



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:58 am BST

PDB ID : 4GZY  
Title : Crystal structures of bacterial RNA Polymerase paused elongation complexes  
Authors : Weixlbaumer, A.; Leon, K.; Landick, R.; Darst, S.A.  
Deposited on : 2012-09-06  
Resolution : 3.51 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.

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

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

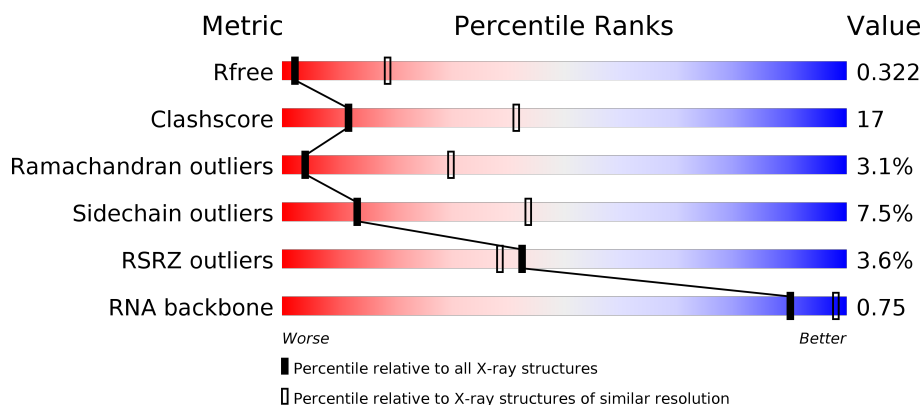
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 on 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	315	
1	B	315	
2	C	1119	
3	D	1534	

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>5%</div><div>55%</div><div>31%</div><div>8%</div><div>6%</div></div>
5	N	13	<div><div></div><div>69%</div><div>69%</div><div>15%</div><div>15%</div></div>
6	R	29	<div><div></div><div>3%</div><div>10%</div><div>17%</div><div>69%</div></div>
7	T	22	<div><div></div><div>27%</div><div>64%</div><div>36%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1083	Total	C	N	O	S	0	0	0
			8548	5412	1524	1588	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1358	Total	C	N	O	S	0	0	0
			10714	6780	1900	2001	33			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1525	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1526	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1527	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1528	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1529	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1530	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1531	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1532	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1533	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1534	HIS	-	EXPRESSION TAG	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	11	Total	C	N	O	P	0	0	0
			225	107	43	64	11			

- Molecule 6 is a RNA chain called RNA transcript.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	9	Total	C	N	O	P	0	0	0
			191	85	31	66	9			

- Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	22	Total	C	N	O	P	0	0	0
			447	213	81	131	22			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		

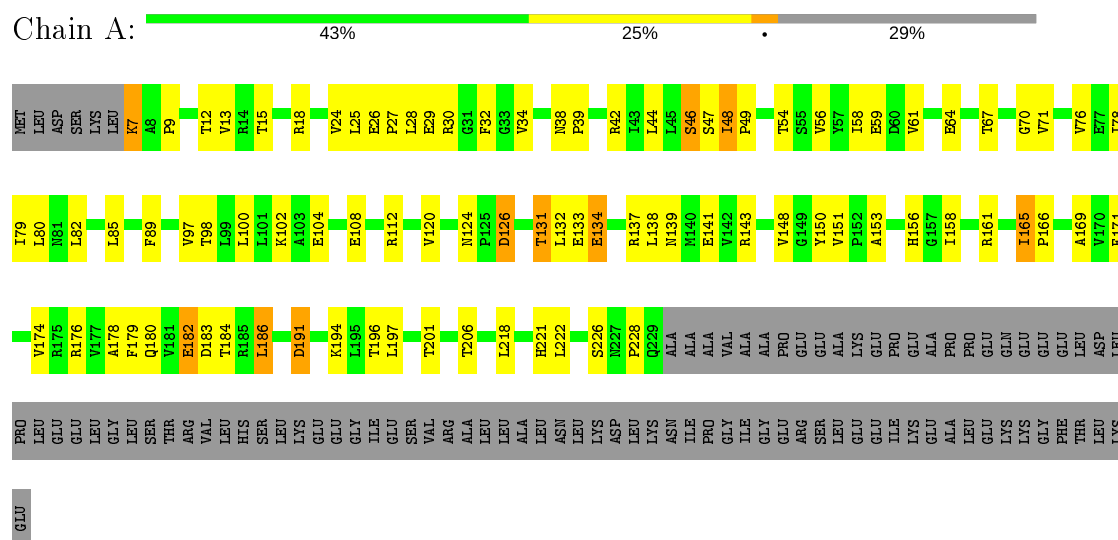
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

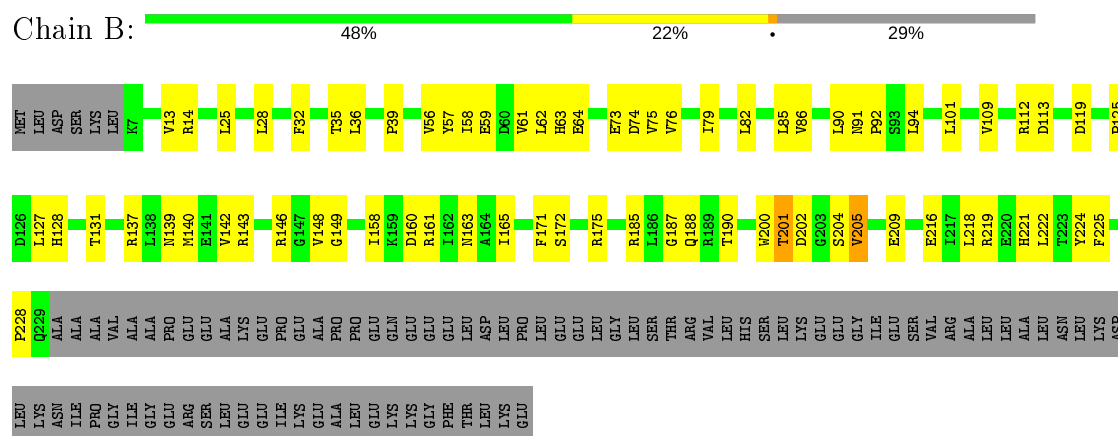
### 3 Residue-property plots

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

#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



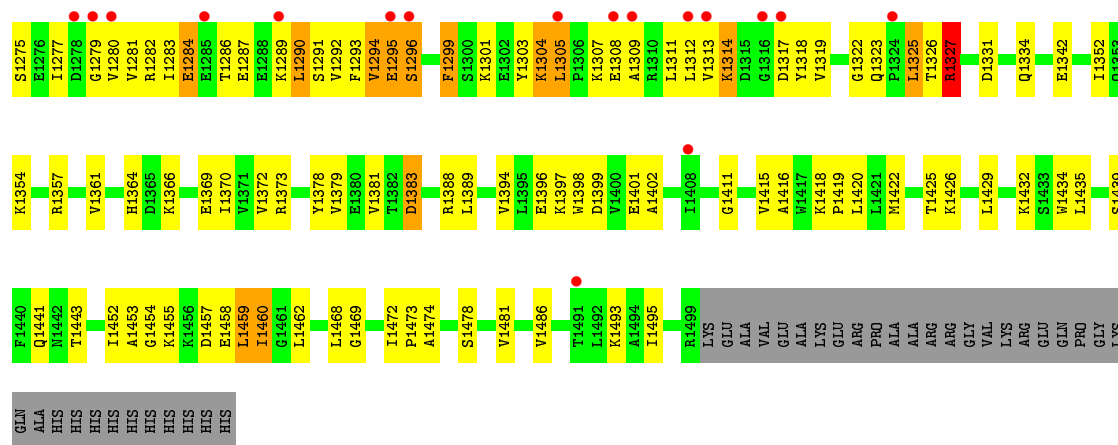
#### • Molecule 2: DNA-directed RNA polymerase subunit beta



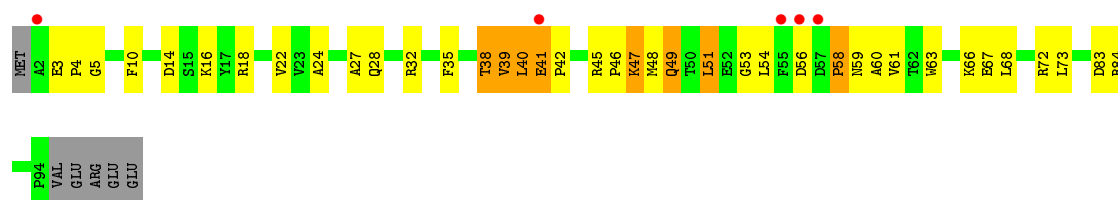




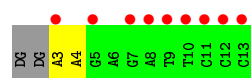




- Molecule 4: DNA-directed RNA polymerase subunit omega



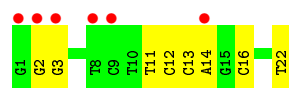
- Molecule 5: non-template DNA



- Molecule 6: RNA transcript



- Molecule 7: template DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.21Å 207.21Å 203.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.77 – 3.51 49.77 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.77-3.51) 87.9 (49.77-3.51)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.76 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
R, $R_{free}$	0.263 , 0.322 0.265 , 0.322	Depositor DCC
$R_{free}$ test set	3199 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.9	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.28	0/1791	0.49	0/2436
1	B	0.29	0/1791	0.48	0/2436
2	C	0.30	0/8711	0.52	1/11784 (0.0%)
3	D	0.30	0/10897	0.50	1/14726 (0.0%)
4	E	0.29	0/768	0.54	0/1035
5	N	0.43	0/252	1.11	0/386
6	R	0.22	0/212	0.77	0/328
7	T	0.43	0/500	1.09	0/768
All	All	0.30	0/24922	0.54	2/33899 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	705	ALA	C-N-CD	5.90	140.78	128.40
2	C	853	LEU	CA-CB-CG	5.11	127.05	115.30

