



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:56 AM UTC

PDB ID : 9BVT / pdb\_00009bvt  
Title : RNA Pol II - High Mn(+2) concentration  
Authors : Calero, G.  
Deposited on : 2024-05-20  
Resolution : 3.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

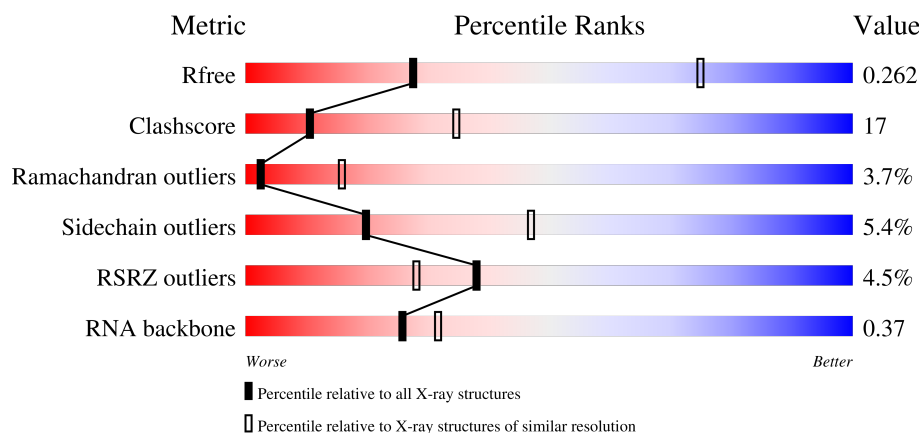
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>4%</div> <div> <div>46%</div> <div>30%</div> <div>•</div> <div>20%</div> </div> </div>
2	B	1224	<div> <div>5%</div> <div> <div>50%</div> <div>33%</div> <div>•</div> <div>13%</div> </div> </div>
3	C	318	<div> <div>•</div> <div> <div>55%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	221	<div> <div>2%</div> <div> <div>47%</div> <div>24%</div> <div>•</div> <div>27%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	X	10	
14	W	13	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 30742 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1378	Total	C	N	O	S	0	0	0
			10848	6846	1894	2047	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1060	Total	C	N	O	S	0	0	0
			8428	5349	1476	1549	54			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	162	Total	C	N	O	S	0	0	0
			1287	799	224	262	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	208	Total	C	N	O	S	0	0	0
			1713	1089	303	312	9			

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

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

- 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	117	Total	C	N	O	S	0	0	0
			951	605	158	184	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 II 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 II subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	43	Total	C	N	O	S	0	0	0
			343	211	69	59	4			

- Molecule 13 is a RNA chain called RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	X	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 14 is a DNA chain called DNA (5'-D(P\*AP\*CP\*GP\*TP\*CP\*CP\*CP\*TP\*CP\*TP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	W	13	Total	C	N	O	P	0	0	0
			260	124	44	79	13			

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Mn	0	0
			2	2		

- Molecule 17 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	55	Total	O	0	0
			55	55		
18	B	45	Total	O	0	0
			45	45		
18	C	7	Total	O	0	0
			7	7		
18	D	5	Total	O	0	0
			5	5		
18	E	6	Total	O	0	0
			6	6		
18	F	4	Total	O	0	0
			4	4		
18	G	4	Total	O	0	0
			4	4		
18	H	2	Total	O	0	0
			2	2		
18	J	1	Total	O	0	0
			1	1		
18	K	6	Total	O	0	0
			6	6		
18	L	3	Total	O	0	0
			3	3		

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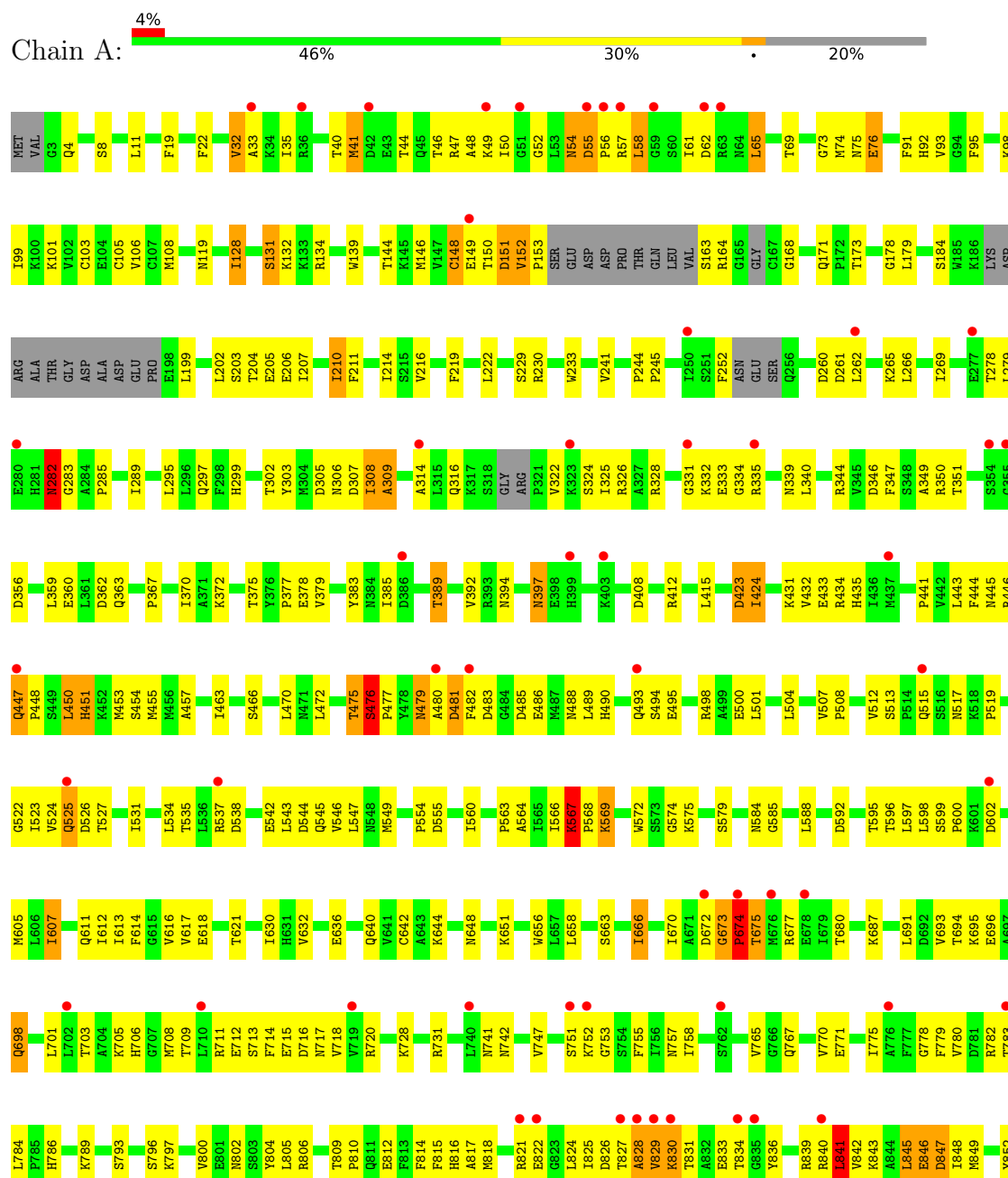
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	X	2	Total	O	0	0
			2	2		
18	W	2	Total	O	0	0
			2	2		

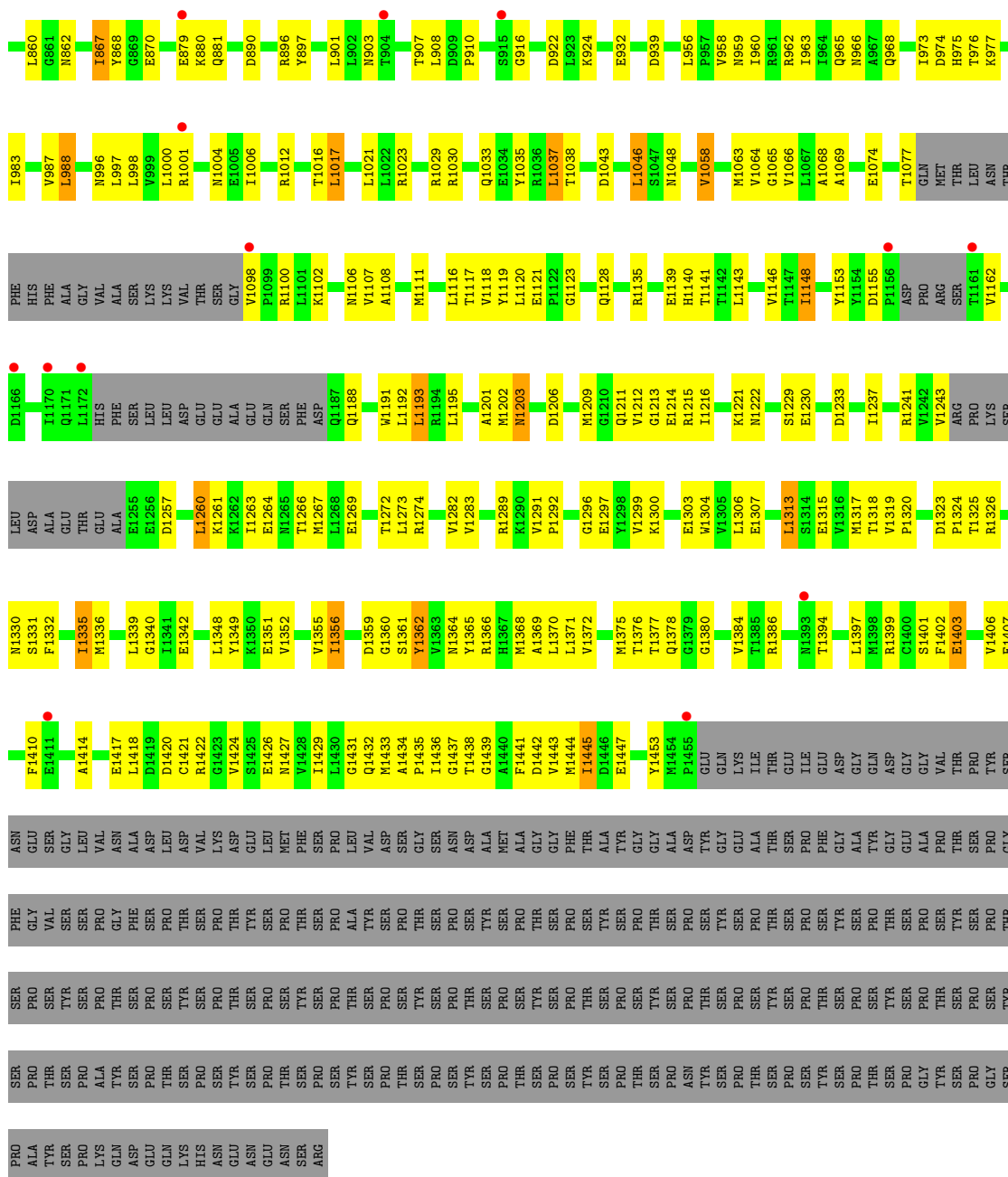


### 3 Residue-property plots

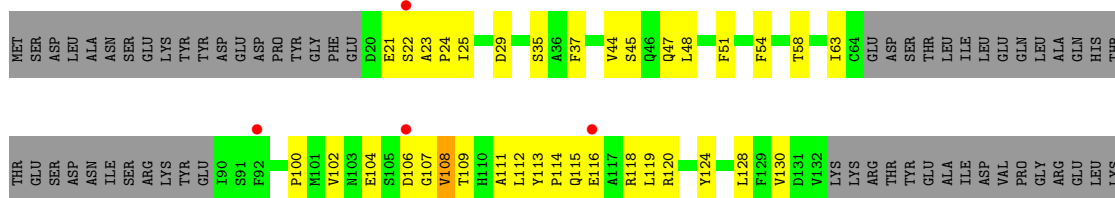
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

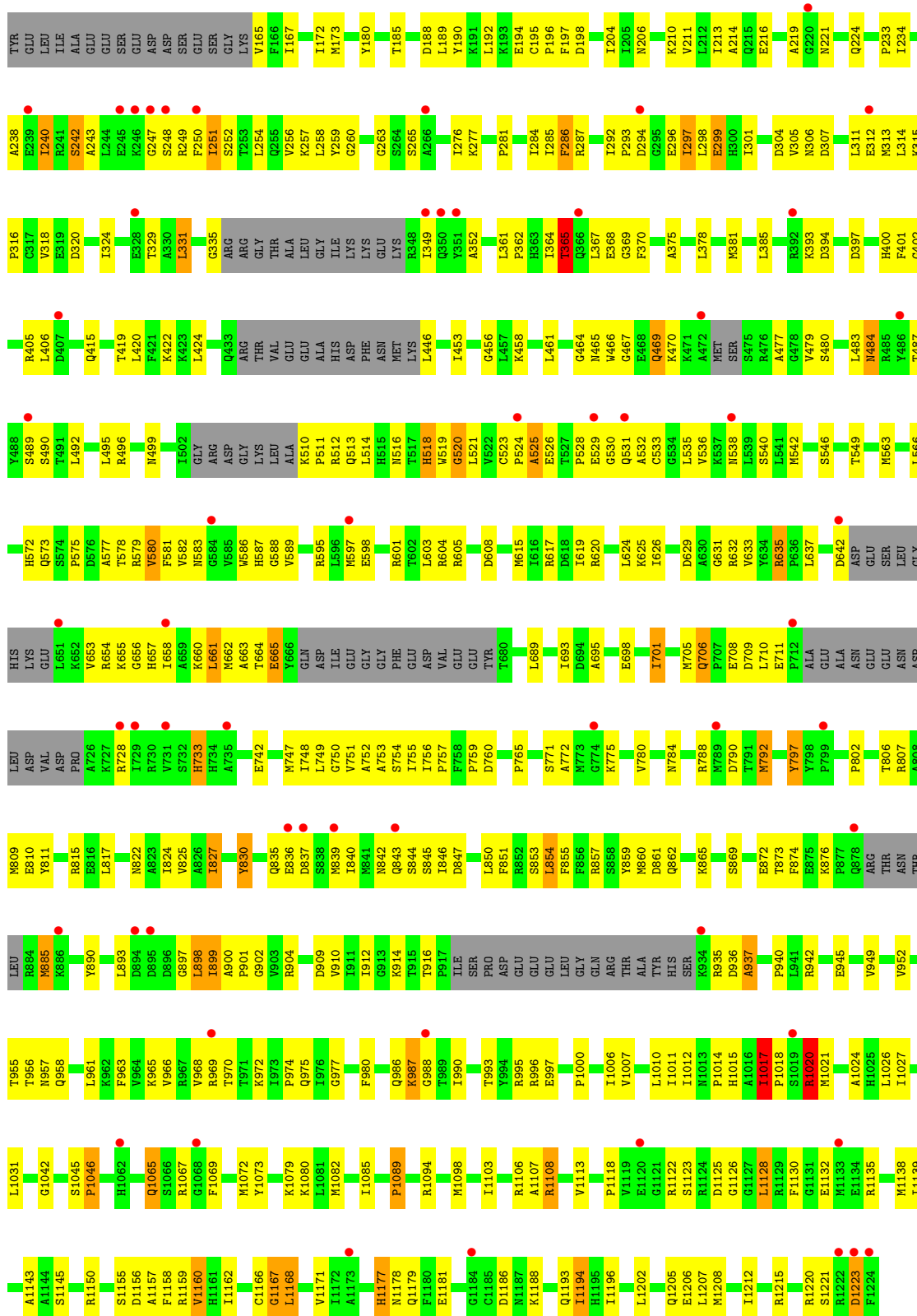
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





