



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 02:17 PM EDT

PDB ID : 9BVT
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

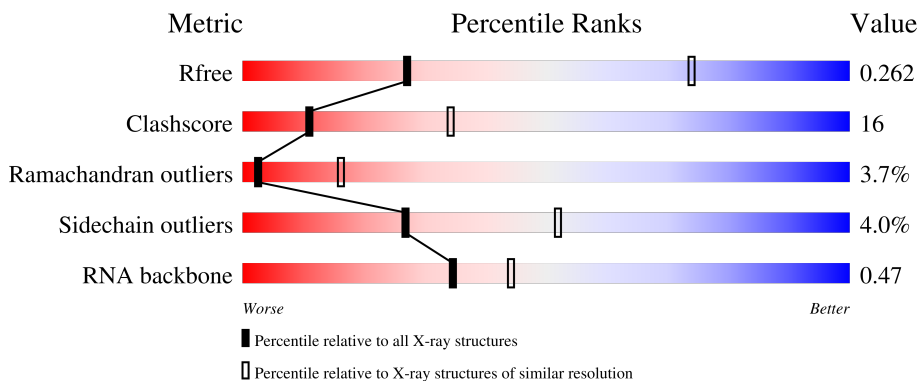
1 Overall quality at a glance

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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RNA backbone	3690	1033 (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 ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1733	48% 29% • 20%
2	B	1224	52% 32% • 13%
3	C	318	55% 26% • 16%
4	D	221	47% 25% • 27%
5	E	215	63% 31% • •
6	F	155	32% 21% • 46%

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Mol	Chain	Length	Quality of chain
7	G	171	 60% 37% .
8	H	146	 52% 27% . 20%
9	I	122	 64% 31% . .
10	J	70	 59% 30% . 7%
11	K	120	 72% 23% . .
12	L	70	 24% 31% 6% 39%
13	X	10	 70% 10% 20%
14	W	13	 62% 38%

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
			Total	C	N	O	S			
1	A	1378	10848	6846	1894	2047	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1060	8428	5349	1476	1549	54	0	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	162	1287	799	224	262	2	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	208	1713	1089	303	312	9	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	84	679	434	115	127	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	117	951	605	158	184	4	0	0	0

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

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

- 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
			Total	C	N	O	P			
13	X	10	217	98	45	65	9	0	0	0

- Molecule 14 is a DNA chain called DNA (5'-D(P*AP*CP*GP*TP*CP*CP*CP*TP*CP*T P*CP*GP*A)-3').

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

- Molecule 15 is ZINC ION (three-letter code: 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 (three-letter code: MN) (formula: Mn).

