



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:53 AM GMT

PDB ID : 3K46  
Title : Crystal structure of full-length E. coli beta-glucuronidase  
Authors : Wallace, B.D.; Lane, K.T.; Redinbo, M.R.  
Deposited on : 2009-10-05  
Resolution : 2.50 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

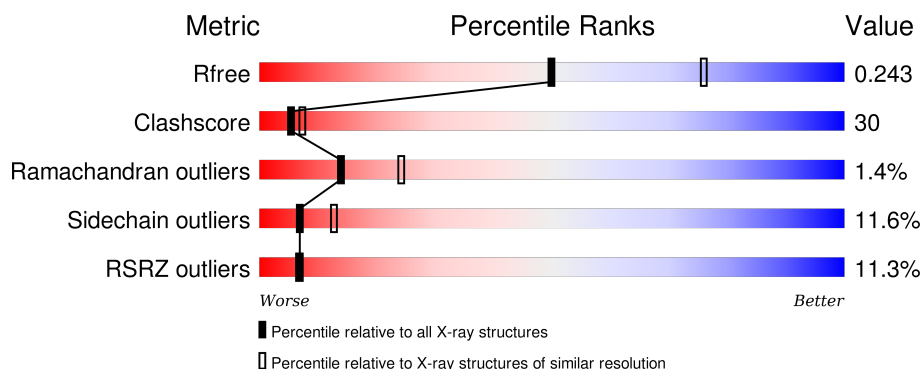
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	605	<div> <div>7%</div> <div>58%</div> <div>32%</div> <div>8%</div> <div>.</div> </div>
1	B	605	<div> <div>16%</div> <div>54%</div> <div>35%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9918 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4781	3035	826	898	22			
1	B	596	Total	C	N	O	S	0	0	0
			4780	3034	826	898	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

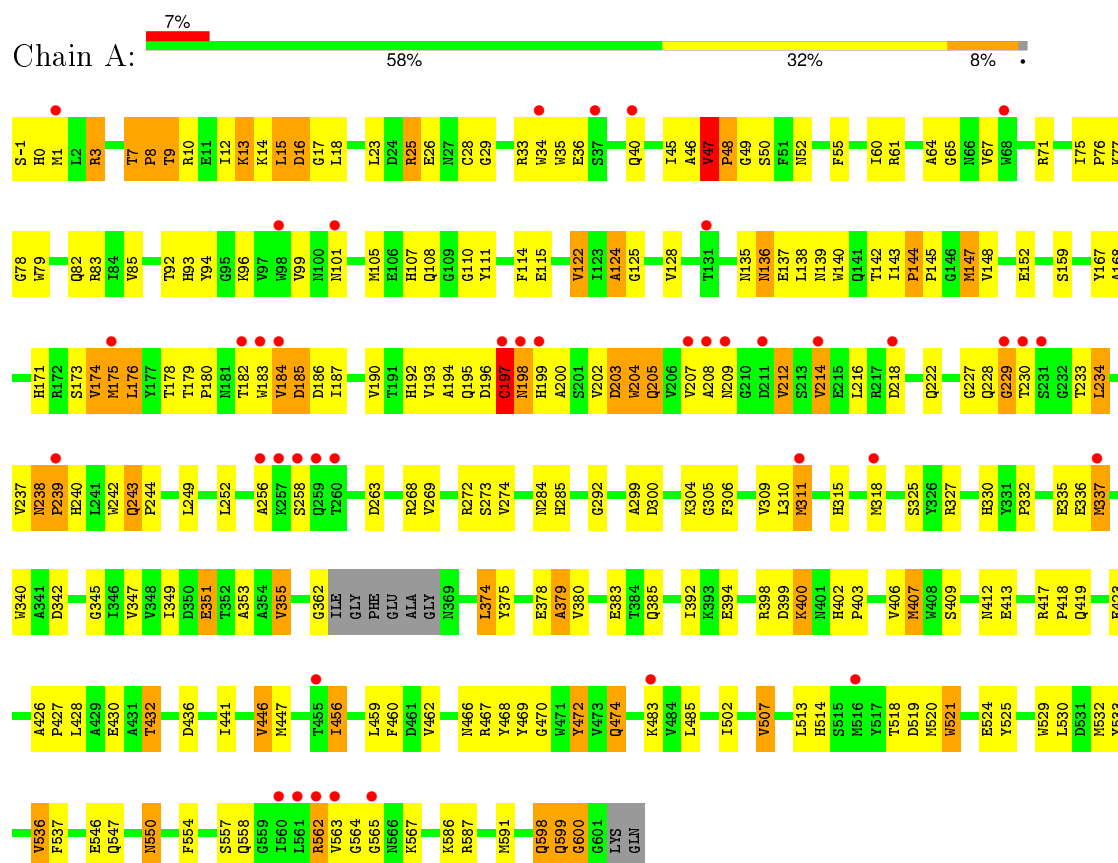
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	245	Total	O	0	0
			245	245		
2	B	112	Total	O	0	0
			112	112		

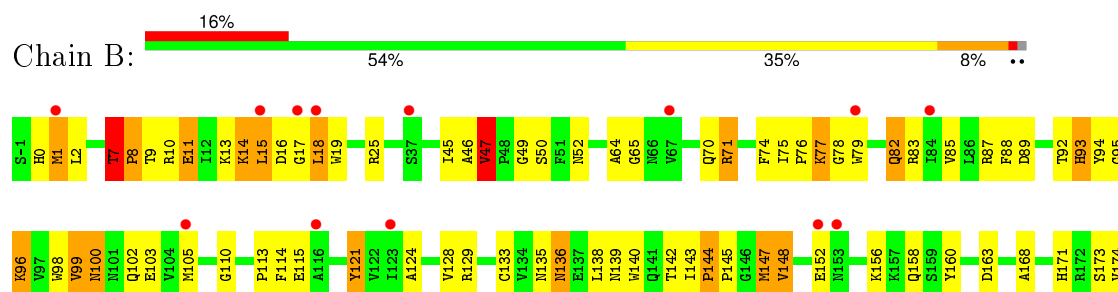
### 3 Residue-property plots

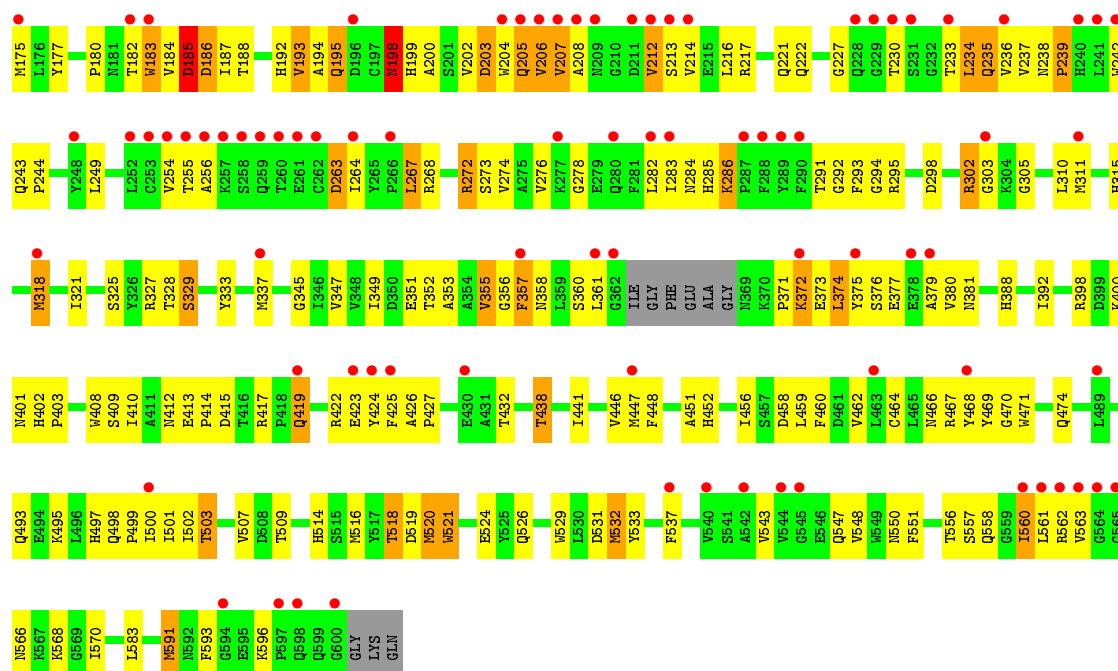
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 1: Beta-glucuronidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.75Å 76.19Å 125.67Å 90.00° 125.00° 90.00°	Depositor
Resolution (Å)	30.62 – 2.50 47.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.62-2.50) 95.5 (47.63-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.214 , 0.267 0.219 , 0.243	Depositor DCC
$R_{free}$ test set	2212 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 63.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43538 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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	0.63	10/4909 (0.2%)	0.69	9/6680 (0.1%)
1	B	0.55	8/4908 (0.2%)	0.66	5/6679 (0.1%)
All	All	0.59	18/9817 (0.2%)	0.67	14/13359 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	520	MET	CG-SD	6.37	1.97	1.81
1	B	516	MET	CG-SD	6.34	1.97	1.81
1	B	591	MET	CG-SD	6.33	1.97	1.81
1	A	532	MET	CG-SD	6.11	1.97	1.81
1	B	532	MET	CG-SD	6.08	1.97	1.81
1	B	147	MET	CG-SD	5.91	1.96	1.81
1	A	407	MET	CG-SD	5.87	1.96	1.81
1	A	337	MET	CG-SD	5.87	1.96	1.81
1	A	311	MET	CG-SD	5.86	1.96	1.81
1	A	175	MET	CG-SD	5.82	1.96	1.81
1	A	1	MET	CG-SD	5.73	1.96	1.81
1	B	318	MET	CG-SD	5.61	1.95	1.81
1	B	1	MET	CG-SD	5.48	1.95	1.81
1	A	147	MET	CG-SD	5.47	1.95	1.81
1	B	520	MET	CG-SD	5.46	1.95	1.81
1	B	337	MET	CG-SD	5.46	1.95	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	MET	CG-SD	5.26	1.94	1.81
1	A	591	MET	CG-SD	5.08	1.94	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASP	N-CA-C	8.18	133.09	111.00
1	B	198	ASN	N-CA-C	7.56	131.40	111.00
1	B	198	ASN	N-CA-CB	-7.17	97.70	110.60
1	B	185	ASP	N-CA-CB	-6.38	99.12	110.60
1	A	300	ASP	N-CA-C	5.94	127.04	111.00
1	A	380	VAL	N-CA-C	-5.75	95.48	111.00
1	A	197	CYS	N-CA-C	-5.65	95.73	111.00
1	A	379	ALA	N-CA-C	5.62	126.17	111.00
1	A	16	ASP	N-CA-C	-5.60	95.87	111.00
1	A	550	ASN	N-CA-C	5.39	125.55	111.00
1	A	108	GLN	N-CA-C	5.35	125.45	111.00
1	A	185	ASP	N-CA-C	5.33	125.40	111.00
1	B	100	ASN	CB-CA-C	5.32	121.04	110.40
1	A	48	PRO	N-CA-C	-5.11	98.81	112.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ILE	Mainchain,Peptide
1	A	184	VAL	Peptide
1	A	47	VAL	Mainchain,Peptide
1	B	143	ILE	Peptide
1	B	47	VAL	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	4781	0	4560	249	0
1	B	4780	0	4561	319	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	245	0	0	30	0
2	B	112	0	0	15	0
All	All	9918	0	9121	560	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 30.

All (560) 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:A:207:VAL:HG21	1:A:212:VAL:CG1	1.35	1.51
1:B:283:ILE:O	1:B:286:LYS:HD3	1.25	1.35
1:A:207:VAL:CG2	1:A:212:VAL:HG11	1.65	1.25
1:B:183:TRP:CD2	1:B:207:VAL:HG11	1.79	1.18
1:A:407:MET:HE2	2:A:833:HOH:O	1.04	1.18
1:A:207:VAL:CG2	1:A:212:VAL:CG1	2.23	1.16
1:B:205:GLN:OE1	1:B:207:VAL:HG22	1.46	1.16
1:A:207:VAL:HG21	1:A:212:VAL:HG12	1.12	1.08
1:B:17:GLY:O	1:B:46:ALA:HA	1.53	1.06
1:B:198:ASN:HB2	1:B:237:VAL:O	1.58	1.03
1:A:207:VAL:HG21	1:A:212:VAL:HG11	1.12	1.02
1:B:183:TRP:CG	1:B:207:VAL:HG11	1.95	1.01