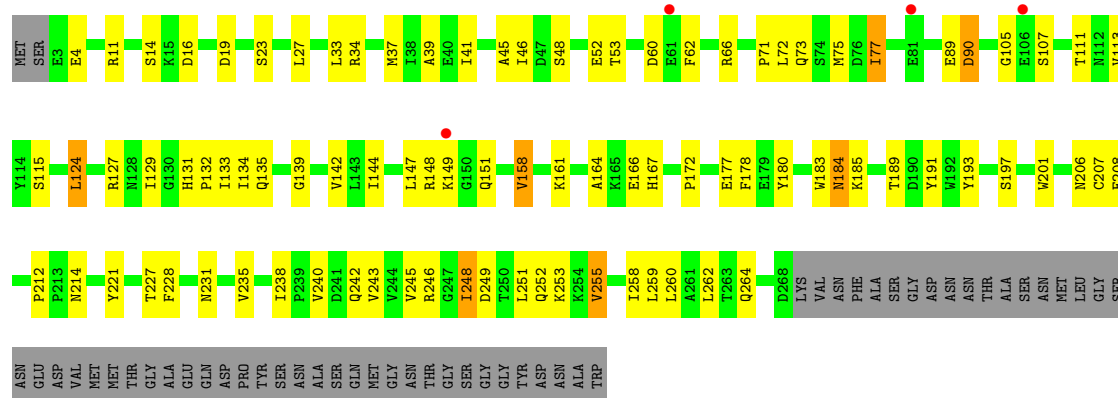
- Molecule 2: DNA-directed RNA polymerase subunit beta





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





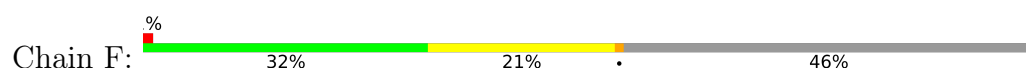
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



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

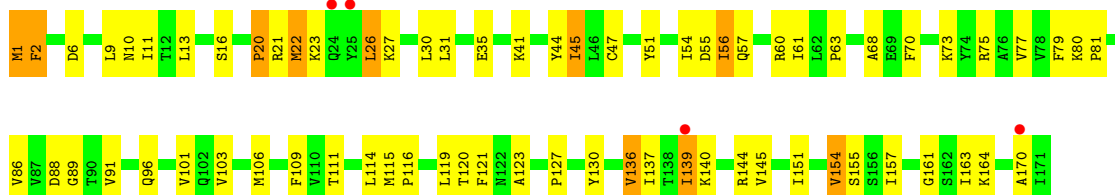


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

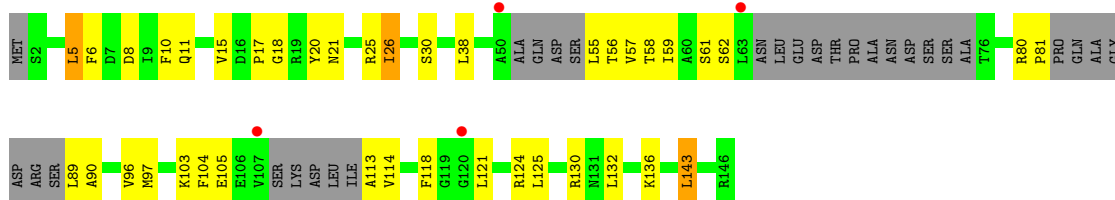




- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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



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

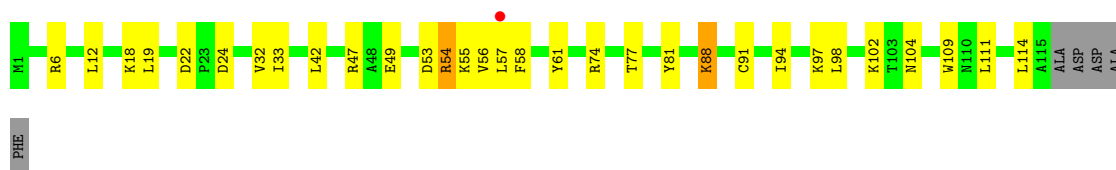


- Molecule 10: DNA-directed RNA polymerases II subunit RPABC5

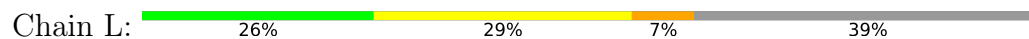


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

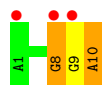




- Molecule 12: DNA-directed RNA polymerases II subunit RPABC4



- Molecule 13: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3')



- Molecule 14: DNA (5'-D(P\*AP\*CP\*GP\*TP\*CP\*CP\*CP\*TP\*CP\*TP\*CP\*GP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.19Å 393.97Å 283.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.40 49.25 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.0 (49.25-3.40) 98.6 (49.25-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.220 , 0.249 0.242 , 0.262	Depositor DCC
$R_{free}$ test set	8256 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.3	Xtriage
Anisotropy	1.597	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 175.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.066 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.076 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: GOL, MN, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/11037	0.51	7/14916 (0.0%)
2	B	0.24	0/8593	0.47	2/11585 (0.0%)
3	C	0.15	0/2133	0.35	0/2891
4	D	0.14	0/1296	0.34	0/1741
5	E	0.16	0/1747	0.40	0/2349
6	F	0.12	0/691	0.36	0/933
7	G	0.13	0/1368	0.36	0/1844
8	H	0.14	0/965	0.40	0/1302
9	I	0.17	0/989	0.40	0/1331
10	J	0.19	0/541	0.38	0/727
11	K	0.15	0/938	0.34	0/1267
12	L	0.30	0/345	0.50	0/457
13	X	0.18	0/244	0.40	0/380
14	W	0.29	0/289	0.79	1/442 (0.2%)
All	All	0.23	0/31176	0.46	10/42165 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	THR	N-CA-C	-9.80	101.08	113.43
14	W	20	DC	O5'-C5'-C4'	6.96	121.23	110.80
2	B	518	HIS	CB-CA-C	-5.58	101.75	111.23
1	A	836	TYR	N-CA-C	-5.55	106.35	113.23
1	A	841	LEU	N-CA-C	-5.41	105.41	112.23
1	A	831	THR	N-CA-C	-5.35	105.40	112.94
1	A	830	LYS	N-CA-C	-5.33	104.40	112.99
1	A	843	LYS	N-CA-C	-5.29	105.68	111.82
1	A	674	PRO	N-CA-CB	-5.29	97.70	103.25
2	B	1020	ARG	N-CA-C	-5.20	107.60	114.04



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	10848	0	10932	450	0
2	B	8428	0	8465	336	0
3	C	2095	0	2051	75	0
4	D	1287	0	1296	28	0
5	E	1713	0	1739	57	0
6	F	679	0	701	26	0
7	G	1340	0	1357	45	0
8	H	951	0	926	32	0
9	I	971	0	929	25	0
10	J	532	0	542	21	0
11	K	920	0	929	23	0
12	L	343	0	363	24	0
13	X	217	0	110	10	0
14	W	260	0	147	12	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	2	0	0	0	0
17	E	6	0	8	1	0
18	A	55	0	0	2	0
18	B	45	0	0	1	0
18	C	7	0	0	0	0
18	D	5	0	0	0	0
18	E	6	0	0	0	0
18	F	4	0	0	0	0
18	G	4	0	0	0	0
18	H	2	0	0	0	0
18	J	1	0	0	0	0
18	K	6	0	0	0	0
18	L	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	2	0	0	0	0
18	X	2	0	0	0	0
All	All	30742	0	30495	1023	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 17.