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	1759	0	1805	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1759	0	1805	53	0
2	C	8548	0	8650	377	0
3	D	10714	0	10936	395	0
4	E	754	0	769	24	0
5	N	225	0	124	1	0
6	R	191	0	95	7	0
7	T	447	0	248	6	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	851	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:610:ARG:HH11	2:C:610:ARG:HG3	1.16	1.08
3:D:346:ARG:NH1	3:D:347:VAL:O	1.89	1.05
2:C:405:ARG:NH1	2:C:442:GLU:OE2	1.90	1.04
2:C:274:ARG:NH1	2:C:284:ARG:HH12	1.54	1.03
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.25	0.98
4:E:39:VAL:O	4:E:72:ARG:NH1	1.98	0.96
2:C:194:VAL:HG21	2:C:224:GLU:HG3	1.49	0.94
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.02	0.92
2:C:978:ARG:HG3	2:C:978:ARG:HH11	1.34	0.91
2:C:274:ARG:HH12	2:C:284:ARG:NH1	1.66	0.91
2:C:274:ARG:HH12	2:C:284:ARG:HH12	1.13	0.90
2:C:829:GLN:HE21	2:C:831:ARG:HH11	1.17	0.87
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ1	1.40	0.86
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.09	0.86
3:D:1106:VAL:HG12	3:D:1220:ALA:HA	1.57	0.83
2:C:290:LEU:HD11	2:C:301:GLU:H	1.43	0.82
2:C:239:PHE:HB2	2:C:251:ASP:HB3	1.62	0.81
3:D:486:ARG:HH21	3:D:489:ARG:HH11	1.29	0.80
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.63	0.80
1:B:91:ASN:ND2	1:B:119:ASP:OD2	2.14	0.80
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.64	0.80
2:C:288:ARG:HH11	2:C:288:ARG:H	1.30	0.79
3:D:1108:ARG:HH22	3:D:1460:ILE:HD11	1.47	0.79
1:B:188:GLN:O	3:D:646:LYS:NZ	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.66	0.78
3:D:770:LEU:HD12	3:D:1211:MET:HA	1.64	0.78
3:D:135:LEU:HD23	3:D:148:GLU:HB2	1.64	0.77
2:C:274:ARG:HH12	2:C:284:ARG:NH2	1.82	0.77
2:C:224:GLU:HB3	2:C:227:PHE:HB3	1.67	0.77
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.65	0.77
2:C:274:ARG:HH12	2:C:284:ARG:CZ	1.96	0.77
2:C:309:TYR:CZ	2:C:321:GLU:HB3	2.20	0.77
2:C:272:ALA:HB1	2:C:276:LYS:HZ1	1.50	0.76
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.67	0.76
3:D:501:ALA:O	3:D:505:SER:OG	2.02	0.76
3:D:557:LEU:HD21	3:D:566:ILE:HG22	1.68	0.76
2:C:274:ARG:NH1	2:C:284:ARG:NH1	2.29	0.76
2:C:334:ARG:HH12	2:C:415:PRO:HG2	1.48	0.76
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.66	0.75
2:C:1103:ASP:HB3	2:C:1105:LYS:NZ	2.01	0.75
2:C:274:ARG:HH21	2:C:278:GLU:HB2	1.51	0.74
2:C:437:ARG:NH1	2:C:491:GLU:OE1	2.14	0.74
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.19	0.74
3:D:700:VAL:HG12	3:D:749:VAL:HG12	1.70	0.74
2:C:1008:ARG:HD2	2:C:1026:GLN:HB3	1.68	0.74
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.68	0.74
2:C:584:GLU:HB3	2:C:666:LEU:H	1.52	0.74
2:C:274:ARG:HH12	2:C:284:ARG:HH22	1.35	0.74
3:D:983:LEU:HD13	3:D:988:ARG:HB2	1.69	0.74
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.67	0.73
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.17	0.73
2:C:205:GLU:HB2	2:C:209:ARG:HH12	1.54	0.73
3:D:213:VAL:HG11	3:D:385:VAL:HA	1.70	0.73
2:C:1105:LYS:H	2:C:1105:LYS:HZ2	1.35	0.73
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.71	0.72
1:A:58:ILE:HB	1:A:61:VAL:HB	1.71	0.72
2:C:204:GLN:NE2	2:C:222:MET:O	2.22	0.72
3:D:1147:ARG:HD3	3:D:1188:VAL:HG21	1.71	0.72
1:A:112:ARG:NH2	1:A:126:ASP:OD1	2.23	0.72
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.72	0.71
1:A:80:LEU:HD21	2:C:573:ARG:HH11	1.55	0.71
2:C:224:GLU:O	2:C:228:ALA:N	2.24	0.71
2:C:755:LEU:HD11	2:C:825:VAL:HG11	1.73	0.71
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.55	0.71
1:A:182:GLU:HB2	1:A:194:LYS:HD3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1273:VAL:HG12	3:D:1274:ILE:H	1.56	0.70
2:C:332:ARG:NH2	2:C:338:GLU:OE1	2.25	0.70
2:C:1005:MET:HB2	3:D:724:GLN:HE22	1.56	0.70
2:C:734:LEU:HG	2:C:737:LEU:HD12	1.73	0.70
3:D:362:GLU:O	3:D:364:GLY:N	2.23	0.70
2:C:610:ARG:HG3	2:C:610:ARG:NH1	1.90	0.70
1:B:185:ARG:NH1	3:D:692:GLU:OE1	2.24	0.70
3:D:1161:GLU:HB2	3:D:1164:ARG:HB2	1.74	0.69
3:D:1418:LYS:HD3	3:D:1419:PRO:HD2	1.74	0.69
3:D:112:ILE:HD11	3:D:461:ILE:HG21	1.73	0.69
3:D:136:ASP:HB2	3:D:137:PRO:HD2	1.74	0.69
1:A:104:GLU:OE1	1:A:137:ARG:NH1	2.25	0.69
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.74	0.69
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.03	0.69
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.75	0.69
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.73	0.69
3:D:133:ILE:HG23	3:D:454:ALA:HB1	1.75	0.69
3:D:501:ALA:HB1	3:D:1453:ALA:HB2	1.75	0.69
2:C:302:VAL:O	2:C:306:THR:OG1	2.11	0.68
3:D:1267:ARG:NH2	3:D:1331:ASP:OD2	2.25	0.68
3:D:691:LEU:HD23	3:D:720:LEU:HD21	1.74	0.68
2:C:670:GLN:NE2	2:C:699:PHE:O	2.27	0.68
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.75	0.68
2:C:829:GLN:NE2	2:C:831:ARG:HH11	1.89	0.68
3:D:486:ARG:HE	3:D:489:ARG:HD2	1.58	0.68
3:D:1283:ILE:HD11	3:D:1290:LEU:HD12	1.76	0.67
3:D:154:THR:HG23	3:D:157:GLU:H	1.59	0.67
2:C:978:ARG:HH11	2:C:978:ARG:CG	2.06	0.67
2:C:726:ILE:HD13	2:C:754:ILE:HD13	1.76	0.67
3:D:525:ARG:NH1	3:D:541:ASN:OD1	2.26	0.67
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.75	0.67
2:C:292:ARG:HB3	2:C:299:LYS:HB3	1.76	0.67
2:C:89:THR:HG22	2:C:129:ILE:HA	1.76	0.67
2:C:260:LEU:HD22	2:C:288:ARG:HH22	1.59	0.67
2:C:292:ARG:HG2	2:C:299:LYS:HE3	1.77	0.67
2:C:292:ARG:NH1	2:C:294:GLU:HB2	2.10	0.67
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.77	0.67
1:A:54:THR:HG21	1:A:158:ILE:HD12	1.77	0.66
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.77	0.66
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.60	0.66
2:C:274:ARG:NH1	2:C:284:ARG:HH22	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1453:ALA:O	3:D:1455:LYS:N	2.29	0.66
3:D:114:THR:O	3:D:495:ARG:NH1	2.29	0.66
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.78	0.65
2:C:829:GLN:HE21	2:C:831:ARG:NH1	1.91	0.65
2:C:388:ARG:NH1	7:T:22:DT:OP1	2.29	0.65
2:C:808:ARG:HD3	2:C:820:ARG:HD2	1.78	0.65
2:C:56:GLU:HA	2:C:356:ARG:HH12	1.61	0.65
2:C:292:ARG:HG3	2:C:292:ARG:HH11	1.62	0.65
3:D:1495:ILE:HG23	4:E:84:ARG:HD3	1.78	0.65
2:C:1031:ARG:HB3	7:T:16:DC:OP1	1.97	0.65
2:C:1008:ARG:HH12	2:C:1011:GLY:N	1.95	0.64
2:C:144:PRO:HA	2:C:163:ILE:HG23	1.79	0.64
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.78	0.64
2:C:1008:ARG:NH2	3:D:624:ASP:OD1	2.30	0.64
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.79	0.64
2:C:720:GLU:O	2:C:820:ARG:NH2	2.31	0.64
3:D:165:LYS:HE3	3:D:200:ASP:HB2	1.80	0.64
2:C:48:PHE:HB3	2:C:52:PHE:HD2	1.63	0.64
2:C:428:ARG:NH1	3:D:1086:LEU:HD11	2.12	0.64
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.78	0.64
3:D:808:THR:H	3:D:809:PRO:HD2	1.63	0.64
3:D:629:SER:HB3	3:D:726:ILE:HG12	1.79	0.63
2:C:292:ARG:HH12	2:C:294:GLU:HB2	1.63	0.63
3:D:100:ALA:HB2	3:D:513:ILE:HG13	1.81	0.63
3:D:813:LEU:HD12	3:D:814:ALA:H	1.64	0.63
2:C:205:GLU:HB2	2:C:209:ARG:NH1	2.14	0.63
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.81	0.63
2:C:680:ASP:H	3:D:943:THR:HG21	1.63	0.62
2:C:845:ASN:HD22	2:C:884:GLN:HE22	1.46	0.62
1:A:221:HIS:HB3	1:B:36:LEU:HD11	1.81	0.62
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.82	0.62
2:C:395:LYS:HD3	2:C:397:GLU:OE2	1.99	0.62
1:A:70:GLY:HA2	1:A:133:GLU:HB3	1.80	0.62
2:C:473:ARG:HA	2:C:531:PHE:HA	1.82	0.62
3:D:1296:SER:HB3	3:D:1299:PHE:HD2	1.64	0.62
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.80	0.62
3:D:368:VAL:HB	3:D:377:VAL:HG12	1.81	0.62
3:D:764:LEU:O	3:D:768:ASN:ND2	2.32	0.62
4:E:38:THR:HG23	4:E:41:GLU:HG2	1.80	0.62
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.63	0.62
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:LEU:HD21	2:C:300:ASP:HB2	1.83	0.61
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.32	0.61
2:C:336:VAL:HA	2:C:339:LEU:HD12	1.82	0.61
3:D:1273:VAL:HG21	3:D:1305:LEU:HD12	1.82	0.61
3:D:553:ARG:NH2	3:D:570:GLU:OE2	2.34	0.61
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.82	0.61
3:D:808:THR:H	3:D:809:PRO:CD	2.13	0.61
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.82	0.61
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.66	0.61
3:D:477:LEU:HA	3:D:480:GLU:HB3	1.82	0.61
3:D:1174:LEU:HD22	3:D:1183:ILE:HD11	1.83	0.61
1:B:175:ARG:N	1:B:200:TRP:O	2.33	0.61
3:D:1274:ILE:HG21	3:D:1334:GLN:HB3	1.83	0.61
2:C:326:ASP:HB2	2:C:331:ARG:NH1	2.16	0.61
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.82	0.61
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.83	0.60
1:A:176:ARG:NH2	2:C:863:ASP:OD1	2.34	0.60
2:C:185:LYS:NZ	2:C:190:LYS:HE2	2.16	0.60
2:C:437:ARG:HD3	2:C:467:ILE:HB	1.82	0.60
2:C:642:ARG:NE	2:C:657:ASP:OD2	2.35	0.60
2:C:1008:ARG:HH12	2:C:1010:THR:C	2.05	0.60
3:D:1319:VAL:HG23	3:D:1323:GLN:HE21	1.67	0.60
3:D:852:ALA:HB1	3:D:857:ILE:HD11	1.83	0.60
2:C:292:ARG:HG3	2:C:292:ARG:NH1	2.17	0.60
1:A:108:GLU:HG2	1:A:131:THR:HG22	1.84	0.59
2:C:987:ILE:HA	3:D:948:THR:HG21	1.83	0.59
2:C:7:GLY:HA3	2:C:904:PRO:HG2	1.85	0.59
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.85	0.59
2:C:540:PHE:O	2:C:545:ASN:ND2	2.36	0.59
2:C:787:ASP:OD1	2:C:791:ARG:NH2	2.35	0.59
2:C:824:ARG:NH2	2:C:826:TYR:OH	2.35	0.59
3:D:164:GLY:HA3	3:D:397:LYS:HE3	1.85	0.59
3:D:1108:ARG:HH12	3:D:1460:ILE:CG1	2.16	0.59
3:D:629:SER:OG	3:D:630:VAL:N	2.34	0.59
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.84	0.59
2:C:971:LYS:HA	2:C:988:VAL:HA	1.85	0.58
3:D:1258:ARG:NH1	3:D:1262:LEU:HD11	2.17	0.58
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.32	0.58
2:C:101:ILE:HD12	2:C:107:LEU:HD22	1.86	0.58
3:D:820:GLU:HB2	3:D:836:VAL:HG21	1.86	0.58
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:LEU:HD22	3:D:153:LEU:HD23	1.85	0.58
2:C:115:LEU:HA	2:C:375:SER:HB2	1.85	0.58
2:C:674:VAL:HG22	2:C:869:VAL:HB	1.86	0.58
3:D:32:ILE:HG21	3:D:37:LEU:HD13	1.86	0.58
2:C:1009:SER:HA	3:D:625:TYR:HA	1.86	0.58
2:C:863:ASP:OD1	2:C:864:GLY:N	2.37	0.58
1:A:7:LYS:HD3	1:A:186:LEU:HD22	1.86	0.57
2:C:324:ASP:O	2:C:330:ASN:ND2	2.32	0.57
6:R:22:U:H2'	6:R:23:G:C8	2.39	0.57
2:C:122:THR:HB	2:C:124:ASP:OD2	2.04	0.57
2:C:145:GLY:H	2:C:163:ILE:HG23	1.69	0.57
2:C:64:LEU:HD13	2:C:359:MET:SD	2.44	0.57
2:C:1082:PRO:HB2	2:C:1085:PHE:HB3	1.86	0.57
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.87	0.57
2:C:158:TYR:HD1	2:C:314:THR:HG22	1.69	0.57
3:D:210:ARG:HB3	3:D:388:HIS:HB2	1.85	0.57