1:B:194:ALA:O	2:B:655:HOH:O	1.78	1.00
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.25	1.00
1:B:263:ASP:OD2	2:B:658:HOH:O	1.81	0.99
1:A:-1:SER:O	2:A:687:HOH:O	1.80	0.99
1:B:286:LYS:HE2	1:B:286:LYS:O	1.61	0.98
1:A:239:PRO:HD2	2:A:697:HOH:O	1.64	0.96
1:B:286:LYS:HE2	1:B:286:LYS:N	1.82	0.95
1:B:183:TRP:CD1	1:B:184:VAL:O	2.21	0.94
1:B:286:LYS:HE2	1:B:286:LYS:H	1.32	0.94
1:A:25:ARG:HG3	1:A:25:ARG:HH11	1.34	0.93
1:B:195:GLN:HA	1:B:195:GLN:NE2	1.84	0.93
1:A:362:GLY:O	2:A:758:HOH:O	1.86	0.92
1:B:283:ILE:O	1:B:286:LYS:CD	2.16	0.92
1:A:175:MET:HE3	2:A:834:HOH:O	1.68	0.91
1:A:407:MET:CE	2:A:833:HOH:O	1.71	0.91
1:B:198:ASN:CB	1:B:237:VAL:O	2.19	0.91
1:B:183:TRP:CG	1:B:207:VAL:CG1	2.55	0.89
1:B:138:LEU:HD22	1:B:142:THR:HG21	1.54	0.89
1:A:175:MET:CE	2:A:834:HOH:O	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:O	2:A:832:HOH:O	1.91	0.87
1:B:286:LYS:O	1:B:286:LYS:CE	2.23	0.87
1:A:-1:SER:C	2:A:687:HOH:O	2.10	0.87
1:B:285:HIS:N	1:B:286:LYS:NZ	2.23	0.86
1:B:283:ILE:H	1:B:286:LYS:HE3	1.37	0.86
1:B:198:ASN:HD21	1:B:236:VAL:HG12	1.42	0.85
1:A:202:VAL:HG13	2:A:744:HOH:O	1.75	0.84
1:A:243:GLN:HA	1:A:243:GLN:HE21	1.41	0.84
1:B:198:ASN:CG	1:B:237:VAL:O	2.16	0.84
1:A:311:MET:HE3	1:A:337:MET:HA	1.57	0.84
1:A:207:VAL:CG1	1:A:256:ALA:CB	2.57	0.82
1:A:187:ILE:HA	1:A:205:GLN:HB2	1.61	0.82
1:B:183:TRP:CD2	1:B:207:VAL:CG1	2.62	0.81
1:B:374:LEU:O	1:B:380:VAL:HG12	1.80	0.81
1:B:283:ILE:N	1:B:286:LYS:HE3	1.94	0.81
1:A:207:VAL:CG1	1:A:256:ALA:HB1	2.11	0.80
1:A:199:HIS:CD2	1:A:200:ALA:H	2.00	0.80
1:B:205:GLN:CD	1:B:207:VAL:HG22	2.02	0.79
1:B:286:LYS:HE2	1:B:286:LYS:CA	2.13	0.79
1:B:186:ASP:HB3	1:B:206:VAL:HG13	1.63	0.78
1:B:272:ARG:HA	1:B:284:ASN:OD1	1.85	0.77
1:B:142:THR:HG22	1:B:144:PRO:O	1.85	0.76
1:A:207:VAL:HG11	1:A:256:ALA:CB	2.16	0.76
1:B:0:HIS:HB2	1:B:185:ASP:HB2	1.67	0.75
1:B:286:LYS:HE2	1:B:286:LYS:C	2.06	0.75
1:B:14:LYS:HZ2	1:B:14:LYS:HB3	1.51	0.75
1:A:192:HIS:O	1:A:199:HIS:HB3	1.87	0.75
1:B:285:HIS:N	1:B:286:LYS:HZ2	1.85	0.74
1:A:139:ASN:O	1:A:142:THR:HG22	1.87	0.74
1:B:212:VAL:CG2	1:B:230:THR:HA	2.17	0.74
1:A:207:VAL:HG11	1:A:256:ALA:HB1	1.69	0.74
1:A:311:MET:HE1	1:A:340:TRP:HB2	1.70	0.74
1:A:194:ALA:O	2:A:627:HOH:O	2.06	0.73
1:B:193:VAL:O	1:B:285:HIS:NE2	2.19	0.73
1:B:52:ASN:HD21	1:B:168:ALA:H	1.37	0.73
1:A:207:VAL:CG2	1:A:212:VAL:HG12	2.06	0.73
1:B:193:VAL:HG13	1:B:273:SER:HB3	1.71	0.73
1:A:23:LEU:HD11	1:A:60:ILE:HG12	1.69	0.72
1:A:52:ASN:HD21	1:A:168:ALA:H	1.37	0.72
1:A:182:THR:O	1:A:208:ALA:O	2.06	0.72
1:B:285:HIS:N	1:B:286:LYS:HZ3	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:H	1:A:110:GLY:CA	2.03	0.72
1:A:140:TRP:HB3	1:A:379:ALA:O	1.91	0.71
1:B:212:VAL:HG22	1:B:230:THR:HA	1.73	0.71
1:B:140:TRP:HB3	1:B:379:ALA:O	1.91	0.71
1:A:351:GLU:HG2	1:A:409:SER:HB3	1.73	0.71
1:A:207:VAL:HG23	1:A:212:VAL:HG11	1.71	0.70
1:A:82:GLN:OE1	1:A:82:GLN:HA	1.90	0.70
1:B:184:VAL:HG12	1:B:185:ASP:H	1.55	0.70
1:B:192:HIS:O	1:B:199:HIS:HB3	1.90	0.70
1:B:283:ILE:N	1:B:286:LYS:CE	2.54	0.70
1:A:554:PHE:O	1:A:565:GLY:O	2.09	0.70
1:B:7:THR:HB	1:B:8:PRO:HD2	1.72	0.70
1:A:13:LYS:HG3	1:A:15:LEU:HD21	1.72	0.70
1:B:203:ASP:CG	1:B:233:THR:HB	2.11	0.70
1:B:237:VAL:HG22	1:B:238:ASN:H	1.55	0.70
1:A:25:ARG:CG	1:A:25:ARG:HH11	2.04	0.70
1:A:192:HIS:HB2	1:A:199:HIS:CD2	2.26	0.70
1:A:507:VAL:HG22	1:A:529:TRP:CD1	2.26	0.70
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.00	0.70
1:A:412:ASN:HD21	1:A:466:ASN:HD21	1.39	0.70
1:A:0:HIS:ND1	1:A:186:ASP:HB2	2.07	0.70
1:B:203:ASP:HB3	1:B:233:THR:HB	1.74	0.69
1:B:392:ILE:HG21	1:B:432:THR:HG21	1.74	0.69
1:B:200:ALA:HB1	1:B:234:LEU:CD2	2.23	0.69
1:B:94:TYR:HB3	1:B:135:ASN:HB3	1.74	0.69
1:A:207:VAL:CG1	1:A:256:ALA:HB2	2.21	0.69
1:B:286:LYS:H	1:B:286:LYS:CE	2.06	0.69
1:B:244:PRO:HB2	1:B:593:PHE:HE1	1.57	0.69
1:B:205:GLN:HE22	1:B:207:VAL:CG2	2.07	0.68
1:B:193:VAL:HA	1:B:199:HIS:HB3	1.75	0.68
1:A:311:MET:CE	1:A:340:TRP:HB2	2.23	0.67
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.75	0.67
1:A:202:VAL:HG22	1:A:234:LEU:CD2	2.25	0.67
1:B:198:ASN:ND2	1:B:236:VAL:HG12	2.09	0.67
1:B:471:TRP:CD1	1:B:507:VAL:HG12	2.30	0.67
1:B:286:LYS:N	1:B:286:LYS:CE	2.55	0.67