All (1023) 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)
13:X:10:A:N6	14:W:20:DC:H42	1.49	1.09
1:A:33:ALA:HB3	1:A:56:PRO:O	1.64	0.97
2:B:952:VAL:HG23	2:B:966:VAL:HG22	1.55	0.89
13:X:10:A:N6	14:W:20:DC:N4	2.21	0.87
1:A:56:PRO:HD2	1:A:58:LEU:HB2	1.56	0.85
1:A:32:VAL:HG11	1:A:57:ARG:HB3	1.58	0.85
1:A:815:PHE:HA	1:A:818:MET:HE3	1.57	0.85
1:A:747:VAL:HG22	1:A:753:GLY:HA3	1.59	0.84
1:A:975:HIS:CE1	8:H:136:LYS:HE3	2.12	0.84
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.17	0.84
1:A:262:LEU:HD13	1:A:328:ARG:NH1	1.93	0.83
1:A:802:ASN:HA	1:A:806:ARG:HH21	1.43	0.83
9:I:83:ASN:HB2	9:I:103:CYS:HA	1.61	0.83
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.14	0.82
13:X:10:A:H61	14:W:19:DC:H42	1.25	0.82
1:A:33:ALA:CB	1:A:56:PRO:O	2.28	0.82
1:A:840:ARG:HH22	1:A:1106:ASN:HD21	1.27	0.81
1:A:32:VAL:HG11	1:A:57:ARG:CB	2.11	0.81
2:B:657:HIS:HA	2:B:660:LYS:HB2	1.63	0.80
7:G:9:LEU:HD23	7:G:30:LEU:HD12	1.63	0.80
1:A:607:ILE:HG22	1:A:612:ILE:HA	1.64	0.80
5:E:175:LEU:HD23	5:E:213:ILE:HB	1.64	0.80
1:A:779:PHE:HE2	2:B:516:ASN:HB2	1.47	0.79
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.64	0.79
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.63	0.79
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.65	0.79
12:L:34:CYS:CB	12:L:51:CYS:SG	2.70	0.79
2:B:104:GLU:OE2	12:L:54:ARG:CZ	2.31	0.78
9:I:85:PHE:HB2	9:I:99:LEU:HD21	1.65	0.78
3:C:183:TRP:HZ3	3:C:212:PRO:HA	1.47	0.77
3:C:242:GLN:HA	3:C:245:VAL:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:LEU:HD12	2:B:484:ASN:H	1.48	0.77
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.67	0.77
1:A:1119:TYR:CD2	1:A:1326:ARG:HG2	2.21	0.76
1:A:537:ARG:CG	8:H:20:TYR:HE2	1.98	0.76
8:H:38:LEU:HD13	8:H:125:LEU:HB3	1.67	0.76
1:A:779:PHE:CE2	2:B:516:ASN:HB2	2.20	0.75
1:A:569:LYS:HD2	3:C:221:TYR:O	1.85	0.75
1:A:757:ASN:HA	2:B:1021:MET:HE2	1.68	0.75
3:C:45:ALA:HA	3:C:72:LEU:HD23	1.67	0.75
2:B:108:VAL:HG23	2:B:109:THR:H	1.51	0.75
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.51	0.75
1:A:537:ARG:HG3	8:H:20:TYR:HE2	1.51	0.75
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.68	0.75
1:A:525:GLN:HE22	2:B:836:GLU:HA	1.52	0.75
2:B:496:ARG:NH2	2:B:540:SER:O	2.20	0.74
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.69	0.74
2:B:873:THR:HG22	2:B:874:PHE:N	2.03	0.74
1:A:1120:LEU:HD11	1:A:1304:TRP:HB2	1.68	0.74
1:A:93:VAL:HG21	1:A:305:ASP:HB3	1.68	0.74
1:A:975:HIS:NE2	8:H:136:LYS:HE3	2.03	0.74
8:H:10:PHE:O	8:H:55:LEU:N	2.21	0.73
12:L:55:ILE:HD12	12:L:56:LEU:H	1.53	0.73
13:X:10:A:H61	14:W:19:DC:N4	1.86	0.73
1:A:663:SER:HB2	18:A:1901:HOH:O	1.87	0.73
3:C:11:ARG:HB3	3:C:19:ASP:HB3	1.70	0.72
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.22	0.72
1:A:881:GLN:NE2	1:A:1021:LEU:HD21	2.03	0.72
1:A:881:GLN:HE21	1:A:1021:LEU:HD21	1.55	0.72
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.55	0.72
2:B:1082:MET:HA	3:C:189:THR:HA	1.72	0.71
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.23	0.71
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.23	0.71
4:D:66:ARG:HD2	4:D:133:THR:HG22	1.72	0.71
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.74	0.70
1:A:1063:MET:HE3	1:A:1436:ILE:HG13	1.73	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.70
6:F:128:LYS:NZ	6:F:151:LEU:O	2.24	0.70
12:L:47:ARG:HH11	12:L:54:ARG:HE	1.37	0.70
2:B:1017:ILE:HG13	2:B:1018:PRO:HD3	1.74	0.70
1:A:58:LEU:HD23	1:A:244:PRO:HD3	1.72	0.70
6:F:105:ALA:HA	7:G:16:SER:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HH21	9:I:97:MET:HG2	1.58	0.69
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.24	0.69
6:F:76:LYS:HA	6:F:79:ARG:HG3	1.75	0.69
1:A:814:PHE:O	1:A:817:ALA:HB3	1.93	0.69
2:B:1162:ILE:HG12	2:B:1194:ILE:HD11	1.73	0.69
1:A:821:ARG:HD2	2:B:514:LEU:HB2	1.75	0.68
1:A:32:VAL:CG1	1:A:57:ARG:CB	2.71	0.68
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.27	0.68
1:A:1043:ASP:HA	1:A:1046:LEU:HB2	1.75	0.68
9:I:100:PHE:HB3	9:I:109:ILE:HD11	1.76	0.68
1:A:350:ARG:NH1	1:A:447:GLN:OE1	2.23	0.68
1:A:1289:ARG:NH1	1:A:1326:ARG:HH12	1.91	0.68
2:B:969:ARG:HH22	3:C:60:ASP:HB2	1.58	0.68
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.76	0.68
13:X:10:A:H61	14:W:20:DC:N4	1.91	0.68
1:A:566:ILE:O	1:A:568:PRO:HD2	1.93	0.67
1:A:32:VAL:CG1	1:A:57:ARG:HB2	2.24	0.67
7:G:57:GLN:HE22	7:G:73:LYS:HE3	1.59	0.67
1:A:476:SER:HB2	1:A:477:PRO:HD3	1.75	0.67
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.76	0.67
2:B:637:LEU:HD11	2:B:742:GLU:HA	1.75	0.67
2:B:287:ARG:NH1	2:B:324:ILE:O	2.27	0.67
6:F:110:ASP:O	6:F:123:LYS:NZ	2.23	0.67
1:A:1324:PRO:HB2	5:E:142:VAL:HG21	1.75	0.67
4:D:168:LYS:NZ	4:D:172:LEU:O	2.28	0.67
5:E:124:VAL:CG2	5:E:125:PRO:HD3	2.24	0.66
1:A:524:VAL:HG22	1:A:525:GLN:HG3	1.76	0.66
6:F:111:LEU:HD23	6:F:113:GLY:H	1.60	0.66
2:B:969:ARG:NH2	3:C:60:ASP:HB2	2.10	0.66
4:D:69:ALA:HA	4:D:72:ARG:HD2	1.77	0.66
1:A:379:VAL:HA	1:A:431:LYS:HG2	1.76	0.66
3:C:191:TYR:HD1	3:C:201:TRP:CD1	2.14	0.66
1:A:335:ARG:CZ	2:B:1206:GLU:OE2	2.44	0.66
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.78	0.66
10:J:2:ILE:HD13	10:J:57:ILE:HD13	1.77	0.66
7:G:96:GLN:HG2	7:G:121:PHE:CE2	2.30	0.66
8:H:15:VAL:HG12	8:H:26:ILE:HD11	1.78	0.66
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.77	0.65
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.78	0.65
1:A:73:GLY:O	1:A:75:ASN:N	2.30	0.65
1:A:360:GLU:OE2	1:A:651:LYS:NZ	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD12	3:C:72:LEU:HD21	1.77	0.65
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.79	0.65
4:D:55:ALA:O	4:D:57:LEU:N	2.30	0.65
9:I:70:ARG:HD2	9:I:84:VAL:HG12	1.79	0.65
1:A:1261:LYS:NZ	2:B:265:SER:OG	2.29	0.65
2:B:620:ARG:NH2	9:I:89:GLN:OE1	2.30	0.65
1:A:605:MET:HE3	1:A:621:THR:HG21	1.77	0.64
2:B:298:LEU:HD23	2:B:311:LEU:HD23	1.78	0.64
5:E:171:LYS:HD3	5:E:173:SER:H	1.61	0.64
1:A:54:ASN:C	1:A:56:PRO:HD3	2.22	0.64
2:B:368:GLU:O	2:B:370:PHE:N	2.29	0.64
3:C:238:ILE:HD11	3:C:246:ARG:HH21	1.61	0.64
2:B:853:SER:HB3	2:B:972:LYS:HB2	1.80	0.64
1:A:544:ASP:OD1	1:A:545:GLN:N	2.30	0.64
2:B:1181:GLU:HB2	2:B:1188:LYS:HE2	1.80	0.64
3:C:34:ARG:HD2	3:C:178:PHE:HD2	1.63	0.64
7:G:23:LYS:HE3	7:G:56:ILE:HG12	1.78	0.64
2:B:104:GLU:OE1	12:L:54:ARG:NH1	2.31	0.64
5:E:175:LEU:HD12	5:E:176:PRO:HD2	1.78	0.64
1:A:1422:ARG:NH2	2:B:1223:ASP:O	2.31	0.63
1:A:728:LYS:HA	1:A:731:ARG:HD3	1.79	0.63
12:L:31:CYS:SG	12:L:32:ALA:N	2.71	0.63
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.80	0.63
10:J:18:TRP:CE2	10:J:22:LEU:HD11	2.34	0.63
1:A:673:GLY:O	1:A:675:THR:N	2.32	0.63
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.10	0.63
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.80	0.63
5:E:39:LEU:HA	5:E:42:PHE:HB3	1.80	0.63
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.81	0.63
2:B:873:THR:HG22	2:B:874:PHE:H	1.64	0.63
5:E:202:SER:OG	5:E:206:GLY:N	2.30	0.63
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.81	0.63
4:D:194:LEU:HB3	7:G:86:VAL:HG21	1.82	0.62
1:A:834:THR:HB	1:A:1077:THR:HG22	1.80	0.62
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.82	0.62
2:B:581:PHE:HB2	2:B:625:LYS:HA	1.80	0.62
1:A:11:LEU:HD12	2:B:1193:GLN:O	2.00	0.62
2:B:23:ALA:HB3	2:B:655:LYS:HE3	1.82	0.62
2:B:601:ARG:HH11	2:B:605:ARG:HH12	1.46	0.62
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.81	0.61
1:A:349:ALA:HB3	1:A:489:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:N	1:A:56:PRO:HD3	2.14	0.61
1:A:751:SER:O	1:A:752:LYS:HG2	2.00	0.61
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.82	0.61
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.31	0.61
1:A:755:PHE:HA	1:A:758:ILE:HD12	1.81	0.61
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.82	0.61
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.82	0.61
1:A:767:GLN:NE2	1:A:797:LYS:O	2.34	0.61
1:A:825:ILE:CD1	2:B:513:GLN:HG3	2.30	0.61
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.81	0.61
5:E:124:VAL:HG23	5:E:125:PRO:HD3	1.83	0.61
12:L:31:CYS:HB3	12:L:36:SER:H	1.66	0.61
1:A:596:THR:HG22	1:A:600:PRO:HD3	1.83	0.61
3:C:183:TRP:NE1	3:C:207:CYS:SG	2.70	0.61
2:B:424:LEU:HG	2:B:453:ILE:HD11	1.81	0.60
1:A:566:ILE:O	8:H:96:VAL:HB	2.01	0.60
2:B:316:PRO:O	2:B:320:ASP:N	2.31	0.60
1:A:32:VAL:HG12	1:A:57:ARG:HB2	1.83	0.60
1:A:383:TYR:HB3	6:F:115:THR:HA	1.82	0.60
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.84	0.60
2:B:104:GLU:CD	12:L:54:ARG:NH1	2.60	0.60
2:B:499:ASN:HA	2:B:536:VAL:HG12	1.83	0.60
2:B:865:LYS:HE2	2:B:869:SER:HA	1.81	0.60
2:B:1205:GLN:HA	2:B:1208:MET:HE3	1.84	0.60
1:A:525:GLN:NE2	2:B:836:GLU:HA	2.17	0.60
1:A:1443:VAL:HG23	7:G:61:ILE:HB	1.83	0.60
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.82	0.60
3:C:135:GLN:NE2	3:C:235:VAL:O	2.34	0.60
17:E:301:GOL:H32	6:F:80:ALA:HB3	1.83	0.60
2:B:1024:ALA:HA	2:B:1027:ILE:HG12	1.84	0.60
1:A:910:PRO:HB3	1:A:916:GLY:HA3	1.84	0.60
2:B:617:ARG:NH1	2:B:619:ILE:HG13	2.16	0.60
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.35	0.60
1:A:262:LEU:CD1	1:A:328:ARG:NH1	2.63	0.60
1:A:592:ASP:H	1:A:595:THR:HG21	1.67	0.60
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.27	0.59
2:B:248:SER:OG	2:B:249:ARG:N	2.35	0.59
4:D:202:ILE:HD11	4:D:206:GLU:HB3	1.84	0.59
1:A:408:ASP:N	1:A:408:ASP:OD1	2.36	0.59
1:A:765:VAL:HB	1:A:800:VAL:HG23	1.85	0.59
2:B:397:ASP:HB3	2:B:400:HIS:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:840:ILE:HG12	2:B:1011:ILE:HB	1.83	0.59
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.83	0.59
7:G:119:LEU:HD12	7:G:130:TYR:HB3	1.84	0.59
2:B:312:GLU:HG2	2:B:315:LYS:HE2	1.84	0.59
1:A:412:ARG:NH1	1:A:433:GLU:OE2	2.36	0.59
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.85	0.59
3:C:148:ARG:NH1	10:J:64:ASN:O	2.35	0.59
1:A:825:ILE:HD12	2:B:513:GLN:HG3	1.85	0.59
1:A:695:LYS:HA	1:A:698:GLN:HG3	1.85	0.59
1:A:708:MET:SD	1:A:708:MET:N	2.75	0.59
1:A:262:LEU:HD11	1:A:328:ARG:HD2	1.84	0.58
1:A:1364:ASN:OD1	1:A:1366:ARG:NH1	2.35	0.58
2:B:885:MET:SD	2:B:885:MET:N	2.76	0.58
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.84	0.58
11:K:56:VAL:HG23	11:K:77:THR:HG22	1.85	0.58
1:A:32:VAL:CG1	1:A:57:ARG:HB3	2.30	0.58
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.86	0.58
2:B:510:LYS:HB3	2:B:511:PRO:HD2	1.85	0.58
2:B:331:LEU:HB2	2:B:352:ALA:HB3	1.85	0.58
7:G:1:MET:HE2	7:G:2:PHE:H	1.69	0.58
3:C:115:SER:HB3	3:C:142:VAL:HG12	1.86	0.58
1:A:179:LEU:O	1:A:297:GLN:NE2	2.37	0.58
1:A:447:GLN:NE2	14:W:20:DC:O2	2.36	0.58
1:A:476:SER:HB2	1:A:477:PRO:CD	2.33	0.58
2:B:952:VAL:CG2	2:B:966:VAL:HG22	2.29	0.58
1:A:299:HIS:HA	1:A:302:THR:HG22	1.86	0.58
4:D:29:LEU:HD23	4:D:33:PHE:HB3	1.86	0.58
1:A:840:ARG:HB3	1:A:1402:PHE:HZ	1.69	0.58
2:B:297:ILE:HG13	2:B:298:LEU:HD12	1.86	0.58
3:C:37:MET:HA	3:C:41:ILE:HD11	1.86	0.58
7:G:31:LEU:HD11	7:G:51:TYR:HE2	1.68	0.58
1:A:1434:ALA:O	1:A:1436:ILE:N	2.36	0.58
2:B:520:GLY:HA3	2:B:635:ARG:HH11	1.68	0.58
2:B:520:GLY:H	2:B:748:ILE:HG22	1.68	0.58
1:A:55:ASP:CG	1:A:55:ASP:O	2.46	0.57
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.19	0.57
1:A:867:ILE:HD12	1:A:1000:LEU:HD11	1.86	0.57
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.86	0.57
1:A:229:SER:OG	1:A:1414:ALA:O	2.20	0.57
1:A:846:GLU:HG2	1:A:1424:VAL:HG11	1.84	0.57
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:SER:CB	18:A:1901:HOH:O	2.49	0.57
1:A:670:ILE:HG22	1:A:805:LEU:HD11	1.86	0.57
7:G:1:MET:HE1	7:G:80:LYS:N	2.19	0.57
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.39	0.57
1:A:1263:ILE:HA	1:A:1266:THR:HB	1.86	0.57
2:B:22:SER:C	2:B:654:ARG:HH12	2.11	0.57
2:B:566:LEU:H	2:B:566:LEU:HD23	1.69	0.57
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.37	0.57
7:G:61:ILE:HD13	7:G:68:ALA:HB2	1.87	0.57
1:A:1035:TYR:HB3	1:A:1037:LEU:HD13	1.86	0.57
1:A:1063:MET:HE3	1:A:1436:ILE:HA	1.87	0.57
2:B:750:GLY:O	2:B:754:SER:OG	2.22	0.57
1:A:447:GLN:O	1:A:448:PRO:C	2.47	0.57
3:C:4:GLU:OE1	11:K:104:ASN:ND2	2.28	0.57
10:J:9:SER:OG	10:J:45:CYS:SG	2.60	0.57
2:B:824:ILE:HD12	2:B:1089:PRO:HB3	1.87	0.56
1:A:445:ASN:HB2	1:A:455:MET:HG3	1.86	0.56
1:A:1117:THR:HG22	1:A:1307:GLU:HG3	1.87	0.56
1:A:1348:LEU:HD21	1:A:1375:MET:HE3	1.87	0.56
1:A:1427:ASN:O	1:A:1431:GLY:N	2.38	0.56
2:B:873:THR:CG2	2:B:874:PHE:N	2.68	0.56
1:A:537:ARG:HG3	8:H:20:TYR:CE2	2.39	0.56
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.86	0.56
1:A:1148:ILE:HG13	9:I:49:ILE:HB	1.88	0.56
3:C:183:TRP:O	3:C:185:LYS:N	2.35	0.56
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.69	0.56
11:K:54:ARG:HD2	11:K:55:LYS:HD2	1.87	0.56
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.87	0.56
1:A:840:ARG:HD2	1:A:1384:VAL:O	2.05	0.56
2:B:661:LEU:O	2:B:664:THR:N	2.38	0.56
3:C:148:ARG:NH1	10:J:63:TYR:O	2.39	0.56
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.88	0.56
9:I:5:ARG:NH2	9:I:36:GLU:OE2	2.38	0.56
2:B:44:VAL:HG22	2:B:47:GLN:HB3	1.88	0.56
5:E:88:VAL:HG13	5:E:92:THR:OG1	2.06	0.56
1:A:8:SER:OG	2:B:1178:ASN:ND2	2.38	0.56
1:A:316:GLN:HB2	1:A:322:VAL:HB	1.87	0.56
1:A:567:LYS:HZ1	8:H:90:ALA:HB3	1.71	0.56
1:A:1263:ILE:HG22	1:A:1267:MET:HG3	1.87	0.56
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.87	0.56
6:F:85:MET:HE3	6:F:90:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:SER:O	1:A:328:ARG:HG3	2.05	0.56
1:A:494:SER:OG	1:A:495:GLU:N	2.40	0.55
1:A:802:ASN:CA	1:A:806:ARG:HH21	2.17	0.55
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.71	0.55
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.23	0.55
1:A:447:GLN:NE2	14:W:20:DC:H1'	2.22	0.55
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.41	0.55
1:A:842:VAL:O	1:A:846:GLU:HB2	2.06	0.55
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.15	0.55
3:C:113:VAL:HG23	3:C:144:ILE:HB	1.88	0.55
1:A:1299:VAL:HG22	1:A:1300:LYS:H	1.72	0.55
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.41	0.55
1:A:1068:ALA:CB	1:A:1370:LEU:HD23	2.36	0.55
1:A:1116:LEU:HD21	1:A:1313:LEU:HB2	1.87	0.55
1:A:446:ARG:HH21	1:A:448:PRO:HD3	1.71	0.55
2:B:364:ILE:O	2:B:365:THR:HB	2.06	0.55
1:A:809:THR:HG22	2:B:728:ARG:HH21	1.71	0.55
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.89	0.54
2:B:216:GLU:HA	2:B:406:LEU:HA	1.87	0.54
2:B:839:MET:HE2	2:B:988:GLY:HA3	1.88	0.54
1:A:49:LYS:HE2	1:A:61:ILE:HG22	1.89	0.54
1:A:91:PHE:CE2	1:A:204:THR:OG1	2.58	0.54
1:A:537:ARG:NE	8:H:20:TYR:CE2	2.71	0.54
2:B:104:GLU:OE2	12:L:54:ARG:NH2	2.40	0.54
2:B:406:LEU:O	2:B:406:LEU:HD12	2.07	0.54
2:B:810:GLU:HA	2:B:815:ARG:NH1	2.23	0.54
3:C:77:ILE:HG12	3:C:161:LYS:HE3	1.88	0.54
11:K:22:ASP:HB2	11:K:32:VAL:HG23	1.89	0.54
2:B:213:ILE:HD12	2:B:499:ASN:HB2	1.88	0.54
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.90	0.54
1:A:542:GLU:HG2	1:A:543:LEU:H	1.72	0.54
2:B:286:PHE:HE1	2:B:375:ALA:HB1	1.73	0.54
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.39	0.54
2:B:287:ARG:NH2	2:B:294:ASP:HB3	2.21	0.54
9:I:26:LEU:HD23	9:I:37:GLU:CA	2.37	0.54
2:B:405:ARG:NH1	2:B:629:ASP:OD2	2.40	0.54
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.90	0.54
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.89	0.54
2:B:285:ILE:HD13	2:B:378:LEU:HD11	1.90	0.54
1:A:108:MET:HA	1:A:210:ILE:HG12	1.90	0.54
1:A:512:VAL:HA	1:A:519:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG23	1:A:712:GLU:H	1.72	0.54
1:A:825:ILE:HD11	2:B:512:ARG:O	2.07	0.54
2:B:465:ASN:O	2:B:467:GLY:N	2.40	0.54
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.41	0.54
4:D:24:ALA:H	4:D:28:GLN:HB3	1.73	0.54
2:B:873:THR:CG2	2:B:874:PHE:H	2.21	0.53
1:A:340:LEU:HD13	1:A:1429:ILE:HG13	1.90	0.53
2:B:546:SER:HG	2:B:631:GLY:H	1.54	0.53
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.09	0.53
2:B:1158:PHE:HD2	2:B:1160:VAL:HG22	1.74	0.53
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.23	0.53
2:B:185:THR:H	2:B:188:ASP:HB2	1.73	0.53
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.89	0.53
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.32	0.53
1:A:793:SER:O	1:A:797:LYS:HB2	2.09	0.53
4:D:124:GLU:N	4:D:124:GLU:OE1	2.41	0.53
4:D:176:GLU:O	4:D:180:LEU:HB2	2.09	0.53
