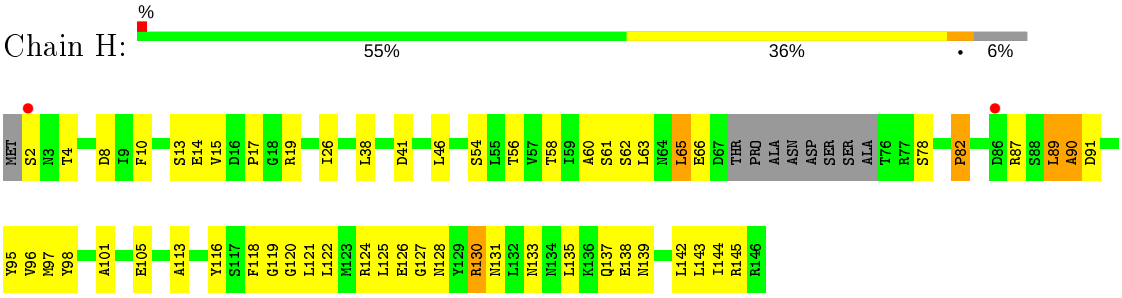
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



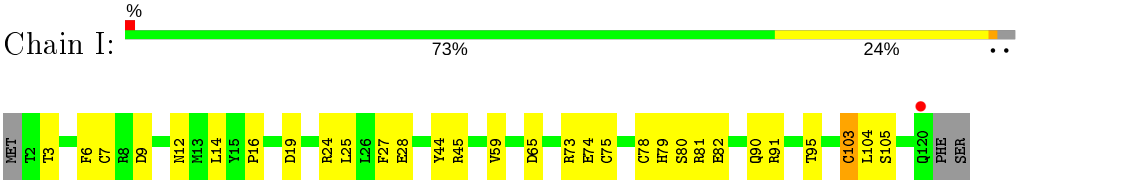
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



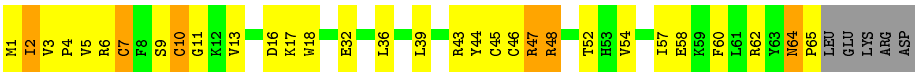
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



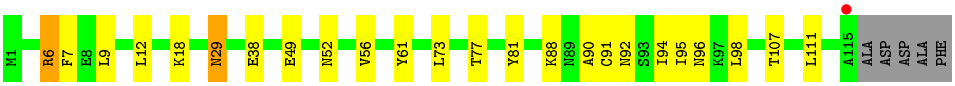
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



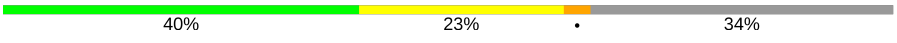
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

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) 98.9 (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 0.218 , 0.271	Depositor DCC
R_{free} test set	2493 reflections (2.01%)	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)	0.24 , 109.4	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	0.94	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/11488	0.44	0/15539
2	B	0.25	0/9317	0.46	1/12566 (0.0%)
3	C	0.24	0/2133	0.43	0/2891
4	D	0.24	0/1426	0.41	0/1919
5	E	0.38	1/1796 (0.1%)	0.41	0/2416
6	F	0.24	0/717	0.41	0/967
7	G	0.25	0/1368	0.45	0/1844
8	H	0.24	0/1119	0.46	0/1515
9	I	0.25	0/989	0.46	0/1331
10	J	0.25	0/541	0.47	0/727
11	K	0.25	0/938	0.42	0/1267
12	L	0.23	0/365	0.46	0/485
All	All	0.26	1/32197 (0.0%)	0.44	1/43467 (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
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	12.32	1.57	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	758	PHE	CB-CG-CD1	-5.04	117.27	120.80

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	331	0
2	B	9138	0	9158	285	0
3	C	2095	0	2052	70	0
4	D	1415	0	1368	45	0
5	E	1760	0	1788	36	0
6	F	705	0	731	22	0
7	G	1340	0	1357	33	0
8	H	1101	0	1067	36	0
9	I	971	0	929	19	0
10	J	532	0	544	33	0
11	K	920	0	929	17	0
12	L	363	0	386	11	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	851	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 13.