1:B:328:THR:O	1:B:351:GLU:HB3	1.94	0.67
1:A:198:ASN:HB3	1:A:237:VAL:O	1.95	0.67
1:A:-1:SER:CA	2:A:687:HOH:O	2.41	0.66
1:B:452:HIS:ND1	2:B:619:HOH:O	2.29	0.66
1:B:375:TYR:HA	1:B:380:VAL:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LYS:HB3	1:B:14:LYS:NZ	2.09	0.65
1:B:93:HIS:H	1:B:110:GLY:CA	2.09	0.65
1:B:548:VAL:HG11	1:B:570:ILE:HD11	1.79	0.65
1:B:200:ALA:HA	1:B:235:GLN:O	1.97	0.65
1:A:35:TRP:HD1	1:A:101:ASN:HA	1.62	0.65
1:B:284:ASN:C	1:B:286:LYS:HZ2	1.99	0.65
1:B:244:PRO:HB2	1:B:593:PHE:CE1	2.32	0.65
1:A:485:LEU:HD23	1:A:536:VAL:HG11	1.79	0.65
1:B:15:LEU:HD13	1:B:15:LEU:O	1.97	0.65
1:A:342:ASP:OD2	1:A:402:HIS:HD2	1.79	0.64
1:A:598:GLN:CD	1:A:598:GLN:H	2.00	0.64
1:B:185:ASP:N	1:B:185:ASP:OD1	2.30	0.64
1:B:402:HIS:NE2	2:B:625:HOH:O	2.30	0.64
1:A:207:VAL:HG13	1:A:256:ALA:HB2	1.78	0.64
1:B:203:ASP:CB	1:B:233:THR:HB	2.27	0.64
1:B:507:VAL:HG13	1:B:529:TRP:CD1	2.33	0.64
1:B:193:VAL:HA	1:B:199:HIS:CB	2.28	0.63
1:A:105:MET:CE	1:A:115:GLU:HA	2.28	0.63
1:B:183:TRP:NE1	1:B:184:VAL:O	2.30	0.63
1:B:2:LEU:HG	1:B:185:ASP:O	1.99	0.63
1:B:282:LEU:HA	1:B:286:LYS:HE3	1.80	0.63
1:B:447:MET:HE1	1:B:470:GLY:HA2	1.80	0.63
1:A:392:ILE:HG21	1:A:432:THR:HG22	1.81	0.62
1:B:284:ASN:N	1:B:286:LYS:HZ2	1.97	0.62
1:B:502:ILE:HG13	1:B:537:PHE:CE2	2.34	0.62
1:A:436:ASP:O	2:A:757:HOH:O	2.15	0.62
1:A:23:LEU:HD23	1:A:67:VAL:HG12	1.82	0.62
1:A:93:HIS:H	1:A:110:GLY:HA2	1.64	0.62
1:B:560:ILE:H	1:B:560:ILE:HD12	1.65	0.62
1:A:193:VAL:HG23	1:A:285:HIS:NE2	2.15	0.62
1:A:249:LEU:HD13	1:A:268:ARG:HE	1.63	0.62
1:B:7:THR:HB	1:B:8:PRO:CD	2.29	0.62
1:A:502:ILE:HG13	1:A:537:PHE:CE2	2.34	0.61
1:A:355:VAL:HG13	1:A:412:ASN:HB3	1.81	0.61
1:B:425:PHE:CB	1:B:456:ILE:HD11	2.31	0.61
1:A:26:GLU:HB2	1:A:28:CYS:SG	2.40	0.61
1:A:33:ARG:NH1	2:A:805:HOH:O	2.33	0.61
1:B:556:THR:OG1	1:B:562:ARG:HG3	2.01	0.61
1:A:228:GLN:O	1:A:229:GLY:C	2.39	0.61
1:A:186:ASP:O	1:A:205:GLN:HB2	2.01	0.60
1:B:243:GLN:HA	1:B:243:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:MET:HA	1:B:321:ILE:HG22	1.83	0.60
1:A:77:LYS:HG3	1:A:125:GLY:HA2	1.81	0.60
1:A:105:MET:HE3	1:A:115:GLU:HA	1.83	0.60
1:A:183:TRP:CD1	1:A:184:VAL:N	2.70	0.60
1:A:207:VAL:O	1:A:207:VAL:HG12	2.00	0.60
1:A:514:HIS:HD2	1:A:524:GLU:OE1	1.83	0.60
1:A:10:ARG:HH21	1:B:76:PRO:HB3	1.66	0.60
1:B:243:GLN:NE2	1:B:284:ASN:HD22	1.99	0.60
1:B:238:ASN:HB3	1:B:239:PRO:HD2	1.84	0.60
1:A:107:HIS:HE1	1:A:394:GLU:OE1	1.84	0.60
1:B:192:HIS:NE2	1:B:202:VAL:HG23	2.17	0.60
1:B:283:ILE:C	1:B:286:LYS:HD3	2.17	0.60
1:A:202:VAL:HG22	1:A:234:LEU:HD23	1.82	0.60
1:A:13:LYS:HG3	1:A:15:LEU:CD2	2.31	0.60
1:B:147:MET:HE1	1:B:371:PRO:HD2	1.83	0.60
1:A:428:LEU:O	1:A:432:THR:HG23	2.02	0.59
1:B:203:ASP:OD1	1:B:214:VAL:HG11	2.01	0.59
1:A:218:ASP:HB2	1:A:222:GLN:HG2	1.84	0.59
1:B:82:GLN:CD	1:B:82:GLN:H	2.03	0.59
1:B:422:ARG:NH2	1:B:458:ASP:OD1	2.35	0.59
1:B:285:HIS:H	1:B:286:LYS:NZ	1.99	0.59
1:A:142:THR:HG23	1:A:144:PRO:O	2.01	0.59
1:B:200:ALA:HB1	1:B:234:LEU:HD23	1.85	0.59
1:A:468:TYR:O	1:A:469:TYR:HB2	2.02	0.59
1:B:282:LEU:HB3	1:B:286:LYS:NZ	2.18	0.59
1:B:413:GLU:HB3	1:B:446:VAL:HG22	1.84	0.59
1:A:502:ILE:HG13	1:A:537:PHE:CZ	2.37	0.59
1:A:299:ALA:CB	1:A:310:LEU:HD11	2.32	0.59
1:A:17:GLY:CA	1:A:47:VAL:H	2.15	0.59
1:B:205:GLN:NE2	1:B:207:VAL:HG22	2.17	0.59
1:B:180:PRO:HD3	2:B:697:HOH:O	2.02	0.58
1:A:349:ILE:HG12	1:A:407:MET:HE3	1.85	0.58
1:B:242:TRP:CZ2	1:B:345:GLY:HA2	2.39	0.58
1:B:283:ILE:C	1:B:286:LYS:NZ	2.57	0.58
1:B:18:LEU:HA	1:B:45:ILE:O	2.03	0.58
1:A:398:ARG:HD2	1:A:399:ASP:OD1	2.04	0.58
1:A:139:ASN:H	1:A:142:THR:CG2	2.16	0.58
1:A:139:ASN:H	1:A:142:THR:HG22	1.68	0.57
1:A:76:PRO:O	1:A:79:TRP:HB2	2.04	0.57
1:B:214:VAL:HG12	1:B:214:VAL:O	2.03	0.57
1:B:14:LYS:C	1:B:16:ASP:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:NH1	1:B:503:THR:HB	2.19	0.57
1:B:212:VAL:HA	1:B:255:THR:O	2.03	0.57
1:A:243:GLN:NE2	1:A:284:ASN:HD22	2.02	0.57
1:B:227:GLY:HA3	1:B:233:THR:CG2	2.34	0.57
1:B:238:ASN:HB3	1:B:239:PRO:CD	2.35	0.57
1:B:195:GLN:HA	1:B:195:GLN:HE21	1.66	0.57
1:A:249:LEU:O	2:A:690:HOH:O	2.18	0.57
1:B:14:LYS:HB2	1:B:71:ARG:HE	1.69	0.57
1:B:183:TRP:CD1	1:B:207:VAL:CG1	2.87	0.57
1:B:311:MET:O	1:B:315:HIS:HD2	1.88	0.57