2:C:246:ASP:N	2:C:246:ASP:OD1	2.38	0.57
2:C:576:ALA:N	2:C:662:GLU:OE1	2.37	0.57
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.87	0.57
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.87	0.57
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.69	0.56
2:C:243:ARG:HE	2:C:254:VAL:HG21	1.70	0.56
2:C:1008:ARG:HD3	2:C:1028:GLY:H	1.70	0.56
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.85	0.56
2:C:1050:GLN:HG3	3:D:1469:GLY:O	2.05	0.56
2:C:111:ASP:HB3	2:C:112:GLU:OE2	2.05	0.56
2:C:1051:GLU:HG3	2:C:1055:LEU:HD23	1.87	0.56
3:D:1458:GLU:O	3:D:1460:ILE:HG22	2.05	0.56
2:C:284:ARG:HG3	2:C:285:LEU:N	2.21	0.56
3:D:1283:ILE:HD13	3:D:1311:LEU:HD22	1.87	0.56
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.86	0.56
3:D:1289:LYS:HZ3	3:D:1304:LYS:HB2	1.70	0.56
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.86	0.56
1:A:59:GLU:HB2	1:A:139:ASN:HB3	1.88	0.56
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.70	0.55
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.21	0.55
2:C:194:VAL:HG12	2:C:221:LEU:HB2	1.86	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HD23	1.89	0.55
3:D:1281:VAL:HG11	3:D:1313:VAL:HG22	1.89	0.55
3:D:96:ALA:HB2	3:D:555:LYS:HG3	1.86	0.55
2:C:537:LYS:HG2	2:C:905:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:ILE:HG22	2:C:66:LEU:HD23	1.89	0.55
3:D:827:ILE:HG23	3:D:828:LYS:HG3	1.89	0.55
2:C:846:LYS:NZ	6:R:29:U:OP1	2.35	0.55
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.87	0.55
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.88	0.55
2:C:1105:LYS:HZ2	2:C:1105:LYS:N	2.03	0.55
3:D:53:ILE:HA	3:D:86:ARG:HD3	1.89	0.55
2:C:462:ASP:O	2:C:464:LEU:N	2.38	0.55
2:C:571:LEU:HD13	2:C:670:GLN:HE21	1.72	0.55
3:D:616:GLN:OE1	3:D:621:LYS:NZ	2.38	0.55
1:B:32:PHE:HA	1:B:35:THR:HB	1.89	0.55
2:C:140:ILE:HG12	2:C:333:ILE:HG12	1.89	0.55
2:C:468:ARG:HB3	2:C:485:TYR:HB3	1.88	0.55
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.89	0.55
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.89	0.55
3:D:165:LYS:HG2	3:D:199:LEU:HB3	1.88	0.55
3:D:660:LYS:HG3	3:D:694:VAL:HG12	1.89	0.55
3:D:770:LEU:HD23	3:D:777:PRO:HA	1.89	0.55
3:D:130:SER:OG	3:D:131:LYS:N	2.40	0.54
1:B:76:VAL:HG13	3:D:872:ARG:HH21	1.72	0.54
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.88	0.54
3:D:1128:VAL:HG12	3:D:1129:THR:H	1.72	0.54
3:D:1286:THR:OG1	3:D:1287:GLU:N	2.39	0.54
3:D:187:LYS:HG3	3:D:199:LEU:HA	1.88	0.54
1:B:163:ASN:OD1	1:B:163:ASN:N	2.41	0.54
3:D:1282:ARG:HB2	3:D:1293:PHE:O	2.06	0.54
1:B:86:VAL:HG21	1:B:204:SER:HB2	1.90	0.54
1:B:149:GLY:HA2	1:B:172:SER:HB2	1.90	0.54
2:C:54:ILE:CG2	2:C:66:LEU:HD23	2.37	0.54
2:C:52:PHE:HE1	2:C:98:LEU:HD13	1.72	0.54
3:D:1283:ILE:HG13	3:D:1292:VAL:HG22	1.90	0.54
3:D:345:TYR:CZ	3:D:377:VAL:HB	2.43	0.54
6:R:26:U:H2'	6:R:27:G:C8	2.43	0.54
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.88	0.54
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.90	0.54
3:D:608:SER:HB3	3:D:1443:THR:HB	1.89	0.54
1:A:7:LYS:NZ	1:A:7:LYS:HB3	2.23	0.54
2:C:18:LEU:HD22	2:C:404:LEU:HD21	1.89	0.54
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.23	0.54
3:D:171:LEU:N	3:D:391:ALA:O	2.36	0.54
3:D:783:ARG:HD3	3:D:1029:ARG:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:949:LYS:HD3	3:D:796:ARG:NH1	2.23	0.54
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.72	0.54
3:D:100:ALA:HB3	3:D:128:TYR:CE1	2.42	0.53
3:D:1106:VAL:HG11	3:D:1474:ALA:HB2	1.90	0.53
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.90	0.53
3:D:658:LEU:HA	3:D:661:MET:HE2	1.89	0.53
2:C:390:GLN:HB3	6:R:25:G:H5'	1.90	0.53
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.88	0.53
2:C:1082:PRO:HB3	3:D:1469:GLY:HA3	1.89	0.53
2:C:1105:LYS:HZ1	2:C:1107:ASN:HB2	1.73	0.53
2:C:1101:THR:HG21	2:C:1111:ILE:HD11	1.89	0.53
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	1.89	0.53
2:C:272:ALA:C	2:C:276:LYS:HZ2	2.11	0.53
3:D:1155:VAL:HG23	3:D:1156:LEU:H	1.73	0.53
2:C:1085:PHE:HD1	3:D:1468:LEU:HD22	1.74	0.53
3:D:568:ARG:NH1	3:D:571:LYS:HE3	2.22	0.53
3:D:52:PRO:HG2	3:D:80:VAL:HG13	1.88	0.53
2:C:334:ARG:NH1	2:C:415:PRO:HG2	2.21	0.53
3:D:1435:LEU:HD21	3:D:1468:LEU:HD21	1.91	0.53
1:A:133:GLU:HG2	1:A:134:GLU:H	1.73	0.53
3:D:172:PRO:HG2	3:D:175:VAL:HG21	1.89	0.53
3:D:458:ALA:HB2	3:D:575:GLN:HE22	1.73	0.53
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.42	0.53
2:C:185:LYS:HZ2	2:C:190:LYS:HE2	1.73	0.53
3:D:87:ARG:HD2	3:D:88:TYR:CE1	2.44	0.53
2:C:284:ARG:NH1	2:C:285:LEU:H	2.05	0.53
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.89	0.53
3:D:1275:SER:OG	3:D:1322:GLY:N	2.42	0.53
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.90	0.53
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.90	0.53
2:C:1007:ALA:HB2	3:D:648:MET:HG2	1.90	0.53
1:B:149:GLY:H	1:B:171:PHE:HB2	1.74	0.53
3:D:176:ASP:O	3:D:390:PRO:HD2	2.08	0.53
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.44	0.53
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.91	0.52
2:C:300:ASP:OD2	2:C:303:PHE:HB2	2.10	0.52
3:D:165:LYS:H	3:D:199:LEU:HD13	1.74	0.52
1:B:205:VAL:HG13	1:B:209:GLU:HB2	1.90	0.52
2:C:91:GLN:HA	2:C:119:PRO:HA	1.90	0.52
2:C:184:MET:HB2	2:C:193:LEU:HB2	1.91	0.52
3:D:964:LEU:HD13	3:D:1058:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.39	0.52
3:D:1128:VAL:HB	3:D:1131:SER:OG	2.10	0.52
3:D:39:PRO:HD3	3:D:53:ILE:HG21	1.91	0.52
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.92	0.52
3:D:802:ALA:HB3	3:D:824:ASN:HB3	1.92	0.52
2:C:236:ILE:HA	2:C:251:ASP:OD2	2.09	0.52
2:C:66:LEU:HD12	2:C:98:LEU:HD11	1.90	0.52
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.24	0.52
3:D:805:GLU:HG2	3:D:809:PRO:HG2	1.91	0.52
2:C:1:MET:O	2:C:899:GLN:HA	2.10	0.52
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.91	0.52
3:D:832:ARG:NE	3:D:833:GLU:OE2	2.43	0.52
2:C:408:ARG:NH2	2:C:456:ALA:O	2.43	0.52
2:C:437:ARG:HG2	2:C:469:THR:HG23	1.92	0.52
2:C:806:LEU:HB2	2:C:822:VAL:HG22	1.91	0.52
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.92	0.52
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.91	0.52
2:C:165:LEU:HG	2:C:166:PRO:HA	1.91	0.52
1:A:80:LEU:HD21	2:C:573:ARG:HD2	1.92	0.52
2:C:756:VAL:O	2:C:789:SER:HB3	2.10	0.52
3:D:367:ILE:HG13	3:D:377:VAL:HG13	1.91	0.52
3:D:50:PHE:CD1	3:D:522:PRO:HD3	2.45	0.52
2:C:1008:ARG:HH12	2:C:1010:THR:CA	2.23	0.52
2:C:756:VAL:HB	2:C:790:LEU:HB3	1.91	0.52
2:C:841:ASN:HD21	2:C:884:GLN:HE21	1.56	0.52
2:C:842:ARG:HB3	2:C:842:ARG:HH11	1.75	0.52
3:D:806:PHE:CD1	3:D:812:ALA:HB3	2.45	0.52
1:B:73:GLU:OE2	1:B:128:HIS:NE2	2.40	0.51
2:C:205:GLU:CB	2:C:209:ARG:HH12	2.22	0.51
3:D:560:GLN:HG3	3:D:561:GLY:H	1.74	0.51
1:A:34:VAL:HG21	2:C:939:ARG:HE	1.75	0.51
2:C:288:ARG:H	2:C:288:ARG:NH1	2.04	0.51
2:C:425:PHE:H	2:C:428:ARG:HD2	1.75	0.51
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.92	0.51
2:C:733:ALA:HB1	2:C:754:ILE:HD12	1.91	0.51
3:D:1108:ARG:NH2	3:D:1460:ILE:HD11	2.19	0.51
3:D:522:PRO:O	3:D:525:ARG:N	2.30	0.51
3:D:988:ARG:HA	3:D:991:GLN:HB2	1.92	0.51
2:C:679:PHE:CE2	2:C:853:LEU:HD21	2.45	0.51
3:D:1107:VAL:O	3:D:1218:GLY:N	2.42	0.51
2:C:95:TYR:HD1	2:C:112:GLU:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.11	0.51
3:D:842:VAL:HG12	3:D:865:THR:HB	1.93	0.51
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.90	0.51
1:B:185:ARG:NH2	1:B:187:GLY:HA2	2.26	0.51
1:B:56:VAL:HG22	1:B:142:VAL:HG22	1.92	0.51
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.75	0.51
3:D:100:ALA:HB3	3:D:128:TYR:HE1	1.76	0.51
2:C:468:ARG:NE	2:C:485:TYR:O	2.41	0.51
3:D:800:LYS:HZ3	3:D:804:LEU:HD22	1.76	0.51
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.92	0.51
3:D:1425:THR:O	3:D:1429:LEU:HB2	2.10	0.51
3:D:484:PRO:HB3	3:D:488:ARG:NE	2.25	0.51
3:D:61:GLY:HA3	3:D:64:LYS:NZ	2.26	0.51
2:C:890:LEU:HB2	2:C:914:ILE:HD12	1.91	0.51
3:D:139:GLY:HA2	3:D:452:ILE:HG12	1.93	0.51
3:D:827:ILE:O	3:D:835:SER:OG	2.23	0.51
1:A:100:LEU:HD22	1:A:141:GLU:HG3	1.92	0.51
1:B:59:GLU:HB3	1:B:137:ARG:HH12	1.75	0.51
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.92	0.51
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.93	0.51
1:A:178:ALA:HB2	2:C:864:GLY:HA2	1.92	0.51
2:C:19:THR:HG21	2:C:124:ASP:O	2.11	0.51
2:C:140:ILE:HG13	2:C:410:ILE:HG21	1.93	0.51
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.46	0.51
3:D:54:LYS:HG3	3:D:55:ASP:H	1.76	0.51
4:E:48:MET:HG2	4:E:49:GLN:H	1.75	0.51
1:A:24:VAL:HG22	1:A:196:THR:HG22	1.94	0.50
3:D:101:HIS:ND1	3:D:582:LEU:HD13	2.25	0.50
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.11	0.50
6:R:22:U:H2'	6:R:23:G:H8	1.75	0.50
3:D:160:GLU:HA	3:D:163:TYR:CZ	2.46	0.50
3:D:414:ARG:HG3	3:D:433:GLY:H	1.75	0.50
3:D:800:LYS:NZ	3:D:804:LEU:HD22	2.27	0.50
3:D:832:ARG:O	3:D:834:THR:N	2.42	0.50
1:A:9:PRO:HG2	1:B:224:TYR:CE2	2.47	0.50
2:C:184:MET:HE2	2:C:193:LEU:HD12	1.94	0.50
3:D:1294:VAL:O	3:D:1295:GLU:HB2	2.11	0.50
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.94	0.50
3:D:637:LEU:HB2	3:D:641:GLN:HG3	1.94	0.50
3:D:917:GLN:HB3	3:D:921:ARG:NH1	2.26	0.50
1:B:59:GLU:HG3	1:B:139:ASN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:191:LEU:HD11	3:D:395:VAL:HG13	1.94	0.50
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.93	0.50
7:T:13:DC:H2''	7:T:14:DA:OP2	2.12	0.50
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.94	0.50
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.46	0.50
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.94	0.50
1:B:14:ARG:HH11	1:B:14:ARG:HG3	1.77	0.49
2:C:108:ILE:HG13	2:C:366:SER:HB2	1.94	0.49
6:R:26:U:H2'	6:R:27:G:H8	1.76	0.49
1:A:18:ARG:HG3	1:A:206:THR:HG22	1.94	0.49
2:C:251:ASP:OD1	2:C:252:LYS:N	2.45	0.49
2:C:442:GLU:HG2	2:C:454:SER:CB	2.41	0.49
2:C:1094:ALA:HB2	3:D:520:LEU:HD12	1.92	0.49
1:A:153:ALA:HA	1:A:156:HIS:CE1	2.47	0.49
3:D:119:SER:H	3:D:123:LEU:HD22	1.76	0.49
2:C:1046:ALA:HB2	3:D:1472:ILE:HG13	1.94	0.49
2:C:1103:ASP:H	2:C:1107:ASN:H	1.59	0.49
3:D:1261:GLU:OE2	3:D:1269:LYS:HG3	2.12	0.49
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.94	0.49
1:A:89:PHE:HE1	1:A:97:VAL:HB	1.78	0.49
2:C:338:GLU:HA	2:C:341:THR:HG22	1.94	0.49
2:C:44:ILE:HG23	2:C:344:PHE:CE2	2.47	0.49
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.45	0.49
