



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 PM GMT

PDB ID : 4B3G  
Title : crystal structure of Ighmbp2 helicase in complex with RNA  
Authors : Lim, S.C.; Song, H.  
Deposited on : 2012-07-24  
Resolution : 2.85 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

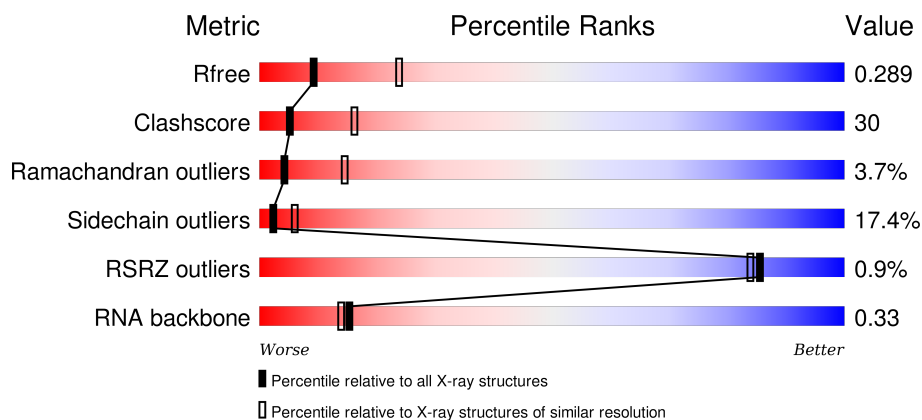
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)
RNA backbone	2183	1020 (3.22-2.50)

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. 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	646	<div> <div></div> <div>43%</div> <div>39%</div> <div>12%</div> <div>5%</div> </div>
1	B	646	<div> <div>49%</div> <div>35%</div> <div>10%</div> <div>6%</div> </div>
2	G	9	<div> <div>44%</div> <div>22%</div> <div>33%</div> </div>
2	H	9	<div> <div>11%</div> <div>44%</div> <div>22%</div> <div>11%</div> <div>11%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9979 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-BINDING PROTEIN SMUBP-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			4756	2998	854	889	15			
1	B	608	Total	C	N	O	S	0	0	0
			4704	2964	844	881	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLN	LEU	CONFLICT	UNP P38935
B	126	GLN	LEU	CONFLICT	UNP P38935

- Molecule 2 is a RNA chain called RNA (5'-(AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	P	0	0	0
			198	90	45	54	9			
2	H	8	Total	C	N	O	P	0	0	0
			176	80	40	48	8			

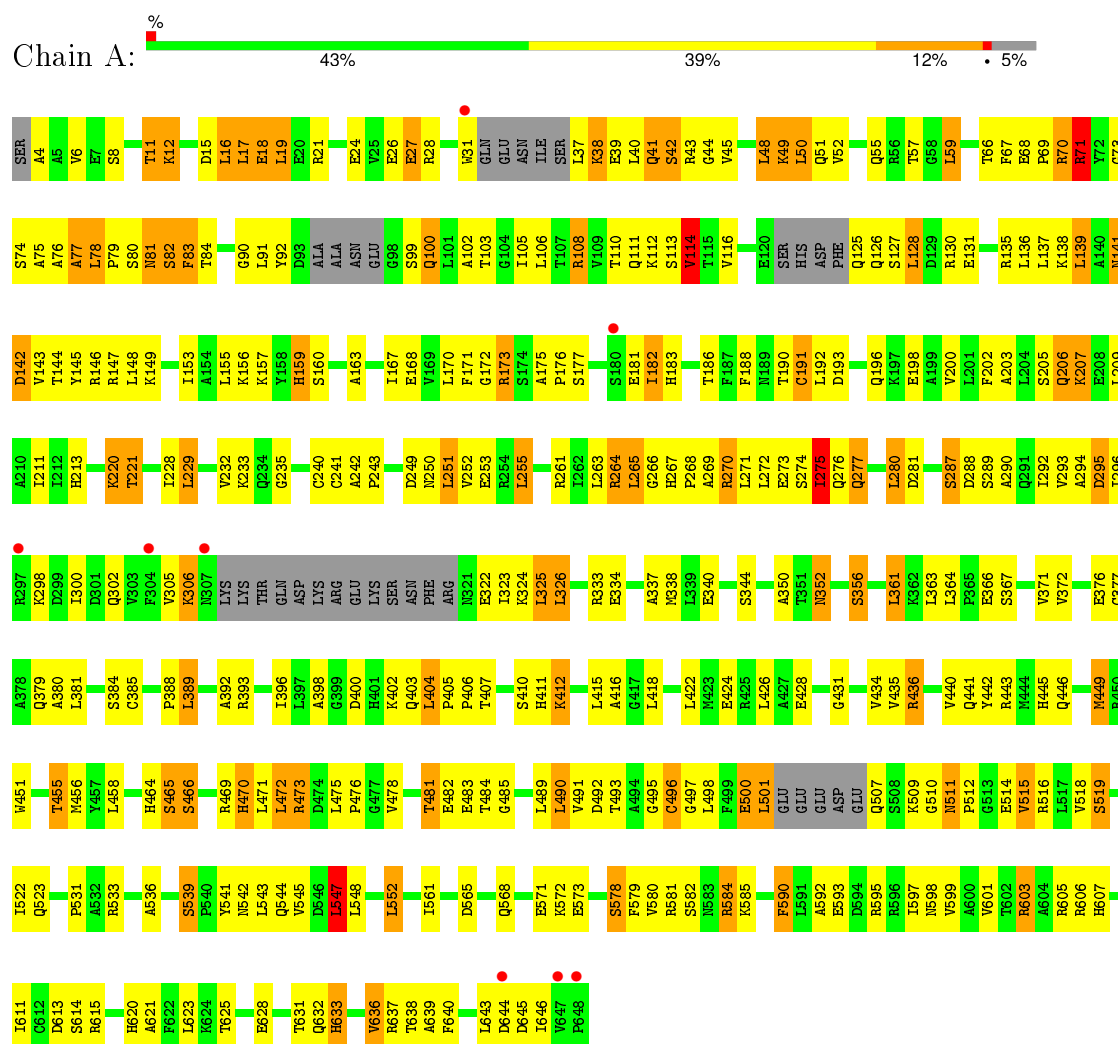
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	69	Total	O	0	0
			69	69		
3	G	5	Total	O	0	0
			5	5		
3	H	4	Total	O	0	0
			4	4		

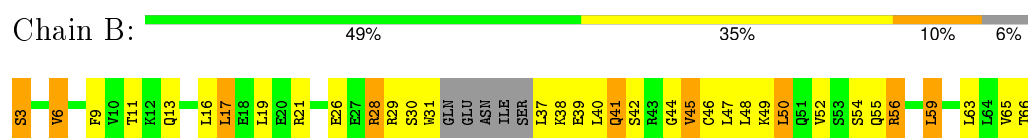
### 3 Residue-property plots

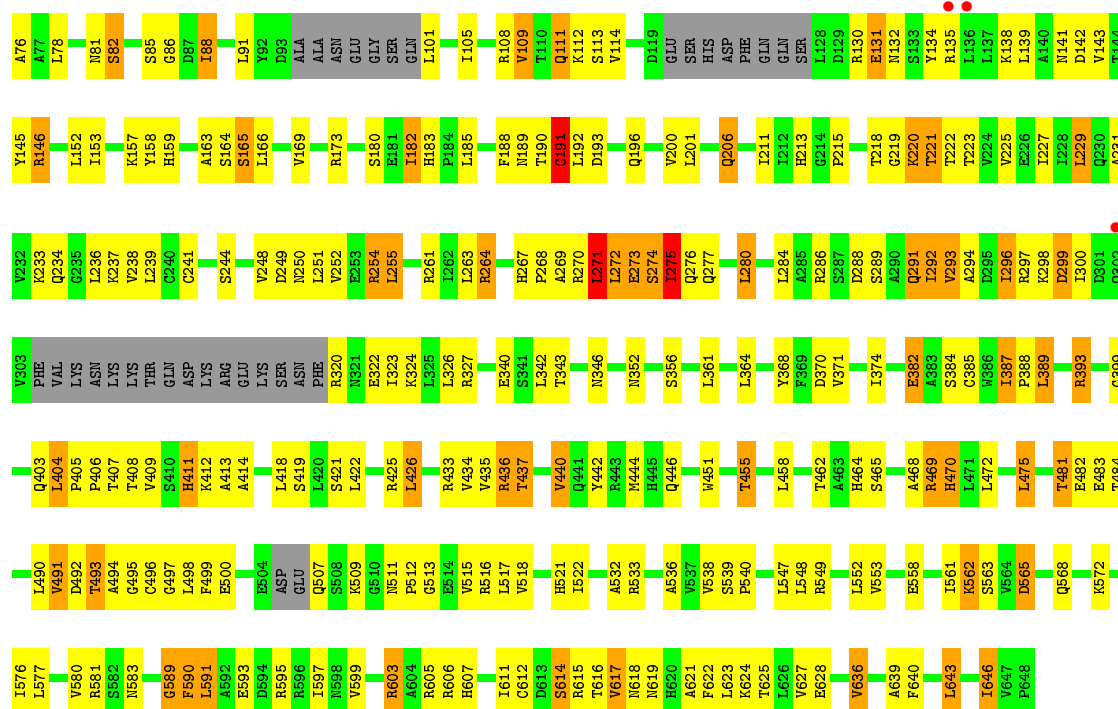
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-BINDING PROTEIN SMUBP-2