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

- Molecule 17 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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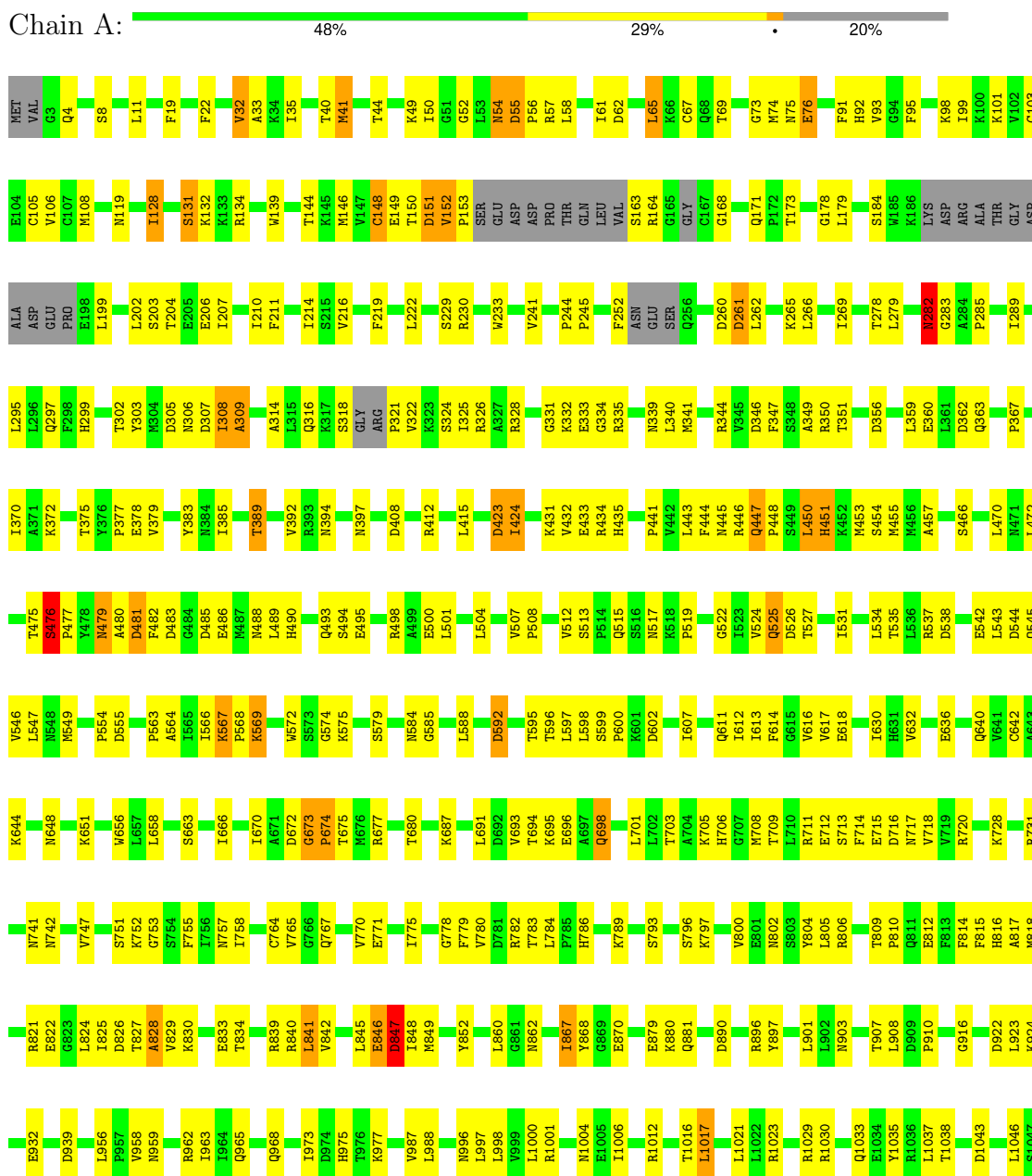
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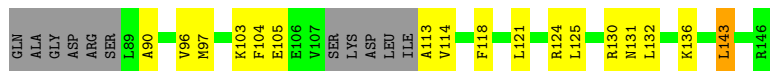
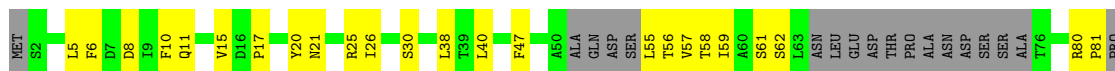
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	X	2	Total O 2 2	0	0
18	W	2	Total O 2 2	0	0

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. 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. 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

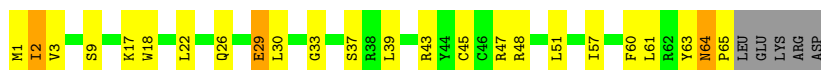




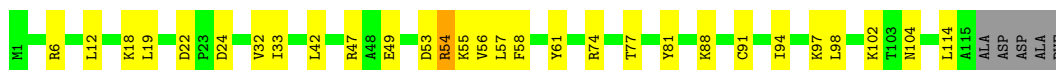
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



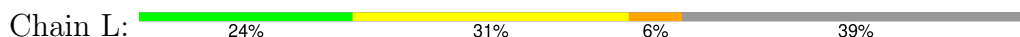
- Molecule 10: DNA-directed RNA polymerase II subunit RPABC5