3:D:1301:LYS:HD2	3:D:1303:TYR:CE1	2.48	0.49
3:D:1108:ARG:HH12	3:D:1460:ILE:HG13	1.76	0.49
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.48	0.49
3:D:1074:SER:HA	3:D:1077:ALA:HB3	1.95	0.49
2:C:428:ARG:NH1	3:D:1086:LEU:HD21	2.27	0.49
3:D:31:THR:OG1	3:D:32:ILE:N	2.45	0.49
3:D:473:LEU:HD23	3:D:499:VAL:HG21	1.95	0.49
2:C:689:VAL:HB	2:C:870:ILE:HB	1.94	0.49
3:D:800:LYS:HZ3	3:D:804:LEU:HD13	1.78	0.49
2:C:1006:HIS:HB2	3:D:628:ARG:HG2	1.95	0.49
2:C:604:ALA:HB3	2:C:612:VAL:HB	1.95	0.49
2:C:474:VAL:HG12	2:C:479:VAL:HA	1.95	0.49
3:D:1258:ARG:NH1	3:D:1262:LEU:HD21	2.28	0.49
1:B:185:ARG:HD3	3:D:692:GLU:OE2	2.13	0.49
2:C:327:HIS:HA	2:C:431:HIS:NE2	2.28	0.48
2:C:739:GLU:HB2	2:C:742:VAL:HB	1.95	0.48
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.95	0.48
1:A:228:PRO:HB3	1:B:13:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HG22	1:A:143:ARG:HG3	1.94	0.48
1:B:85:LEU:HB3	1:B:127:LEU:HD23	1.95	0.48
2:C:858:MET:HG3	2:C:859:PRO:HD2	1.93	0.48
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	2.17	0.48
3:D:690:ALA:O	3:D:694:VAL:HG13	2.13	0.48
3:D:695:ILE:HG13	3:D:696:HIS:H	1.77	0.48
3:D:820:GLU:HB3	3:D:836:VAL:HG11	1.95	0.48
2:C:1008:ARG:HD3	2:C:1028:GLY:N	2.29	0.48
2:C:472:ARG:O	2:C:532:MET:N	2.46	0.48
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.96	0.48
3:D:539:ASP:HB3	3:D:600:LEU:HB3	1.94	0.48
3:D:7:LYS:HA	3:D:1459:LEU:HD13	1.94	0.48
2:C:97:ARG:HG2	2:C:112:GLU:OE2	2.13	0.48
2:C:424:GLY:O	2:C:426:ASP:N	2.41	0.48
3:D:353:VAL:HG22	3:D:368:VAL:HG22	1.94	0.48
3:D:153:LEU:HB2	3:D:157:GLU:HG2	1.95	0.48
3:D:739:ASP:N	3:D:739:ASP:OD1	2.47	0.48
3:D:850:LEU:HD22	3:D:881:LEU:HD12	1.95	0.48
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.48
2:C:810:ASP:HB2	2:C:813:VAL:HG13	1.96	0.48
3:D:101:HIS:HE1	3:D:582:LEU:HD22	1.77	0.48
3:D:1189:ARG:HD2	3:D:1204:CYS:SG	2.54	0.48
3:D:50:PHE:O	3:D:89:ARG:HD2	2.14	0.48
2:C:680:ASP:N	3:D:943:THR:HG21	2.27	0.48
3:D:415:VAL:O	3:D:432:TYR:HA	2.14	0.48
3:D:1284:GLU:HB2	3:D:1291:SER:O	2.14	0.48
3:D:702:LEU:HB3	3:D:745:MET:CE	2.44	0.48
1:A:133:GLU:HG2	1:A:134:GLU:N	2.29	0.47
2:C:45:GLN:O	2:C:48:PHE:HB2	2.14	0.47
1:B:75:VAL:O	1:B:79:ILE:HG13	2.14	0.47
2:C:1056:LYS:O	3:D:624:ASP:HB2	2.14	0.47
2:C:198:ARG:NH1	2:C:202:TYR:O	2.39	0.47
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.95	0.47
3:D:1031:ASN:HB3	3:D:1034:GLN:HB2	1.96	0.47
3:D:123:LEU:HG	3:D:152:LEU:HD13	1.96	0.47
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.61	0.47
2:C:198:ARG:NH1	2:C:203:ASP:HA	2.30	0.47
2:C:713:ARG:HA	2:C:819:VAL:HA	1.97	0.47
3:D:1264:GLU:OE2	3:D:1425:THR:HG22	2.15	0.47
3:D:365:ASP:O	3:D:379:ALA:HB2	2.13	0.47
2:C:47:ALA:CB	2:C:345:ARG:HG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:GLU:H	2:C:614:ARG:HB3	1.80	0.47
2:C:865:THR:HA	2:C:866:PRO:HD3	1.78	0.47
3:D:1394:VAL:HG21	3:D:1432:LYS:NZ	2.30	0.47
3:D:61:GLY:HA3	3:D:64:LYS:HZ3	1.79	0.47
3:D:829:VAL:O	3:D:831:GLY:N	2.43	0.47
3:D:1354:LYS:HA	3:D:1357:ARG:HD2	1.96	0.47
3:D:165:LYS:O	3:D:167:GLU:N	2.48	0.47
2:C:978:ARG:NH1	2:C:978:ARG:CG	2.73	0.47
2:C:891:GLY:O	2:C:991:GLN:HG2	2.15	0.47
3:D:348:GLN:HB3	3:D:350:HIS:CE1	2.50	0.47
3:D:565:ILE:O	3:D:569:ASN:HB2	2.15	0.47
5:N:3:DA:H2"	5:N:4:DA:C8	2.50	0.47
3:D:956:ILE:HA	3:D:1039:CYS:HB3	1.97	0.47
2:C:216:GLU:O	2:C:218:VAL:N	2.48	0.47
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.50	0.46
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.48	0.46
1:A:165:ILE:HA	1:A:166:PRO:HD3	1.83	0.46
2:C:397:GLU:HG2	2:C:403:SER:OG	2.15	0.46
2:C:759:THR:HG22	2:C:787:ASP:HA	1.98	0.46
2:C:910:LYS:O	2:C:914:ILE:HG12	2.15	0.46
2:C:946:ARG:HH11	2:C:946:ARG:HG2	1.80	0.46
3:D:29:PRO:HB3	3:D:548:ILE:HB	1.97	0.46
3:D:607:LEU:HD23	3:D:614:PHE:CE1	2.49	0.46
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.16	0.46
3:D:786:ILE:HG21	3:D:1027:GLY:H	1.81	0.46
1:A:97:VAL:HG21	1:A:120:VAL:HG21	1.97	0.46
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.16	0.46
1:B:58:ILE:HB	1:B:61:VAL:HB	1.98	0.46
3:D:1458:GLU:O	3:D:1460:ILE:N	2.49	0.46
2:C:290:LEU:HD13	2:C:302:VAL:HG12	1.97	0.46
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.97	0.46
2:C:98:LEU:HD21	2:C:373:VAL:HG21	1.98	0.46
3:D:1135:ARG:NH1	3:D:1139:ASP:HB3	2.31	0.46
3:D:1197:ARG:HB3	3:D:1396:GLU:CD	2.36	0.46
1:A:169:ALA:HB1	1:A:171:PHE:CE2	2.51	0.46
2:C:100:LEU:HB3	2:C:368:THR:OG1	2.15	0.46
2:C:478:VAL:HG22	2:C:507:ARG:HG2	1.97	0.46
1:B:94:LEU:HD11	1:B:119:ASP:HB2	1.97	0.46
2:C:198:ARG:HH12	2:C:203:ASP:HA	1.81	0.46
1:A:67:THR:HB	2:C:627:ARG:HD3	1.98	0.46
2:C:851:LYS:HG3	2:C:853:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.98	0.46
1:B:201:THR:HG22	1:B:202:ASP:H	1.81	0.46
2:C:288:ARG:N	2:C:288:ARG:HH11	2.07	0.46
2:C:861:LEU:HD12	2:C:865:THR:HG23	1.97	0.46
3:D:1044:LEU:HA	3:D:1056:PRO:HA	1.97	0.46
1:A:174:VAL:HA	1:A:201:THR:HG22	1.97	0.45
1:A:13:VAL:HG21	1:B:228:PRO:HB3	1.98	0.45
2:C:165:LEU:HA	2:C:165:LEU:HD12	1.87	0.45
2:C:3:ILE:HD11	2:C:665:PHE:CE2	2.50	0.45
2:C:966:LEU:HA	2:C:966:LEU:HD12	1.77	0.45
3:D:182:GLY:HA2	3:D:203:ALA:O	2.16	0.45
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.98	0.45
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.51	0.45
3:D:792:ILE:HD13	3:D:941:PHE:HD2	1.81	0.45
2:C:335:THR:O	2:C:339:LEU:HG	2.16	0.45
2:C:586:ARG:NH1	2:C:590:ASP:OD2	2.49	0.45
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.98	0.45
2:C:146:VAL:HB	2:C:281:LEU:HD11	1.99	0.45
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.98	0.45
2:C:602:GLU:HA	2:C:648:ARG:HA	1.99	0.45
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.98	0.45
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.97	0.45
3:D:805:GLU:HA	3:D:832:ARG:HB3	1.98	0.45
3:D:908:LYS:HB2	3:D:1027:GLY:CA	2.47	0.45
2:C:1040:LEU:HD23	2:C:1049:LEU:HA	1.99	0.45
2:C:97:ARG:HG2	2:C:111:ASP:HB3	1.97	0.45
2:C:327:HIS:C	2:C:329:GLY:H	2.20	0.45
3:D:165:LYS:NZ	3:D:199:LEU:HD22	2.31	0.45
3:D:613:ARG:NH1	3:D:616:GLN:HG2	2.32	0.45
2:C:1009:SER:HB2	3:D:625:TYR:CD1	2.51	0.45
3:D:826:PRO:HD2	3:D:829:VAL:HG21	1.98	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.17	0.45
4:E:72:ARG:HB2	4:E:73:LEU:HD12	1.97	0.45
1:B:109:VAL:HA	1:B:113:ASP:OD2	2.16	0.45
2:C:134:ARG:NH2	2:C:392:SER:O	2.50	0.45
2:C:976:ASP:OD1	2:C:978:ARG:NH1	2.50	0.45
1:A:85:LEU:HD12	1:A:124:ASN:HB3	1.98	0.45
1:A:30:ARG:HH21	1:A:191:ASP:HB3	1.82	0.45
2:C:290:LEU:HA	2:C:290:LEU:HD12	1.60	0.45
2:C:344:PHE:CE1	2:C:378:LEU:HD11	2.52	0.45
3:D:1381:VAL:HB	3:D:1389:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.98	0.45
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.98	0.45
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.99	0.45
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.97	0.45
2:C:235:LEU:HD11	2:C:298:PHE:HE2	1.81	0.45
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.97	0.45
3:D:558:LEU:HD23	3:D:567:ILE:HD13	1.99	0.45
3:D:963:TYR:CE1	3:D:1002:LYS:HB3	2.51	0.45
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.99	0.45
2:C:1089:VAL:HA	2:C:1099:VAL:HG21	1.99	0.45
2:C:288:ARG:H	2:C:288:ARG:HD3	1.81	0.45
3:D:123:LEU:O	3:D:127:LEU:HG	2.16	0.45
3:D:805:GLU:OE2	3:D:816:HIS:NE2	2.49	0.45
3:D:1462:LEU:HG	3:D:1472:ILE:HB	1.99	0.45
3:D:209:ARG:HB2	3:D:389:GLU:HG3	1.99	0.45
3:D:346:ARG:HH22	3:D:349:PRO:HD3	1.82	0.45
3:D:553:ARG:O	3:D:557:LEU:HB2	2.17	0.45
3:D:721:VAL:HG12	3:D:722:GLU:O	2.17	0.45
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.82	0.45
1:A:183:ASP:N	1:A:183:ASP:OD1	2.50	0.45
1:B:143:ARG:HD2	1:B:160:ASP:HB2	1.98	0.45
2:C:139:GLN:HA	2:C:411:SER:O	2.17	0.45
2:C:272:ALA:C	2:C:276:LYS:NZ	2.71	0.45
2:C:716:LYS:HD3	2:C:716:LYS:HA	1.83	0.45
2:C:953:VAL:HB	2:C:962:GLN:OE1	2.17	0.45
3:D:179:VAL:HG11	3:D:203:ALA:HB3	1.99	0.45
3:D:800:LYS:HG2	3:D:804:LEU:HD22	1.99	0.45
1:B:74:ASP:HB2	3:D:872:ARG:HH22	1.83	0.44
2:C:473:ARG:HG3	2:C:480:THR:HB	1.99	0.44
2:C:428:ARG:HH11	3:D:1086:LEU:HD11	1.81	0.44
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.99	0.44
2:C:1053:LEU:HD13	3:D:617:ASN:HB3	1.99	0.44
3:D:701:LEU:O	3:D:747:VAL:HA	2.17	0.44
3:D:758:GLU:O	3:D:762:GLN:HG2	2.18	0.44
2:C:200:LEU:HA	2:C:298:PHE:HB2	1.99	0.44
2:C:223:ASP:HB2	2:C:224:GLU:H	1.36	0.44
2:C:341:THR:O	2:C:345:ARG:HG3	2.18	0.44
3:D:176:ASP:HB3	3:D:177:ALA:H	1.56	0.44
3:D:510:GLU:HG3	3:D:511:TRP:HD1	1.82	0.44
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.52	0.44
3:D:764:LEU:HD23	3:D:766:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:O	1:A:46:SER:HB3	2.18	0.44
2:C:1036:GLU:OE1	2:C:1036:GLU:N	2.47	0.44
2:C:1055:LEU:HD11	2:C:1066:ALA:HB2	1.99	0.44
3:D:708:LEU:HD21	3:D:1091:SER:HB2	1.99	0.44
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.52	0.44
2:C:290:LEU:HD22	2:C:302:VAL:HG12	2.00	0.44
2:C:858:MET:HE3	2:C:858:MET:HB2	1.91	0.44
3:D:486:ARG:HH21	3:D:489:ARG:NH1	2.04	0.44
2:C:146:VAL:HB	2:C:281:LEU:HD21	1.99	0.44
3:D:101:HIS:HD2	3:D:104:PHE:CE2	2.35	0.44
3:D:1136:LYS:HB3	3:D:1139:ASP:OD2	2.17	0.44
3:D:1213:ARG:NH2	4:E:10:PHE:O	2.51	0.44
3:D:602:SER:O	3:D:606:ILE:HG12	2.17	0.44
2:C:710:ILE:HG22	2:C:823:VAL:HB	1.99	0.44
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.38	0.44
2:C:673:LEU:HA	2:C:991:GLN:HA	1.99	0.44
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.99	0.44
3:D:714:GLN:HB2	3:D:716:PHE:CE2	2.53	0.44
2:C:78:PHE:HA	2:C:79:PRO:HD3	1.90	0.44
2:C:695:LEU:HD21	2:C:833:LEU:HB3	2.00	0.44
3:D:1294:VAL:HG12	3:D:1295:GLU:N	2.32	0.44
3:D:1307:LYS:HB3	3:D:1308:GLU:OE2	2.18	0.44
3:D:165:LYS:HZ2	3:D:199:LEU:HD22	1.81	0.44
3:D:42:ASP:HA	3:D:46:ASP:HB2	2.00	0.44
3:D:967:ALA:HB1	3:D:995:LEU:HD21	2.00	0.44
2:C:1070:ILE:HD11	2:C:1076:VAL:HG22	2.00	0.44
2:C:246:ASP:HA	2:C:247:PRO:HD3	1.72	0.44
2:C:48:PHE:HB3	2:C:52:PHE:CD2	2.49	0.44
2:C:71:TYR:HA	2:C:96:ALA:HA	2.00	0.44
3:D:1422:MET:HB2	3:D:1426:LYS:HD3	2.00	0.44
3:D:1311:LEU:HA	3:D:1325:LEU:O	2.18	0.44
3:D:355:VAL:HG11	3:D:385:VAL:HG11	2.00	0.44
3:D:65:ARG:HA	3:D:65:ARG:HD2	1.69	0.44
1:B:57:TYR:CD2	1:B:161:ARG:HG3	2.53	0.43
2:C:358:ARG:HD3	2:C:371:LYS:O	2.17	0.43
2:C:136:ILE:HD11	2:C:386:PHE:CE1	2.53	0.43
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.53	0.43
3:D:136:ASP:CB	3:D:137:PRO:HD2	2.45	0.43
1:A:79:ILE:HA	1:A:82:LEU:HD12	2.00	0.43