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.74	0.53
1:A:472:LEU:HD13	2:B:835:GLN:HE21	1.73	0.53
1:A:598:LEU:O	8:H:25:ARG:NH2	2.40	0.53
1:A:1139:GLU:HG3	1:A:1282:VAL:HG22	1.89	0.53
1:A:392:VAL:HG13	1:A:415:LEU:HD21	1.91	0.53
1:A:525:GLN:OE1	2:B:836:GLU:HG2	2.08	0.53
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.53	0.53
7:G:111:THR:HB	7:G:114:LEU:HD23	1.91	0.53
1:A:335:ARG:HH21	2:B:1202:LEU:HD21	1.74	0.52
2:B:579:ARG:HG2	2:B:586:TRP:CZ2	2.44	0.52
1:A:441:PRO:HG2	1:A:498:ARG:HB3	1.89	0.52
1:A:1342:GLU:HG3	5:E:198:ILE:HG12	1.92	0.52
2:B:521:LEU:HD21	2:B:635:ARG:HG2	1.90	0.52
7:G:145:VAL:HG12	7:G:163:ILE:HD11	1.90	0.52
11:K:54:ARG:HH11	11:K:55:LYS:HD2	1.74	0.52
1:A:965:GLN:HA	1:A:968:GLN:HB2	1.91	0.52
3:C:48:SER:HB2	3:C:158:VAL:HG22	1.90	0.52
3:C:133:ILE:H	3:C:133:ILE:HD12	1.73	0.52
8:H:5:LEU:HB2	8:H:59:ILE:HD11	1.92	0.52
1:A:57:ARG:HB3	1:A:69:THR:CG2	2.40	0.52
1:A:903:ASN:O	1:A:907:THR:OG1	2.23	0.52
2:B:519:TRP:C	2:B:521:LEU:H	2.18	0.52
3:C:180:TYR:HB3	3:C:228:PHE:HD1	1.73	0.52
5:E:117:THR:HB	5:E:118:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:CG2	2.90	0.52
4:D:160:VAL:O	4:D:164:ILE:HG12	2.09	0.52
1:A:432:VAL:O	1:A:432:VAL:HG13	2.10	0.52
1:A:713:SER:O	1:A:717:ASN:ND2	2.41	0.52
1:A:840:ARG:HH22	1:A:1106:ASN:ND2	2.02	0.52
1:A:1100:ARG:HH22	1:A:1111:MET:HE2	1.75	0.52
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.92	0.52
2:B:936:ASP:OD1	2:B:937:ALA:N	2.42	0.52
7:G:81:PRO:HG3	7:G:106:MET:SD	2.50	0.52
7:G:154:VAL:HG22	7:G:155:SER:H	1.74	0.52
2:B:519:TRP:O	2:B:521:LEU:N	2.40	0.52
2:B:844:SER:HB3	2:B:995:ARG:HG2	1.92	0.52
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.92	0.52
9:I:26:LEU:HD13	9:I:35:VAL:HG11	1.92	0.52
1:A:1141:THR:HB	1:A:1273:LEU:HB2	1.92	0.52
1:A:1317:MET:HB3	5:E:142:VAL:HG11	1.91	0.52
10:J:17:LYS:HB3	10:J:39:LEU:HD13	1.91	0.52
4:D:40:HIS:CD2	4:D:41:GLN:HG3	2.45	0.52
10:J:37:SER:OG	10:J:47:ARG:NH2	2.32	0.52
1:A:4:GLN:HB3	2:B:1159:ARG:HH21	1.75	0.52
1:A:687:LYS:O	1:A:691:LEU:N	2.42	0.52
3:C:34:ARG:HD2	3:C:178:PHE:CD2	2.44	0.52
1:A:663:SER:HB2	2:B:827:ILE:O	2.10	0.51
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.45	0.51
2:B:190:TYR:OH	2:B:196:PRO:HG3	2.10	0.51
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.45	0.51
9:I:103:CYS:SG	9:I:108:HIS:N	2.82	0.51
1:A:397:ASN:OD1	1:A:397:ASN:N	2.42	0.51
5:E:18:THR:OG1	5:E:140:LEU:O	2.28	0.51
1:A:306:ASN:HB2	1:A:324:SER:HB2	1.92	0.51
2:B:37:PHE:HE2	2:B:542:MET:HA	1.75	0.51
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.93	0.51
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.92	0.51
1:A:347:PHE:H	2:B:1107:ALA:HA	1.75	0.51
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.75	0.51
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.33	0.51
1:A:1433:MET:HE2	2:B:1145:SER:HB3	1.92	0.51
1:A:1399:ARG:NH2	1:A:1417:GLU:OE1	2.44	0.51
3:C:107:SER:HB3	3:C:111:THR:HB	1.92	0.51
7:G:55:ASP:OD1	7:G:56:ILE:N	2.43	0.51
1:A:211:PHE:HA	1:A:214:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.92	0.51
1:A:1397:LEU:HD13	1:A:1429:ILE:HG21	1.92	0.51
2:B:573:GLN:NE2	18:B:1403:HOH:O	2.44	0.51
3:C:105:GLY:HA2	3:C:111:THR:HG21	1.92	0.51
1:A:106:VAL:O	1:A:171:GLN:NE2	2.43	0.51
1:A:525:GLN:HE22	2:B:836:GLU:CA	2.23	0.51
1:A:481:ASP:OD1	1:A:481:ASP:N	2.44	0.51
2:B:575:PRO:C	2:B:577:ALA:H	2.19	0.51
7:G:13:LEU:HD11	7:G:26:LEU:HD13	1.92	0.51
2:B:304:ASP:O	2:B:306:ASN:N	2.38	0.50
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.50
1:A:996:ASN:O	1:A:998:LEU:N	2.45	0.50
2:B:119:LEU:O	2:B:965:LYS:NZ	2.41	0.50
6:F:106:PRO:HD3	7:G:16:SER:HA	1.94	0.50
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.77	0.50
2:B:876:LYS:HE2	2:B:893:LEU:HB2	1.93	0.50
2:B:977:GLY:H	2:B:990:ILE:HB	1.75	0.50
6:F:101:ILE:HD13	6:F:120:ILE:HG22	1.94	0.50
1:A:716:ASP:O	1:A:720:ARG:HG2	2.11	0.50
2:B:511:PRO:HG2	2:B:512:ARG:HG3	1.94	0.50
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.46	0.50
1:A:1229:SER:OG	1:A:1233:ASP:OD2	2.26	0.50
5:E:179:GLN:HB2	5:E:182:ASP:OD1	2.12	0.50
7:G:127:PRO:HG2	7:G:139:ILE:HG21	1.94	0.50
10:J:3:VAL:HG21	10:J:18:TRP:CD2	2.46	0.50
11:K:47:ARG:HD3	11:K:61:TYR:HD1	1.77	0.50
1:A:49:LYS:HZ3	1:A:61:ILE:HB	1.76	0.50
1:A:98:LYS:HA	1:A:101:LYS:HB2	1.94	0.50
1:A:1001:ARG:HB3	6:F:80:ALA:O	2.12	0.50
9:I:85:PHE:CB	9:I:99:LEU:HD21	2.40	0.50
1:A:278:THR:O	1:A:282:ASN:ND2	2.44	0.50
1:A:542:GLU:O	1:A:546:VAL:HG23	2.12	0.50
2:B:902:GLY:O	12:L:65:VAL:HG11	2.12	0.50
2:B:1207:LEU:HD22	2:B:1212:ILE:HD11	1.94	0.50
2:B:299:GLU:N	2:B:299:GLU:OE1	2.45	0.50
2:B:514:LEU:HD21	2:B:524:PRO:HA	1.94	0.50
2:B:898:LEU:HB3	12:L:58:LYS:HE2	1.93	0.50
2:B:980:PHE:HE2	2:B:990:ILE:HD11	1.76	0.50
5:E:198:ILE:HD12	5:E:198:ILE:H	1.75	0.50
9:I:26:LEU:HA	9:I:37:GLU:HA	1.93	0.50
10:J:33:GLY:O	10:J:47:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LYS:NZ	1:A:602:ASP:OD2	2.45	0.49
1:A:741:ASN:OD1	1:A:742:ASN:N	2.45	0.49
1:A:1441:PHE:CE1	6:F:92:ARG:HD3	2.47	0.49
2:B:100:PRO:HG2	2:B:180:TYR:CE2	2.47	0.49
2:B:195:CYS:HB3	2:B:198:ASP:HB2	1.93	0.49
2:B:912:ILE:HD11	2:B:966:VAL:HG21	1.94	0.49
1:A:841:LEU:HD21	1:A:1371:LEU:HD13	1.94	0.49
2:B:706:GLN:HB3	2:B:709:ASP:HB2	1.93	0.49
2:B:862:GLN:HB3	2:B:963:PHE:CD1	2.47	0.49
3:C:249:ASP:O	3:C:253:LYS:HG2	2.12	0.49
6:F:147:SER:HB3	6:F:150:GLU:HG2	1.93	0.49
7:G:89:GLY:HA3	7:G:103:VAL:HG22	1.94	0.49
1:A:579:SER:HB3	1:A:611:GLN:HA	1.94	0.49
1:A:778:GLY:H	2:B:516:ASN:HD21	1.59	0.49
1:A:840:ARG:CB	1:A:1402:PHE:HZ	2.25	0.49
1:A:896:ARG:HD3	1:A:1030:ARG:HD2	1.93	0.49
2:B:483:LEU:CD1	2:B:484:ASN:H	2.22	0.49
4:D:6:SER:OG	4:D:7:THR:N	2.45	0.49
1:A:260:ASP:OD1	1:A:261:ASP:N	2.45	0.49
1:A:485:ASP:OD1	13:X:10:A:H4'	2.12	0.49
1:A:1291:VAL:CG2	1:A:1292:PRO:HD2	2.43	0.49
2:B:749:LEU:HD13	2:B:754:SER:HA	1.94	0.49
2:B:957:ASN:OD1	2:B:958:GLN:HG3	2.12	0.49
1:A:41:MET:HE1	1:A:47:ARG:HA	1.94	0.49
1:A:476:SER:O	1:A:477:PRO:C	2.55	0.49
1:A:1128:GLN:H	1:A:1128:GLN:CD	2.20	0.49
3:C:73:GLN:N	3:C:131:HIS:O	2.43	0.49
5:E:195:VAL:HG12	5:E:196:VAL:H	1.77	0.49
1:A:55:ASP:H	1:A:58:LEU:HB3	1.78	0.49
1:A:149:GLU:HB2	1:A:164:ARG:HH11	1.77	0.49
1:A:731:ARG:HB3	1:A:755:PHE:CZ	2.48	0.49
1:A:922:ASP:OD1	1:A:924:LYS:HG2	2.12	0.49
1:A:1261:LYS:HA	1:A:1264:GLU:HB2	1.93	0.49
1:A:131:SER:OG	1:A:132:LYS:N	2.45	0.49
1:A:351:THR:HB	2:B:1103:ILE:HG13	1.95	0.49
1:A:446:ARG:HE	1:A:448:PRO:HD2	1.76	0.49
2:B:563:MET:HE1	2:B:587:HIS:HB3	1.95	0.49
2:B:806:THR:H	2:B:809:MET:HE2	1.78	0.49
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.94	0.49
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.94	0.49
1:A:49:LYS:HD2	1:A:55:ASP:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:O	1:A:146:MET:HG2	2.13	0.49
1:A:1342:GLU:HG2	5:E:212:ARG:HE	1.76	0.49
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.93	0.49
2:B:490:SER:HB3	2:B:775:LYS:HA	1.94	0.49
2:B:492:LEU:HA	2:B:495:LEU:HD12	1.95	0.49
2:B:885:MET:HA	2:B:936:ASP:HB2	1.95	0.49
3:C:14:SER:HA	11:K:114:LEU:HD12	1.95	0.49
4:D:23:ASN:HB2	4:D:28:GLN:O	2.13	0.49
5:E:94:LYS:HA	5:E:97:VAL:HG12	1.94	0.49
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.93	0.49
1:A:1068:ALA:HB3	1:A:1370:LEU:HD23	1.95	0.49
2:B:1103:ILE:O	2:B:1122:ARG:NE	2.46	0.49
3:C:191:TYR:CD1	3:C:201:TRP:CD1	2.97	0.49
2:B:874:PHE:HB3	2:B:897:GLY:HA3	1.93	0.49
9:I:17:ARG:HD2	9:I:18:GLU:H	1.78	0.49
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.75	0.49
13:X:10:A:N6	14:W:19:DC:H42	2.01	0.49
2:B:603:LEU:HG	2:B:608:ASP:HB2	1.95	0.48
2:B:604:ARG:NH2	2:B:615:MET:HG2	2.28	0.48
8:H:6:PHE:CD2	8:H:130:ARG:HG3	2.48	0.48
1:A:335:ARG:HE	2:B:1202:LEU:CD2	2.26	0.48
1:A:778:GLY:N	2:B:516:ASN:HD21	2.11	0.48
1:A:779:PHE:CE2	2:B:516:ASN:CB	2.96	0.48
1:A:1155:ASP:CG	1:A:1162:VAL:H	2.21	0.48
2:B:242:SER:OG	2:B:252:SER:O	2.20	0.48
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.48
3:C:183:TRP:CZ3	3:C:212:PRO:HA	2.38	0.48
3:C:184:ASN:ND2	3:C:189:THR:O	2.45	0.48
1:A:596:THR:HG23	1:A:598:LEU:H	1.77	0.48
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.42	0.48
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.48	0.48
3:C:246:ARG:HA	3:C:249:ASP:HB3	1.96	0.48
7:G:139:ILE:HG12	7:G:140:LYS:HG2	1.95	0.48
14:W:22:DT:H2'	14:W:23:DC:O4'	2.13	0.48
1:A:55:ASP:C	1:A:57:ARG:H	2.20	0.48
2:B:519:TRP:O	2:B:521:LEU:HG	2.13	0.48
2:B:642:ASP:OD1	2:B:642:ASP:N	2.46	0.48
5:E:84:ASP:OD1	5:E:85:GLU:HG3	2.13	0.48
5:E:112:TYR:HB3	5:E:116:ILE:HD11	1.96	0.48
1:A:41:MET:HA	1:A:50:ILE:HG22	1.95	0.48
1:A:771:GLU:H	1:A:822:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:O	1:A:847:ASP:N	2.46	0.48
2:B:756:ILE:HB	2:B:759:PRO:HG3	1.95	0.48
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.95	0.48
9:I:92:ARG:HB3	9:I:95:THR:HG23	1.95	0.48
1:A:385:ILE:O	1:A:389:THR:OG1	2.28	0.48
2:B:44:VAL:HG13	2:B:48:LEU:HG	1.96	0.48
2:B:335:GLY:HA3	2:B:349:ILE:HD11	1.95	0.48
3:C:71:PRO:HB2	3:C:133:ILE:HD13	1.95	0.48
5:E:54:GLN:NE2	5:E:84:ASP:HB3	2.27	0.48
5:E:178:ILE:O	5:E:214:CYS:HA	2.14	0.48
1:A:335:ARG:HE	2:B:1202:LEU:HD23	1.79	0.48
1:A:1141:THR:HB	1:A:1274:ARG:H	1.79	0.48
9:I:69:PRO:HG2	9:I:85:PHE:CZ	2.48	0.48
1:A:331:GLY:O	1:A:333:GLU:N	2.47	0.48
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.79	0.48
1:A:1436:ILE:O	1:A:1438:THR:N	2.47	0.48
1:A:55:ASP:N	1:A:56:PRO:CD	2.77	0.47
1:A:148:CYS:O	1:A:149:GLU:HG3	2.13	0.47
1:A:537:ARG:CG	8:H:20:TYR:CE2	2.87	0.47
1:A:1193:LEU:HG	1:A:1260:LEU:HD21	1.96	0.47
3:C:33:LEU:O	3:C:37:MET:HG3	2.14	0.47
3:C:73:GLN:HB3	3:C:131:HIS:H	1.79	0.47
7:G:1:MET:HB2	7:G:1:MET:HE3	1.65	0.47
7:G:57:GLN:NE2	7:G:73:LYS:HE3	2.28	0.47
1:A:829:VAL:HG21	2:B:512:ARG:HH21	1.79	0.47
1:A:1221:LYS:HG2	1:A:1222:ASN:H	1.78	0.47
2:B:853:SER:OG	2:B:854:LEU:N	2.48	0.47
5:E:124:VAL:HG22	5:E:125:PRO:HD3	1.95	0.47
7:G:27:LYS:HG2	7:G:54:ILE:HD11	1.95	0.47
1:A:76:GLU:HB2	2:B:1159:ARG:HH22	1.78	0.47
1:A:703:THR:O	1:A:705:LYS:HD2	2.14	0.47
1:A:1349:TYR:HA	1:A:1372:VAL:HG11	1.96	0.47
3:C:258:ILE:HG23	11:K:19:LEU:HD21	1.95	0.47
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.78	0.47
1:A:535:THR:OG1	1:A:617:VAL:HG12	2.14	0.47
1:A:677:ARG:O	1:A:680:THR:OG1	2.32	0.47
1:A:696:GLU:HG2	1:A:701:LEU:HB3	1.96	0.47
1:A:800:VAL:HG12	1:A:812:GLU:HB3	1.95	0.47
1:A:1376:THR:HG22	5:E:212:ARG:HH22	1.80	0.47
2:B:843:GLN:HB2	2:B:993:THR:HB	1.96	0.47
2:B:904:ARG:NH1	12:L:66:GLN:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:TYR:HD1	3:C:201:TRP:NE1	2.13	0.47
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.96	0.47
7:G:10:ASN:HA	7:G:70:PHE:O	2.15	0.47
8:H:96:VAL:HG12	8:H:97:MET:N	2.30	0.47
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.95	0.47
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.29	0.47
1:A:715:GLU:HA	1:A:718:VAL:HG12	1.96	0.47
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.39	0.47
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.15	0.47
4:D:129:LEU:O	4:D:133:THR:N	2.38	0.47
1:A:108:MET:HE2	1:A:108:MET:HB2	1.75	0.47
1:A:1065:GLY:HA2	1:A:1370:LEU:HD21	1.96	0.47
2:B:299:GLU:HB3	2:B:572:HIS:CE1	2.50	0.47
2:B:580:VAL:HG22	2:B:588:GLY:H	1.79	0.47
2:B:757:PRO:O	2:B:1024:ALA:HB1	2.15	0.47
2:B:859:TYR:O	2:B:965:LYS:HA	2.14	0.47
2:B:1130:PHE:HZ	2:B:1138:MET:HG3	1.80	0.47
8:H:11:GLN:HE21	8:H:55:LEU:HD21	1.80	0.47
1:A:335:ARG:NE	2:B:1206:GLU:OE2	2.48	0.47
1:A:457:ALA:HB2	1:A:501:LEU:HD22	1.95	0.47
1:A:1211:GLN:HA	1:A:1214:GLU:HB2	1.97	0.47
2:B:784:ASN:O	2:B:788:ARG:HB2	2.14	0.47
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.15	0.47
2:B:1220:ARG:HG2	2:B:1221:SER:N	2.30	0.47
4:D:155:ARG:H	4:D:219:THR:HG21	1.79	0.47
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.49	0.47
1:A:57:ARG:HB3	1:A:69:THR:HG23	1.97	0.47
1:A:265:LYS:HD3	1:A:302:THR:HG23	1.97	0.47
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.30	0.47
2:B:420:LEU:HD21	2:B:456:GLY:HA3	1.97	0.47
5:E:207:ARG:O	5:E:207:ARG:HG2	2.15	0.47
1:A:49:LYS:NZ	1:A:55:ASP:HB2	2.30	0.47
1:A:566:ILE:O	1:A:567:LYS:HB2	2.15	0.47
1:A:1407:GLU:HA	1:A:1410:PHE:HB2	1.96	0.47
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.96	0.47
2:B:855:PHE:HB3	2:B:970:THR:HG23	1.97	0.47
4:D:130:LEU:HD13	4:D:142:LYS:HA	1.96	0.47
4:D:160:VAL:HA	4:D:163:VAL:HG12	1.97	0.47
4:D:194:LEU:HD21	7:G:144:ARG:HD3	1.97	0.47
1:A:751:SER:O	1:A:752:LYS:CG	2.62	0.47
1:A:531:ILE:HG23	1:A:617:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:PHE:HB3	9:I:97:MET:HE1	1.98	0.46
2:B:102:VAL:HB	2:B:112:LEU:HD22	1.97	0.46
4:D:174:PRO:HA	4:D:177:VAL:HB	1.97	0.46
1:A:173:THR:OG1	1:A:184:SER:OG	2.31	0.46
1:A:262:LEU:CD1	1:A:328:ARG:HH11	2.29	0.46
1:A:1143:LEU:HD21	1:A:1216:ILE:HD11	1.96	0.46
8:H:104:PHE:CD2	8:H:136:LYS:HG2	2.50	0.46
1:A:482:PHE:CE2	2:B:836:GLU:HG3	2.50	0.46
1:A:1215:ARG:HH12	1:A:1272:THR:C	2.22	0.46
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.48	0.46
2:B:35:SER:HA	2:B:811:TYR:HE2	1.79	0.46
2:B:520:GLY:O	2:B:540:SER:OG	2.33	0.46
2:B:780:VAL:HG12	2:B:817:LEU:HD23	1.96	0.46
1:A:377:PRO:HG2	1:A:493:GLN:HG3	1.96	0.46
1:A:1029:ARG:NH1	1:A:1033:GLN:OE1	2.44	0.46
1:A:1325:THR:OG1	5:E:146:HIS:O	2.28	0.46
1:A:1369:ALA:HA	1:A:1372:VAL:HG22	1.97	0.46
2:B:315:LYS:HB2	2:B:316:PRO:HD3	1.98	0.46
2:B:771:SER:OG	2:B:772:ALA:N	2.48	0.46
3:C:180:TYR:HB3	3:C:228:PHE:CD1	2.50	0.46
1:A:782:ARG:HB3	1:A:789:LYS:HA	1.98	0.46
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.15	0.46
3:C:208:GLU:H	3:C:208:GLU:CD	2.24	0.46
1:A:1352:VAL:HG12	1:A:1368:MET:HE2	1.98	0.46
2:B:293:PRO:HD2	2:B:296:GLU:HB3	1.97	0.46
2:B:313:MET:HE3	2:B:313:MET:HB2	1.73	0.46
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.98	0.46
7:G:1:MET:HE1	7:G:80:LYS:H	1.80	0.46
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.16	0.46
1:A:613:ILE:HG22	1:A:614:PHE:HD2	1.81	0.46
1:A:640:GLN:H	1:A:640:GLN:CD	2.24	0.46
1:A:784:LEU:C	1:A:786:HIS:H	2.24	0.46
1:A:802:ASN:HA	1:A:806:ARG:NH2	2.22	0.46
1:A:1001:ARG:O	6:F:80:ALA:HB1	2.15	0.46
2:B:286:PHE:HE2	2:B:301:ILE:HD11	1.81	0.46
3:C:16:ASP:C	3:C:240:VAL:HG11	2.41	0.46
3:C:124:LEU:HD13	3:C:127:ARG:H	1.81	0.46
5:E:124:VAL:HG23	5:E:125:PRO:CD	2.45	0.46
11:K:53:ASP:O	11:K:56:VAL:HG12	2.16	0.46
1:A:597:LEU:HD21	8:H:103:LYS:HG2	1.98	0.46
2:B:706:GLN:OE1	2:B:708:GLU:N	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:ARG:NH2	14:W:24:DT:OP1	2.49	0.46
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.51	0.45
5:E:84:ASP:OD1	5:E:85:GLU:N	2.49	0.45
1:A:62:ASP:OD1	1:A:65:LEU:HB2	2.17	0.45
1:A:672:ASP:O	1:A:673:GLY:C	2.60	0.45
1:A:1356:ILE:HD12	1:A:1368:MET:HE3	1.98	0.45
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.15	0.45
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.98	0.45
8:H:80:ARG:HG2	8:H:81:PRO:HD2	1.98	0.45
1:A:1202:MET:O	1:A:1206:ASP:HA	2.17	0.45
2:B:361:LEU:N	2:B:362:PRO:HD3	2.31	0.45
1:A:41:MET:HB2	1:A:49:LYS:HA	1.98	0.45
1:A:55:ASP:C	1:A:57:ARG:N	2.73	0.45
1:A:244:PRO:N	1:A:245:PRO:HD2	2.31	0.45
1:A:833:GLU:O	1:A:834:THR:C	2.59	0.45
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.51	0.45
1:A:1336:MET:HE3	1:A:1380:GLY:HA2	1.98	0.45
3:C:27:LEU:HD13	3:C:228:PHE:CE1	2.52	0.45
5:E:147:HIS:HB3	5:E:150:VAL:HG12	1.99	0.45
10:J:30:LEU:HD23	10:J:30:LEU:HA	1.79	0.45
1:A:32:VAL:HG12	1:A:33:ALA:N	2.32	0.45
1:A:1318:THR:OG1	5:E:141:VAL:HG21	2.17	0.45
2:B:214:ALA:HB1	2:B:406:LEU:HD13	1.98	0.45
2:B:1166:CYS:O	2:B:1168:LEU:N	2.46	0.45
1:A:262:LEU:HD21	1:A:325:ILE:HG12	1.97	0.45
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.47	0.45
1:A:1436:ILE:O	1:A:1439:GLY:N	2.39	0.45
2:B:415:GLN:O	2:B:419:THR:OG1	2.30	0.45
2:B:234:ILE:HG12	2:B:257:LYS:HD3	1.99	0.45
2:B:276:ILE:HD13	2:B:276:ILE:HA	1.80	0.45
2:B:287:ARG:HH21	2:B:294:ASP:HB3	1.81	0.45
2:B:807:ARG:H	2:B:1045:SER:HB3	1.80	0.45
2:B:942:ARG:NH2	14:W:23:DC:OP1	2.46	0.45
3:C:48:SER:HB3	12:L:66:GLN:NE2	2.31	0.45
4:D:198:LEU:O	4:D:200:ASN:N	2.50	0.45
12:L:61:THR:C	12:L:63:ARG:H	2.24	0.45
1:A:617:VAL:C	1:A:618:GLU:OE1	2.60	0.45
1:A:1360:GLY:O	1:A:1362:TYR:N	2.50	0.45
2:B:528:PRO:HG3	2:B:536:VAL:CG2	2.45	0.45