All (851) 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
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
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.20	0.74
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: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
8:H:2:SER:N	8:H:62:SER:HG	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187:THR:HG22	4:D:189:ASP:H	1.57	0.70
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
8:H:61:SER:OG	8:H:62:SER:N	2.22	0.69
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
1:A:966:ASN:O	1:A:970:THR:OG1	2.09	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:1081:LEU:HD11	1:A:1098:VAL:H	1.58	0.67
1:A:278:THR:O	1:A:282:ASN:ND2	2.23	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:1170:ILE:HG22	1:A:1174:PHE:HE2	1.61	0.65
1:A:306:ASN:ND2	1:A:321:PRO:O	2.29	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
10:J:48:ARG:O	10:J:52:THR:OG1	2.15	0.65
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.30	0.65
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.78	0.65
1:A:1013:ASP:OD1	5:E:207:ARG:NH1	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:O	2:B:1183:LYS:NZ	2.29	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
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:836:TYR:OH	1:A:1403:GLU:OE2	2.17	0.63
1:A:767:GLN:HE21	1:A:774:ARG:HB2	1.62	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
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:225:ASN:OD1	1:A:228:PHE:N	2.24	0.63
1:A:43:GLU:HB2	1:A:46:THR:HB	1.81	0.63
2:B:680:THR:OG1	2:B:681:TRP:N	2.32	0.63
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.17	0.62
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.31	0.62
1:A:316:GLN:O	1:A:318:SER:N	2.32	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
3:C:184:ASN:HD21	3:C:189:THR:H	1.45	0.62
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.80	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:N	1:A:108:MET:SD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.81	0.61
2:B:756:ILE:HG22	2:B:983:ARG:HB3	1.83	0.61
5:E:202:SER:HB3	5:E:204:THR:HG22	1.81	0.61
7:G:117:GLN:OE1	7:G:117:GLN:N	2.33	0.61
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.83	0.61
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.81	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
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:888:GLY:O	1:A:940:ARG:NH2	2.33	0.60
1:A:433:GLU:OE1	2:B:1108:ARG:NH1	2.34	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:OD1	1:A:408:ASP:N	2.36	0.58
1:A:1411:GLU:O	1:A:1415:SER:OG	2.22	0.58
1:A:830:LYS:O	1:A:834:THR:OG1	2.21	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:NE2	2:B:770:GLN:O	2.36	0.58
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.86	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	11:K:29:ASN:ND2	2.37	0.57
1:A:403:LYS:HG3	1:A:404:TYR:HD2	1.69	0.57
1:A:335:ARG:HH12	2:B:1202:LEU:HD13	1.70	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
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
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
3:C:56:THR:HG21	3:C:145:CYS:SG	2.47	0.55
1:A:609:ASP:OD1	1:A:969:GLN:NE2	2.32	0.55
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.86	0.55
2:B:916:THR:HB	2:B:935:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:H	1:A:114:LEU:HD21	1.72	0.55
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.71	0.55
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.72	0.55
8:H:65:LEU:HD23	8:H:65:LEU:H	1.71	0.55
1:A:1415:SER:O	1:A:1417:GLU:N	2.39	0.55
1:A:58:LEU:HD12	1:A:244:PRO:HD3	1.86	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:1163:CYS:SG	2:B:1164:GLY:N	2.80	0.55
2:B:165:VAL:HG21	2:B:445:LYS:HE2	1.87	0.55
2:B:115:GLN:NE2	2:B:193:LYS:O	2.36	0.55
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.88	0.55
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.36	0.55
2:B:637:LEU:HB2	2:B:693:ILE:HD13	1.89	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:1072:MET:HG3	2:B:1085:ILE:HB	1.88	0.54
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.89	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
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:1125:ALA:HB1	1:A:1303:GLU:HB2	1.87	0.54
1:A:362:ASP:N	1:A:362:ASP:OD1	2.40	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
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
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:1191:TRP:NE1	1:A:1256:GLU:OE1	2.41	0.54
1:A:136:ALA:O	1:A:140:THR:OG1	2.23	0.54
1:A:42:ASP:O	1:A:44:THR:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1221:SER:OG	2:B:1221:SER:O	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:159:ASP:OD1	5:E:162:ARG:NH2	2.41	0.54
5:E:33:GLU:OE1	5:E:33:GLU:N	2.41	0.54
1:A:58:LEU:HD23	1:A:58:LEU:H	1.71	0.53
1:A:63:ARG:HG2	1:A:74:MET:HE1	1.89	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:1345:ARG:NH1	1:A:1373:ASP:OD2	2.41	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:1117:THR:HG23	1:A:1307:GLU:HG2	1.89	0.53
1:A:975:HIS:HA	1:A:1036:ARG:HG3	1.90	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