2:C:585:GLU:O	2:C:589:ARG:HG2	2.19	0.43
3:D:1131:SER:OG	3:D:1133:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:408:GLU:HG2	3:D:408:GLU:H	1.59	0.43
3:D:650:LEU:HD21	3:D:677:LEU:HD23	2.00	0.43
1:B:62:LEU:HD23	1:B:163:ASN:HD22	1.83	0.43
2:C:184:MET:O	2:C:190:LYS:HA	2.18	0.43
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.01	0.43
2:C:666:LEU:HG	2:C:668:LEU:HG	2.00	0.43
2:C:21:ILE:HD11	2:C:455:LEU:HD22	2.00	0.43
2:C:233:GLU:N	2:C:233:GLU:OE1	2.41	0.43
2:C:47:ALA:HB2	2:C:345:ARG:HG2	2.00	0.43
2:C:627:ARG:HG3	2:C:628:PHE:CD2	2.54	0.43
2:C:722:ILE:HD12	2:C:823:VAL:HG21	2.00	0.43
3:D:1280:VAL:O	3:D:1294:VAL:HG13	2.17	0.43
3:D:798:GLU:HG2	3:D:799:LYS:H	1.83	0.43
3:D:919:PHE:HA	3:D:927:THR:OG1	2.19	0.43
1:A:102:LYS:HA	1:A:138:LEU:O	2.19	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	2.01	0.43
2:C:853:LEU:HB2	2:C:858:MET:CE	2.49	0.43
3:D:1118:ILE:HA	3:D:1118:ILE:HD12	1.84	0.43
3:D:563:PRO:HG2	3:D:566:ILE:HG13	2.01	0.43
3:D:568:ARG:HH11	3:D:571:LYS:HE3	1.83	0.43
3:D:739:ASP:OD2	3:D:741:ASP:OD2	2.36	0.43
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.53	0.43
2:C:1075:ASP:OD1	2:C:1076:VAL:N	2.52	0.43
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.00	0.43
3:D:1123:PHE:HB3	3:D:1132:LEU:HG	2.00	0.43
2:C:147:TYR:HA	2:C:323:ASP:OD2	2.18	0.43
2:C:18:LEU:HB3	2:C:408:ARG:HD2	2.00	0.43
2:C:429:ASP:OD1	3:D:1079:LYS:HD3	2.19	0.43
2:C:715:THR:OG1	2:C:718:GLY:O	2.36	0.43
2:C:810:ASP:O	2:C:812:GLY:N	2.50	0.43
3:D:1135:ARG:HB3	3:D:1140:ILE:HD11	2.00	0.43
3:D:1274:ILE:HA	3:D:1325:LEU:HD21	2.00	0.43
3:D:975:GLU:HG3	3:D:979:GLU:OE2	2.18	0.43
2:C:501:THR:HA	2:C:502:PRO:HD3	1.88	0.43
2:C:759:THR:HB	2:C:785:VAL:HG22	2.01	0.43
1:A:38:ASN:O	1:A:42:ARG:HG2	2.18	0.43
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.34	0.43
2:C:219:GLN:O	2:C:223:ASP:OD2	2.37	0.43
2:C:334:ARG:HH22	2:C:415:PRO:HG2	1.84	0.43
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.19	0.43
3:D:165:LYS:HD2	3:D:397:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:486:ARG:HA	3:D:489:ARG:HB3	2.00	0.43
3:D:645:PRO:HA	3:D:721:VAL:O	2.19	0.43
4:E:45:ARG:HH21	4:E:63:TRP:HH2	1.66	0.43
2:C:238:LEU:HD21	2:C:242:LEU:HD13	2.01	0.43
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.00	0.43
2:C:676:ILE:HG23	2:C:988:VAL:HG13	1.99	0.43
3:D:1366:LYS:O	3:D:1370:ILE:HG13	2.19	0.43
1:B:143:ARG:CZ	1:B:158:ILE:HG21	2.49	0.42
3:D:531:ASP:C	3:D:533:GLY:H	2.23	0.42
3:D:628:ARG:NH1	7:T:16:DC:H2"	2.34	0.42
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.54	0.42
2:C:34:VAL:HB	2:C:38:LYS:HZ2	1.84	0.42
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.00	0.42
3:D:895:VAL:HG21	3:D:922:LEU:HD21	2.00	0.42
2:C:876:VAL:HG11	3:D:949:ILE:HG21	2.01	0.42
4:E:54:LEU:HG	4:E:58:PRO:CG	2.44	0.42
1:B:92:PRO:HA	1:B:146:ARG:HH12	1.85	0.42
2:C:274:ARG:HH22	2:C:284:ARG:HA	1.84	0.42
2:C:334:ARG:HE	2:C:339:LEU:HD23	1.85	0.42
2:C:37:GLU:OE2	2:C:38:LYS:HG2	2.20	0.42
2:C:512:ARG:HD3	2:C:512:ARG:HA	1.84	0.42
2:C:52:PHE:CE1	2:C:98:LEU:HD13	2.53	0.42
3:D:1018:ASN:O	3:D:1021:TYR:N	2.51	0.42
3:D:1037:GLN:HG2	3:D:1042:ARG:HG2	2.00	0.42
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.85	0.42
3:D:1277:ILE:HG13	3:D:1277:ILE:H	1.68	0.42
3:D:1435:LEU:HB2	3:D:1457:ASP:OD1	2.20	0.42
3:D:520:LEU:HG	3:D:521:PRO:HD2	2.01	0.42
3:D:630:VAL:O	3:D:725:SER:HB3	2.18	0.42
2:C:379:GLU:O	2:C:383:ARG:HB3	2.19	0.42
2:C:893:ALA:HB2	2:C:918:LEU:HD23	2.00	0.42
3:D:1128:VAL:HG12	3:D:1129:THR:N	2.33	0.42
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.54	0.42
3:D:500:ARG:HG2	3:D:1388:ARG:NH1	2.35	0.42
3:D:966:GLU:HA	3:D:969:ARG:HG2	2.01	0.42
2:C:700:TYR:HB2	2:C:833:LEU:HB2	2.01	0.42
2:C:718:GLY:HA3	2:C:761:PHE:CG	2.54	0.42
3:D:1209:LEU:HD11	4:E:16:LYS:HD2	2.01	0.42
3:D:1296:SER:HB3	3:D:1299:PHE:CD2	2.49	0.42
3:D:864:VAL:HG22	3:D:877:PRO:HD3	2.01	0.42
3:D:93:ILE:HB	3:D:517:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.55	0.42
2:C:211:LEU:HD13	2:C:221:LEU:HD21	2.01	0.42
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.55	0.42
3:D:1312:LEU:HD21	3:D:1327:ARG:HH21	1.85	0.42
2:C:1085:PHE:HB2	3:D:1468:LEU:HB3	2.01	0.42
3:D:212:ARG:HB3	3:D:388:HIS:CD2	2.54	0.42
2:C:889:HIS:CE1	3:D:951:ILE:H	2.37	0.42
4:E:3:GLU:O	4:E:5:GLY:N	2.52	0.42
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.70	0.42
2:C:113:VAL:O	2:C:115:LEU:N	2.49	0.42
2:C:313:LEU:HD22	2:C:321:GLU:O	2.20	0.42
2:C:393:GLN:HG2	6:R:25:G:O2'	2.20	0.42
2:C:475:VAL:HG23	2:C:480:THR:OG1	2.19	0.42
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.84	0.42
2:C:905:ILE:HG22	2:C:906:PHE:CD2	2.54	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.91	0.42
3:D:167:GLU:OE1	3:D:198:ARG:NH2	2.53	0.42
3:D:458:ALA:HB2	3:D:575:GLN:NE2	2.33	0.42
3:D:583:ASP:OD2	3:D:604:THR:HG21	2.19	0.42
4:E:24:ALA:O	4:E:28:GLN:HG3	2.20	0.42
1:A:180:GLN:HB2	1:A:196:THR:OG1	2.19	0.42
2:C:1014:SER:HB3	2:C:1017:THR:O	2.19	0.42
2:C:469:THR:O	2:C:485:TYR:HA	2.20	0.42
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.50	0.42
2:C:127:PHE:O	2:C:129:ILE:HD12	2.20	0.42
3:D:719:VAL:O	3:D:721:VAL:HG23	2.20	0.42
3:D:877:PRO:O	3:D:880:ILE:HG22	2.20	0.42
2:C:295:ASP:C	2:C:297:GLU:H	2.23	0.42
2:C:350:ARG:HB3	2:C:377:PRO:HB3	2.00	0.42
2:C:521:PRO:HB2	3:D:1055:VAL:HG21	2.02	0.42
3:D:1401:GLU:OE2	3:D:1402:ALA:N	2.53	0.42
3:D:352:ASN:HB2	3:D:369:ALA:O	2.20	0.42
2:C:1071:ILE:HA	2:C:1071:ILE:HD13	1.91	0.41
2:C:127:PHE:HB2	2:C:129:ILE:HD11	2.01	0.41
2:C:906:PHE:HZ	3:D:1070:TYR:HD1	1.67	0.41
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.55	0.41
3:D:212:ARG:H	3:D:388:HIS:HD2	1.68	0.41
3:D:28:LYS:C	3:D:548:ILE:HG21	2.40	0.41
3:D:494:LYS:HB2	3:D:494:LYS:NZ	2.35	0.41
1:B:101:LEU:HD23	1:B:140:MET:HG2	2.02	0.41
2:C:205:GLU:HG3	2:C:205:GLU:H	1.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:ASP:OD1	2:C:224:GLU:HG2	2.20	0.41
2:C:48:PHE:O	2:C:52:PHE:HB2	2.20	0.41
3:D:433:GLY:HA3	3:D:447:VAL:O	2.19	0.41
3:D:607:LEU:HD23	3:D:614:PHE:HE1	1.85	0.41
2:C:265:ARG:NH1	2:C:267:TYR:HD1	2.18	0.41
3:D:1378:TYR:O	3:D:1420:LEU:HB3	2.21	0.41
3:D:1394:VAL:HB	3:D:1397:LYS:HG2	2.02	0.41
3:D:184:GLU:HA	3:D:202:VAL:HA	2.03	0.41
3:D:416:ALA:HB3	3:D:419:ASP:OD1	2.20	0.41
3:D:703:ASN:HB3	3:D:746:ALA:HB3	2.02	0.41
7:T:11:DT:H2''	7:T:12:DC:O5'	2.20	0.41
2:C:18:LEU:HD21	2:C:542:VAL:HG11	2.02	0.41
2:C:710:ILE:HD11	2:C:758:ARG:NH2	2.28	0.41
3:D:1209:LEU:HD12	3:D:1213:ARG:HD3	2.01	0.41
3:D:1401:GLU:CD	3:D:1415:VAL:HG22	2.40	0.41
1:B:190:THR:HG21	3:D:720:LEU:O	2.20	0.41
1:A:25:LEU:HD22	1:B:225:PHE:CE1	2.55	0.41
2:C:1005:MET:HB2	3:D:724:GLN:NE2	2.31	0.41
2:C:384:GLU:HA	2:C:388:ARG:NH2	2.33	0.41
2:C:555:ALA:HB2	3:D:1070:TYR:HE2	1.86	0.41
2:C:580:MET:HG3	2:C:902:ILE:HG12	2.02	0.41
3:D:655:PRO:HA	3:D:658:LEU:HD12	2.01	0.41
3:D:717:GLN:HA	3:D:718:PRO:HD3	1.87	0.41
1:A:34:VAL:HG21	2:C:939:ARG:NE	2.36	0.41
2:C:726:ILE:HA	2:C:727:PRO:HD3	1.81	0.41
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	2.03	0.41
3:D:646:LYS:HE3	3:D:722:GLU:HG2	2.02	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HD2	2.03	0.41
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.56	0.41
2:C:409:ARG:HA	2:C:454:SER:HA	2.03	0.41
3:D:1279:GLY:O	3:D:1319:VAL:HG12	2.21	0.41
3:D:1398:TRP:CE3	3:D:1398:TRP:HA	2.56	0.41
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.82	0.41
3:D:165:LYS:CG	3:D:199:LEU:HB3	2.49	0.41
3:D:131:LYS:HB2	3:D:568:ARG:HG2	2.03	0.41
3:D:826:PRO:HB2	3:D:829:VAL:HG23	2.01	0.41
3:D:880:ILE:HA	3:D:880:ILE:HD12	1.93	0.41
3:D:1284:GLU:HG2	3:D:1291:SER:HB2	2.02	0.41
3:D:1364:HIS:ND1	3:D:1366:LYS:HG3	2.35	0.41
3:D:756:GLN:O	3:D:760:ARG:HG2	2.21	0.41
4:E:59:ASN:OD1	4:E:60:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:VAL:HG22	2:C:121:MET:HE1	2.03	0.41
2:C:196:LEU:HA	2:C:199:VAL:HG23	2.02	0.41
2:C:290:LEU:HD11	2:C:301:GLU:N	2.23	0.41
2:C:607:ASP:OD1	2:C:608:GLY:N	2.49	0.41
3:D:1295:GLU:HB3	3:D:1296:SER:H	1.53	0.41
2:C:1081:VAL:HB	2:C:1086:ARG:NH1	2.36	0.41
2:C:443:THR:HG22	2:C:453:THR:HG22	2.02	0.41
2:C:743:VAL:HG11	2:C:755:LEU:HD12	2.02	0.41
3:D:111:LYS:HE2	3:D:111:LYS:HB2	1.88	0.41
3:D:832:ARG:HA	3:D:832:ARG:HD2	1.86	0.41
4:E:51:LEU:HG	4:E:53:GLY:H	1.86	0.41
2:C:436:GLY:HA2	2:C:538:GLN:O	2.21	0.41
2:C:586:ARG:HH12	2:C:590:ASP:CG	2.25	0.41
3:D:1108:ARG:NH1	3:D:1460:ILE:HG13	2.36	0.41
3:D:704:ARG:NH2	3:D:743:ASP:OD2	2.53	0.41
3:D:861:GLN:N	3:D:861:GLN:OE1	2.54	0.41
1:B:25:LEU:HD23	1:B:28:LEU:HD21	2.04	0.40
2:C:200:LEU:HD23	2:C:298:PHE:HB3	2.03	0.40
2:C:34:VAL:HG11	2:C:38:LYS:HZ1	1.85	0.40
2:C:474:VAL:HG12	2:C:479:VAL:HG13	2.03	0.40
2:C:729:LEU:HA	2:C:729:LEU:HD23	1.93	0.40
3:D:1119:SER:HB2	3:D:1185:GLU:CB	2.51	0.40
3:D:1128:VAL:HG23	3:D:1133:ARG:HH22	1.85	0.40
2:C:1085:PHE:CD1	3:D:1468:LEU:HB3	2.55	0.40
7:T:2:DG:H2"	7:T:3:DG:C8	2.56	0.40
1:A:179:PHE:HB3	1:A:197:LEU:HD12	2.03	0.40
1:B:185:ARG:HB3	1:B:190:THR:HA	2.03	0.40
2:C:259:GLY:CA	2:C:291:ALA:HB2	2.51	0.40
2:C:559:LEU:HD12	2:C:559:LEU:O	2.21	0.40
2:C:589:ARG:HB3	2:C:596:TYR:CZ	2.56	0.40
3:D:367:ILE:HG13	3:D:368:VAL:H	1.85	0.40
4:E:22:VAL:CG1	4:E:68:LEU:HD21	2.51	0.40
2:C:205:GLU:OE1	2:C:206:THR:HG23	2.20	0.40
2:C:350:ARG:CB	2:C:377:PRO:HB3	2.51	0.40
2:C:503:LEU:HD21	2:C:508:ILE:HD13	2.03	0.40
2:C:690:ILE:HG12	2:C:691:SER:N	2.37	0.40
3:D:549:ASN:O	3:D:553:ARG:HB2	2.21	0.40
2:C:831:ARG:HH21	2:C:1000:MET:HG3	1.86	0.40
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	2.02	0.40
3:D:192:ALA:HB2	3:D:393:ILE:HD12	2.04	0.40
3:D:760:ARG:HD3	4:E:61:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:HA	1:A:27:PRO:HA	1.88	0.40
2:C:222:MET:HG2	2:C:222:MET:O	2.19	0.40
2:C:69:LEU:O	2:C:97:ARG:HB2	2.22	0.40
3:D:116:LEU:HA	3:D:116:LEU:HD23	1.85	0.40
3:D:57:GLU:HG2	3:D:58:CYS:N	2.37	0.40
3:D:849:ALA:O	3:D:853:VAL:HG23	2.21	0.40
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.95	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	221/315 (70%)	193 (87%)	19 (9%)	9 (4%)	3	23
1	B	221/315 (70%)	199 (90%)	21 (10%)	1 (0%)	29	68
2	C	1077/1119 (96%)	901 (84%)	149 (14%)	27 (2%)	5	34
3	D	1352/1534 (88%)	1112 (82%)	189 (14%)	51 (4%)	3	25
4	E	91/99 (92%)	74 (81%)	14 (15%)	3 (3%)	4	28
All	All	2962/3382 (88%)	2479 (84%)	392 (13%)	91 (3%)	4	30