2:B:846:ILE:HA	2:B:850:LEU:HB3	1.98	0.45
2:B:893:LEU:HD23	2:B:899:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:HD12	3:C:129:ILE:HD11	1.99	0.45
1:A:481:ASP:HB2	2:B:837:ASP:OD2	2.16	0.45
1:A:987:VAL:HG23	1:A:988:LEU:HD12	1.99	0.45
2:B:368:GLU:C	2:B:370:PHE:H	2.24	0.45
3:C:62:PHE:O	3:C:66:ARG:HG3	2.17	0.45
4:D:207:LEU:HG	4:D:211:LEU:HD23	1.99	0.45
8:H:18:GLY:C	8:H:20:TYR:H	2.25	0.45
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.52	0.45
2:B:113:TYR:HD1	2:B:114:PRO:HD2	1.81	0.45
2:B:790:ASP:N	2:B:790:ASP:OD1	2.49	0.45
3:C:238:ILE:HD11	3:C:246:ARG:NH2	2.30	0.45
5:E:113:GLN:HA	5:E:137:GLU:HG2	1.99	0.45
1:A:830:LYS:HE3	1:A:830:LYS:HB3	1.74	0.44
1:A:860:LEU:HB2	1:A:862:ASN:ND2	2.31	0.44
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.31	0.44
2:B:529:GLU:O	2:B:529:GLU:HG3	2.17	0.44
3:C:193:TYR:HB3	3:C:197:SER:HA	1.99	0.44
5:E:123:LEU:HD23	5:E:123:LEU:H	1.82	0.44
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.52	0.44
1:A:564:ALA:O	8:H:97:MET:HB2	2.18	0.44
1:A:849:MET:HA	1:A:1064:VAL:HG12	1.99	0.44
1:A:1195:LEU:HD23	1:A:1195:LEU:H	1.81	0.44
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.98	0.44
2:B:324:ILE:HG13	2:B:329:THR:HB	1.98	0.44
2:B:487:THR:HG22	2:B:489:SER:H	1.82	0.44
5:E:83:CYS:HB2	5:E:110:PHE:HZ	1.82	0.44
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.98	0.44
1:A:356:ASP:HB3	1:A:359:LEU:HB2	2.00	0.44
1:A:360:GLU:HB2	1:A:363:GLN:HG2	1.99	0.44
2:B:118:ARG:NH1	2:B:788:ARG:HD2	2.32	0.44
2:B:165:VAL:HG21	2:B:446:LEU:HD12	1.99	0.44
2:B:465:ASN:HA	2:B:477:ALA:HA	1.99	0.44
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.83	0.44
3:C:89:GLU:O	3:C:90:ASP:HB2	2.17	0.44
13:X:9:G:H1	14:W:20:DC:N4	2.16	0.44
2:B:986:GLN:HE22	2:B:1020:ARG:HD2	1.82	0.44
8:H:11:GLN:HG2	8:H:55:LEU:HG	1.99	0.44
1:A:362:ASP:OD1	1:A:362:ASP:N	2.42	0.44
1:A:447:GLN:HB2	1:A:448:PRO:HD3	1.98	0.44
7:G:35:GLU:OE2	7:G:47:CYS:HA	2.17	0.44
7:G:44:TYR:HB2	7:G:79:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:HB	1:A:134:ARG:HB3	1.99	0.44
1:A:483:ASP:HB2	2:B:987:LYS:HB3	2.00	0.44
1:A:1212:VAL:HG23	1:A:1273:LEU:HD21	2.00	0.44
1:A:1229:SER:OG	1:A:1230:GLU:N	2.44	0.44
2:B:219:ALA:HB2	2:B:405:ARG:HG2	2.00	0.44
1:A:555:ASP:OD2	1:A:644:LYS:HG2	2.18	0.44
2:B:210:LYS:HD3	2:B:461:LEU:O	2.17	0.44
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.00	0.44
2:B:510:LYS:C	2:B:512:ARG:H	2.26	0.44
2:B:797:TYR:O	10:J:1:MET:HG2	2.18	0.44
2:B:827:ILE:HD11	2:B:1014:PRO:HA	1.99	0.44
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.17	0.44
5:E:90:VAL:HB	5:E:119:SER:HB3	2.00	0.44
11:K:77:THR:HB	11:K:81:TYR:HD2	1.83	0.44
1:A:92:HIS:HE2	1:A:1410:PHE:HE1	1.65	0.44
1:A:149:GLU:HG2	1:A:152:VAL:HG21	2.00	0.44
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.50	0.44
1:A:693:VAL:HG13	1:A:714:PHE:HE1	1.83	0.44
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	2.00	0.44
2:B:128:LEU:HB2	2:B:167:ILE:HB	2.00	0.44
2:B:847:ASP:OD2	11:K:6:ARG:NH1	2.51	0.44
7:G:23:LYS:O	7:G:27:LYS:HG3	2.18	0.44
8:H:114:VAL:O	8:H:124:ARG:HA	2.18	0.44
1:A:203:SER:O	1:A:206:GLU:HG2	2.17	0.43
1:A:775:ILE:HG12	1:A:797:LYS:HA	2.00	0.43
2:B:956:THR:HG23	12:L:46:VAL:HG21	2.00	0.43
9:I:111:THR:HG21	9:I:118:ARG:HG2	2.00	0.43
13:X:8:G:H2'	13:X:9:G:C8	2.53	0.43
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.99	0.43
11:K:94:ILE:O	11:K:98:LEU:HG	2.18	0.43
11:K:109:TRP:C	11:K:111:LEU:H	2.26	0.43
1:A:210:ILE:HD12	1:A:210:ILE:HA	1.90	0.43
1:A:666:ILE:O	1:A:670:ILE:HG23	2.18	0.43
1:A:852:TYR:CZ	6:F:136:ARG:HG2	2.54	0.43
1:A:423:ASP:CG	1:A:424:ILE:H	2.25	0.43
1:A:475:THR:O	1:A:476:SER:C	2.60	0.43
2:B:393:LYS:NZ	2:B:394:ASP:O	2.27	0.43
2:B:401:PHE:HB2	2:B:518:HIS:CD2	2.53	0.43
2:B:483:LEU:HD12	2:B:484:ASN:N	2.26	0.43
2:B:530:GLY:O	2:B:533:CYS:N	2.50	0.43
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:THR:HG22	8:H:59:ILE:H	1.83	0.43
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.51	0.43
2:B:118:ARG:HG2	2:B:204:ILE:HD13	2.01	0.43
4:D:157:GLN:HA	4:D:160:VAL:HG22	2.01	0.43
7:G:26:LEU:HD12	7:G:26:LEU:HA	1.78	0.43
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.43
1:A:205:GLU:CD	1:A:205:GLU:H	2.27	0.43
1:A:826:ASP:O	1:A:828:ALA:N	2.46	0.43
1:A:1191:TRP:CZ2	1:A:1257:ASP:OD1	2.72	0.43
2:B:257:LYS:HG3	2:B:259:TYR:HE1	1.84	0.43
2:B:530:GLY:C	2:B:532:ALA:N	2.75	0.43
2:B:956:THR:HA	2:B:961:LEU:O	2.19	0.43
5:E:128:PRO:HA	5:E:129:PRO:HA	1.77	0.43
8:H:6:PHE:O	8:H:58:THR:HG23	2.18	0.43
10:J:57:ILE:O	10:J:61:LEU:HG	2.18	0.43
1:A:49:LYS:CE	1:A:55:ASP:HB2	2.49	0.43
1:A:95:PHE:O	1:A:99:ILE:HG13	2.19	0.43
1:A:527:THR:O	1:A:531:ILE:HB	2.19	0.43
1:A:973:ILE:H	1:A:973:ILE:HG13	1.61	0.43
2:B:254:LEU:HD22	2:B:381:MET:HE1	2.01	0.43
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.83	0.43
2:B:698:GLU:HA	2:B:701:ILE:HD11	2.00	0.43
2:B:861:ASP:OD2	2:B:914:LYS:NZ	2.44	0.43
2:B:1179:GLN:HG3	2:B:1188:LYS:HZ1	1.83	0.43
5:E:42:PHE:O	5:E:46:TYR:HB2	2.17	0.43
12:L:33:GLU:H	12:L:33:GLU:CD	2.25	0.43
12:L:48:CYS:O	12:L:52:GLY:N	2.52	0.43
1:A:350:ARG:HH12	1:A:447:GLN:CD	2.19	0.43
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	2.01	0.43
8:H:132:LEU:HD23	8:H:132:LEU:H	1.82	0.43
11:K:58:PHE:HE1	11:K:74:ARG:HB3	1.84	0.43
12:L:30:ILE:HG22	12:L:31:CYS:H	1.83	0.43
2:B:361:LEU:HB3	2:B:364:ILE:HD12	1.99	0.43
2:B:637:LEU:HD12	2:B:637:LEU:HA	1.81	0.43
2:B:837:ASP:O	2:B:988:GLY:HA2	2.19	0.43
3:C:252:GLN:HE22	11:K:102:LYS:HD2	1.84	0.43
2:B:760:ASP:OD1	2:B:760:ASP:N	2.52	0.43
2:B:910:VAL:HA	2:B:940:PRO:HA	2.00	0.43
5:E:123:LEU:O	5:E:126:SER:OG	2.37	0.43
7:G:47:CYS:O	7:G:77:VAL:HG12	2.17	0.43
10:J:26:GLN:O	10:J:29:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HA	1:A:222:LEU:HB3	1.99	0.42
1:A:283:GLY:O	1:A:285:PRO:HD3	2.19	0.42
1:A:451:HIS:HE1	1:A:515:GLN:NE2	2.17	0.42
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.01	0.42
1:A:977:LYS:HA	1:A:977:LYS:HD3	1.74	0.42
1:A:1320:PRO:HD2	5:E:7:ARG:HH22	1.84	0.42
1:A:1445:ILE:H	1:A:1445:ILE:HG13	1.64	0.42
2:B:192:LEU:HD23	2:B:192:LEU:HA	1.84	0.42
2:B:285:ILE:H	2:B:285:ILE:HG13	1.68	0.42
2:B:365:THR:HG23	2:B:367:LEU:H	1.84	0.42
2:B:469:GLN:HB2	2:B:470:LYS:H	1.59	0.42
2:B:752:ALA:O	2:B:754:SER:N	2.52	0.42
9:I:91:ARG:HA	9:I:91:ARG:HH11	1.84	0.42
1:A:453:MET:HB3	1:A:477:PRO:HB3	2.00	0.42
1:A:757:ASN:HD22	2:B:1021:MET:HE3	1.83	0.42
1:A:1445:ILE:HG22	6:F:131:PRO:O	2.19	0.42
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.00	0.42
2:B:542:MET:SD	2:B:747:MET:HG3	2.59	0.42
2:B:617:ARG:CZ	2:B:619:ILE:HG13	2.49	0.42
3:C:259:LEU:HD22	3:C:259:LEU:H	1.85	0.42
4:D:121:LYS:HB3	4:D:121:LYS:HE3	1.74	0.42
7:G:41:LYS:HE2	7:G:41:LYS:HB3	1.93	0.42
12:L:47:ARG:O	12:L:49:LYS:N	2.52	0.42
1:A:879:GLU:HG2	1:A:880:LYS:N	2.34	0.42
1:A:901:LEU:HA	1:A:907:THR:HG23	2.02	0.42
2:B:528:PRO:CD	2:B:536:VAL:HG23	2.49	0.42
2:B:899:ILE:HD13	2:B:949:VAL:HG21	2.01	0.42
3:C:248:ILE:H	3:C:248:ILE:HG13	1.70	0.42
4:D:188:ALA:HA	4:D:191:ALA:HB3	2.01	0.42
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.85	0.42
7:G:116:PRO:HG3	7:G:164:LYS:HA	2.01	0.42
8:H:8:ASP:OD1	8:H:30:SER:OG	2.35	0.42
1:A:1135:ARG:O	1:A:1139:GLU:HB2	2.20	0.42
1:A:1318:THR:OG1	5:E:141:VAL:CG2	2.68	0.42
2:B:307:ASP:O	2:B:311:LEU:HD12	2.20	0.42
4:D:118:THR:HG22	4:D:121:LYS:HE2	2.01	0.42
1:A:149:GLU:HB2	1:A:164:ARG:NH1	2.34	0.42
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.41	0.42
1:A:1118:VAL:HG13	1:A:1306:LEU:HB2	2.02	0.42
2:B:37:PHE:CE2	2:B:542:MET:HA	2.54	0.42
2:B:299:GLU:HB3	2:B:572:HIS:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HG11	2.00	0.42
9:I:91:ARG:HA	9:I:91:ARG:NH1	2.34	0.42
1:A:476:SER:O	1:A:479:ASN:N	2.52	0.42
2:B:54:PHE:HA	2:B:58:THR:OG1	2.20	0.42
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.02	0.42
2:B:635:ARG:HH22	2:B:742:GLU:CD	2.27	0.42
2:B:1166:CYS:C	2:B:1168:LEU:H	2.26	0.42
5:E:163:GLU:O	5:E:167:ARG:HG2	2.20	0.42
6:F:116:ASP:OD1	6:F:117:PRO:HD2	2.19	0.42
10:J:1:MET:O	10:J:2:ILE:HG22	2.19	0.42
1:A:149:GLU:HG2	1:A:152:VAL:CG2	2.50	0.42
1:A:451:HIS:HB2	1:A:454:SER:OG	2.19	0.42
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.59	0.42
1:A:840:ARG:HB3	1:A:1402:PHE:CZ	2.53	0.42
1:A:842:VAL:HG12	1:A:1069:ALA:CB	2.50	0.42
1:A:862:ASN:OD1	5:E:174:GLN:HA	2.19	0.42
2:B:851:PHE:HD1	2:B:1094:ARG:HB2	1.85	0.42
2:B:1031:LEU:HD21	2:B:1042:GLY:HA3	2.02	0.42
7:G:1:MET:CE	7:G:2:PHE:H	2.30	0.42
8:H:105:GLU:HB2	8:H:113:ALA:HB3	2.02	0.42
1:A:216:VAL:HA	1:A:219:PHE:CE1	2.54	0.42
1:A:453:MET:HE3	1:A:513:SER:HB2	2.02	0.42
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.50	0.42
2:B:294:ASP:HB2	2:B:318:VAL:HG13	2.02	0.42
2:B:480:SER:O	2:B:480:SER:OG	2.34	0.42
2:B:661:LEU:O	2:B:663:ALA:N	2.53	0.42
5:E:109:ILE:HG12	5:E:133:GLU:HB2	2.02	0.42
7:G:22:MET:HE2	7:G:22:MET:HB3	1.82	0.42
1:A:103:CYS:O	1:A:108:MET:HE1	2.20	0.42
1:A:230:ARG:HB2	1:A:233:TRP:CD2	2.55	0.42
2:B:221:ASN:ND2	2:B:243:ALA:O	2.51	0.42
2:B:251:ILE:H	2:B:251:ILE:HG13	1.67	0.42
2:B:581:PHE:O	2:B:626:ILE:N	2.51	0.42
2:B:846:ILE:HG22	2:B:850:LEU:HB3	2.02	0.42
3:C:258:ILE:HD11	11:K:42:LEU:HD21	2.01	0.42
5:E:83:CYS:HB2	5:E:110:PHE:CZ	2.54	0.42
5:E:103:LYS:HA	5:E:103:LYS:HD2	1.81	0.42
8:H:57:VAL:HA	8:H:143:LEU:O	2.20	0.42
1:A:592:ASP:H	1:A:595:THR:CG2	2.32	0.42
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.65	0.42
2:B:21:GLU:HA	2:B:656:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASP:CG	2:B:658:ILE:HG12	2.45	0.42
2:B:108:VAL:HG23	2:B:109:THR:N	2.27	0.42
2:B:128:LEU:HB3	2:B:167:ILE:HD12	2.01	0.42
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.85	0.42
2:B:1167:GLY:N	2:B:1215:ARG:HG2	2.35	0.42
6:F:75:PRO:HB2	6:F:77:ASP:OD1	2.20	0.42
1:A:821:ARG:HH21	2:B:525:ALA:N	2.18	0.41
1:A:1153:TYR:HB2	1:A:1192:LEU:HB3	2.01	0.41
2:B:362:PRO:C	2:B:364:ILE:H	2.28	0.41
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.29	0.41
2:B:969:ARG:NH2	3:C:60:ASP:CB	2.81	0.41
2:B:1006:ILE:HG13	10:J:43:ARG:HD2	2.02	0.41
3:C:164:ALA:HA	3:C:167:HIS:O	2.20	0.41
7:G:88:ASP:OD1	7:G:144:ARG:HG3	2.20	0.41
1:A:423:ASP:OD1	1:A:424:ILE:N	2.46	0.41
1:A:534:LEU:O	1:A:574:GLY:HA3	2.20	0.41
1:A:1188:GLN:HA	1:A:1243:VAL:HA	2.01	0.41
2:B:51:PHE:HE2	2:B:172:ILE:HG23	1.85	0.41
2:B:461:LEU:HD23	2:B:461:LEU:HA	1.81	0.41
2:B:546:SER:OG	2:B:632:ARG:N	2.49	0.41
2:B:661:LEU:O	2:B:664:THR:HG23	2.20	0.41
2:B:842:ASN:HB3	2:B:845:SER:HB2	2.02	0.41
2:B:975:GLN:O	2:B:990:ILE:HD12	2.20	0.41
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.20	0.41
1:A:517:ASN:O	1:A:517:ASN:ND2	2.53	0.41
1:A:809:THR:HB	1:A:810:PRO:HD2	2.03	0.41
2:B:824:ILE:HA	2:B:1089:PRO:HA	2.02	0.41
3:C:131:HIS:HA	3:C:132:PRO:HD3	1.95	0.41
4:D:61:GLU:HA	4:D:64:VAL:HG12	2.02	0.41
1:A:308:ILE:HG22	1:A:309:ALA:H	1.85	0.41
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.02	0.41
1:A:870:GLU:OE1	5:E:202:SER:HB2	2.21	0.41
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.35	0.41
1:A:1209:MET:HA	1:A:1212:VAL:HG12	2.02	0.41
1:A:1366:ARG:H	1:A:1366:ARG:HG2	1.71	0.41
2:B:595:ARG:HA	2:B:598:GLU:HG3	2.02	0.41
2:B:601:ARG:O	2:B:605:ARG:HG3	2.21	0.41
2:B:752:ALA:O	2:B:755:ILE:HG12	2.20	0.41
2:B:1017:ILE:N	2:B:1018:PRO:CD	2.77	0.41
3:C:183:TRP:CD1	3:C:183:TRP:N	2.87	0.41
5:E:96:PHE:O	5:E:99:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG11	1:A:57:ARG:O	2.19	0.41
1:A:105:CYS:SG	1:A:139:TRP:HA	2.61	0.41
1:A:314:ALA:O	1:A:322:VAL:HG12	2.19	0.41
1:A:372:LYS:O	1:A:435:HIS:NE2	2.54	0.41
1:A:535:THR:O	1:A:575:LYS:NZ	2.50	0.41
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.84	0.41
1:A:974:ASP:OD2	1:A:976:THR:OG1	2.31	0.41
2:B:197:PHE:CD2	2:B:817:LEU:HD11	2.55	0.41
2:B:523:CYS:SG	2:B:750:GLY:N	2.94	0.41
2:B:665:GLU:H	2:B:665:GLU:HG2	1.49	0.41
12:L:54:ARG:H	12:L:54:ARG:HD2	1.85	0.41
1:A:537:ARG:HG2	8:H:20:TYR:HE2	1.84	0.41
1:A:959:ASN:O	1:A:963:ILE:HG13	2.20	0.41
2:B:406:LEU:HD12	2:B:406:LEU:C	2.45	0.41
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.03	0.41
3:C:134:ILE:HG21	3:C:139:GLY:HA2	2.03	0.41
3:C:183:TRP:HE1	3:C:207:CYS:CB	2.32	0.41
3:C:251:LEU:O	3:C:255:VAL:HG12	2.21	0.41
5:E:144:ILE:O	5:E:150:VAL:HG11	2.21	0.41
9:I:7:CYS:HB2	9:I:14:LEU:HD21	2.02	0.41
11:K:58:PHE:CE1	11:K:74:ARG:HB3	2.55	0.41
1:A:663:SER:HB3	2:B:1085:ILE:HD12	2.02	0.41
1:A:783:THR:HG21	1:A:796:SER:O	2.20	0.41
1:A:1330:ASN:O	1:A:1332:PHE:N	2.53	0.41
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.02	0.41
2:B:113:TYR:CE1	2:B:192:LEU:HD21	2.55	0.41
2:B:916:THR:O	2:B:935:ARG:HB3	2.21	0.41
5:E:71:LYS:C	5:E:73:PRO:HD3	2.46	0.41
13:X:8:G:H2'	13:X:9:G:H8	1.85	0.41
1:A:46:THR:C	1:A:48:ALA:H	2.28	0.41
1:A:846:GLU:HA	1:A:1066:VAL:HB	2.02	0.41
2:B:206:ASN:OD1	2:B:458:LYS:HE2	2.21	0.41
3:C:262:LEU:HD11	11:K:88:LYS:HG2	2.02	0.41
9:I:19:ASP:CB	9:I:24:ARG:HG2	2.50	0.41
1:A:99:ILE:HG23	1:A:211:PHE:HE2	1.86	0.41
1:A:303:TYR:O	1:A:325:ILE:HG13	2.21	0.41
1:A:446:ARG:HD2	1:A:480:ALA:CB	2.42	0.41
1:A:588:LEU:HD13	1:A:632:VAL:HG21	2.03	0.41
1:A:765:VAL:HB	1:A:800:VAL:CG2	2.50	0.41
1:A:1121:GLU:H	1:A:1121:GLU:HG3	1.73	0.41
1:A:1155:ASP:O	1:A:1241:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:NH2	2:B:956:THR:O	2.49	0.41
2:B:546:SER:OG	2:B:631:GLY:N	2.35	0.41
2:B:597:MET:HE2	2:B:597:MET:HB3	1.92	0.41
2:B:1079:LYS:HE3	2:B:1079:LYS:HB2	1.77	0.41
3:C:260:LEU:HD23	3:C:264:GLN:HE21	1.86	0.41
5:E:67:GLU:OE1	5:E:67:GLU:N	2.49	0.41
7:G:20:PRO:HB2	7:G:21:ARG:H	1.64	0.41
7:G:101:VAL:HG12	7:G:103:VAL:HG23	2.03	0.41
7:G:111:THR:O	7:G:115:MET:HG3	2.21	0.41
1:A:91:PHE:HD2	1:A:297:GLN:NE2	2.18	0.41
1:A:443:LEU:HB3	1:A:490:HIS:HB2	2.03	0.41
1:A:907:THR:HG22	1:A:908:LEU:N	2.36	0.41
2:B:464:GLY:O	2:B:479:VAL:HG12	2.21	0.41
2:B:619:ILE:H	2:B:619:ILE:HD12	1.86	0.41
2:B:972:LYS:HD3	2:B:1098:MET:HE3	2.03	0.41
1:A:457:ALA:O	1:A:507:VAL:HG23	2.21	0.40
1:A:466:SER:HB3	2:B:1103:ILE:HD12	2.03	0.40
1:A:747:VAL:HG22	1:A:753:GLY:CA	2.40	0.40
1:A:783:THR:HG21	1:A:796:SER:HB2	2.03	0.40
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	2.19	0.40
3:C:240:VAL:O	3:C:243:VAL:HG12	2.21	0.40
5:E:3:GLN:HG3	5:E:5:ASN:H	1.85	0.40
5:E:52:ARG:N	5:E:53:PRO:CD	2.84	0.40
7:G:6:ASP:OD2	7:G:75:ARG:NH2	2.35	0.40
7:G:109:PHE:O	7:G:161:GLY:N	2.40	0.40
1:A:19:PHE:HZ	1:A:1397:LEU:HD21	1.86	0.40
1:A:500:GLU:O	1:A:504:LEU:HB2	2.21	0.40
1:A:618:GLU:OE1	1:A:618:GLU:N	2.54	0.40
1:A:106:VAL:HG21	1:A:214:ILE:CD1	2.50	0.40
1:A:1119:TYR:CE2	1:A:1326:ARG:HG2	2.56	0.40
2:B:535:LEU:HD23	2:B:535:LEU:HA	1.84	0.40
2:B:901:PRO:HD2	12:L:59:ALA:O	2.22	0.40
2:B:901:PRO:HB2	12:L:60:ARG:HG2	2.04	0.40
10:J:2:ILE:HD12	10:J:2:ILE:HA	1.96	0.40
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.96	0.40
1:A:554:PRO:HD2	1:A:648:ASN:OD1	2.22	0.40
1:A:575:LYS:H	1:A:575:LYS:HG3	1.65	0.40
1:A:1203:ASN:OD1	1:A:1203:ASN:N	2.54	0.40
2:B:51:PHE:CD2	2:B:173:MET:HG2	2.56	0.40
2:B:130:VAL:O	2:B:165:VAL:N	2.55	0.40
2:B:792:MET:HE3	2:B:855:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:GLN:O	2:B:836:GLU:C	2.65	0.40
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.53	0.40
1:A:472:LEU:CD1	2:B:835:GLN:HE21	2.35	0.40
1:A:826:ASP:HA	1:A:830:LYS:HG3	2.02	0.40
1:A:1006:ILE:HD12	1:A:1006:ILE:H	1.86	0.40
2:B:124:TYR:HB2	2:B:204:ILE:HB	2.04	0.40
3:C:260:LEU:O	3:C:264:GLN:HG3	2.21	0.40
7:G:121:PHE:CE2	7:G:123:ALA:HB2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1358/1733 (78%)	1135 (84%)	169 (12%)	54 (4%)	2	15
2	B	1036/1224 (85%)	869 (84%)	129 (12%)	38 (4%)	2	16
3	C	264/318 (83%)	239 (90%)	19 (7%)	6 (2%)	5	23
4	D	156/221 (71%)	133 (85%)	15 (10%)	8 (5%)	1	10
5	E	202/215 (94%)	181 (90%)	17 (8%)	4 (2%)	6	25
6	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	10	35
7	G	169/171 (99%)	141 (83%)	19 (11%)	9 (5%)	1	10
8	H	107/146 (73%)	84 (78%)	19 (18%)	4 (4%)	2	16
9	I	117/122 (96%)	99 (85%)	12 (10%)	6 (5%)	1	10
10	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	3	17
11	K	113/120 (94%)	102 (90%)	10 (9%)	1 (1%)	14	42
12	L	41/70 (59%)	21 (51%)	15 (37%)	5 (12%)	0	1
All	All	3708/4565 (81%)	3131 (84%)	439 (12%)	138 (4%)	2	16