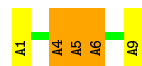


#### • Molecule 1: DNA-BINDING PROTEIN SMUBP-2





Chain G:



• Molecule 2: RNA (5'-(AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP)-3')

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.29 Å 87.29 Å 372.69 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.85 19.97 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.97-2.85) 99.3 (19.97-2.85)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.83 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.206 , 0.292 0.205 , 0.289	Depositor DCC
$R_{free}$ test set	1973 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.7	EDS
Estimated twinning fraction	0.075 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 39342 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.45	0/4824	0.66	1/6528 (0.0%)
1	B	0.48	0/4771	0.67	0/6458
2	G	0.68	0/224	1.12	0/347
2	H	0.88	0/199	1.19	1/308 (0.3%)
All	All	0.48	0/10018	0.70	2/13641 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	LEU	CA-CB-CG	5.67	128.34	115.30
2	H	5	A	C8-N9-C4	-5.34	103.66	105.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	271	LEU	Peptide

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4756	0	4878	339	0
1	B	4704	0	4816	257	0
2	G	198	0	100	9	0
2	H	176	0	89	10	0
3	A	67	0	0	15	1
3	B	69	0	0	10	0
3	G	5	0	0	1	0
3	H	4	0	0	0	0
All	All	9979	0	9883	601	1

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 30.