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	THR
2	C	2	GLU
2	C	111	ASP
2	C	164	PRO
2	C	213	ALA
2	C	217	LEU
2	C	223	ASP

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Mol	Chain	Res	Type
2	C	320	HIS
2	C	369	PRO
3	D	136	ASP
3	D	176	ASP
3	D	363	ALA
3	D	806	PHE
3	D	808	THR
3	D	830	ALA
3	D	1273	VAL
3	D	1294	VAL
3	D	1295	GLU
3	D	1327	ARG
3	D	1454	GLY
1	A	47	SER
1	A	161	ARG
2	C	248	PRO
2	C	262	ALA
2	C	274	ARG
2	C	476	GLY
2	C	517	ARG
2	C	795	GLY
3	D	50	PHE
3	D	200	ASP
3	D	522	PRO
3	D	594	PRO
3	D	616	GLN
3	D	823	LEU
3	D	1411	GLY
3	D	1459	LEU
4	E	58	PRO
1	A	48	ILE
1	A	186	LEU
1	A	226	SER
2	C	96	ALA
2	C	188	LYS
2	C	272	ALA
2	C	815	LEU
2	C	984	GLU
3	D	166	GLN
3	D	345	TYR
3	D	417	PRO
3	D	735	ALA

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Mol	Chain	Res	Type
3	D	822	ALA
3	D	832	ARG
3	D	1208	ASP
4	E	4	PRO
1	A	29	GLU
1	A	191	ASP
2	C	114	PHE
3	D	82	LYS
3	D	109	PRO
3	D	132	TYR
3	D	146	PRO
3	D	374	GLU
3	D	406	ASP
3	D	425	GLY
3	D	595	GLY
3	D	696	HIS
3	D	711	LEU
3	D	750	PRO
3	D	1205	TYR
3	D	1269	LYS
3	D	1284	GLU
3	D	1317	ASP
4	E	42	PRO
1	A	134	GLU
2	C	751	PRO
2	C	905	ILE
3	D	560	GLN
3	D	621	LYS
3	D	1314	LYS
1	B	125	PRO
2	C	152	PRO
2	C	231	PRO
2	C	463	GLU
3	D	55	ASP
3	D	124	GLU
3	D	705	ALA
2	C	811	PRO
3	D	683	ILE
3	D	809	PRO
3	D	1032	PRO
3	D	1057	VAL
2	C	244	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	196/273 (72%)	187 (95%)	9 (5%)	27	61
1	B	196/273 (72%)	191 (97%)	5 (3%)	46	74
2	C	912/941 (97%)	837 (92%)	75 (8%)	11	40
3	D	1147/1289 (89%)	1058 (92%)	89 (8%)	12	42
4	E	82/88 (93%)	70 (85%)	12 (15%)	3	18
All	All	2533/2864 (88%)	2343 (92%)	190 (8%)	13	43