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: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:898:ARG:NH1	1:A:899:VAL:O	2.42	0.52
1:A:690:VAL:O	1:A:694:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:746:SER:HB3	2:B:1046:PRO:HG2	1.90	0.52
2:B:445:LYS:HG3	2:B:446:LEU:HA	1.91	0.52
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.09	0.52
1:A:443:LEU:HD11	1:A:455:MET:HB3	1.91	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: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
1:A:506:ALA:HB3	1:A:509:LEU:HG	1.92	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:1348:LEU:HD23	1:A:1372:VAL:HG23	1.90	0.52
1:A:739:ASP:OD1	8:H:19:ARG:NH1	2.38	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: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
2:B:51:PHE:O	2:B:55:VAL:HG23	2.10	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
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
7:G:34:VAL:O	7:G:37:SER:OG	2.22	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
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
3:C:69:LEU:O	10:J:6:ARG:NH1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1376:THR:O	1:A:1378:GLN:N	2.36	0.51
1:A:367:PRO:HB3	1:A:465:TYR:O	2.10	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:1121:GLU:HB3	1:A:1124:HIS:ND1	2.26	0.51
1:A:123:ARG:HA	1:A:126:LEU:HD12	1.92	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
4:D:140:ASP:O	4:D:144:THR:OG1	2.20	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: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:21:LEU:HD11	1:A:1414:ALA:HA	1.92	0.50
1:A:986:ILE:HD11	1:A:1032:LEU:HD21	1.94	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
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
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:1407:GLU:N	1:A:1407:GLU:OE2	2.39	0.50
1:A:896:ARG:HH21	1:A:1030:ARG:HH21	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1037:LEU:O	10:J:47:ARG:NH1	2.45	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: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: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:813:PHE:HE1	2:B:759:PRO:HB2	1.77	0.49
1:A:1004:ASN:O	1:A:1008:GLN:HG2	2.12	0.49
1:A:828:ALA:O	1:A:831:THR:HG22	2.13	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
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:ND2	3:C:24:ASN:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:108:MET:HE1	1:A:171:GLN:HB3	1.95	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
2:B:185:THR:OG1	2:B:188:ASP:OD1	2.29	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:475:THR:O	1:A:479:ASN:N	2.47	0.48
1:A:95:PHE:O	1:A:99:ILE:HG13	2.14	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:1073:TYR:CE2	2:B:1080:LYS:HG2	2.49	0.48
2:B:723:VAL:HA	2:B:724:ASP:HB3	1.94	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:N	1:A:853:ASP:OD1	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:877:HIS:ND1	1:A:1056:SER:HA	2.29	0.47
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
2:B:804:GLY:O	2:B:805:THR:OG1	2.27	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:57:LEU:O	4:D:61:GLU:HG3	2.15	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
4:D:33:PHE:HZ	7:G:80:LYS:HZ2	1.62	0.47
10:J:16:ASP:OD1	10:J:16:ASP:N	2.48	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
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
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:41:MET:HB3	1:A:48:ALA:O	2.15	0.47
1:A:694:THR:O	1:A:698:GLN:HG3	2.15	0.47
4:D:25:ALA:HB2	7:G:84:GLY:HA3	1.96	0.47
8:H:130:ARG:HB2	8:H:133:ASN:HB2	1.97	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
8:H:58:THR:HB	8:H:143:LEU:HB2	1.97	0.47
2:B:1006:ILE:HG23	10:J:45:CYS:HB3	1.97	0.47
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.97	0.47
4:D:187:THR:HG22	4:D:189:ASP:N	2.27	0.47
5:E:84:ASP:HA	5:E:113:GLN:HE21	1.80	0.47
1:A:1248:LEU:HD12	1:A:1249:ASP:N	2.30	0.46
1:A:515:GLN:HB2	1:A:1071:SER:HB3	1.98	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
2:B:46:GLN:HG2	2:B:408:LEU:HD21	1.96	0.46
6:F:128:LYS:HD3	6:F:149:GLU:HA	1.97	0.46
1:A:1451:VAL:HG22	7:G:20:PRO:HA	1.96	0.46
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	2:B:834:ASN:OD1	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:1135:ARG:O	2:B:1139:ILE:HG13	2.15	0.46
2:B:475:SER:OG	2:B:476:ARG:O	2.24	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:N	2:B:199:MET:SD	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
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.97	0.46
4:D:68:ARG:O	4:D:72:ARG:HG3	2.16	0.46
1:A:1436:ILE:O	1:A:1438:THR:N	2.49	0.46
1:A:565:ILE:HD11	1:A:567:LYS:HE2	1.96	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
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
1:A:1308:THR:OG1	1:A:1309:ASP:N	2.49	0.46
2:B:651:LEU:HD12	2:B:651:LEU:H	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:1441:PHE:CE2	6:F:89:GLU:HG3	2.52	0.46
1:A:438:ASP:N	1:A:438:ASP:OD1	2.48	0.46
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.97	0.46
1:A:567:LYS:HE3	8:H:46:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:ASP:HB2	3:C:29:MET:HB2	1.98	0.45