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	76	GLU
1	A	119	ASN
1	A	131	SER
1	A	424	ILE
1	A	476	SER
1	A	567	LYS
1	A	674	PRO
1	A	1437	GLY
2	B	277	LYS
2	B	365	THR
2	B	1156	ASP
4	D	55	ALA
4	D	56	ARG
7	G	63	PRO
8	H	17	PRO
10	J	2	ILE
1	A	40	THR
1	A	55	ASP
1	A	74	MET
1	A	148	CYS
1	A	178	GLY
1	A	282	ASN
1	A	309	ALA
1	A	706	HIS
1	A	827	THR
1	A	846	GLU
1	A	997	LEU
1	A	1107	VAL
1	A	1108	ALA
1	A	1123	GLY
1	A	1365	TYR
1	A	1377	THR
2	B	108	VAL
2	B	250	PHE
2	B	305	VAL
2	B	369	GLY
2	B	422	LYS
2	B	466	TRP
2	B	1046	PRO
2	B	1177	HIS
2	B	1186	ASP

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Mol	Chain	Res	Type
3	C	149	LYS
4	D	119	ARG
5	E	3	GLN
7	G	20	PRO
7	G	139	ILE
7	G	154	VAL
8	H	61	SER
8	H	62	SER
9	I	58	VAL
1	A	332	LYS
1	A	394	ASN
1	A	584	ASN
1	A	828	ALA
1	A	1331	SER
1	A	1361	SER
2	B	106	ASP
2	B	260	GLY
2	B	531	GLN
2	B	662	MET
2	B	711	GLU
2	B	792	MET
2	B	1157	ALA
3	C	184	ASN
3	C	227	THR
4	D	8	PHE
4	D	44	GLU
4	D	199	ASN
7	G	2	PHE
9	I	59	VAL
9	I	60	GLN
12	L	43	THR
12	L	56	LEU
12	L	62	LYS
1	A	54	ASN
1	A	128	ILE
1	A	423	ASP
1	A	447	GLN
1	A	475	THR
1	A	599	SER
1	A	673	GLY
1	A	694	THR
1	A	847	ASP