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	THR
1	A	15	THR
1	A	32	PHE
1	A	46	SER
1	A	126	ASP
1	A	131	THR
1	A	165	ILE
1	A	182	GLU
1	B	63	HIS
1	B	112	ARG
1	B	148	VAL
1	B	201	THR
1	B	205	VAL
2	C	8	ARG
2	C	30	LEU
2	C	38	LYS
2	C	39	ARG
2	C	49	ARG
2	C	52	PHE
2	C	81	ASP
2	C	98	LEU
2	C	102	HIS

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Mol	Chain	Res	Type
2	C	104	ASP
2	C	118	ILE
2	C	127	PHE
2	C	135	VAL
2	C	154	ARG
2	C	157	ARG
2	C	189	ARG
2	C	193	LEU
2	C	205	GLU
2	C	214	TYR
2	C	223	ASP
2	C	243	ARG
2	C	267	TYR
2	C	274	ARG
2	C	279	GLU
2	C	281	LEU
2	C	284	ARG
2	C	288	ARG
2	C	289	THR
2	C	295	ASP
2	C	300	ASP
2	C	307	LEU
2	C	321	GLU
2	C	350	ARG
2	C	351	LEU
2	C	367	LEU
2	C	375	SER
2	C	376	ARG
2	C	378	LEU
2	C	388	ARG
2	C	391	LEU
2	C	394	PHE
2	C	403	SER
2	C	405	ARG
2	C	473	ARG
2	C	481	ASP
2	C	506	ASN
2	C	533	ASP
2	C	565	GLN
2	C	589	ARG
2	C	605	LYS
2	C	610	ARG