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



- Molecule 12: DNA-directed RNA polymerase 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 i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.33Å)	Xtrriage
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	8254 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	92.3	Xtrriage
Anisotropy	1.597	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 145.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
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	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30742	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/11037	0.54	0/14916
2	B	0.28	0/8593	0.55	0/11585
3	C	0.25	0/2133	0.49	0/2891
4	D	0.25	0/1296	0.49	0/1741
5	E	0.26	0/1747	0.53	0/2349
6	F	0.24	0/691	0.51	0/933
7	G	0.26	0/1368	0.49	0/1844
8	H	0.25	0/965	0.55	0/1302
9	I	0.25	0/989	0.57	0/1331
10	J	0.27	0/541	0.55	0/727
11	K	0.25	0/938	0.48	0/1267
12	L	0.31	0/345	0.59	0/457
13	X	0.25	0/244	0.72	0/380
14	W	0.62	0/289	1.12	0/442
All	All	0.28	0/31176	0.54	0/42165

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	10848	0	10932	439	0
2	B	8428	0	8465	316	0
3	C	2095	0	2051	76	0
4	D	1287	0	1296	28	0
5	E	1713	0	1739	56	0
6	F	679	0	701	26	0
7	G	1340	0	1357	42	0
8	H	951	0	926	32	0
9	I	971	0	929	24	0
10	J	532	0	542	21	0
11	K	920	0	929	22	0
12	L	343	0	363	23	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
18	W	2	0	0	0	0
18	X	2	0	0	0	0
All	All	30742	0	30495	989	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 16.