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Mol	Chain	Res	Type
1	A	958	VAL
1	A	1140	HIS
1	A	1362	TYR
1	A	1378	GLN
1	A	1394	THR
2	B	830	TYR
2	B	1017	ILE
2	B	1108	ARG
2	B	1143	ALA
3	C	75	MET
3	C	90	ASP
4	D	36	LYS
4	D	198	LEU
9	I	47	GLU
12	L	39	SER
12	L	48	CYS
1	A	334	GLY
1	A	479	ASN
1	A	525	GLN
1	A	585	GLY
2	B	24	PRO
2	B	111	ALA
2	B	525	ALA
2	B	937	ALA
2	B	987	LYS
2	B	1089	PRO
2	B	1125	ASP
2	B	1223	ASP
3	C	214	ASN
7	G	170	ALA
11	K	54	ARG
1	A	151	ASP
2	B	107	GLY
2	B	753	ALA
2	B	1155	SER
6	F	73	ALA
7	G	136	VAL
7	G	157	ILE
8	H	21	ASN
10	J	29	GLU
1	A	569	LYS
1	A	1435	PRO

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Mol	Chain	Res	Type
2	B	247	GLY
1	A	52	GLY
1	A	152	VAL
7	G	45	ILE
2	B	974	PRO
2	B	1167	GLY
5	E	27	GLY
5	E	125	PRO
9	I	57	GLY
9	I	84	VAL
2	B	520	GLY
5	E	129	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1204/1520 (79%)	1134 (94%)	70 (6%)	18	45
2	B	918/1061 (86%)	864 (94%)	54 (6%)	18	44
3	C	234/274 (85%)	227 (97%)	7 (3%)	36	59
4	D	144/200 (72%)	133 (92%)	11 (8%)	12	38
5	E	192/197 (98%)	185 (96%)	7 (4%)	31	56
6	F	74/137 (54%)	73 (99%)	1 (1%)	59	70
7	G	152/152 (100%)	141 (93%)	11 (7%)	13	39
8	H	104/128 (81%)	99 (95%)	5 (5%)	23	50
9	I	113/116 (97%)	107 (95%)	6 (5%)	20	47
10	J	60/65 (92%)	58 (97%)	2 (3%)	33	57
11	K	99/102 (97%)	96 (97%)	3 (3%)	36	59
12	L	38/57 (67%)	35 (92%)	3 (8%)	11	36
All	All	3332/4009 (83%)	3152 (95%)	180 (5%)	20	47