All (601) 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)
1:B:254:ARG:NH1	1:B:254:ARG:HB3	1.61	1.15
1:B:70:ARG:HH11	1:B:70:ARG:HG2	1.12	1.14
1:B:481:THR:HG22	1:B:484:THR:H	1.15	1.11
1:B:469:ARG:HG2	1:B:469:ARG:HH11	1.12	1.07
1:A:76:ALA:H	1:A:77:ALA:HB2	1.20	1.07
1:A:37:LEU:HD12	1:A:40:LEU:HD21	1.32	1.05
1:B:254:ARG:HH11	1:B:254:ARG:HB3	0.88	1.02
1:A:127:SER:HA	1:A:128:LEU:HB3	1.41	1.01
1:A:269:ALA:HB3	1:A:270:ARG:HB2	1.43	1.00
1:A:436:ARG:HG2	1:A:436:ARG:HH11	1.26	1.00
1:A:371:VAL:HB	3:A:2045:HOH:O	1.62	0.97
1:B:458:LEU:HG	3:B:2052:HOH:O	1.64	0.97
1:A:287:SER:HB3	1:A:288:ASP:HA	1.46	0.96
1:B:254:ARG:CB	1:B:254:ARG:HH11	1.76	0.95
1:A:43:ARG:H	1:A:44:GLY:HA3	1.32	0.94
1:B:451:TRP:O	1:B:455:THR:HB	1.71	0.91
1:A:127:SER:HA	1:A:128:LEU:CB	2.00	0.91
1:B:221:THR:HG21	1:B:250:ASN:HD21	1.35	0.91
1:A:75:ALA:HB1	1:A:76:ALA:HA	1.53	0.90
1:A:48:LEU:HD22	1:A:48:LEU:H	1.37	0.90
1:B:274:SER:O	1:B:276:GLN:N	2.05	0.90
1:A:493:THR:HG23	1:A:498:LEU:HB2	1.53	0.90
1:B:59:LEU:HD21	1:B:268:PRO:HB2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ILE:HD13	1:B:646:ILE:H	1.36	0.89
1:B:70:ARG:HG2	1:B:70:ARG:NH1	1.83	0.88
1:B:481:THR:HG23	1:B:483:GLU:H	1.39	0.88
1:A:493:THR:HB	1:A:613:ASP:HA	1.53	0.87
1:A:403:GLN:HE21	1:A:599:VAL:HG22	1.39	0.87
1:A:436:ARG:CG	1:A:436:ARG:HH11	1.88	0.86
1:B:481:THR:CG2	1:B:483:GLU:H	1.89	0.86
1:A:481:THR:HG22	1:A:483:GLU:H	1.40	0.84
1:B:213:HIS:HB3	1:B:437:THR:HB	1.59	0.83
1:B:47:LEU:HD12	1:B:78:LEU:HD22	1.59	0.83
1:A:76:ALA:HB3	1:A:77:ALA:HA	1.62	0.82
1:B:59:LEU:O	1:B:59:LEU:HD13	1.79	0.81
1:A:113:SER:O	1:A:114:VAL:HG12	1.80	0.80
1:B:469:ARG:HG2	1:B:469:ARG:NH1	1.88	0.80
1:B:45:VAL:HB	1:B:138:LYS:HB3	1.63	0.80
1:A:108:ARG:HH11	1:A:108:ARG:CG	1.94	0.79
1:B:267:HIS:HD2	1:B:269:ALA:H	1.30	0.79
1:A:213:HIS:HE1	1:A:400:ASP:OD1	1.66	0.79
1:A:290:ALA:HB1	3:A:2038:HOH:O	1.81	0.78
1:A:145:TYR:HB3	1:A:149:LYS:NZ	1.98	0.78
1:B:59:LEU:CD2	1:B:268:PRO:HB2	2.14	0.78
1:A:76:ALA:N	1:A:77:ALA:HB2	1.96	0.78
1:B:324:LYS:HA	1:B:327:ARG:HD2	1.66	0.78
1:A:127:SER:CA	1:A:128:LEU:HB3	2.15	0.77
1:A:69:PRO:HG2	1:A:77:ALA:HB3	1.67	0.76
1:A:273:GLU:HA	1:A:276:GLN:HE21	1.47	0.75
1:A:145:TYR:HB3	1:A:149:LYS:HZ2	1.51	0.75
1:B:289:SER:HB3	1:B:292:ILE:HG12	1.67	0.75
1:A:410:SER:OG	1:A:412:LYS:HG2	1.87	0.74
1:B:231:ALA:O	1:B:236:LEU:HB2	1.85	0.74
1:B:481:THR:HG22	1:B:484:THR:N	1.98	0.74
1:A:59:LEU:O	1:A:59:LEU:HD13	1.88	0.74
1:A:441:GLN:NE2	1:A:449:MET:HG3	2.03	0.74
1:A:75:ALA:HB1	1:A:76:ALA:CA	2.18	0.73
1:A:126:GLN:HG3	1:A:127:SER:H	1.54	0.73
1:A:242:ALA:HB1	1:A:243:PRO:HD2	1.68	0.73
1:B:590:PHE:HB3	2:H:3:A:OP1	1.88	0.73
1:A:209:LEU:HD23	1:A:434:VAL:HG21	1.70	0.72
1:B:297:ARG:HA	1:B:300:ILE:HG22	1.70	0.72
1:A:592:ALA:HA	1:A:620:HIS:CE1	2.24	0.72
1:A:412:LYS:HD3	1:A:412:LYS:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:CD	1:A:412:LYS:H	2.03	0.72
1:B:384:SER:O	1:B:387:ILE:HG13	1.90	0.71
1:A:17:LEU:HD11	1:A:145:TYR:HD1	1.55	0.71
1:B:271:LEU:HD23	1:B:272:LEU:H	1.54	0.71
1:A:43:ARG:N	1:A:44:GLY:HA3	2.01	0.71
1:A:220:LYS:HD3	1:A:398:ALA:HB1	1.73	0.71
2:H:2:A:H4'	2:H:3:A:OP1	1.89	0.70
1:A:42:SER:HB2	1:A:48:LEU:HD11	1.72	0.70
1:A:48:LEU:HD22	1:A:48:LEU:N	2.07	0.70
1:A:182:ILE:HD12	1:A:205:SER:HB3	1.74	0.69
1:A:261:ARG:HD3	1:A:344:SER:O	1.91	0.69
1:A:492:ASP:OD2	1:A:614:SER:HB2	1.92	0.69
1:B:193:ASP:H	1:B:196:GLN:NE2	1.89	0.69
1:A:18:GLU:OE2	1:A:149:LYS:HE2	1.91	0.69
1:A:515:VAL:O	1:A:518:VAL:HG22	1.91	0.69
2:G:9:A:H3'	2:G:9:A:N3	2.07	0.69
1:B:549:ARG:O	1:B:553:VAL:HG23	1.92	0.69
1:B:271:LEU:CG	1:B:272:LEU:H	2.06	0.69
1:A:493:THR:HB	1:A:613:ASP:CA	2.22	0.69
2:G:4:A:H5'	2:G:5:A:OP1	1.93	0.69
1:A:159:HIS:CG	1:A:160:SER:H	2.10	0.68
1:A:6:VAL:HG12	1:A:171:PHE:CD2	2.29	0.68
1:B:558:GLU:HG2	3:B:2064:HOH:O	1.93	0.68
1:A:510:GLY:O	1:A:511:ASN:HB2	1.93	0.67
1:A:269:ALA:CB	1:A:270:ARG:HB2	2.22	0.67
1:B:271:LEU:O	1:B:272:LEU:HB2	1.93	0.67
1:A:515:VAL:HG21	1:A:547:LEU:HD12	1.75	0.67
1:B:41:GLN:HG3	1:B:42:SER:N	2.08	0.67
1:B:48:LEU:HD23	1:B:135:ARG:HD3	1.75	0.67
1:B:109:VAL:HG23	1:B:109:VAL:O	1.93	0.67
1:A:44:GLY:O	1:A:81:ASN:HB2	1.94	0.67
1:A:451:TRP:O	1:A:455:THR:HB	1.94	0.66
1:A:252:VAL:HG21	1:A:264:ARG:HG3	1.76	0.66
1:A:436:ARG:HG2	1:A:436:ARG:NH1	2.04	0.66
1:A:385:CYS:O	1:A:389:LEU:HB2	1.95	0.66
1:B:271:LEU:CD2	1:B:272:LEU:H	2.08	0.66
1:A:640:PHE:HD1	1:A:646:ILE:HG21	1.61	0.66
1:A:287:SER:CB	1:A:288:ASP:HA	2.18	0.66
1:B:442:TYR:HE2	1:B:464:HIS:CD2	2.14	0.66
1:A:142:ASP:O	1:A:146:ARG:HG3	1.96	0.66
1:A:458:LEU:N	1:A:458:LEU:HD23	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:VAL:HG21	1:B:548:LEU:CD2	2.26	0.65
1:B:252:VAL:HG11	1:B:275:ILE:HG12	1.79	0.65
1:B:69:PRO:HG2	1:B:76:ALA:O	1.96	0.65
1:A:412:LYS:HD3	1:A:412:LYS:N	2.10	0.65
1:B:68:GLU:OE1	1:B:112:LYS:HE3	1.96	0.65
1:A:518:VAL:HG12	1:A:611:ILE:HD12	1.77	0.65
1:B:193:ASP:H	1:B:196:GLN:HE21	1.44	0.65
1:A:220:LYS:NZ	1:A:220:LYS:HB3	2.12	0.65
1:A:584:ARG:H	1:A:584:ARG:NE	1.95	0.65
1:B:267:HIS:CD2	1:B:269:ALA:H	2.15	0.64
1:B:274:SER:O	1:B:275:ILE:HG22	1.98	0.64
2:H:2:A:C4'	2:H:3:A:OP1	2.46	0.64
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.62	0.64
1:B:300:ILE:HD11	3:B:2019:HOH:O	1.97	0.64
1:B:48:LEU:C	1:B:49:LYS:HG2	2.19	0.64
1:A:405:PRO:HG3	1:A:595:ARG:CZ	2.27	0.63
1:B:292:ILE:O	1:B:296:ILE:HG13	1.98	0.63
1:B:617:VAL:HG13	1:B:623:LEU:HD23	1.80	0.63
1:B:16:LEU:HD22	1:B:413:ALA:HA	1.80	0.63
1:A:590:PHE:C	1:A:592:ALA:H	2.02	0.63
2:H:2:A:O2'	2:H:3:A:N9	2.30	0.63
1:A:455:THR:HG22	1:A:456:MET:HG2	1.81	0.63
1:A:544:GLN:HE21	1:A:578:SER:HB3	1.63	0.62
1:A:631:THR:HG22	1:A:636:VAL:HG11	1.80	0.62
1:B:158:TYR:CE2	1:B:163:ALA:HB3	2.34	0.62
1:B:37:LEU:HD23	1:B:39:GLU:HB3	1.81	0.62
1:B:69:PRO:HG3	1:B:78:LEU:HD23	1.80	0.62
1:B:617:VAL:HG13	1:B:623:LEU:HB3	1.81	0.62
1:B:497:GLY:HA2	1:B:499:PHE:CE2	2.34	0.62
1:B:109:VAL:O	1:B:109:VAL:CG2	2.47	0.62
1:A:17:LEU:HD12	1:A:149:LYS:HE3	1.82	0.62
1:A:159:HIS:CG	1:A:160:SER:N	2.67	0.62
1:A:548:LEU:O	1:A:552:LEU:HB2	2.00	0.62
1:A:243:PRO:HB3	1:A:380:ALA:HB2	1.81	0.61
1:A:296:ILE:HD11	3:A:2040:HOH:O	2.00	0.61
1:B:492:ASP:OD1	1:B:614:SER:OG	2.17	0.61
1:A:83:PHE:CE1	1:A:138:LYS:HG3	2.35	0.61
1:A:492:ASP:CG	1:A:614:SER:HB2	2.21	0.61
1:A:584:ARG:H	1:A:584:ARG:CD	2.14	0.61
1:B:498:LEU:HG	1:B:513:GLY:HA3	1.83	0.61
1:B:422:LEU:HD11	1:B:426:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:SER:O	1:B:563:SER:HA	2.00	0.61
1:B:30:SER:HB2	3:B:2004:HOH:O	2.00	0.61
1:B:268:PRO:O	1:B:271:LEU:HB3	2.01	0.61