11:K:61:TYR:HB3	11:K:73:LEU:HD13	1.97	0.45
3:C:167:HIS:CD2	12:L:70:ARG:HG3	2.51	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:250:ILE:H	1:A:250:ILE:HD12	1.81	0.45
1:A:46:THR:O	1:A:48:ALA:N	2.49	0.45
2:B:216:GLU:OE1	2:B:500:THR:OG1	2.33	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
1:A:810:PRO:HB2	2:B:705:MET:HE2	1.99	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
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: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: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
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.97	0.45
1:A:449:SER:HB2	2:B:1133:MET:HB3	1.99	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:1418:LEU:HD12	1:A:1419:ASP:H	1.82	0.45
1:A:607:ILE:HG13	1:A:612:ILE:HA	1.98	0.45
2:B:1180:PHE:H	2:B:1188:LYS:HE3	1.80	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
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.98	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
2:B:827:ILE:HG23	2:B:1012:ILE:HG13	1.99	0.45
2:B:338:GLY:HA3	2:B:347:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:J:17:LYS:HB3	10:J:39:LEU:HD22	1.99	0.45
10:J:6:ARG:HG2	10:J:13:VAL:HA	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:1187:ASN:O	2:B:1191:ILE:HD11	2.17	0.45
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.99	0.45
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.99	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:1177:LEU:HB2	1:A:1181:ALA:HA	1.98	0.44
1:A:67:CYS:HB2	1:A:71:GLN:N	2.32	0.44
1:A:773:LYS:HD2	1:A:773:LYS:H	1.82	0.44
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.14	0.44
2:B:542:MET:HG3	2:B:747:MET:HB3	2.00	0.44
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.99	0.44
3:C:22:LEU:HB3	3:C:25:VAL:HG21	1.99	0.44
4:D:206:GLU:HG2	4:D:209:ARG:HD2	1.98	0.44
7:G:129:SER:HB3	7:G:138:THR:HG23	1.98	0.44
2:B:901:PRO:HD2	12:L:59:ALA:O	2.17	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:1171:VAL:HG11	2:B:1191:ILE:HG21	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
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
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:CE	1:A:577:ILE:HD13	2.48	0.44
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.00	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: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:259:TYR:HB2	2:B:268:THR:HG23	2.00	0.44
7:G:151:ILE:HD11	7:G:160:ILE:HD11	2.00	0.44
1:A:1158:PRO:HG3	1:A:1188:GLN:HE22	1.82	0.44
1:A:752:LYS:HB2	2:B:1015:HIS:HD2	1.83	0.44
2:B:309:GLN:OE1	2:B:392:ARG:NH2	2.49	0.44
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:HA	10:J:2:ILE:HD12	1.85	0.44
1:A:1325:THR:HG23	5:E:147:HIS:HA	1.99	0.44
1:A:825:ILE:O	1:A:829:VAL:HG23	2.18	0.44
9:I:6:PHE:HA	9:I:14:LEU:HG	1.99	0.44
3:C:66:ARG:HH21	10:J:4:PRO:HA	1.82	0.44
2:B:1201:LYS:O	2:B:1205:GLN:HG3	2.18	0.43
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
4:D:63:LEU:HD13	4:D:66:ARG:HD2	2.00	0.43
1:A:1248:LEU:HD12	1:A:1249:ASP:H	1.83	0.43
1:A:18:GLN:O	2:B:1215:ARG:N	2.43	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: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
2:B:193:LYS:NZ	12:L:32:ALA:O	2.37	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
4:D:152:SER:HG	4:D:221:TYR:HH	1.56	0.43
7:G:23:LYS:HE3	7:G:56:ILE:HD13	2.01	0.43
1:A:1175:SER:HA	1:A:1176:LEU:HA	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:A:883:LEU:HD12	1.83	0.43
2:B:999:MET:HG3	2:B:1008:PRO:HD2	1.99	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
1:A:440:ASP:O	1:A:460:VAL:HG23	2.19	0.43
3:C:244:VAL:O	3:C:248:ILE:HG13	2.19	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
1:A:931:GLU:OE2	1:A:991:LYS:NZ	2.49	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:1076:HIS:O	3:C:31:ASN:ND2	2.52	0.43
2:B:918:ILE:HB	2:B:935:ARG:HG3	2.00	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:232:SER:OG	2:B:234:ILE:O	2.28	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:N	7:G:6:ASP:OD1	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:42:PRO:HA	3:C:163:ILE:HG22	2.01	0.42
3:C:18:VAL:HG12	3:C:20:PHE:CD1	2.55	0.42
4:D:119:ARG:HD3	4:D:221:TYR:HD2	1.84	0.42
4:D:53:SER:O	4:D:57:LEU:HG	2.19	0.42
9:I:103:CYS:SG	9:I:105:SER:N	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:78:CYS:SG	9:I:80:SER:OG	2.77	0.42
1:A:1188:GLN:HA	1:A:1243:VAL:HA	2.00	0.42
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.87	0.42
2:B:547:VAL:H	2:B:612:GLU:CD	2.23	0.42
2:B:645:SER:O	2:B:647:GLY:N	2.49	0.42
1:A:445:ASN:HB2	1:A:454:SER:O	2.20	0.42
1:A:345:VAL:HA	2:B:1155:SER:HB2	2.00	0.42
2:B:816:GLU:HB3	2:B:817:LEU:HD12	2.00	0.42
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.34	0.42
3:C:51:VAL:HB	12:L:65:VAL:HG23	1.99	0.42
8:H:98:TYR:OH	8:H:138:GLU:OE1	2.35	0.42
2:B:830:TYR:HB3	2:B:831:SER:H	1.55	0.42
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.59	0.42
1:A:719:VAL:HA	1:A:722:LEU:HD12	2.01	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
3:C:251:LEU:O	3:C:255:VAL:HG23	2.18	0.42
3:C:56:THR:HG22	3:C:57:VAL:H	1.85	0.42
4:D:115:HIS:HB3	4:D:116:SER:H	1.55	0.42