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	41	MET
1	A	44	THR
1	A	58	LEU
1	A	65	LEU
1	A	150	THR
1	A	199	LEU
1	A	210	ILE
1	A	252	PHE
1	A	282	ASN
1	A	295	LEU
1	A	307	ASP
1	A	308	ILE
1	A	389	THR
1	A	397	ASN
1	A	450	LEU
1	A	451	HIS
1	A	463	ILE
1	A	476	SER
1	A	481	ASP
1	A	523	ILE
1	A	538	ASP
1	A	547	LEU
1	A	560	ILE
1	A	567	LYS
1	A	607	ILE
1	A	658	LEU
1	A	666	ILE
1	A	674	PRO
1	A	698	GLN
1	A	780	VAL
1	A	829	VAL
1	A	839	ARG
1	A	841	LEU
1	A	845	LEU
1	A	867	ILE
1	A	932	GLU
1	A	960	ILE
1	A	966	ASN
1	A	983	ILE
1	A	988	LEU
1	A	1017	LEU
1	A	1037	LEU

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Mol	Chain	Res	Type
1	A	1038	THR
1	A	1046	LEU
1	A	1048	ASN
1	A	1058	VAL
1	A	1098	VAL
1	A	1148	ILE
1	A	1193	LEU
1	A	1203	ASN
1	A	1237	ILE
1	A	1260	LEU
1	A	1283	VAL
1	A	1297	GLU
1	A	1303	GLU
1	A	1313	LEU
1	A	1315	GLU
1	A	1319	VAL
1	A	1335	ILE
1	A	1355	VAL
1	A	1356	ILE
1	A	1359	ASP
1	A	1401	SER
1	A	1403	GLU
1	A	1418	LEU
1	A	1432	GLN
1	A	1445	ILE
1	A	1447	GLU
1	A	1453	TYR
2	B	25	ILE
2	B	45	SER
2	B	63	ILE
2	B	115	GLN
2	B	116	GLU
2	B	189	LEU
2	B	194	GLU
2	B	224	GLN
2	B	240	ILE
2	B	242	SER
2	B	251	ILE
2	B	286	PHE
2	B	297	ILE
2	B	299	GLU
2	B	331	LEU

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Mol	Chain	Res	Type
2	B	365	THR
2	B	469	GLN
2	B	484	ASN
2	B	549	THR
2	B	578	THR
2	B	580	VAL
2	B	582	VAL
2	B	583	ASN
2	B	624	LEU
2	B	635	ARG
2	B	661	LEU
2	B	665	GLU
2	B	693	ILE
2	B	701	ILE
2	B	706	GLN
2	B	733	HIS
2	B	751	VAL
2	B	797	TYR
2	B	827	ILE
2	B	854	LEU
2	B	885	MET
2	B	898	LEU
2	B	899	ILE
2	B	909	ASP
2	B	968	VAL
2	B	1012	ILE
2	B	1017	ILE
2	B	1020	ARG
2	B	1065	GLN
2	B	1113	VAL
2	B	1123	SER
2	B	1128	LEU
2	B	1132	GLU
2	B	1160	VAL
2	B	1168	LEU
2	B	1171	VAL
2	B	1177	HIS
2	B	1194	ILE
2	B	1196	ILE
3	C	23	SER
3	C	77	ILE
3	C	124	LEU

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Mol	Chain	Res	Type
3	C	158	VAL
3	C	166	GLU
3	C	248	ILE
3	C	255	VAL
4	D	5	THR
4	D	27	LEU
4	D	50	LEU
4	D	65	GLU
4	D	129	LEU
4	D	133	THR
4	D	134	THR
4	D	156	ASP
4	D	169	SER
4	D	211	LEU
4	D	221	TYR
5	E	60	PHE
5	E	80	VAL
5	E	126	SER
5	E	141	VAL
5	E	195	VAL
5	E	196	VAL
5	E	202	SER
6	F	136	ARG
7	G	1	MET
7	G	11	ILE
7	G	22	MET
7	G	26	LEU
7	G	45	ILE
7	G	56	ILE
7	G	91	VAL
7	G	120	THR
7	G	136	VAL
7	G	137	ILE
7	G	151	ILE
8	H	5	LEU
8	H	26	ILE
8	H	56	THR
8	H	89	LEU
8	H	143	LEU
9	I	59	VAL
9	I	62	ILE
9	I	68	LEU

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Mol	Chain	Res	Type
9	I	75	CYS
9	I	83	ASN
9	I	117	LYS
10	J	2	ILE
10	J	51	LEU
11	K	33	ILE
11	K	57	LEU
11	K	88	LYS
12	L	30	ILE
12	L	55	ILE
12	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	GLN
1	A	339	ASN
1	A	515	GLN
1	A	545	GLN
1	A	548	ASN
1	A	626	ASN
1	A	881	GLN
1	A	1211	GLN
1	A	1354	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	306	ASN
2	B	309	GLN
2	B	484	ASN
2	B	518	HIS
2	B	538	ASN
2	B	573	GLN
2	B	657	HIS
2	B	686	ASN
2	B	770	GLN
2	B	800	GLN
2	B	986	GLN
2	B	1076	HIS
2	B	1093	GLN

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Mol	Chain	Res	Type
2	B	1097	HIS
2	B	1161	HIS
2	B	1211	ASN
3	C	31	ASN
3	C	135	GLN
4	D	143	ASN
5	E	113	GLN
7	G	57	GLN
8	H	133	ASN
9	I	51	ASN
9	I	83	ASN
9	I	108	HIS
11	K	40	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	X	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	X	8	G
13	X	10	A

There are no RNA pucker outliers to report.

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
17	GOL	E	301	-	5,5,5	0.96	0	5,5,5	1.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	GOL	E	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	E	301	GOL	O1-C1-C2-O2
17	E	301	GOL	O1-C1-C2-C3
17	E	301	GOL	C1-C2-C3-O3
17	E	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	E	301	GOL	1	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1378/1733 (79%)	0.24	69 (5%) 34 25	80, 141, 219, 306	0
2	B	1060/1224 (86%)	0.32	62 (5%) 29 22	85, 149, 236, 363	0
3	C	266/318 (83%)	0.06	4 (1%) 72 57	100, 145, 209, 266	0
4	D	162/221 (73%)	0.21	4 (2%) 58 43	121, 165, 221, 274	0
5	E	208/215 (96%)	0.22	10 (4%) 35 26	102, 175, 245, 299	0
6	F	84/155 (54%)	-0.11	1 (1%) 76 63	84, 115, 168, 174	0
7	G	171/171 (100%)	0.24	4 (2%) 61 46	103, 143, 203, 251	0
8	H	117/146 (80%)	0.46	4 (3%) 48 35	150, 190, 258, 281	0
9	I	119/122 (97%)	0.39	6 (5%) 34 25	145, 194, 274, 300	0
10	J	65/70 (92%)	0.05	2 (3%) 51 38	117, 147, 212, 240	0
11	K	115/120 (95%)	-0.14	1 (0%) 81 68	102, 140, 203, 245	0
12	L	43/70 (61%)	0.36	0 100 100	120, 167, 250, 291	0
13	X	10/10 (100%)	1.32	3 (30%) 1 2	192, 251, 294, 332	0
14	W	13/13 (100%)	1.18	2 (15%) 5 7	193, 206, 258, 325	0
All	All	3811/4588 (83%)	0.24	172 (4%) 38 28	80, 150, 232, 363	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	120	GLY	7.8
2	B	836	GLU	6.6
1	A	537	ARG	6.3
1	A	56	PRO	6.2
9	I	52	ILE	5.7
2	B	839	MET	5.6
2	B	1222	ARG	5.2
2	B	1224	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	447	GLN	4.9
13	X	1	A	4.6
1	A	57	ARG	4.5
1	A	752	LYS	4.5
1	A	740	LEU	4.2
2	B	350	GLN	4.2
3	C	61	GLU	4.1
5	E	194	GLU	3.9
1	A	331	GLY	3.8
1	A	840	ARG	3.8
2	B	1173	ALA	3.7
1	A	751	SER	3.7
2	B	248	SER	3.7
5	E	26	ARG	3.7
7	G	170	ALA	3.7
1	A	59	GLY	3.6
1	A	1411	GLU	3.6
4	D	40	HIS	3.6
1	A	55	ASP	3.6
1	A	678	GLU	3.5
1	A	672	ASP	3.5
1	A	879	GLU	3.4
1	A	250	ILE	3.4
1	A	904	THR	3.4
9	I	69	PRO	3.4
1	A	49	LYS	3.4
1	A	149	GLU	3.3
1	A	323	LYS	3.3
1	A	480	ALA	3.3
1	A	1455	PRO	3.3
2	B	489	SER	3.3
2	B	969	ARG	3.3
2	B	658	ILE	3.3
1	A	1001	ARG	3.3
2	B	584	GLY	3.3
2	B	531	GLN	3.3
8	H	50	ALA	3.2
1	A	1172	LEU	3.2
2	B	351	TYR	3.2
1	A	719	VAL	3.1
10	J	6	ARG	3.1
14	W	20	DC	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	525	GLN	3.1
1	A	355	GLY	3.1
1	A	762	SER	3.1
2	B	486	TYR	3.1
1	A	1170	ILE	3.0
1	A	776	ALA	3.0
1	A	493	GLN	3.0
2	B	731	VAL	3.0
2	B	116	GLU	3.0
2	B	407	ASP	3.0
2	B	728	ARG	3.0
1	A	386	ASP	3.0
3	C	149	LYS	3.0
2	B	843	GLN	2.9
5	E	131	THR	2.9
6	F	72	LYS	2.9
8	H	107	VAL	2.9
5	E	12	LEU	2.9
5	E	109	ILE	2.9
9	I	13	MET	2.9
1	A	1098	VAL	2.9
1	A	829	VAL	2.8
2	B	246	LYS	2.8
8	H	63	LEU	2.8
5	E	215	MET	2.8
2	B	837	ASP	2.8
1	A	1161	THR	2.7
2	B	774	GLY	2.7
1	A	36	ARG	2.7
1	A	335	ARG	2.7
1	A	399	HIS	2.7
2	B	22	SER	2.7
2	B	220	GLY	2.6
2	B	789	MET	2.6
1	A	42	ASP	2.6
4	D	220	LEU	2.6
1	A	821	ARG	2.6
9	I	15	TYR	2.6
13	X	9	G	2.6
5	E	133	GLU	2.6
1	A	834	THR	2.6
2	B	366	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	702	LEU	2.5
2	B	529	GLU	2.5
7	G	139	ILE	2.5
1	A	783	THR	2.5
1	A	827	THR	2.5
1	A	1156	PRO	2.5
2	B	328	GLU	2.5
1	A	676	MET	2.5
2	B	597	MET	2.5
2	B	392	ARG	2.5
1	A	33	ALA	2.4
2	B	349	ILE	2.4
1	A	602	ASP	2.4
2	B	894	ASP	2.4
2	B	524	PRO	2.4
2	B	247	GLY	2.4
2	B	895	ASP	2.4
10	J	28	ASP	2.4
2	B	266	ALA	2.4
13	X	8	G	2.4
4	D	122	GLU	2.4
2	B	799	PRO	2.4
2	B	651	LEU	2.4
1	A	835	GLY	2.4
2	B	886	LYS	2.4
2	B	250	PHE	2.4
14	W	21	DC	2.4
11	K	57	LEU	2.4
3	C	81	GLU	2.4
1	A	674	PRO	2.3
2	B	735	ALA	2.3
1	A	482	PHE	2.3
2	B	934	LYS	2.3
5	E	149	LEU	2.3
2	B	312	GLU	2.3
1	A	314	ALA	2.3
1	A	828	ALA	2.3
4	D	25	ALA	2.3
1	A	62	ASP	2.3
1	A	515	GLN	2.3
7	G	24	GLN	2.3
1	A	822	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	472	ALA	2.2
2	B	988	GLY	2.2
1	A	830	LYS	2.2
1	A	915	SER	2.2
9	I	102	VAL	2.2
1	A	51	GLY	2.2
2	B	92	PHE	2.2
7	G	25	TYR	2.2
2	B	729	ILE	2.2
2	B	1184	GLY	2.2
2	B	245	GLU	2.1
2	B	1068	GLY	2.1
1	A	1393	ASN	2.1
2	B	294	ASP	2.1
2	B	1223	ASP	2.1
1	A	354	SER	2.1
2	B	239	GLU	2.1
2	B	712	PRO	2.1
2	B	1019	SER	2.1
2	B	538	ASN	2.1
9	I	4	PHE	2.1
1	A	262	LEU	2.1
1	A	403	LYS	2.1
2	B	1120	GLU	2.1
1	A	710	LEU	2.1
1	A	1166	ASP	2.1
1	A	437	MET	2.1
2	B	1133	MET	2.1
2	B	106	ASP	2.1
5	E	107	THR	2.1
2	B	878	GLN	2.1
3	C	106	GLU	2.1
2	B	642	ASP	2.0
1	A	63	ARG	2.0
2	B	1062	HIS	2.0
5	E	58	MET	2.0
1	A	277	GLU	2.0
1	A	280	GLU	2.0

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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
17	GOL	E	301	6/6	0.90	0.28	177,189,192,193	0
16	MN	A	1804	1/1	0.97	0.11	30,30,30,30	1
15	ZN	L	101	1/1	0.98	0.04	166,166,166,166	0
16	MN	A	1803	1/1	0.98	0.18	30,30,30,30	0
15	ZN	I	201	1/1	0.98	0.05	150,150,150,150	0
15	ZN	I	202	1/1	0.98	0.04	215,215,215,215	0
15	ZN	B	1301	1/1	0.99	0.08	135,135,135,135	0
15	ZN	C	401	1/1	0.99	0.05	114,114,114,114	0
15	ZN	A	1801	1/1	0.99	0.03	159,159,159,159	0
15	ZN	A	1802	1/1	0.99	0.03	116,116,116,116	0
15	ZN	J	101	1/1	1.00	0.02	133,133,133,133	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.