All (989) 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: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
7:G:1:MET:HE2	7:G:2:PHE:H	1.43	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:183:TRP:HE1	3:C:207:CYS:HG	1.31	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:F:110:ASP:O	6:F:123:LYS:NZ	2.23	0.65
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
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:757:ASN:HA	2:B:1021:MET:HE2	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:PHE:HD1	1:A:818:MET:HE3	1.62	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:HG22	1:A:600:PRO:HD3	1.83	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: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
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
2:B:248:SER:OG	2:B:249:ARG:N	2.35	0.59
1:A:54:ASN:C	1:A:56:PRO:HD3	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
1:A:815:PHE:CD1	1:A:818:MET:HE3	2.39	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: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
1:A:1063:MET:HE3	1:A:1436:ILE:HG13	1.86	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
2:B:750:GLY:O	2:B:754:SER:OG	2.22	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:1427:ASN:O	1:A:1431:GLY:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:567:LYS:HZ1	8:H:90:ALA:HB3	1.71	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: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
2:B:104:GLU:CD	12:L:54:ARG:NH1	2.60	0.55
3:C:113:VAL:HG23	3:C:144:ILE:HB	1.88	0.55
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.51	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:1004:ASN:CG	5:E:167:ARG:HD2	2.27	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
1:A:49:LYS:HE2	1:A:61:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:55:ASP:CG	1:A:55:ASP:O	2.46	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:SER:C	2:B:654:ARG:HH12	2.11	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
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
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:447:GLN:O	1:A:448:PRO:C	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.15	0.50
2:B:303:TYR:HH	2:B:586:TRP:HZ3	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
6:F:85:MET:HE1	6:F:153:VAL:HG22	1.94	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
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:453:MET:HE3	1:A:513:SER:HB2	1.95	0.49
3:C:73:GLN:N	3:C:131:HIS:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:TRP:NE1	3:C:207:CYS:SG	2.70	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: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
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:313:MET:HE3	2:B:386:LEU:HD22	1.95	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
1:A:1229:SER:OG	1:A:1230:GLU:N	2.44	0.48
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
7:G:1:MET:HE1	7:G:80:LYS:N	2.29	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:1012:ARG:O	1:A:1016:THR:OG1	2.23	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: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:519:TRP:C	2:B:521:LEU:H	2.18	0.47
2:B:853:SER:OG	2:B:854:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:1065:GLY:HA2	1:A:1370:LEU:HD21	1.96	0.47
2:B:20:ASP:N	2:B:655:LYS:HZ2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1325:THR:OG1	5:E:146:HIS:O	2.28	0.47
1:A:531:ILE:HG23	1:A:617:VAL:HG13	1.96	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: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:815:PHE:HA	1:A:818:MET:CE	2.45	0.46
1:A:1029:ARG:NH1	1:A:1033:GLN:OE1	2.44	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
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.32	0.46
1:A:49:LYS:HZ3	1:A:61:ILE:N	2.13	0.46
1:A:677:ARG:O	1:A:680:THR:OG1	2.32	0.46
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.80	0.46
2:B:293:PRO:HD2	2:B:296:GLU:HB3	1.97	0.46
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:244:PRO:N	1:A:245:PRO:HD2	2.31	0.45
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.51	0.45
2:B:575:PRO:C	2:B:577:ALA:H	2.19	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
8:H:40:LEU:HD11	8:H:97:MET:HE2	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:1020:ARG:O	2:B:1021:MET:HB2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
7:G:22:MET:HE1	7:G:70:PHE:CZ	2.52	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:476:SER:O	1:A:477:PRO:C	2.55	0.44
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
1:A:173:THR:HG1	1:A:184:SER:HG	1.60	0.44
2:B:986:GLN:HE22	2:B:1020:ARG:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1179:GLN:HG3	2:B:1188:LYS:HZ1	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
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
2:B:219:ALA:HB2	2:B:405:ARG:HG2	2.00	0.44
1:A:535:THR:O	1:A:575:LYS:NZ	2.50	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
1:A:1155:ASP:CG	1:A:1162:VAL:H	2.21	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
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
1:A:55:ASP:C	1:A:57:ARG:H	2.20	0.43
1:A:815:PHE:HA	1:A:818:MET:HE2	1.98	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
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
2:B:393:LYS:NZ	2:B:394:ASP:O	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:318:SER:HG	1:A:321:PRO:N	2.17	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: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:698:GLU:HA	2:B:701:ILE:HD11	2.00	0.43
5:E:42:PHE:O	5:E:46:TYR:HB2	2.17	0.43
12:L:48:CYS:O	12:L:52:GLY:N	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:771:GLU:H	1:A:822:GLU:CD	2.22	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
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.39	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:575:LYS:NZ	1:A:602:ASP:OD2	2.45	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
2:B:577:ALA:HB1	2:B:589:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:49:LYS:HZ1	1:A:55:ASP:HB2	1.85	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
1:A:1043:ASP:N	1:A:1043:ASP:OD1	2.52	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
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: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: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
1:A:103:CYS:HB3	1:A:108:MET:HE1	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:1215:ARG:HH12	1:A:1272:THR:C	2.22	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
3:C:208:GLU:H	3:C:208:GLU:CD	2.24	0.41
5:E:96:PHE:O	5:E:99:HIS:HB2	2.20	0.41
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:868:TYR:HD2	1:A:1058:VAL:HG11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:55:ASP:C	1:A:57:ARG:N	2.73	0.41
1:A:640:GLN:H	1:A:640:GLN:CD	2.24	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:784:LEU:C	1:A:786:HIS:H	2.24	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
3:C:16:ASP:C	3:C:240:VAL:HG11	2.41	0.41
13:X:8:G:H2'	13:X:9:G:H8	1.85	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:341:MET:HE1	1:A:1429:ILE:CD1	2.51	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:672:ASP:O	1:A:673:GLY:C	2.60	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:617:VAL:C	1:A:618:GLU:OE1	2.60	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:833:GLU:O	1:A:834:THR:C	2.59	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
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.53	0.40
12:L:61:THR:C	12:L:63:ARG:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:TYR:HB2	2:B:204:ILE:HB	2.04	0.40
2:B:806:THR:H	2:B:809:MET:HE2	1.85	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 [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	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	11
5	E	202/215 (94%)	181 (90%)	17 (8%)	4 (2%)	6	25
6	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	11	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	11
10	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	3	18
11	K	113/120 (94%)	102 (90%)	10 (9%)	1 (1%)	14	41
12	L	41/70 (59%)	21 (51%)	15 (37%)	5 (12%)	0	2
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
3	C	149	LYS

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Mol	Chain	Res	Type
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
1	A	958	VAL

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Mol	Chain	Res	Type
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
2	B	247	GLY

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Mol	Chain	Res	Type
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 [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	1204/1520 (79%)	1156 (96%)	48 (4%)	27	52
2	B	918/1061 (86%)	879 (96%)	39 (4%)	25	51
3	C	234/274 (85%)	229 (98%)	5 (2%)	48	69
4	D	144/200 (72%)	134 (93%)	10 (7%)	13	38
5	E	192/197 (98%)	187 (97%)	5 (3%)	41	64
6	F	74/137 (54%)	73 (99%)	1 (1%)	62	77
7	G	152/152 (100%)	146 (96%)	6 (4%)	27	53
8	H	104/128 (81%)	100 (96%)	4 (4%)	28	54
9	I	113/116 (97%)	108 (96%)	5 (4%)	24	50
10	J	60/65 (92%)	57 (95%)	3 (5%)	20	46
11	K	99/102 (97%)	97 (98%)	2 (2%)	50	70
12	L	38/57 (67%)	34 (90%)	4 (10%)	5	21
All	All	3332/4009 (83%)	3200 (96%)	132 (4%)	27	52