1:A:492:ASP:OD1	1:A:614:SER:HB2	2.01	0.61
1:B:280:LEU:O	1:B:284:LEU:HG	2.00	0.61
1:A:127:SER:CA	1:A:128:LEU:CB	2.76	0.61
1:A:83:PHE:CZ	1:A:138:LYS:HG3	2.35	0.61
1:A:4:ALA:HB2	1:A:173:ARG:NH2	2.14	0.61
1:A:51:GLN:HB2	1:A:70:ARG:HD2	1.83	0.60
1:B:538:VAL:HB	1:B:577:LEU:HD23	1.84	0.60
1:A:372:VAL:HG23	1:A:392:ALA:HB2	1.83	0.60
1:B:507:GLN:HA	2:H:3:A:C8	2.36	0.60
1:B:494:ALA:HB1	1:B:615:ARG:HE	1.66	0.60
1:A:147:ARG:HH22	2:G:9:A:H5'	1.65	0.60
1:B:81:ASN:O	1:B:82:SER:O	2.19	0.60
1:A:147:ARG:HD3	1:A:356:SER:HB3	1.83	0.60
1:B:9:PHE:HZ	1:B:382:GLU:HG2	1.66	0.60
1:B:385:CYS:O	1:B:389:LEU:HB2	2.02	0.60
1:A:78:LEU:HD12	1:A:110:THR:O	2.02	0.59
1:A:196:GLN:O	1:A:200:VAL:HG23	2.02	0.59
1:A:213:HIS:CE1	1:A:400:ASP:OD1	2.52	0.59
1:A:476:PRO:HG2	1:B:234:GLN:HG2	1.83	0.59
2:G:9:A:N6	3:G:2005:HOH:O	2.36	0.59
1:A:170:LEU:HD21	1:A:209:LEU:HD13	1.83	0.59
1:B:597:ILE:HG13	1:B:623:LEU:HD11	1.85	0.59
1:A:431:GLY:O	1:A:435:VAL:HG12	2.03	0.59
1:B:292:ILE:HG13	1:B:293:VAL:N	2.16	0.58
1:B:407:THR:HB	2:H:5:A:N3	2.18	0.58
1:B:646:ILE:CD1	1:B:646:ILE:H	2.12	0.58
1:B:271:LEU:HG	1:B:272:LEU:H	1.68	0.58
1:B:272:LEU:O	1:B:275:ILE:HG22	2.04	0.58
1:A:518:VAL:HG23	1:A:519:SER:N	2.19	0.58
1:B:225:VAL:O	1:B:229:LEU:HD22	2.04	0.58
1:A:70:ARG:HG3	1:A:73:GLY:HA2	1.84	0.58
1:A:52:VAL:HG22	1:A:67:PHE:CE1	2.38	0.58
1:A:290:ALA:O	1:A:294:ALA:HB2	2.03	0.58
1:B:271:LEU:CG	1:B:272:LEU:N	2.66	0.58
1:A:539:SER:CB	1:A:544:GLN:HG2	2.33	0.58
1:B:393:ARG:CB	1:B:393:ARG:HH11	2.17	0.58
1:A:31:TRP:HH2	1:A:44:GLY:HA2	1.68	0.58
1:A:37:LEU:HD12	1:A:40:LEU:CD2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:CG2	1:B:250:ASN:HD21	2.11	0.57
1:A:403:GLN:HE22	1:A:603:ARG:HH12	1.50	0.57
1:A:305:VAL:HA	1:A:306:LYS:O	2.03	0.57
1:B:300:ILE:HD12	3:B:2018:HOH:O	2.04	0.57
1:B:252:VAL:CG1	1:B:275:ILE:HG12	2.34	0.57
1:A:481:THR:HB	1:A:484:THR:OG1	2.05	0.57
1:B:442:TYR:CE2	1:B:464:HIS:CD2	2.92	0.57
1:A:472:LEU:HD13	1:A:606:ARG:HB2	1.85	0.57
1:A:31:TRP:CH2	1:A:44:GLY:HA2	2.39	0.57
1:A:76:ALA:HB3	1:A:77:ALA:CA	2.34	0.57
1:A:481:THR:CG2	1:A:483:GLU:H	2.13	0.57
1:A:458:LEU:H	1:A:458:LEU:HD23	1.66	0.57
1:A:268:PRO:HA	1:A:271:LEU:HD12	1.85	0.57
1:A:541:TYR:O	1:A:545:VAL:HG23	2.05	0.57
1:B:66:THR:CG2	1:B:113:SER:HB2	2.34	0.57
1:B:491:VAL:HG13	1:B:611:ILE:HG12	1.87	0.57
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.68	0.57
1:A:458:LEU:HD21	3:A:2048:HOH:O	2.04	0.57
1:A:366:GLU:O	1:A:367:SER:HB2	2.05	0.57
1:B:213:HIS:O	1:B:215:PRO:HD3	2.04	0.56
1:A:633:HIS:H	1:A:633:HIS:CD2	2.23	0.56
1:A:644:ASP:HB3	3:A:2031:HOH:O	2.05	0.56
1:A:76:ALA:CB	1:A:77:ALA:HA	2.35	0.56
1:A:544:GLN:HE21	1:A:578:SER:CB	2.18	0.56
1:B:48:LEU:O	1:B:49:LYS:HG2	2.06	0.56
1:B:238:VAL:HG22	1:B:371:VAL:HG13	1.88	0.56
1:B:189:ASN:HB3	1:B:192:LEU:HD13	1.87	0.56
1:A:518:VAL:HG21	1:A:548:LEU:CD2	2.35	0.56
1:B:190:THR:C	1:B:191:CYS:SG	2.85	0.56
1:B:206:GLN:HE21	1:B:206:GLN:HA	1.70	0.56
1:A:203:ALA:HB1	1:A:396:ILE:HD12	1.88	0.56
1:B:263:LEU:HD11	1:B:280:LEU:HA	1.87	0.56
1:B:446:GLN:HG2	1:B:468:ALA:O	2.06	0.56
1:B:52:VAL:HG22	1:B:131:GLU:CB	2.36	0.56
1:A:228:ILE:O	1:A:232:VAL:HG23	2.06	0.56
1:A:38:LYS:HA	1:A:41:GLN:HG3	1.89	0.55
1:B:455:THR:HG23	1:B:622:PHE:CE1	2.41	0.55
1:A:443:ARG:HG3	1:A:605:ARG:HG2	1.87	0.55
1:A:209:LEU:CD2	1:A:434:VAL:HG21	2.37	0.55
1:B:13:GLN:HB3	1:B:152:LEU:HD11	1.88	0.55
1:A:240:CYS:SG	1:A:251:LEU:HD23	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLN:O	1:B:56:ARG:HB2	2.07	0.55
1:A:182:ILE:CD1	1:A:205:SER:HB3	2.35	0.55
1:A:139:LEU:N	1:A:139:LEU:HD13	2.22	0.54
1:A:69:PRO:CG	1:A:77:ALA:HB3	2.35	0.54
1:A:481:THR:HG22	1:A:483:GLU:N	2.16	0.54
1:A:571:GLU:O	1:A:572:LYS:HG2	2.07	0.54
1:A:125:GLN:O	1:A:126:GLN:HB2	2.07	0.54
1:B:393:ARG:NH1	1:B:393:ARG:HB3	2.23	0.54
1:B:289:SER:C	1:B:291:GLN:N	2.57	0.54
1:B:158:TYR:CZ	1:B:163:ALA:HB3	2.42	0.54
1:A:221:THR:HG23	3:A:2014:HOH:O	2.07	0.54
1:A:597:ILE:O	1:A:601:VAL:HG23	2.07	0.54
1:B:91:LEU:O	1:B:101:LEU:HA	2.07	0.54
1:B:640:PHE:CD1	1:B:646:ILE:HG13	2.43	0.54
1:B:249:ASP:OD2	1:B:271:LEU:O	2.26	0.54
1:B:271:LEU:HG	1:B:272:LEU:N	2.23	0.54
1:A:172:GLY:O	1:A:173:ARG:C	2.45	0.54
1:B:411:HIS:CD2	2:H:2:A:N7	2.76	0.54
1:B:225:VAL:O	1:B:225:VAL:HG12	2.08	0.54
1:A:464:HIS:O	1:A:466:SER:N	2.41	0.54
1:B:475:LEU:HD13	1:B:606:ARG:CZ	2.37	0.54
1:B:153:ILE:O	1:B:157:LYS:HG2	2.07	0.54
1:B:114:VAL:O	1:B:114:VAL:HG13	2.08	0.54
1:B:254:ARG:NH1	1:B:254:ARG:CB	2.52	0.54
1:A:490:LEU:HD23	1:A:636:VAL:HB	1.90	0.53
1:B:45:VAL:HG11	3:B:2020:HOH:O	2.07	0.53
1:A:636:VAL:HG23	1:A:637:ARG:N	2.24	0.53
1:A:153:ILE:O	1:A:156:LYS:HB3	2.09	0.53
1:A:170:LEU:CD2	1:A:209:LEU:HD22	2.39	0.53
1:B:48:LEU:CD2	1:B:135:ARG:HD3	2.37	0.53
1:B:225:VAL:HG13	1:B:255:LEU:CD1	2.38	0.53
1:B:490:LEU:HD12	1:B:636:VAL:HB	1.91	0.53
1:B:239:LEU:CB	3:B:2037:HOH:O	2.57	0.53
1:A:472:LEU:CD1	1:A:606:ARG:HB2	2.39	0.53
1:A:384:SER:O	1:A:388:PRO:HD2	2.07	0.53
1:B:493:THR:HB	1:B:612:CYS:O	2.08	0.53
1:B:19:LEU:HD21	1:B:412:LYS:HB3	1.89	0.53
1:B:481:THR:HG23	1:B:482:GLU:N	2.24	0.53
1:A:75:ALA:HB1	1:A:76:ALA:CB	2.39	0.53
1:B:220:LYS:HE2	1:B:399:GLY:HA2	1.90	0.53
1:B:572:LYS:O	1:B:605:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:CD2	1:A:136:LEU:HB2	2.38	0.53
1:A:16:LEU:HD11	1:A:416:ALA:HB1	1.90	0.53
1:A:182:ILE:HA	3:A:2020:HOH:O	2.09	0.53
1:B:239:LEU:CB	3:B:2016:HOH:O	2.56	0.52
1:B:67:PHE:N	1:B:67:PHE:CD1	2.78	0.52
1:B:405:PRO:HG3	1:B:595:ARG:NH2	2.25	0.52
1:A:489:LEU:HD21	1:A:491:VAL:HG12	1.91	0.52
1:A:110:THR:HG22	1:A:111:GLN:N	2.23	0.52
1:A:17:LEU:CD1	1:A:145:TYR:HD1	2.22	0.52
1:B:536:ALA:HB2	1:B:572:LYS:HG3	1.92	0.52
1:A:81:ASN:C	1:A:83:PHE:H	2.11	0.52
1:B:403:GLN:HE21	1:B:599:VAL:HG22	1.74	0.52
1:B:274:SER:C	1:B:276:GLN:H	2.09	0.52
1:A:147:ARG:HH22	2:G:9:A:C5'	2.22	0.52
1:A:221:THR:HG21	1:A:250:ASN:HD21	1.75	0.52
1:A:496:CYS:SG	1:A:639:ALA:HB3	2.50	0.52
1:A:293:VAL:HG22	1:A:296:ILE:HD12	1.91	0.52
1:B:374:ILE:HD11	1:B:388:PRO:HG2	1.90	0.52
1:A:75:ALA:CB	1:A:76:ALA:CA	2.87	0.52
1:A:16:LEU:HD11	1:A:416:ALA:CB	2.39	0.52
1:B:646:ILE:N	1:B:646:ILE:HD13	2.17	0.51
1:A:305:VAL:HA	1:A:306:LYS:C	2.30	0.51
1:B:70:ARG:NH1	1:B:70:ARG:CG	2.64	0.51
1:A:402:LYS:HD3	1:A:456:MET:O	2.10	0.51
1:B:81:ASN:O	1:B:82:SER:C	2.48	0.51
1:B:91:LEU:HD11	1:B:134:TYR:HB3	1.92	0.51
1:B:277:GLN:O	1:B:286:ARG:NH2	2.42	0.51
1:A:326:LEU:HD13	1:A:326:LEU:H	1.74	0.51
2:G:5:A:H2'	2:G:6:A:O4'	2.10	0.51
1:B:66:THR:HG23	1:B:113:SER:HB2	1.93	0.51
1:A:366:GLU:O	1:A:367:SER:CB	2.58	0.51