1:A:35:TRP:CD1	1:A:101:ASN:HA	2.40	0.57
1:B:205:GLN:NE2	1:B:207:VAL:CG2	2.67	0.57
1:B:138:LEU:HD22	1:B:142:THR:CG2	2.29	0.57
1:A:94:TYR:OH	1:A:96:LYS:HE3	2.05	0.57
1:B:222:GLN:NE2	2:B:691:HOH:O	2.38	0.57
1:B:283:ILE:N	1:B:286:LYS:HZ1	2.02	0.56
1:B:148:VAL:HG12	1:B:158:GLN:OE1	2.06	0.56
1:B:198:ASN:HD21	1:B:236:VAL:CG1	2.14	0.56
1:B:188:THR:HB	1:B:204:TRP:HB3	1.87	0.56
1:B:292:GLY:HA3	1:B:325:SER:O	2.05	0.56
1:A:184:VAL:HG12	1:A:185:ASP:HB3	1.88	0.56
1:A:470:GLY:O	1:A:474:GLN:HB2	2.05	0.56
1:B:200:ALA:HB1	1:B:234:LEU:HD21	1.86	0.56
1:A:309:VAL:HG23	2:A:638:HOH:O	2.06	0.56
1:B:75:ILE:O	1:B:124:ALA:O	2.24	0.56
1:A:244:PRO:O	1:A:345:GLY:O	2.24	0.56
1:B:283:ILE:C	1:B:286:LYS:HZ2	2.09	0.56
1:A:183:TRP:CD1	1:A:207:VAL:HA	2.41	0.56
1:A:77:LYS:HZ1	1:B:8:PRO:HA	1.71	0.56
1:B:267:LEU:HG	1:B:268:ARG:N	2.21	0.56
1:A:193:VAL:HG23	1:A:285:HIS:HE2	1.69	0.55
1:B:70:GLN:NE2	1:B:129:ARG:HD2	2.22	0.55
1:B:1:MET:HA	1:B:1:MET:HE3	1.88	0.55
1:B:89:ASP:OD2	1:B:173:SER:HB2	2.05	0.55
1:B:441:ILE:HG22	1:B:460:PHE:HD1	1.71	0.55
1:A:10:ARG:HH11	1:B:77:LYS:HE2	1.72	0.55
1:A:17:GLY:HA3	1:A:47:VAL:H	1.70	0.55
1:A:564:GLY:HA2	2:A:625:HOH:O	2.06	0.55
1:B:282:LEU:C	1:B:286:LYS:HZ1	2.09	0.55
1:B:183:TRP:CG	1:B:207:VAL:HG12	2.41	0.55
1:A:10:ARG:NH2	1:B:76:PRO:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLY:HA2	1:A:305:GLY:HA3	1.87	0.55
1:A:36:GLU:HA	1:A:101:ASN:OD1	2.07	0.55
1:B:283:ILE:H	1:B:286:LYS:CE	2.09	0.54
1:A:65:GLY:H	1:A:136:ASN:HD21	1.55	0.54
1:B:351:GLU:HA	1:B:409:SER:HB3	1.89	0.54
1:A:447:MET:HE1	1:A:470:GLY:HA2	1.90	0.54
1:B:468:TYR:O	1:B:469:TYR:HB2	2.08	0.54
1:A:468:TYR:HA	2:A:803:HOH:O	2.07	0.54
1:B:83:ARG:HH12	1:B:184:VAL:HA	1.71	0.54
1:A:77:LYS:NZ	1:B:8:PRO:HA	2.22	0.54
1:A:50:SER:HB3	1:A:52:ASN:HD22	1.73	0.54
1:B:105:MET:HE1	1:B:114:PHE:O	2.08	0.54
1:A:413:GLU:HB3	1:A:446:VAL:HG13	1.89	0.54
1:B:205:GLN:NE2	1:B:212:VAL:HG11	2.22	0.54
1:A:204:TRP:CD1	1:A:204:TRP:C	2.81	0.53
1:B:273:SER:O	1:B:283:ILE:HA	2.07	0.53
1:B:7:THR:C	1:B:9:THR:H	2.11	0.53
1:B:413:GLU:CB	1:B:446:VAL:HG22	2.38	0.53
1:A:187:ILE:HA	1:A:205:GLN:CB	2.37	0.53
1:B:19:TRP:CZ2	1:B:174:VAL:HG11	2.43	0.53
1:B:388:HIS:CD2	1:B:392:ILE:HD11	2.44	0.53
1:B:93:HIS:H	1:B:110:GLY:HA3	1.73	0.53
1:B:82:GLN:N	1:B:82:GLN:CD	2.62	0.53
1:B:388:HIS:O	1:B:392:ILE:HG13	2.08	0.53
1:A:93:HIS:H	1:A:110:GLY:HA3	1.74	0.53
1:A:3:ARG:CZ	1:A:335:GLU:HG3	2.38	0.53
1:A:193:VAL:HG22	1:A:273:SER:HB3	1.89	0.53
1:A:29:GLY:HA2	1:A:34:TRP:CE2	2.44	0.53
1:B:0:HIS:HB2	1:B:185:ASP:CB	2.39	0.52
1:B:212:VAL:HG21	1:B:230:THR:HA	1.90	0.52
1:A:25:ARG:CG	1:A:25:ARG:NH1	2.71	0.52
1:B:283:ILE:N	1:B:286:LYS:NZ	2.58	0.52
1:A:204:TRP:HD1	1:A:205:GLN:N	2.07	0.52
1:A:52:ASN:H	1:A:52:ASN:ND2	2.08	0.52
1:B:413:GLU:CA	1:B:446:VAL:HG22	2.40	0.52
1:B:187:ILE:CG2	1:B:188:THR:N	2.73	0.52
1:B:138:LEU:CD2	1:B:142:THR:HG21	2.33	0.52
1:A:426:ALA:HA	1:A:459:LEU:HD13	1.91	0.52
1:A:203:ASP:C	1:A:203:ASP:OD2	2.48	0.52
1:B:183:TRP:CE3	1:B:207:VAL:HG11	2.39	0.52
1:A:83:ARG:NH2	1:A:184:VAL:HG11	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:TRP:CE2	1:A:533:TYR:HE1	2.29	0.51
1:A:10:ARG:CZ	1:A:79:TRP:HE1	2.23	0.51
1:B:412:ASN:HD21	1:B:466:ASN:HD21	1.57	0.51
1:A:0:HIS:HB3	1:A:185:ASP:O	2.11	0.51
1:A:82:GLN:HG3	1:A:178:THR:HG23	1.91	0.51
1:A:82:GLN:O	1:A:179:THR:O	2.29	0.51
1:A:65:GLY:HA2	1:A:137:GLU:OE2	2.10	0.51
1:A:529:TRP:NE1	1:A:533:TYR:HE1	2.08	0.51
1:B:15:LEU:CD1	1:B:15:LEU:O	2.59	0.51
1:A:342:ASP:CG	1:A:403:PRO:HD2	2.31	0.51
1:A:547:GLN:NE2	2:A:648:HOH:O	2.41	0.51
1:A:76:PRO:HD2	1:A:79:TRP:CE3	2.46	0.51
1:B:79:TRP:O	1:B:82:GLN:HG2	2.10	0.51
1:B:105:MET:HE3	1:B:115:GLU:HA	1.92	0.51
1:A:29:GLY:HA2	1:A:34:TRP:CD2	2.45	0.51
1:B:10:ARG:CZ	1:B:79:TRP:HE1	2.24	0.51
1:A:417:ARG:N	1:A:418:PRO:CD	2.74	0.51
1:A:227:GLY:HA3	1:A:233:THR:HG21	1.92	0.51
1:A:306:PHE:CZ	1:A:336:GLU:HG3	2.46	0.50
1:B:284:ASN:O	1:B:286:LYS:HG3	2.10	0.50
1:B:227:GLY:HA3	1:B:233:THR:HG23	1.93	0.50
1:B:286:LYS:HE3	1:B:286:LYS:O	2.11	0.50
1:A:598:GLN:O	1:A:599:GLN:C	2.50	0.50
1:B:14:LYS:C	1:B:16:ASP:N	2.65	0.50
1:B:351:GLU:OE1	1:B:412:ASN:HB2	2.12	0.50
1:A:10:ARG:HD3	1:B:77:LYS:HE2	1.92	0.50