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Mol	Chain	Res	Type
2	C	620	LEU
2	C	626	ARG
2	C	627	ARG
2	C	676	ILE
2	C	690	ILE
2	C	699	PHE
2	C	703	ILE
2	C	717	LEU
2	C	728	HIS
2	C	807	ARG
2	C	835	VAL
2	C	842	ARG
2	C	858	MET
2	C	899	GLN
2	C	953	VAL
2	C	966	LEU
2	C	978	ARG
2	C	1000	MET
2	C	1001	VAL
2	C	1008	ARG
2	C	1021	LEU
2	C	1035	MET
2	C	1099	VAL
2	C	1105	LYS
3	D	17	LYS
3	D	41	ARG
3	D	57	GLU
3	D	60	CYS
3	D	68	PHE
3	D	74	GLU
3	D	75	ARG
3	D	79	GLU
3	D	80	VAL
3	D	82	LYS
3	D	87	ARG
3	D	124	GLU
3	D	137	PRO
3	D	142	LEU
3	D	149	LYS
3	D	166	GLN
3	D	176	ASP
3	D	178	LEU

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Mol	Chain	Res	Type
3	D	340	THR
3	D	347	VAL
3	D	382	GLU
3	D	392	SER
3	D	400	VAL
3	D	405	ASP
3	D	408	GLU
3	D	414	ARG
3	D	430	ASP
3	D	431	VAL
3	D	435	VAL
3	D	450	TYR
3	D	494	LYS
3	D	520	LEU
3	D	686	GLU
3	D	724	GLN
3	D	734	GLU
3	D	754	PHE
3	D	804	LEU
3	D	808	THR
3	D	813	LEU
3	D	817	GLU
3	D	823	LEU
3	D	828	LYS
3	D	833	GLU
3	D	892	ASP
3	D	935	LYS
3	D	943	THR
3	D	971	LEU
3	D	983	LEU
3	D	985	ASP
3	D	1001	GLU
3	D	1008	PHE
3	D	1012	GLU
3	D	1013	GLU
3	D	1029	ARG
3	D	1041	LEU
3	D	1044	LEU
3	D	1058	ARG
3	D	1070	TYR
3	D	1083	ASP
3	D	1106	VAL

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Mol	Chain	Res	Type
3	D	1108	ARG
3	D	1109	GLU
3	D	1115	THR
3	D	1131	SER
3	D	1135	ARG
3	D	1151	ARG
3	D	1162	GLU
3	D	1170	ASP
3	D	1197	ARG
3	D	1207	TYR
3	D	1209	LEU
3	D	1235	GLN
3	D	1262	LEU
3	D	1290	LEU
3	D	1296	SER
3	D	1299	PHE
3	D	1304	LYS
3	D	1305	LEU
3	D	1314	LYS
3	D	1318	TYR
3	D	1325	LEU
3	D	1327	ARG
3	D	1342	GLU
3	D	1373	ARG
3	D	1383	ASP
3	D	1441	GLN
3	D	1460	ILE
3	D	1478	SER
3	D	1493	LYS
4	E	14	ASP
4	E	32	ARG
4	E	35	PHE
4	E	38	THR
4	E	39	VAL
4	E	40	LEU
4	E	41	GLU
4	E	47	LYS
4	E	49	GLN
4	E	51	LEU
4	E	56	ASP
4	E	83	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
2	C	141	HIS
2	C	431	HIS
2	C	609	ASN
2	C	670	GLN
2	C	829	GLN
2	C	884	GLN
3	D	101	HIS
3	D	388	HIS
3	D	552	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/29 (27%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	22	U

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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	223/315 (70%)	-0.31	0	100	100	45, 90, 147, 194	0
1	B	223/315 (70%)	-0.38	0	100	100	40, 86, 139, 173	0
2	C	1083/1119 (96%)	-0.11	19 (1%)	68	62	32, 101, 186, 255	0
3	D	1358/1534 (88%)	0.02	68 (5%)	28	25	34, 102, 194, 264	0
4	E	93/99 (93%)	0.10	5 (5%)	25	23	58, 107, 184, 204	0
5	N	11/13 (84%)	2.78	9 (81%)	0	0	369, 412, 462, 465	0
6	R	9/29 (31%)	1.02	1 (11%)	5	6	178, 188, 215, 227	0
7	T	22/22 (100%)	1.70	6 (27%)	0	0	202, 334, 453, 466	0
All	All	3022/3446 (87%)	-0.05	108 (3%)	42	38	32, 100, 193, 466	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	56	ASP	10.4
3	D	802	ALA	10.0
3	D	810	GLU	9.9
2	C	417	GLY	6.8
7	T	9	DC	6.2
4	E	57	ASP	5.7
3	D	1090	ASP	5.3
3	D	1296	SER	5.3
7	T	1	DG	5.2
3	D	1324	PRO	4.9
3	D	1309	ALA	4.8
2	C	416	GLY	4.8
3	D	70	GLY	4.7
3	D	1295	GLU	4.7
2	C	270	GLY	4.5
3	D	365	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
3	D	194	GLY	4.3
5	N	13	DC	4.3
3	D	1308	GLU	4.1
3	D	366	LYS	4.0
7	T	14	DA	4.0
3	D	1279	GLY	4.0
3	D	1280	VAL	4.0
3	D	369	ALA	4.0
3	D	367	ILE	3.9
5	N	12	DC	3.9
3	D	66	GLN	3.9
5	N	11	DC	3.9
3	D	1289	LYS	3.8
3	D	1408	ILE	3.8
3	D	79	GLU	3.7
3	D	341	GLU	3.7
2	C	1022	GLY	3.7
2	C	320	HIS	3.6
2	C	105	THR	3.6
2	C	365	ASP	3.6
3	D	63	TYR	3.6
2	C	726	ILE	3.5
7	T	2	DG	3.4
3	D	1313	VAL	3.3
7	T	3	DG	3.3
3	D	368	VAL	3.2
2	C	366	SER	3.2
3	D	1491	THR	3.2
3	D	58	CYS	3.1
3	D	801	GLY	3.1
3	D	81	THR	3.1
2	C	167	LYS	3.0
3	D	1273	VAL	3.0
2	C	361	MET	3.0
3	D	1316	GLY	3.0
3	D	165	LYS	2.9
3	D	372	ASP	2.9
2	C	103	LYS	2.9
3	D	67	ARG	2.9
3	D	378	ILE	2.9
3	D	215	TYR	2.9
4	E	55	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
5	N	5	DG	2.9
3	D	371	ILE	2.9
3	D	2	LYS	2.8
5	N	8	DA	2.8
3	D	343	LYS	2.8
3	D	1312	LEU	2.8
3	D	1305	LEU	2.8
3	D	351	MET	2.7
2	C	418	LEU	2.7
2	C	112	GLU	2.7
3	D	62	LYS	2.7
2	C	741	GLY	2.7
3	D	65	ARG	2.7
3	D	370	ALA	2.6
5	N	10	DT	2.6
3	D	798	GLU	2.6
3	D	342	PRO	2.6
2	C	222	MET	2.6
3	D	211	VAL	2.5
3	D	350	HIS	2.5
3	D	1278	ASP	2.5
3	D	193	PRO	2.5
3	D	393	ILE	2.5
3	D	1317	ASP	2.5
3	D	1130	ARG	2.5
3	D	803	GLY	2.4
5	N	7	DG	2.4
3	D	28	LYS	2.4
3	D	57	GLU	2.4
5	N	9	DT	2.4
7	T	8	DT	2.4
3	D	384	VAL	2.4
3	D	385	VAL	2.4
4	E	2	ALA	2.3
5	N	3	DA	2.3
2	C	786	LYS	2.3
2	C	106	GLY	2.2
3	D	78	VAL	2.2
3	D	481	MET	2.2
3	D	71	LYS	2.2
3	D	61	GLY	2.1
3	D	69	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	44	LEU	2.1
3	D	73	CYS	2.1
2	C	1023	GLY	2.1
3	D	55	ASP	2.1
6	R	24	U	2.1
4	E	41	GLU	2.1
3	D	1087	ARG	2.0
3	D	1285	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
8	ZN	D	1601	1/1	0.82	0.27	188,188,188,188	0
9	MG	D	1603	1/1	0.96	0.28	46,46,46,46	0
8	ZN	D	1602	1/1	0.98	0.12	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.