1:A:289:SER:HB3	1:A:292:ILE:HG12	1.92	0.51
1:A:500:GLU:HG2	1:A:582:SER:O	2.11	0.51
1:B:342:LEU:HB3	1:B:364:LEU:HD11	1.93	0.51
1:A:579:PHE:O	1:A:580:VAL:HB	2.10	0.51
1:B:3:SER:O	1:B:6:VAL:HG13	2.11	0.51
1:B:111:GLN:HE21	1:B:111:GLN:HA	1.75	0.51
1:A:155:LEU:O	1:A:155:LEU:HD12	2.11	0.51
1:B:225:VAL:HG13	1:B:255:LEU:HD13	1.93	0.51
1:B:481:THR:HG22	1:B:483:GLU:H	1.74	0.50
1:A:50:LEU:HD23	1:A:136:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:N	1:A:326:LEU:HD13	2.26	0.50
1:A:141:ASN:HD22	1:A:143:VAL:H	1.59	0.50
1:A:41:GLN:O	1:A:43:ARG:N	2.43	0.50
1:A:44:GLY:O	1:A:81:ASN:CB	2.59	0.50
1:A:640:PHE:CD1	1:A:646:ILE:HG21	2.45	0.50
1:B:188:PHE:HZ	1:B:233:LYS:HD2	1.76	0.50
1:A:80:SER:HB2	1:A:83:PHE:HB2	1.94	0.50
1:B:522:ILE:CD1	1:B:576:ILE:HD12	2.42	0.50
1:A:249:ASP:HA	1:A:252:VAL:HB	1.92	0.50
1:A:241:CYS:HA	1:A:350:ALA:O	2.12	0.50
1:A:114:VAL:HG13	1:A:114:VAL:O	2.11	0.50
1:B:356:SER:HA	1:B:387:ILE:HG22	1.92	0.50
1:A:451:TRP:CH2	1:A:598:ASN:HA	2.46	0.50
1:A:49:LYS:NZ	1:A:71:ARG:HH21	2.09	0.50
1:A:157:LYS:HG2	1:A:157:LYS:O	2.12	0.50
1:A:496:CYS:HB2	1:A:498:LEU:CD2	2.43	0.49
1:B:273:GLU:C	1:B:274:SER:O	2.50	0.49
1:A:542:ASN:ND2	2:G:4:A:H5'	2.27	0.49
1:A:472:LEU:HD21	1:A:607:HIS:CB	2.43	0.49
1:A:590:PHE:C	1:A:592:ALA:N	2.66	0.49
1:A:4:ALA:HB2	1:A:173:ARG:HH22	1.78	0.49
1:B:561:ILE:C	1:B:562:LYS:HG2	2.32	0.49
1:B:593:GLU:O	1:B:593:GLU:HG3	2.13	0.49
1:A:141:ASN:ND2	1:A:143:VAL:HG22	2.28	0.49
1:A:404:LEU:HB2	1:A:568:GLN:NE2	2.27	0.49
1:B:496:CYS:SG	1:B:639:ALA:HB3	2.52	0.49
1:A:127:SER:HB2	1:A:128:LEU:O	2.13	0.49
1:A:434:VAL:O	1:A:434:VAL:HG22	2.13	0.49
1:A:221:THR:HG22	3:A:2029:HOH:O	2.13	0.49
1:B:211:ILE:HB	1:B:435:VAL:HA	1.93	0.49
1:B:500:GLU:CD	1:B:583:ASN:HD22	2.16	0.49
1:A:90:GLY:O	1:A:91:LEU:HB3	2.12	0.49
1:B:193:ASP:OD2	1:B:442:TYR:OH	2.23	0.49
1:B:422:LEU:CD1	1:B:426:LEU:HD11	2.42	0.49
1:A:190:THR:HG23	1:B:464:HIS:CE1	2.48	0.49
1:A:514:GLU:O	1:A:515:VAL:C	2.51	0.49
1:A:275:ILE:O	1:A:275:ILE:HG23	2.12	0.49
1:B:532:ALA:HB3	1:B:558:GLU:HG3	1.94	0.48
1:B:40:LEU:HD12	1:B:40:LEU:O	2.12	0.48
1:A:519:SER:O	1:A:522:ILE:HB	2.13	0.48
1:B:507:GLN:HA	2:H:3:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HG13	2:H:8:A:C2	2.48	0.48
1:A:455:THR:HG22	1:A:456:MET:N	2.28	0.48
1:A:142:ASP:HB2	1:A:146:ARG:HE	1.78	0.48
1:A:472:LEU:HD21	1:A:607:HIS:HB3	1.95	0.48
1:B:241:CYS:HB3	1:B:352:ASN:HD22	1.78	0.48
1:A:442:TYR:CE2	1:A:464:HIS:CD2	3.02	0.48
1:A:501:LEU:HD21	1:A:512:PRO:HD3	1.94	0.48
1:B:404:LEU:HB2	1:B:568:GLN:NE2	2.28	0.48
1:A:470:HIS:O	1:A:471:LEU:HD23	2.14	0.48
1:A:175:ALA:HB1	1:A:176:PRO:CD	2.43	0.48
1:B:356:SER:HA	1:B:387:ILE:CG2	2.44	0.48
1:B:640:PHE:CE1	1:B:646:ILE:HG13	2.49	0.48
3:A:2017:HOH:O	1:B:294:ALA:HB2	2.14	0.48
1:B:70:ARG:HH11	1:B:70:ARG:CG	1.99	0.47
1:A:289:SER:HA	1:A:292:ILE:HG23	1.96	0.47
1:A:411:HIS:HB2	2:G:1:A:N1	2.29	0.47
1:B:618:ASN:OD1	1:B:624:LYS:HA	2.14	0.47
1:B:261:ARG:O	1:B:346:ASN:HB2	2.14	0.47
1:A:80:SER:O	1:A:82:SER:N	2.47	0.47
1:A:108:ARG:NH1	1:A:108:ARG:CG	2.63	0.47
2:H:2:A:O2'	2:H:3:A:C8	2.63	0.47
1:A:440:VAL:HG22	1:A:442:TYR:CE1	2.50	0.47
1:A:412:LYS:HE3	3:A:2049:HOH:O	2.15	0.47
1:B:490:LEU:HD13	1:B:490:LEU:O	2.15	0.47
1:B:408:THR:OG1	1:B:414:ALA:HB2	2.15	0.47
1:A:12:LYS:O	1:A:12:LYS:HD3	2.15	0.47
1:A:12:LYS:O	1:A:15:ASP:HB2	2.14	0.47
1:A:45:VAL:HG12	1:A:45:VAL:O	2.15	0.47
1:A:69:PRO:HB2	1:A:77:ALA:CB	2.44	0.47
1:B:271:LEU:HB3	1:B:276:GLN:OE1	2.14	0.47
1:B:28:ARG:C	1:B:30:SER:H	2.17	0.47
1:B:435:VAL:HG12	1:B:436:ARG:N	2.30	0.47
1:A:177:SER:CB	1:A:207:LYS:HD3	2.44	0.47
1:A:16:LEU:HB3	1:A:418:LEU:HG	1.97	0.47
1:A:12:LYS:HD3	1:A:12:LYS:C	2.35	0.47
1:A:68:GLU:HB3	1:A:112:LYS:O	2.15	0.47
1:A:518:VAL:CG2	1:A:519:SER:N	2.78	0.47
1:A:470:HIS:HB2	1:A:606:ARG:NH1	2.30	0.47
1:B:540:PRO:HG2	1:B:591:LEU:HD21	1.95	0.47
1:A:424:GLU:O	1:A:428:GLU:HG2	2.15	0.47
1:B:603:ARG:N	1:B:603:ARG:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:O	1:A:114:VAL:CG1	2.63	0.46
1:A:470:HIS:C	1:A:471:LEU:HD23	2.35	0.46
1:B:481:THR:CG2	1:B:483:GLU:N	2.70	0.46
1:A:202:PHE:CD1	1:A:436:ARG:NH1	2.83	0.46
1:A:243:PRO:HB3	1:A:380:ALA:CB	2.44	0.46
1:A:193:ASP:OD1	1:A:196:GLN:HG3	2.15	0.46
1:B:509:LYS:HE2	1:B:581:ARG:NH2	2.30	0.46
1:B:244:SER:O	1:B:248:VAL:HG23	2.15	0.46
1:A:39:GLU:C	1:A:41:GLN:N	2.68	0.46
1:A:21:ARG:HD3	1:A:145:TYR:CD2	2.51	0.46
1:B:297:ARG:HA	1:B:300:ILE:CG2	2.42	0.46
1:A:547:LEU:HG	3:A:2060:HOH:O	2.15	0.46
1:A:8:SER:HA	1:A:11:THR:HG23	1.98	0.46
1:A:381:LEU:HD23	1:A:406:PRO:HB2	1.97	0.46
1:B:469:ARG:CG	1:B:469:ARG:HH11	2.03	0.46
1:B:455:THR:HG23	1:B:622:PHE:HE1	1.81	0.46
1:B:289:SER:C	1:B:291:GLN:H	2.19	0.46
1:A:431:GLY:C	1:A:435:VAL:HG12	2.35	0.46
1:B:188:PHE:CZ	1:B:233:LYS:HD2	2.51	0.46
1:B:621:ALA:O	1:B:624:LYS:N	2.49	0.46
1:A:379:GLN:O	1:A:379:GLN:HG2	2.16	0.46
1:A:8:SER:CA	1:A:11:THR:HG23	2.46	0.46
1:B:418:LEU:HA	1:B:418:LEU:HD23	1.74	0.46
1:B:3:SER:HB2	1:B:6:VAL:HG13	1.97	0.46
1:B:299:ASP:HB3	1:B:326:LEU:HG	1.98	0.46
1:A:81:ASN:C	1:A:83:PHE:N	2.70	0.46
1:A:403:GLN:NE2	1:A:599:VAL:HG22	2.20	0.46
1:A:389:LEU:HA	1:A:389:LEU:HD12	1.80	0.45
1:A:4:ALA:HB1	1:A:173:ARG:NH1	2.31	0.45
1:A:263:LEU:HD11	1:A:280:LEU:HA	1.98	0.45
1:A:42:SER:OG	1:A:48:LEU:HD21	2.16	0.45
1:B:599:VAL:O	1:B:603:ARG:HD2	2.16	0.45
1:A:376:GLU:HA	1:A:376:GLU:OE1	2.16	0.45
1:A:163:ALA:O	1:A:167:ILE:HG13	2.17	0.45
1:B:229:LEU:HA	1:B:229:LEU:HD12	1.61	0.45
1:B:55:GLN:O	1:B:56:ARG:CB	2.63	0.45
1:A:265:LEU:O	1:A:266:GLY:O	2.33	0.45
1:A:493:THR:HB	1:A:613:ASP:CB	2.46	0.45
1:B:52:VAL:HG22	1:B:131:GLU:HB3	1.99	0.45
1:B:249:ASP:OD1	1:B:264:ARG:NH1	2.48	0.45
1:B:406:PRO:HG2	1:B:419:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:O	1:A:325:LEU:HB2	2.17	0.45
1:A:6:VAL:HG12	1:A:171:PHE:CE2	2.51	0.45
1:A:638:THR:O	1:A:639:ALA:C	2.54	0.45
1:A:26:GLU:C	1:A:28:ARG:H	2.20	0.45
1:A:183:HIS:HB3	3:A:2023:HOH:O	2.16	0.45
1:A:55:GLN:OE1	1:A:128:LEU:HD23	2.17	0.45
1:A:403:GLN:NE2	1:A:603:ARG:HH12	2.14	0.45
1:A:192:LEU:HG	1:A:196:GLN:HB2	1.99	0.45
1:B:237:LYS:HD2	1:B:368:TYR:OH	2.17	0.45
1:B:59:LEU:O	1:B:59:LEU:CD1	2.60	0.45
1:A:441:GLN:HE21	1:A:449:MET:HG3	1.79	0.44
1:A:445:HIS:ND1	1:A:446:GLN:N	2.65	0.44
1:A:110:THR:HG22	1:A:112:LYS:H	1.82	0.44
1:B:165:SER:O	1:B:169:VAL:HG23	2.17	0.44
1:A:495:GLY:HA2	1:A:615:ARG:HE	1.81	0.44
1:B:185:LEU:HD12	1:B:201:LEU:HD12	2.00	0.44
1:A:263:LEU:HD21	1:A:280:LEU:HG	1.98	0.44
1:B:393:ARG:NH1	1:B:393:ARG:CB	2.79	0.44
1:B:521:HIS:HE1	1:B:607:HIS:NE2	2.16	0.44
1:A:621:ALA:O	1:A:625:THR:HG23	2.18	0.44