1:B:65:GLY:H	1:B:136:ASN:HD21	1.60	0.50
1:A:92:THR:HA	1:A:110:GLY:HA2	1.94	0.50
1:B:242:TRP:HB2	2:B:662:HOH:O	2.12	0.50
1:B:49:GLY:HA2	1:B:305:GLY:HA3	1.94	0.50
1:A:15:LEU:HD22	1:A:173:SER:CB	2.42	0.50
1:B:71:ARG:CG	1:B:71:ARG:NH1	2.72	0.49
1:A:140:TRP:CE3	1:A:379:ALA:O	2.64	0.49
1:B:358:ASN:HD21	1:B:448:PHE:HZ	1.60	0.49
1:A:138:LEU:HA	1:A:142:THR:HG21	1.93	0.49
1:B:425:PHE:HB3	1:B:456:ILE:HD11	1.93	0.49
1:A:14:LYS:HB2	1:A:174:VAL:O	2.11	0.49
1:B:291:THR:HG21	1:B:591:MET:HE2	1.93	0.49
1:A:562:ARG:C	1:A:562:ARG:HD2	2.32	0.49
1:B:518:THR:OG1	1:B:518:THR:O	2.29	0.49
1:A:513:LEU:HD23	1:A:521:TRP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:THR:HG21	1:B:526:GLN:NE2	2.27	0.49
1:B:233:THR:HG22	1:B:234:LEU:N	2.28	0.49
1:A:238:ASN:H	1:A:239:PRO:HD3	1.77	0.49
1:B:1:MET:HA	1:B:1:MET:CE	2.42	0.49
1:B:294:GLY:O	1:B:550:ASN:HA	2.12	0.49
1:B:425:PHE:HB2	1:B:456:ILE:HD11	1.95	0.49
1:A:135:ASN:ND2	1:A:137:GLU:H	2.11	0.49
1:B:186:ASP:O	1:B:187:ILE:HG13	2.13	0.49
1:B:194:ALA:CB	1:B:199:HIS:HD2	2.26	0.49
1:A:195:GLN:HG3	2:A:627:HOH:O	2.12	0.49
1:B:377:GLU:HA	1:B:381:ASN:HB3	1.94	0.49
1:B:17:GLY:O	1:B:46:ALA:CA	2.44	0.49
1:B:375:TYR:HA	1:B:380:VAL:CG1	2.42	0.49
1:B:11:GLU:HB2	1:B:177:TYR:HB3	1.94	0.49
1:A:93:HIS:N	1:A:110:GLY:HA2	2.28	0.49
1:A:351:GLU:HG2	1:A:409:SER:CB	2.41	0.49
1:B:293:PHE:CD1	1:B:551:PHE:HA	2.48	0.49
1:B:360:SER:HB2	1:B:417:ARG:HH21	1.78	0.48
1:B:284:ASN:CA	1:B:286:LYS:HZ2	2.26	0.48
1:B:7:THR:C	1:B:9:THR:N	2.66	0.48
1:B:75:ILE:HD11	1:B:128:VAL:HG22	1.95	0.48
1:B:563:VAL:H	1:B:566:ASN:HA	1.78	0.48
1:B:401:ASN:O	1:B:403:PRO:HD3	2.13	0.48
1:A:205:GLN:OE1	1:A:212:VAL:HG21	2.13	0.48
1:B:102:GLN:HG2	1:B:121:TYR:CG	2.49	0.48
1:B:96:LYS:HD3	1:B:98:TRP:CZ2	2.49	0.48
1:B:0:HIS:CD2	1:B:185:ASP:OD1	2.65	0.48
1:B:255:THR:OG1	1:B:264:ILE:HG12	2.13	0.48
1:A:92:THR:OG1	1:A:171:HIS:ND1	2.42	0.48
1:B:182:THR:O	1:B:208:ALA:O	2.31	0.48
1:A:7:THR:C	1:A:9:THR:N	2.65	0.48
1:B:203:ASP:C	1:B:203:ASP:OD2	2.50	0.48
1:A:456:ILE:HG23	1:A:460:PHE:HE2	1.77	0.48
1:B:500:ILE:O	1:B:543:VAL:HA	2.14	0.48
1:B:254:VAL:O	1:B:264:ILE:HA	2.14	0.48
1:B:328:THR:HA	1:B:333:TYR:CZ	2.49	0.48
1:A:426:ALA:HB3	1:A:427:PRO:HD3	1.96	0.48
1:A:306:PHE:CE1	1:A:336:GLU:HG3	2.49	0.48
1:B:207:VAL:HG21	1:B:256:ALA:HB2	1.96	0.48
1:A:200:ALA:HB1	1:A:234:LEU:HD13	1.95	0.48
1:A:327:ARG:NH2	1:A:412:ASN:ND2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:THR:OG1	1:B:353:ALA:N	2.47	0.48
1:A:355:VAL:CG1	1:A:412:ASN:HB3	2.44	0.47
1:A:183:TRP:O	1:A:263:ASP:OD2	2.32	0.47
1:B:19:TRP:HZ2	1:B:174:VAL:HG11	1.78	0.47
1:A:135:ASN:HD21	1:A:137:GLU:HB2	1.79	0.47
1:B:351:GLU:HG2	1:B:352:THR:N	2.30	0.47
1:B:562:ARG:C	1:B:562:ARG:HD2	2.34	0.47
1:B:183:TRP:CD1	1:B:207:VAL:HG12	2.49	0.47
1:B:413:GLU:N	1:B:414:PRO:HD3	2.28	0.47
1:A:140:TRP:CD2	1:A:379:ALA:O	2.68	0.47
1:B:194:ALA:HB2	1:B:199:HIS:CD2	2.49	0.47
1:A:122:VAL:HG23	1:A:128:VAL:HG11	1.96	0.47
1:A:204:TRP:CD1	1:A:205:GLN:N	2.82	0.47
1:B:193:VAL:CG1	1:B:273:SER:HB3	2.42	0.47
1:A:92:THR:HA	1:A:110:GLY:CA	2.44	0.47
1:B:52:ASN:ND2	1:B:168:ALA:H	2.07	0.47
1:B:95:GLY:HA2	1:B:133:CYS:O	2.15	0.47
1:B:92:THR:HA	1:B:110:GLY:CA	2.44	0.47
1:B:327:ARG:NH2	1:B:412:ASN:ND2	2.63	0.47
1:B:50:SER:HB2	1:B:303:GLY:HA3	1.97	0.47
1:B:183:TRP:CE2	1:B:207:VAL:CG1	2.97	0.47
1:B:237:VAL:HG22	1:B:238:ASN:N	2.28	0.47
1:B:171:HIS:O	1:B:305:GLY:HA2	2.15	0.47
1:A:75:ILE:O	1:A:124:ALA:O	2.33	0.47
2:A:638:HOH:O	1:B:302:ARG:NH2	2.47	0.47
1:A:75:ILE:N	1:A:75:ILE:HD12	2.30	0.47
1:B:180:PRO:HG3	1:B:263:ASP:OD2	2.15	0.46
1:B:227:GLY:HA3	1:B:233:THR:HG21	1.97	0.46
1:A:599:GLN:O	1:A:600:GLY:C	2.53	0.46
1:B:45:ILE:HG12	1:B:46:ALA:N	2.30	0.46
1:B:45:ILE:HG12	1:B:46:ALA:H	1.80	0.46
1:B:145:PRO:HD2	1:B:355:VAL:O	2.15	0.46
1:A:342:ASP:OD2	1:A:402:HIS:CD2	2.66	0.46
1:B:274:VAL:HA	1:B:282:LEU:O	2.16	0.46
1:B:204:TRP:CD1	1:B:205:GLN:N	2.84	0.46
1:B:243:GLN:HA	1:B:243:GLN:NE2	2.30	0.46
1:A:3:ARG:NH1	1:A:335:GLU:HG3	2.30	0.46
1:B:205:GLN:HG3	1:B:254:VAL:HG11	1.98	0.46
1:A:15:LEU:O	1:A:16:ASP:C	2.52	0.46
1:B:520:MET:O	1:B:521:TRP:HB2	2.15	0.46
1:A:400:LYS:H	1:A:400:LYS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASP:OD1	1:A:403:PRO:HD2	2.16	0.46