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.54	0.42
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.83	0.42
1:A:606:LEU:HG	1:A:613:ILE:HD13	2.02	0.42
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.20	0.42
2:B:644:GLU:HG2	2:B:654:ARG:HH22	1.83	0.42
2:B:637:LEU:HD12	2:B:693:ILE:HD13	2.00	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
1:A:1036:ARG:H	1:A:1036:ARG:HG2	1.71	0.42
1:A:132:LYS:NZ	1:A:1411:GLU:HB3	2.35	0.42
1:A:34:LYS:HE2	1:A:34:LYS:HB2	1.83	0.42
1:A:583:PRO:O	1:A:610:GLY:HA3	2.20	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:HA	6:F:138:LEU:HD23	1.82	0.42
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.19	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:22:PHE:CD2	2:B:1213:THR:HG22	2.55	0.42
8:H:118:PHE:HB2	8:H:121:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:63:LEU:HB3	8:H:90:ALA:HB3	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
2:B:61:ASP:N	2:B:61:ASP:OD1	2.53	0.42
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.55	0.42
3:C:110:THR:HA	3:C:147:LEU:O	2.20	0.42
3:C:56:THR:HA	3:C:151:GLN:NE2	2.35	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:1208:THR:N	1:A:1211:GLN:OE1	2.49	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:346:ASP:HB3	2:B:1108:ARG:H	1.86	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
1:A:383:TYR:HB3	6:F:115:THR:HA	2.02	0.41
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.21	0.41
1:A:540:PHE:HB3	1:A:571:LEU:HD23	2.01	0.41
2:B:1106:ARG:NH2	2:B:1118:PRO:HB3	2.36	0.41
2:B:424:LEU:O	2:B:428:ILE:HG13	2.19	0.41
3:C:98:VAL:HG23	3:C:122:SER:HB3	2.01	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.95	0.41
7:G:43:GLY:HA3	7:G:80:LYS:HB3	2.02	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
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.85	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
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:112:TYR:O	5:E:137:GLU:HB2	2.20	0.41
5:E:95:THR:O	5:E:99:HIS:HB3	2.20	0.41
6:F:97:ARG:NH2	6:F:106:PRO:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:32:ALA:HB3	12:L:55:ILE:HD12	2.03	0.41
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.20	0.41
5:E:153:HIS:C	5:E:154:ILE:HD12	2.40	0.41
1:A:1211:GLN:HG3	1:A:1211:GLN:H	1.59	0.41
2:B:758:PHE:CZ	2:B:1044:ALA:HB1	2.56	0.41
2:B:648:HIS:CG	2:B:649:LYS:H	2.39	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:1042:PHE:CE2	1:A:1046:LEU:HD11	2.56	0.41
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.21	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
2:B:1165:ILE:H	2:B:1165:ILE:HD12	1.85	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:499:ASN:OD1	2:B:500:THR:N	2.54	0.41
2:B:498:THR:O	2:B:536:VAL:HA	2.21	0.41
4:D:3:VAL:HB	4:D:4:SER:H	1.66	0.41
2:B:308:TRP:CH2	9:I:45:ARG:HD3	2.55	0.41
10:J:45:CYS:SG	10:J:46:CYS:N	2.94	0.41
11:K:7:PHE:C	11:K:9:LEU:H	2.24	0.41
1:A:1015:VAL:HB	1:A:1016:THR:H	1.75	0.41
1:A:108:MET:H	1:A:108:MET:HE2	1.86	0.41
1:A:770:VAL:HG12	1:A:771:GLU:HG3	2.03	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
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	2.03	0.41
8:H:89:LEU:O	8:H:91:ASP:N	2.45	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:1116:LEU:HG	1:A:1308:THR:CG2	2.51	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:477:PRO:HG3	1:A:521:MET:HE2	2.02	0.41
1:A:517:ASN:ND2	1:A:517:ASN:O	2.53	0.41
4:D:52:LEU:O	4:D:53:SER:OG	2.36	0.41
5:E:171:LYS:HA	5:E:171:LYS:HD3	1.90	0.41
1:A:1444:MET:HB3	7:G:58:ARG:HB3	2.03	0.41
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.21	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:628:THR:OG1	2:B:628:THR:O	2.38	0.40
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.86	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
2:B:108:VAL:HB	2:B:109:THR:H	1.71	0.40
2:B:1173:ALA:HB1	2:B:1175:LEU:HD21	2.04	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
4:D:158:GLU:CD	4:D:158:GLU:H	2.24	0.40
5:E:78:LEU:HA	5:E:107:THR:HB	2.03	0.40
11:K:29:ASN:ND2	11:K:77:THR:O	2.54	0.40
1:A:1247:SER:H	1:A:1248:LEU:HA	1.86	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
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:146:LYS:HB2	10:J:57:ILE:HD11	2.02	0.40
3:C:73:GLN:HA	3:C:133:ILE:HD11	2.03	0.40
1:A:1116:LEU:HD23	1:A:1311:VAL:HA	2.02	0.40
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	2.04	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
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:HG2	4:D:121:LYS:H	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%)	3 28
2	B	1142/1224 (93%)	943 (83%)	155 (14%)	44 (4%)	3 28
3	C	264/318 (83%)	221 (84%)	35 (13%)	8 (3%)	4 33
4	D	180/221 (81%)	155 (86%)	19 (11%)	6 (3%)	4 32
5	E	213/215 (99%)	188 (88%)	21 (10%)	4 (2%)	8 42
6	F	85/155 (55%)	77 (91%)	7 (8%)	1 (1%)	13 50
7	G	169/171 (99%)	156 (92%)	11 (6%)	2 (1%)	13 50
8	H	133/146 (91%)	103 (77%)	22 (16%)	8 (6%)	1 20
9	I	117/122 (96%)	98 (84%)	15 (13%)	4 (3%)	3 31
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2 24
11	K	113/120 (94%)	105 (93%)	8 (7%)	0	100 100
12	L	44/70 (63%)	25 (57%)	14 (32%)	5 (11%)	0 7
All	All	3951/4565 (86%)	3344 (85%)	465 (12%)	142 (4%)	3 30