1:A:253:GLU:HB3	1:A:275:ILE:CD1	2.48	0.44
1:A:76:ALA:CB	1:A:77:ALA:CA	2.95	0.43
1:A:473:ARG:HA	1:A:478:VAL:HG12	2.00	0.43
1:A:584:ARG:H	1:A:584:ARG:HE	1.63	0.43
1:B:562:LYS:HB3	1:B:562:LYS:HE2	1.60	0.43
1:B:200:VAL:HA	1:B:227:ILE:HD13	2.00	0.43
1:A:337:ALA:O	1:A:340:GLU:HB3	2.17	0.43
1:A:202:PHE:CE1	1:A:436:ARG:NH1	2.81	0.43
1:A:407:THR:HB	2:G:5:A:C2	2.53	0.43
1:B:623:LEU:O	1:B:627:VAL:HG13	2.18	0.43
1:B:500:GLU:OE1	1:B:581:ARG:HD2	2.18	0.43
1:A:361:LEU:HA	1:A:361:LEU:HD12	1.74	0.43
1:A:277:GLN:HG3	1:A:277:GLN:H	1.21	0.43
1:B:517:LEU:HD21	1:B:643:LEU:HD22	2.00	0.43
1:A:496:CYS:HB2	1:A:498:LEU:HD22	2.00	0.43
1:A:481:THR:CG2	1:A:482:GLU:N	2.81	0.43
1:B:589:GLY:O	1:B:590:PHE:HB3	2.18	0.43
1:B:538:VAL:O	1:B:577:LEU:HA	2.18	0.43
1:A:186:THR:N	3:A:2025:HOH:O	2.49	0.43
1:A:323:ILE:O	1:A:324:LYS:C	2.56	0.43
1:A:59:LEU:CD2	1:A:268:PRO:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLU:HA	1:A:573:GLU:OE1	2.19	0.43
1:A:75:ALA:HB1	1:A:76:ALA:HB2	2.00	0.43
1:B:455:THR:CG2	1:B:455:THR:O	2.65	0.43
1:A:367:SER:HA	3:A:2043:HOH:O	2.18	0.43
1:A:500:GLU:O	1:A:501:LEU:HB3	2.18	0.43
1:A:295:ASP:O	1:A:298:LYS:HB2	2.18	0.43
1:B:112:LYS:O	1:B:112:LYS:HD3	2.17	0.43
1:B:54:SER:HB3	1:B:66:THR:HB	2.00	0.43
1:B:142:ASP:CB	1:B:146:ARG:HH21	2.31	0.43
1:B:549:ARG:CA	1:B:553:VAL:HG23	2.49	0.43
1:B:500:GLU:CD	1:B:581:ARG:HH11	2.22	0.43
1:A:422:LEU:O	1:A:426:LEU:HG	2.19	0.43
1:A:404:LEU:HA	1:A:404:LEU:HD12	1.73	0.43
1:B:223:THR:O	1:B:227:ILE:HG12	2.19	0.43
1:B:616:THR:O	1:B:619:ASN:HB2	2.18	0.43
1:A:76:ALA:CA	1:A:77:ALA:HB2	2.49	0.43
1:A:451:TRP:HH2	1:A:598:ASN:HA	1.83	0.43
1:A:275:ILE:O	1:A:275:ILE:CG2	2.67	0.43
1:A:295:ASP:HB2	1:A:298:LYS:HG3	2.01	0.43
1:A:255:LEU:HD12	1:A:255:LEU:HA	1.64	0.43
1:A:17:LEU:CD1	1:A:145:TYR:CD1	3.01	0.43
1:A:168:GLU:HA	1:A:173:ARG:HB2	2.01	0.43
1:B:182:ILE:HD11	1:B:201:LEU:HG	2.01	0.43
1:A:352:ASN:HD22	1:A:352:ASN:N	2.17	0.43
1:A:27:GLU:HA	1:A:27:GLU:OE1	2.19	0.43
1:A:267:HIS:ND1	1:A:269:ALA:HB2	2.34	0.42
1:B:405:PRO:HB2	1:B:406:PRO:HD2	2.01	0.42
1:A:144:THR:O	1:A:148:LEU:HG	2.18	0.42
1:A:59:LEU:CD1	1:A:59:LEU:O	2.61	0.42
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.64	0.42
1:A:233:LYS:C	1:A:235:GLY:H	2.22	0.42
1:B:481:THR:CG2	1:B:482:GLU:N	2.82	0.42
1:A:42:SER:O	1:A:43:ARG:HD3	2.19	0.42
1:A:49:LYS:HG2	1:A:70:ARG:O	2.19	0.42
1:B:182:ILE:O	1:B:183:HIS:C	2.57	0.42
1:A:81:ASN:O	1:A:83:PHE:N	2.43	0.42
1:A:539:SER:HB2	1:A:544:GLN:HG2	2.01	0.42
1:B:364:LEU:N	1:B:364:LEU:HD22	2.34	0.42
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.74	0.42
1:A:126:GLN:HG3	1:A:127:SER:N	2.29	0.42
1:A:405:PRO:HG3	1:A:595:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HD23	1:A:489:LEU:C	2.38	0.42
3:A:2064:HOH:O	1:B:261:ARG:NH1	2.52	0.42
1:A:497:GLY:HA2	1:A:615:ARG:HH22	1.84	0.42
1:B:387:ILE:HB	1:B:388:PRO:HD3	2.01	0.42
1:B:549:ARG:C	1:B:553:VAL:HG23	2.39	0.42
1:B:141:ASN:OD1	1:B:143:VAL:HG13	2.20	0.42
1:B:271:LEU:HD23	1:B:272:LEU:N	2.26	0.42
1:B:225:VAL:O	1:B:225:VAL:CG1	2.68	0.42
1:B:603:ARG:NH2	3:B:2049:HOH:O	2.30	0.42
1:A:544:GLN:NE2	1:A:578:SER:OG	2.52	0.42
1:B:13:GLN:O	1:B:17:LEU:HD22	2.20	0.42
1:A:45:VAL:HG13	1:A:138:LYS:HB2	2.01	0.42
1:A:108:ARG:NH1	1:A:108:ARG:HG3	2.29	0.42
1:B:470:HIS:CG	1:B:606:ARG:HG2	2.55	0.42
1:A:177:SER:HB2	1:A:207:LYS:HD3	2.01	0.42
1:B:85:SER:HA	1:B:86:GLY:HA2	1.72	0.42
1:A:599:VAL:O	1:A:603:ARG:HD2	2.20	0.42
1:A:271:LEU:HA	1:A:271:LEU:HD23	1.78	0.42
1:A:495:GLY:C	1:A:497:GLY:H	2.23	0.42
1:A:509:LYS:HE3	1:A:581:ARG:NH2	2.35	0.42
1:B:298:LYS:HE2	1:B:298:LYS:HB2	1.73	0.42
1:A:127:SER:HA	1:A:128:LEU:HB2	1.94	0.41
1:A:41:GLN:O	1:A:44:GLY:HA3	2.20	0.41
1:A:473:ARG:HG2	1:A:485:GLY:HA2	2.02	0.41
1:A:145:TYR:HB3	1:A:149:LYS:HZ1	1.79	0.41
1:B:38:LYS:HA	1:B:41:GLN:HB3	2.02	0.41
1:A:91:LEU:HA	1:A:135:ARG:O	2.20	0.41
1:B:218:THR:HA	1:B:440:VAL:O	2.20	0.41
1:A:404:LEU:HA	1:A:405:PRO:HD3	1.76	0.41
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.81	0.41
1:A:377:CYS:C	1:A:379:GLN:H	2.24	0.41
1:B:511:ASN:O	1:B:515:VAL:HG23	2.20	0.41
1:A:71:ARG:C	1:A:71:ARG:HE	2.23	0.41
1:A:191:CYS:SG	1:B:191:CYS:HA	2.60	0.41
1:A:443:ARG:CG	1:A:605:ARG:HG2	2.51	0.41
1:A:422:LEU:HD11	1:A:426:LEU:HD11	2.02	0.41
1:B:455:THR:HG23	1:B:455:THR:O	2.20	0.41
1:B:320:ARG:O	1:B:324:LYS:HE2	2.20	0.41
1:B:26:GLU:HG3	1:B:26:GLU:O	2.19	0.41
1:A:334:GLU:O	1:A:338:MET:HG2	2.20	0.41
1:B:9:PHE:CZ	1:B:382:GLU:HG2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:LYS:HE2	1:B:581:ARG:CZ	2.50	0.41
1:A:411:HIS:O	1:A:415:LEU:HG	2.21	0.41
1:B:30:SER:O	1:B:31:TRP:C	2.58	0.41
1:A:531:PRO:HB2	1:A:533:ARG:HG2	2.01	0.41
1:B:299:ASP:CB	1:B:326:LEU:HG	2.50	0.41
1:A:188:PHE:CE2	1:A:229:LEU:HB3	2.55	0.41
1:A:585:LYS:NZ	1:A:585:LYS:CB	2.84	0.41
1:A:75:ALA:CB	1:A:76:ALA:HA	2.25	0.41
1:A:92:TYR:CZ	1:A:100:GLN:OE1	2.74	0.41
1:A:483:GLU:C	1:A:485:GLY:H	2.23	0.41
1:A:220:LYS:HZ3	1:A:220:LYS:HB3	1.85	0.41
1:A:510:GLY:N	1:A:543:LEU:HD23	2.35	0.41
1:B:494:ALA:HA	1:B:495:GLY:HA2	1.67	0.41
1:B:44:GLY:O	1:B:81:ASN:CG	2.60	0.41
1:A:66:THR:HG22	1:A:67:PHE:N	2.35	0.41
1:A:175:ALA:HB1	1:A:176:PRO:HD2	2.03	0.41
1:A:333:ARG:HD3	1:A:333:ARG:HA	1.84	0.41
1:A:632:GLN:HE21	1:A:632:GLN:HB3	1.62	0.41
1:B:409:VAL:O	1:B:409:VAL:HG12	2.21	0.41
1:B:422:LEU:O	1:B:425:ARG:HB3	2.21	0.41
1:B:17:LEU:HA	1:B:17:LEU:HD12	1.75	0.41
1:A:68:GLU:HA	1:A:69:PRO:HD3	1.87	0.40
1:B:280:LEU:HD22	1:B:280:LEU:O	2.21	0.40
1:A:211:ILE:HG22	1:A:435:VAL:HG23	2.02	0.40
1:A:536:ALA:HB2	1:A:572:LYS:HG3	2.03	0.40
1:A:465:SER:O	1:A:466:SER:HB3	2.21	0.40
1:B:111:GLN:CA	1:B:111:GLN:HE21	2.32	0.40
1:B:145:TYR:CD1	1:B:145:TYR:N	2.89	0.40
1:B:130:ARG:HA	1:B:134:TYR:OH	2.21	0.40
1:B:237:LYS:HD2	1:B:368:TYR:CZ	2.56	0.40
1:B:105:ILE:HD11	1:B:270:ARG:CZ	2.51	0.40
1:B:512:PRO:O	1:B:516:ARG:HG3	2.21	0.40
1:A:24:GLU:HG2	1:A:28:ARG:NH2	2.36	0.40
1:A:481:THR:HG22	1:A:484:THR:H	1.86	0.40
1:B:69:PRO:CG	1:B:78:LEU:HD23	2.50	0.40
1:B:236:LEU:HD22	1:B:370:ASP:CB	2.52	0.40
1:A:442:TYR:HE2	1:A:464:HIS:CD2	2.39	0.40
1:B:50:LEU:HG	1:B:67:PHE:HB2	2.04	0.40
1:B:565:ASP:O	1:B:568:GLN:HG3	2.22	0.40
1:B:384:SER:O	1:B:388:PRO:HD2	2.21	0.40
1:A:544:GLN:HG3	1:A:548:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:LEU:O	1:B:552:LEU:HB2	2.22	0.40
1:B:615:ARG:HG3	3:B:2067:HOH:O	2.22	0.40
1:B:599:VAL:O	1:B:603:ARG:CD	2.69	0.40
1:A:206:GLN:HB3	1:A:207:LYS:H	1.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2058:HOH:O	3:A:2058:HOH:O[4_555]	2.16	0.04