All (132) 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	65	LEU
1	A	67	CYS
1	A	150	THR
1	A	199	LEU
1	A	252	PHE
1	A	261	ASP
1	A	282	ASN
1	A	295	LEU
1	A	307	ASP
1	A	308	ILE
1	A	389	THR
1	A	450	LEU
1	A	451	HIS
1	A	476	SER
1	A	481	ASP
1	A	538	ASP
1	A	547	LEU
1	A	592	ASP
1	A	658	LEU
1	A	674	PRO
1	A	698	GLN
1	A	764	CYS
1	A	780	VAL
1	A	839	ARG
1	A	841	LEU
1	A	847	ASP
1	A	867	ILE
1	A	923	LEU
1	A	932	GLU
1	A	1017	LEU
1	A	1038	THR
1	A	1048	ASN
1	A	1058	VAL
1	A	1193	LEU
1	A	1203	ASN
1	A	1230	GLU
1	A	1260	LEU
1	A	1297	GLU
1	A	1303	GLU
1	A	1313	LEU

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Mol	Chain	Res	Type
1	A	1359	ASP
1	A	1401	SER
1	A	1402	PHE
1	A	1403	GLU
1	A	1453	TYR
2	B	45	SER
2	B	189	LEU
2	B	194	GLU
2	B	199	MET
2	B	224	GLN
2	B	242	SER
2	B	261	ARG
2	B	286	PHE
2	B	297	ILE
2	B	299	GLU
2	B	326	ASP
2	B	365	THR
2	B	421	PHE
2	B	429	PHE
2	B	484	ASN
2	B	578	THR
2	B	582	VAL
2	B	608	ASP
2	B	635	ARG
2	B	666	TYR
2	B	706	GLN
2	B	733	HIS
2	B	797	TYR
2	B	827	ILE
2	B	854	LEU
2	B	885	MET
2	B	958	GLN
2	B	959	ASP
2	B	1020	ARG
2	B	1065	GLN
2	B	1087	PHE
2	B	1123	SER
2	B	1132	GLU
2	B	1160	VAL
2	B	1168	LEU
2	B	1171	VAL
2	B	1177	HIS

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Mol	Chain	Res	Type
2	B	1187	ASN
2	B	1194	ILE
3	C	77	ILE
3	C	158	VAL
3	C	178	PHE
3	C	248	ILE
3	C	268	ASP
4	D	5	THR
4	D	27	LEU
4	D	50	LEU
4	D	121	LYS
4	D	133	THR
4	D	134	THR
4	D	156	ASP
4	D	169	SER
4	D	186	ASP
4	D	221	TYR
5	E	60	PHE
5	E	80	VAL
5	E	141	VAL
5	E	196	VAL
5	E	202	SER
6	F	136	ARG
7	G	11	ILE
7	G	26	LEU
7	G	45	ILE
7	G	91	VAL
7	G	120	THR
7	G	135	ASP
8	H	47	PHE
8	H	56	THR
8	H	131	ASN
8	H	143	LEU
9	I	6	PHE
9	I	68	LEU
9	I	75	CYS
9	I	83	ASN
9	I	116	ASN
10	J	48	ARG
10	J	51	LEU
10	J	64	ASN
11	K	33	ILE

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Mol	Chain	Res	Type
11	K	57	LEU
12	L	30	ILE
12	L	38	LEU
12	L	55	ILE
12	L	67	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	445	ASN
1	A	515	GLN
1	A	881	GLN
2	B	309	GLN
2	B	484	ASN
2	B	518	HIS
2	B	538	ASN
2	B	986	GLN
2	B	1076	HIS
2	B	1161	HIS
3	C	135	GLN
7	G	57	GLN
11	K	40	HIS

5.3.3 RNA [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.