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%)	1205 (96%)	50 (4%)	31	59
2	B	995/1061 (94%)	957 (96%)	38 (4%)	33	61
3	C	234/274 (85%)	230 (98%)	4 (2%)	60	78
4	D	147/200 (74%)	144 (98%)	3 (2%)	55	75
5	E	197/197 (100%)	193 (98%)	4 (2%)	55	75
6	F	77/137 (56%)	74 (96%)	3 (4%)	32	60
7	G	152/152 (100%)	144 (95%)	8 (5%)	22	54
8	H	121/128 (94%)	118 (98%)	3 (2%)	47	70
9	I	113/116 (97%)	110 (97%)	3 (3%)	44	69
10	J	60/65 (92%)	56 (93%)	4 (7%)	16	47
11	K	99/102 (97%)	96 (97%)	3 (3%)	41	66
12	L	40/57 (70%)	38 (95%)	2 (5%)	24	55
All	All	3490/4009 (87%)	3365 (96%)	125 (4%)	35	63

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	34	LYS
1	A	42	ASP
1	A	58	LEU
1	A	68	GLN
1	A	70	CYS

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Mol	Chain	Res	Type
1	A	71	GLN
1	A	134	ARG
1	A	200	ARG
1	A	215	SER
1	A	261	ASP
1	A	265	LYS
1	A	324	SER
1	A	337	ARG
1	A	378	GLU
1	A	416	ARG
1	A	438	ASP
1	A	445	ASN
1	A	470	LEU
1	A	483	ASP
1	A	498	ARG
1	A	503	GLN
1	A	544	ASP
1	A	573	SER
1	A	590	ARG
1	A	598	LEU
1	A	602	ASP
1	A	618	GLU
1	A	635	ARG
1	A	685	GLU
1	A	764	CYS
1	A	774	ARG
1	A	782	ARG
1	A	821	ARG
1	A	877	HIS
1	A	1001	ARG
1	A	1029	ARG
1	A	1035	TYR
1	A	1140	HIS
1	A	1150	SER
1	A	1176	LEU
1	A	1218	GLN
1	A	1249	ASP
1	A	1255	GLU
1	A	1256	GLU
1	A	1297	GLU
1	A	1359	ASP
1	A	1390	ASN