## 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	602/646 (93%)	485 (81%)	87 (14%)	30 (5%)	3	8
1	B	596/646 (92%)	531 (89%)	51 (9%)	14 (2%)	8	26
All	All	1198/1292 (93%)	1016 (85%)	138 (12%)	44 (4%)	4	14

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	465	SER
1	A	466	SER
1	B	82	SER
1	B	271	LEU
1	B	275	ILE
1	A	71	ARG
1	A	74	SER
1	A	77	ALA

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Mol	Chain	Res	Type
1	A	275	ILE
1	A	511	ASN
1	A	593	GLU
1	B	56	ARG
1	B	146	ARG
1	B	159	HIS
1	B	272	LEU
1	B	274	SER
1	B	589	GLY
1	A	42	SER
1	A	78	LEU
1	A	82	SER
1	A	100	GLN
1	A	102	ALA
1	A	128	LEU
1	A	206	GLN
1	A	207	LYS
1	A	270	ARG
1	A	515	VAL
1	B	191	CYS
1	B	219	GLY
1	B	421	SER
1	A	131	GLU
1	A	173	ARG
1	A	306	LYS
1	A	547	LEU
1	A	27	GLU
1	A	79	PRO
1	A	81	ASN
1	A	114	VAL
1	A	274	SER
1	A	287	SER
1	A	500	GLU
1	B	296	ILE
1	B	580	VAL