1:A:190:VAL:HB	1:A:202:VAL:HB	1.98	0.46
1:A:198:ASN:O	1:A:199:HIS:HB2	2.15	0.46
1:B:547:GLN:NE2	2:B:651:HOH:O	2.49	0.46
1:A:205:GLN:N	1:A:205:GLN:HE21	2.14	0.45
1:A:93:HIS:CE1	1:A:138:LEU:HD21	2.51	0.45
1:B:213:SER:O	1:B:227:GLY:O	2.34	0.45
1:B:282:LEU:CA	1:B:286:LYS:HE3	2.43	0.45
1:A:311:MET:O	1:A:315:HIS:HD2	1.98	0.45
1:B:88:PHE:O	1:B:113:PRO:HA	2.16	0.45
1:B:1:MET:CE	1:B:87:ARG:HH12	2.29	0.45
1:A:105:MET:HE1	1:A:114:PHE:O	2.17	0.45
1:A:65:GLY:H	1:A:136:ASN:ND2	2.15	0.45
1:B:199:HIS:ND1	1:B:200:ALA:N	2.50	0.45
1:B:98:TRP:CH2	1:B:133:CYS:HB2	2.51	0.45
1:A:40:GLN:HG2	2:A:801:HOH:O	2.16	0.45
1:A:240:HIS:N	2:A:697:HOH:O	2.47	0.45
1:B:291:THR:HG21	1:B:591:MET:CE	2.47	0.45
1:B:566:ASN:ND2	1:B:568:LYS:NZ	2.64	0.45
1:B:182:THR:CG2	1:B:182:THR:O	2.64	0.45
1:B:423:GLU:OE1	1:B:424:TYR:N	2.50	0.45
1:B:529:TRP:CZ2	1:B:533:TYR:HE1	2.35	0.45
1:B:102:GLN:HG2	1:B:121:TYR:CD1	2.52	0.45
1:A:274:VAL:HG11	1:A:406:VAL:O	2.17	0.45
1:A:419:GLN:HE21	1:A:419:GLN:HA	1.82	0.45
1:A:546:GLU:OE2	1:A:587:ARG:HD3	2.17	0.45
1:A:185:ASP:N	1:A:185:ASP:OD1	2.50	0.45
1:A:598:GLN:CD	1:A:598:GLN:N	2.69	0.45
1:B:50:SER:OG	1:B:303:GLY:HA3	2.17	0.45
1:B:276:VAL:HG13	1:B:499:PRO:HG2	1.97	0.45
1:A:299:ALA:HB2	1:A:310:LEU:HD11	1.98	0.44
1:A:140:TRP:CB	1:A:379:ALA:O	2.64	0.44
1:B:295:ARG:O	1:B:329:SER:OG	2.28	0.44
1:B:136:ASN:HD22	1:B:136:ASN:H	1.65	0.44
1:A:472:TYR:C	1:A:472:TYR:CD1	2.91	0.44
1:A:430:GLU:HG2	2:A:632:HOH:O	2.17	0.44
1:A:14:LYS:NZ	1:A:14:LYS:HB3	2.33	0.44
1:A:78:GLY:HA3	1:B:78:GLY:HA3	1.99	0.44
1:A:147:MET:O	1:A:159:SER:HB3	2.18	0.44
1:A:183:TRP:CD1	1:A:183:TRP:C	2.89	0.44
1:A:3:ARG:NH2	2:A:820:HOH:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:SER:CB	1:B:303:GLY:HA3	2.47	0.44
1:A:292:GLY:HA3	1:A:325:SER:O	2.17	0.44
1:B:493:GLN:O	1:B:497:HIS:N	2.40	0.44
1:B:9:THR:HA	2:B:697:HOH:O	2.17	0.44
1:B:93:HIS:H	1:B:110:GLY:HA2	1.79	0.44
1:A:432:THR:OG1	1:A:441:ILE:HD12	2.17	0.44
1:A:242:TRP:CZ2	1:A:345:GLY:HA2	2.53	0.44
1:A:203:ASP:CG	1:A:233:THR:HB	2.37	0.44
1:B:561:LEU:HD22	1:B:566:ASN:HD21	1.82	0.44
1:B:139:ASN:H	1:B:142:THR:HB	1.83	0.44
1:A:227:GLY:HA3	1:A:233:THR:CG2	2.47	0.44
1:A:140:TRP:CG	1:A:379:ALA:O	2.71	0.44
1:B:533:TYR:HD2	1:B:537:PHE:CZ	2.35	0.44
1:B:415:ASP:OD2	1:B:417:ARG:NH2	2.51	0.44
1:B:419:GLN:HB2	1:B:419:GLN:HE21	1.62	0.44
1:A:330:HIS:O	1:A:353:ALA:HA	2.18	0.44
1:B:408:TRP:HB2	1:B:441:ILE:HG12	1.99	0.44
1:B:243:GLN:HE22	1:B:284:ASN:HD22	1.62	0.43
1:B:1:MET:HE1	1:B:87:ARG:NH1	2.34	0.43
1:A:47:VAL:HA	1:A:48:PRO:C	2.38	0.43
1:A:237:VAL:HG12	1:A:238:ASN:H	1.83	0.43
1:A:14:LYS:HZ2	1:A:14:LYS:HB3	1.81	0.43
1:A:198:ASN:N	1:A:198:ASN:OD1	2.51	0.43
1:A:243:GLN:HA	1:A:243:GLN:NE2	2.22	0.43
1:B:426:ALA:HA	1:B:459:LEU:HD13	1.99	0.43
1:B:212:VAL:HG23	1:B:214:VAL:HG23	2.00	0.43
1:B:19:TRP:CE2	1:B:71:ARG:HD2	2.53	0.43
1:A:385:GLN:HE22	1:A:427:PRO:HG2	1.83	0.43
1:A:412:ASN:HD21	1:A:466:ASN:ND2	2.12	0.43
1:B:471:TRP:CG	1:B:507:VAL:HG12	2.53	0.43
1:B:529:TRP:CE2	1:B:533:TYR:HE1	2.36	0.43
1:B:302:ARG:HB3	1:B:302:ARG:CZ	2.49	0.43
1:B:372:LYS:HD3	1:B:372:LYS:HA	1.78	0.43
1:A:195:GLN:C	1:A:197:CYS:H	2.22	0.43
1:B:514:HIS:HA	1:B:524:GLU:OE2	2.19	0.43
1:B:471:TRP:HE3	1:B:520:MET:HE1	1.83	0.43
1:B:328:THR:HG1	1:B:351:GLU:H	1.66	0.43
1:B:357:PHE:HB2	2:B:632:HOH:O	2.18	0.43
1:B:295:ARG:HB2	1:B:333:TYR:OH	2.19	0.43
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.69	0.43
1:B:464:CYS:HA	1:B:501:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ALA:CB	1:B:199:HIS:CD2	3.02	0.42
1:A:52:ASN:HB3	1:A:61:ARG:HG3	2.00	0.42
1:A:105:MET:CE	1:A:115:GLU:CA	2.95	0.42
1:B:526:GLN:NE2	2:B:605:HOH:O	2.51	0.42
1:A:7:THR:C	1:A:9:THR:H	2.22	0.42
1:B:160:TYR:OH	1:B:557:SER:HB3	2.19	0.42
1:A:586:LYS:HE3	1:A:586:LYS:HB2	1.67	0.42
1:A:64:ALA:HA	1:A:136:ASN:HD21	1.84	0.42
1:B:451:ALA:HB1	1:B:495:LYS:HD2	2.02	0.42
1:B:556:THR:OG1	1:B:562:ARG:CG	2.65	0.42
1:A:8:PRO:HD3	1:B:74:PHE:CE2	2.54	0.42
1:A:222:GLN:NE2	2:A:705:HOH:O	2.52	0.42
1:A:519:ASP:O	1:A:525:TYR:HB2	2.20	0.42
1:B:1:MET:HE1	1:B:115:GLU:CD	2.40	0.42
1:A:507:VAL:CG2	1:A:529:TRP:CD1	3.01	0.42
1:B:413:GLU:HA	1:B:446:VAL:HG22	2.02	0.42