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Mol	Chain	Res	Type
1	A	1391	ARG
1	A	1442	ASP
2	B	39	ARG
2	B	50	SER
2	B	61	ASP
2	B	175	ARG
2	B	188	ASP
2	B	194	GLU
2	B	199	MET
2	B	232	SER
2	B	261	ARG
2	B	289	LEU
2	B	294	ASP
2	B	351	TYR
2	B	394	ASP
2	B	401	PHE
2	B	417	PHE
2	B	466	TRP
2	B	496	ARG
2	B	537	LYS
2	B	644	GLU
2	B	670	GLU
2	B	678	GLU
2	B	679	TYR
2	B	705	MET
2	B	830	TYR
2	B	959	ASP
2	B	1020	ARG
2	B	1049	ASP
2	B	1092	TYR
2	B	1108	ARG
2	B	1122	ARG
2	B	1125	ASP
2	B	1129	ARG
2	B	1148	LYS
2	B	1156	ASP
2	B	1163	CYS
2	B	1183	LYS
2	B	1221	SER
2	B	1222	ARG
3	C	136	ASP
3	C	140	ASN

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Mol	Chain	Res	Type
3	C	148	ARG
3	C	188	HIS
4	D	70	PHE
4	D	114	MET
4	D	120	GLU
5	E	17	ARG
5	E	70	SER
5	E	74	ASP
5	E	182	ASP
6	F	79	ARG
6	F	90	ARG
6	F	147	SER
7	G	1	MET
7	G	6	ASP
7	G	38	CYS
7	G	42	PHE
7	G	79	PHE
7	G	80	LYS
7	G	106	MET
7	G	118	ASP
8	H	65	LEU
8	H	66	GLU
8	H	130	ARG
9	I	7	CYS
9	I	44	TYR
9	I	103	CYS
10	J	7	CYS
10	J	10	CYS
10	J	47	ARG
10	J	48	ARG
11	K	6	ARG
11	K	29	ASN
11	K	52	ASN
12	L	27	LEU
12	L	54	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	458	HIS
1	A	1140	HIS