### 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	518/551 (94%)	429 (83%)	89 (17%)	2	6
1	B	511/551 (93%)	421 (82%)	90 (18%)	2	6
All	All	1029/1102 (93%)	850 (83%)	179 (17%)	2	6

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	12	LYS
1	A	16	LEU
1	A	17	LEU
1	A	18	GLU
1	A	19	LEU
1	A	38	LYS
1	A	41	GLN
1	A	48	LEU
1	A	49	LYS
1	A	50	LEU
1	A	57	THR
1	A	70	ARG
1	A	71	ARG
1	A	83	PHE
1	A	84	THR
1	A	99	SER
1	A	103	THR
1	A	105	ILE
1	A	106	LEU
1	A	108	ARG
1	A	114	VAL
1	A	116	VAL
1	A	130	ARG
1	A	137	LEU
1	A	139	LEU
1	A	141	ASN
1	A	142	ASP
1	A	181	GLU
1	A	182	ILE
1	A	191	CYS
1	A	198	GLU
1	A	220	LYS
1	A	221	THR

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Mol	Chain	Res	Type
1	A	229	LEU
1	A	251	LEU
1	A	255	LEU
1	A	264	ARG
1	A	265	LEU
1	A	272	LEU
1	A	275	ILE
1	A	277	GLN
1	A	280	LEU
1	A	281	ASP
1	A	295	ASP
1	A	300	ILE
1	A	302	GLN
1	A	325	LEU
1	A	326	LEU
1	A	352	ASN
1	A	356	SER
1	A	361	LEU
1	A	363	LEU
1	A	364	LEU
1	A	389	LEU
1	A	393	ARG
1	A	404	LEU
1	A	412	LYS
1	A	436	ARG
1	A	449	MET
1	A	455	THR
1	A	469	ARG
1	A	470	HIS
1	A	472	LEU
1	A	473	ARG
1	A	475	LEU
1	A	481	THR
1	A	490	LEU
1	A	496	CYS
1	A	501	LEU
1	A	507	GLN
1	A	516	ARG
1	A	519	SER
1	A	523	GLN
1	A	539	SER
1	A	547	LEU

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Mol	Chain	Res	Type
1	A	552	LEU
1	A	561	ILE
1	A	565	ASP
1	A	578	SER
1	A	584	ARG
1	A	590	PHE
1	A	603	ARG
1	A	623	LEU
1	A	628	GLU
1	A	633	HIS
1	A	636	VAL
1	A	643	LEU
1	A	645	ASP
1	B	3	SER
1	B	6	VAL
1	B	11	THR
1	B	17	LEU
1	B	21	ARG
1	B	28	ARG
1	B	29	ARG
1	B	41	GLN
1	B	45	VAL
1	B	46	CYS
1	B	50	LEU
1	B	59	LEU
1	B	63	LEU
1	B	65	VAL
1	B	67	PHE
1	B	70	ARG
1	B	88	ILE
1	B	108	ARG
1	B	109	VAL
1	B	111	GLN
1	B	131	GLU
1	B	132	ASN
1	B	139	LEU
1	B	164	SER
1	B	165	SER
1	B	166	LEU
1	B	173	ARG
1	B	180	SER
1	B	182	ILE

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Mol	Chain	Res	Type
1	B	191	CYS
1	B	206	GLN
1	B	220	LYS
1	B	221	THR
1	B	222	THR
1	B	229	LEU
1	B	251	LEU
1	B	254	ARG
1	B	255	LEU
1	B	264	ARG
1	B	271	LEU
1	B	273	GLU
1	B	275	ILE
1	B	280	LEU
1	B	288	ASP
1	B	291	GLN
1	B	292	ILE
1	B	293	VAL
1	B	299	ASP
1	B	322	GLU
1	B	323	ILE
1	B	340	GLU
1	B	343	THR
1	B	361	LEU
1	B	382	GLU
1	B	387	ILE
1	B	389	LEU
1	B	393	ARG
1	B	404	LEU
1	B	411	HIS
1	B	426	LEU
1	B	433	ARG
1	B	434	VAL
1	B	436	ARG
1	B	437	THR
1	B	440	VAL
1	B	444	MET
1	B	455	THR
1	B	462	THR
1	B	465	SER
1	B	469	ARG
1	B	470	HIS

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Mol	Chain	Res	Type
1	B	472	LEU
1	B	475	LEU
1	B	481	THR
1	B	491	VAL
1	B	493	THR
1	B	533	ARG
1	B	547	LEU
1	B	562	LYS
1	B	565	ASP
1	B	590	PHE
1	B	591	LEU
1	B	603	ARG
1	B	614	SER
1	B	617	VAL
1	B	625	THR
1	B	628	GLU
1	B	636	VAL
1	B	643	LEU
1	B	646	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	111	GLN
1	A	141	ASN
1	A	213	HIS
1	A	245	ASN
1	A	250	ASN
1	A	276	GLN
1	A	291	GLN
1	A	352	ASN
1	A	403	GLN
1	A	446	GLN
1	A	460	GLN
1	A	464	HIS
1	A	521	HIS
1	A	544	GLN
1	A	556	HIS
1	A	568	GLN
1	A	632	GLN
1	A	633	HIS

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Mol	Chain	Res	Type
1	B	111	GLN
1	B	196	GLN
1	B	206	GLN
1	B	213	HIS
1	B	234	GLN
1	B	245	ASN
1	B	250	ASN
1	B	267	HIS
1	B	278	HIS
1	B	291	GLN
1	B	321	ASN
1	B	352	ASN
1	B	379	GLN
1	B	403	GLN
1	B	411	HIS
1	B	446	GLN
1	B	460	GLN
1	B	521	HIS
1	B	568	GLN
1	B	619	ASN
1	B	620	HIS
1	B	632	GLN
1	B	633	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	8/9 (88%)	3 (37%)	0
2	H	8/9 (88%)	5 (62%)	1 (12%)
All	All	16/18 (88%)	8 (50%)	1 (6%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	4	A
2	G	5	A
2	G	6	A
2	H	3	A
2	H	4	A
2	H	5	A
2	H	6	A

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Mol	Chain	Res	Type
2	H	9	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	614/646 (95%)	-0.28	8 (1%) 79 77	39, 63, 106, 143	0
1	B	608/646 (94%)	-0.42	3 (0%) 91 90	33, 53, 101, 126	0
2	G	9/9 (100%)	-0.06	0 100 100	58, 69, 107, 111	0
2	H	8/9 (88%)	-0.06	0 100 100	49, 62, 86, 103	0
All	All	1239/1310 (94%)	-0.34	11 (0%) 85 84	33, 60, 103, 143	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	648	PRO	4.6
1	A	307	ASN	4.6
1	A	31	TRP	4.2
1	A	647	VAL	3.6
1	A	297	ARG	3.2
1	B	302	GLN	2.7
1	B	135	ARG	2.4
1	A	644	ASP	2.4
1	B	136	LEU	2.3
1	A	180	SER	2.2
1	A	304	PHE	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.