1:A:17:GLY:O	1:A:45:ILE:O	2.38	0.42
1:A:183:TRP:HB3	1:A:263:ASP:HB3	2.02	0.42
1:A:45:ILE:HG13	1:A:55:PHE:CZ	2.54	0.42
1:B:99:VAL:O	1:B:100:ASN:C	2.58	0.42
1:B:282:LEU:HB3	1:B:286:LYS:HZ3	1.85	0.42
1:B:285:HIS:CA	1:B:286:LYS:HZ3	2.32	0.42
1:B:263:ASP:CG	2:B:658:HOH:O	2.43	0.42
1:A:311:MET:CE	1:A:340:TRP:CB	2.95	0.42
1:B:327:ARG:HA	1:B:349:ILE:O	2.19	0.42
1:A:269:VAL:HA	2:A:829:HOH:O	2.20	0.42
1:B:233:THR:HG22	1:B:234:LEU:H	1.85	0.42
1:A:243:GLN:HE22	1:A:284:ASN:HD22	1.66	0.42
1:A:145:PRO:HD2	1:A:355:VAL:O	2.19	0.42
1:A:563:VAL:HG23	1:A:567:LYS:HG2	2.01	0.42
1:B:93:HIS:HB2	1:B:135:ASN:O	2.20	0.41
1:B:519:ASP:OD1	1:B:519:ASP:N	2.45	0.41
1:B:543:VAL:O	1:B:596:LYS:NZ	2.46	0.41
1:B:198:ASN:OD1	1:B:237:VAL:O	2.37	0.41
1:B:451:ALA:HB3	2:B:619:HOH:O	2.20	0.41
1:B:469:TYR:OH	2:B:645:HOH:O	2.20	0.41
1:A:214:VAL:HG13	1:A:252:LEU:HD11	2.02	0.41
1:A:238:ASN:N	1:A:238:ASN:OD1	2.54	0.41
1:B:217:ARG:HG2	1:B:221:GLN:HA	2.02	0.41
1:B:284:ASN:N	1:B:286:LYS:NZ	2.64	0.41
1:A:-1:SER:N	2:A:687:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:MET:HE3	1:B:115:GLU:CA	2.49	0.41
1:B:426:ALA:HB3	1:B:427:PRO:HD3	2.02	0.41
1:B:274:VAL:HG23	1:B:438:THR:O	2.21	0.41
1:A:199:HIS:CD2	1:A:200:ALA:N	2.81	0.41
1:A:79:TRP:HZ3	1:A:176:LEU:HD13	1.86	0.41
1:B:467:ARG:HB3	1:B:533:TYR:OH	2.21	0.41
1:A:12:ILE:HG22	1:A:79:TRP:CH2	2.56	0.41
1:A:374:LEU:HD12	1:A:375:TYR:CE2	2.56	0.41
1:B:373:GLU:HB3	1:B:376:SER:HB3	2.03	0.41
1:B:205:GLN:NE2	1:B:212:VAL:CG1	2.83	0.41
1:A:167:TYR:HB2	1:A:304:LYS:HG3	2.02	0.41
1:A:83:ARG:HH22	1:A:184:VAL:HG11	1.84	0.41
1:A:237:VAL:C	1:A:238:ASN:OD1	2.59	0.41
1:A:203:ASP:OD2	1:A:233:THR:N	2.48	0.41
1:A:180:PRO:HD3	2:A:615:HOH:O	2.20	0.41
1:B:596:LYS:HD3	2:B:679:HOH:O	2.20	0.41
1:B:98:TRP:HH2	1:B:133:CYS:HB2	1.86	0.41
1:A:9:THR:HA	2:A:615:HOH:O	2.21	0.41
1:B:183:TRP:CD1	1:B:184:VAL:N	2.89	0.40
1:B:249:LEU:HD13	1:B:268:ARG:HE	1.86	0.40
1:A:413:GLU:CB	1:A:446:VAL:HG13	2.51	0.40
1:B:64:ALA:HA	1:B:136:ASN:HD21	1.86	0.40
1:B:583:LEU:HD23	1:B:583:LEU:C	2.42	0.40
1:B:566:ASN:ND2	1:B:568:LYS:HZ1	2.20	0.40
1:B:192:HIS:H	1:B:192:HIS:CD2	2.39	0.40
1:B:19:TRP:CD1	1:B:47:VAL:CG1	3.04	0.40
1:B:460:PHE:O	1:B:498:GLN:NE2	2.54	0.40
1:B:278:GLY:O	1:B:499:PRO:HD3	2.21	0.40
1:B:216:LEU:HG	1:B:217:ARG:H	1.86	0.40
1:B:19:TRP:CD1	1:B:19:TRP:N	2.89	0.40
1:B:356:GLY:C	1:B:358:ASN:H	2.24	0.40
1:A:83:ARG:HB3	1:A:179:THR:O	2.22	0.40
1:B:83:ARG:NH2	1:B:184:VAL:HG13	2.37	0.40
1:A:15:LEU:HD13	1:A:173:SER:OG	2.21	0.40
1:A:17:GLY:O	1:A:46:ALA:HA	2.22	0.40
1:B:1:MET:HE2	1:B:87:ARG:HH12	1.87	0.40
1:A:111:TYR:HB2	1:A:332:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/605 (98%)	549 (93%)	35 (6%)	9 (2%)	13	22
1	B	592/605 (98%)	544 (92%)	41 (7%)	7 (1%)	16	29
All	All	1185/1210 (98%)	1093 (92%)	76 (6%)	16 (1%)	14	24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	239	PRO
1	B	7	THR
1	B	198	ASN
1	A	600	GLY
1	B	93	HIS
1	A	124	ALA
1	A	550	ASN
1	A	198	ASN
1	B	144	PRO
1	B	357	PHE
1	A	144	PRO
1	B	8	PRO
1	B	239	PRO
1	A	229	GLY
1	A	238	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	506/513 (99%)	449 (89%)	57 (11%)	7	13
1	B	507/513 (99%)	446 (88%)	61 (12%)	6	12
All	All	1013/1026 (99%)	895 (88%)	118 (12%)	7	13

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	THR
1	A	9	THR
1	A	13	LYS
1	A	15	LEU
1	A	18	LEU
1	A	25	ARG
1	A	47	VAL
1	A	71	ARG
1	A	85	VAL
1	A	99	VAL
1	A	122	VAL
1	A	136	ASN
1	A	148	VAL
1	A	152	GLU
1	A	174	VAL
1	A	176	LEU
1	A	196	ASP
1	A	197	CYS
1	A	203	ASP
1	A	204	TRP
1	A	205	GLN
1	A	209	ASN
1	A	212	VAL
1	A	214	VAL
1	A	216	LEU
1	A	230	THR
1	A	234	LEU
1	A	243	GLN
1	A	258	SER
1	A	272	ARG
1	A	347	VAL
1	A	351	GLU
1	A	355	VAL
1	A	374	LEU

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Mol	Chain	Res	Type
1	A	378	GLU
1	A	383	GLU
1	A	400	LYS
1	A	423	GLU
1	A	432	THR
1	A	446	VAL
1	A	456	ILE
1	A	462	VAL
1	A	467	ARG
1	A	472	TYR
1	A	474	GLN
1	A	483	LYS
1	A	507	VAL
1	A	518	THR
1	A	521	TRP
1	A	530	LEU
1	A	536	VAL
1	A	557	SER
1	A	558	GLN
1	A	562	ARG
1	A	598	GLN
1	A	599	GLN
1	B	7	THR
1	B	11	GLU
1	B	13	LYS
1	B	14	LYS
1	B	15	LEU
1	B	18	LEU
1	B	25	ARG
1	B	47	VAL
1	B	71	ARG
1	B	77	LYS
1	B	82	GLN