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Mol	Chain	Res	Type
2	B	449	ASN
2	B	770	GLN
3	C	31	ASN
3	C	123	ASN
4	D	115	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1429/1733 (82%)	-0.50	8 (0%) 89 85	57, 151, 244, 348	0
2	B	1144/1224 (93%)	-0.38	16 (1%) 75 68	78, 157, 266, 369	0
3	C	266/318 (83%)	-0.56	0 100 100	83, 158, 209, 278	0
4	D	184/221 (83%)	-0.56	0 100 100	135, 220, 290, 320	0
5	E	215/215 (100%)	-0.51	1 (0%) 91 87	102, 201, 277, 336	0
6	F	87/155 (56%)	-0.69	0 100 100	71, 124, 184, 213	0
7	G	171/171 (100%)	-0.44	0 100 100	121, 185, 244, 270	0
8	H	137/146 (93%)	-0.47	2 (1%) 73 66	140, 201, 276, 327	0
9	I	119/122 (97%)	-0.65	1 (0%) 86 81	121, 172, 245, 277	0
10	J	65/70 (92%)	-0.51	0 100 100	110, 154, 200, 238	0
11	K	115/120 (95%)	-0.54	1 (0%) 84 79	85, 141, 206, 267	0
12	L	46/70 (65%)	-0.48	0 100 100	123, 198, 252, 288	0
All	All	3978/4565 (87%)	-0.48	29 (0%) 87 83	57, 161, 260, 369	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	441	ASP	4.9
2	B	509	ALA	3.7
8	H	2	SER	3.6
2	B	467	GLY	3.6
1	A	253	ASN	3.4
1	A	159	THR	3.1
2	B	92	PHE	3.0
2	B	1075	GLY	2.8
8	H	86	ASP	2.6
11	K	115	ALA	2.6
2	B	443	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	1173	ALA	2.5
2	B	469	GLN	2.4
5	E	110	PHE	2.4
1	A	257	ARG	2.4
2	B	918	ILE	2.3
9	I	120	GLN	2.3
1	A	154	SER	2.3
1	A	1176	LEU	2.3
2	B	671	GLY	2.3
2	B	882	THR	2.3
1	A	1249	ASP	2.2
1	A	161	LEU	2.2
2	B	442	PHE	2.1
2	B	670	GLU	2.1
2	B	444	MET	2.1
1	A	1253	GLU	2.1
2	B	505	ASP	2.0
2	B	468	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	L	101	1/1	0.96	0.10	135,135,135,135	0
13	ZN	A	1801	1/1	0.96	0.06	233,233,233,233	0
13	ZN	I	201	1/1	0.97	0.08	100,100,100,100	0
13	ZN	A	1802	1/1	0.98	0.06	107,107,107,107	0
14	MG	A	1803	1/1	0.98	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	ZN	C	401	1/1	0.99	0.16	171,171,171,171	0
13	ZN	B	1301	1/1	0.99	0.09	122,122,122,122	0
13	ZN	I	202	1/1	0.99	0.03	193,193,193,193	0
13	ZN	J	101	1/1	0.99	0.21	131,131,131,131	0

6.5 Other polymers (i)

There are no such residues in this entry.