1	B	85	VAL
1	B	96	LYS
1	B	99	VAL
1	B	103	GLU
1	B	121	TYR
1	B	136	ASN
1	B	148	VAL
1	B	152	GLU
1	B	156	LYS

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Mol	Chain	Res	Type
1	B	163	ASP
1	B	175	MET
1	B	183	TRP
1	B	185	ASP
1	B	186	ASP
1	B	193	VAL
1	B	195	GLN
1	B	203	ASP
1	B	205	GLN
1	B	206	VAL
1	B	207	VAL
1	B	212	VAL
1	B	234	LEU
1	B	235	GLN
1	B	263	ASP
1	B	267	LEU
1	B	272	ARG
1	B	286	LYS
1	B	298	ASP
1	B	302	ARG
1	B	310	LEU
1	B	329	SER
1	B	347	VAL
1	B	355	VAL
1	B	361	LEU
1	B	372	LYS
1	B	374	LEU
1	B	398	ARG
1	B	400	LYS
1	B	410	ILE
1	B	419	GLN
1	B	438	THR
1	B	462	VAL
1	B	474	GLN
1	B	503	THR
1	B	518	THR
1	B	521	TRP
1	B	531	ASP
1	B	532	MET
1	B	558	GLN
1	B	560	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	66	ASN
1	A	107	HIS
1	A	108	GLN
1	A	135	ASN
1	A	136	ASN
1	A	199	HIS
1	A	209	ASN
1	A	228	GLN
1	A	243	GLN
1	A	313	HIS
1	A	315	HIS
1	A	330	HIS
1	A	385	GLN
1	A	390	GLN
1	A	402	HIS
1	A	412	ASN
1	A	419	GLN
1	A	493	GLN
1	A	514	HIS
1	A	547	GLN
1	A	550	ASN
1	A	592	ASN
1	B	0	HIS
1	B	52	ASN
1	B	82	GLN
1	B	108	GLN
1	B	135	ASN
1	B	136	ASN
1	B	162	HIS
1	B	221	GLN
1	B	222	GLN
1	B	238	ASN
1	B	243	GLN
1	B	280	GLN
1	B	315	HIS
1	B	330	HIS
1	B	388	HIS
1	B	390	GLN
1	B	412	ASN
1	B	419	GLN
1	B	493	GLN

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Mol	Chain	Res	Type
1	B	498	GLN
1	B	514	HIS
1	B	526	GLN
1	B	547	GLN
1	B	566	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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	597/605 (98%)	0.34	41 (6%)	20 22	18, 52, 114, 147	0
1	B	596/605 (98%)	0.81	94 (15%)	3 2	27, 93, 178, 229	0
All	All	1193/1210 (98%)	0.57	135 (11%)	7 7	18, 74, 153, 229	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	16.0
1	A	230	THR	10.0
1	B	229	GLY	9.7
1	B	207	VAL	9.4
1	B	208	ALA	9.3
1	A	229	GLY	8.5
1	B	204	TRP	6.3
1	B	282	LEU	6.1
1	A	560	ILE	5.9
1	B	283	ILE	5.8
1	B	230	THR	5.8
1	A	209	ASN	5.6
1	B	259	GLN	5.6
1	B	288	PHE	5.4
1	B	205	GLN	5.3
1	B	545	GLY	5.2
1	A	256	ALA	5.1
1	A	561	LEU	5.0
1	A	183	TRP	4.9
1	B	287	PRO	4.9
1	B	256	ALA	4.7
1	B	17	GLY	4.5
1	B	598	GLN	4.5
1	B	560	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	561	LEU	4.4
1	B	1	MET	4.3
1	B	289	TYR	4.3
1	B	563	VAL	4.3
1	B	209	ASN	4.3
1	B	84	ILE	4.3
1	B	253	CYS	4.2
1	A	259	GLN	4.2
1	B	196	ASP	4.2
1	B	182	THR	4.1
1	B	562	ARG	3.9
1	A	257	LYS	3.9
1	B	152	GLU	3.9
1	B	175	MET	3.9
1	B	565	GLY	3.8
1	B	206	VAL	3.7
1	B	258	SER	3.7
1	B	337	MET	3.7
1	A	37	SER	3.7
1	B	544	VAL	3.6
1	B	262	CYS	3.6
1	B	430	GLU	3.5
1	B	260	THR	3.5
1	A	239	PRO	3.5
1	B	311	MET	3.4
1	B	290	PHE	3.4
1	B	214	VAL	3.4
1	B	261	GLU	3.4
1	B	18	LEU	3.4
1	B	242	TRP	3.4
1	B	419	GLN	3.4
1	B	105	MET	3.4
1	A	562	ARG	3.4
1	A	318	MET	3.3
1	A	182	THR	3.3
1	B	257	LYS	3.3
1	A	208	ALA	3.3
1	B	240	HIS	3.2
1	A	198	ASN	3.2
1	B	153	ASN	3.2
1	A	563	VAL	3.2
1	A	337	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	116	ALA	3.1
1	A	311	MET	3.0
1	B	252	LEU	3.0
1	B	236	VAL	3.0
1	B	600	GLY	3.0
1	A	516	MET	3.0
1	A	260	THR	3.0
1	B	361	LEU	3.0
1	B	255	THR	3.0
1	A	565	GLY	3.0
1	A	197	CYS	2.9
1	B	212	VAL	2.9
1	B	537	PHE	2.9
1	B	67	VAL	2.9
1	B	375	TYR	2.8
1	B	564	GLY	2.8
1	B	211	ASP	2.8
1	B	425	PHE	2.7
1	A	1	MET	2.7
1	B	213	SER	2.7
1	B	468	TYR	2.7
1	A	131	THR	2.7
1	B	379	ALA	2.7
1	B	540	VAL	2.7
1	B	447	MET	2.6
1	B	248	TYR	2.6
1	B	597	PRO	2.6
1	B	303	GLY	2.6
1	A	175	MET	2.6
1	A	211	ASP	2.6
1	B	489	LEU	2.6
1	A	184	VAL	2.5
1	B	542	ALA	2.5
1	B	357	PHE	2.5
1	B	423	GLU	2.5
1	B	15	LEU	2.5
1	B	463	LEU	2.5
1	A	214	VAL	2.5
1	B	228	GLN	2.5
1	B	264	ILE	2.5
1	A	98	TRP	2.4
1	A	258	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	378	GLU	2.4
1	A	34	TRP	2.4
1	B	594	GLY	2.4
1	A	218	ASP	2.4
1	A	483	LYS	2.4
1	B	254	VAL	2.3
1	B	123	ILE	2.3
1	B	241	LEU	2.3
1	B	318	MET	2.2
1	B	500	ILE	2.2
1	A	40	GLN	2.2
1	B	424	TYR	2.2
1	B	231	SER	2.2
1	B	362	GLY	2.2
1	A	199	HIS	2.1
1	B	280	GLN	2.1
1	B	37	SER	2.1
1	B	79	TRP	2.1
1	A	231	SER	2.1
1	B	372	LYS	2.1
1	A	101	ASN	2.1
1	B	266	PRO	2.1
1	A	455	THR	2.0
1	A	68	TRP	2.0
1	B	183	TRP	2.0
1	B	277	LYS	2.0
1	B	233	THR	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](#)

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.