



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 AM GMT

PDB ID : 3K4D  
Title : Crystal structure of E. coli beta-glucuronidase with the glucaro-d-lactam inhibitor bound  
Authors : Wallace, B.D.; Redinbo, M.R.  
Deposited on : 2009-10-05  
Resolution : 2.39 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

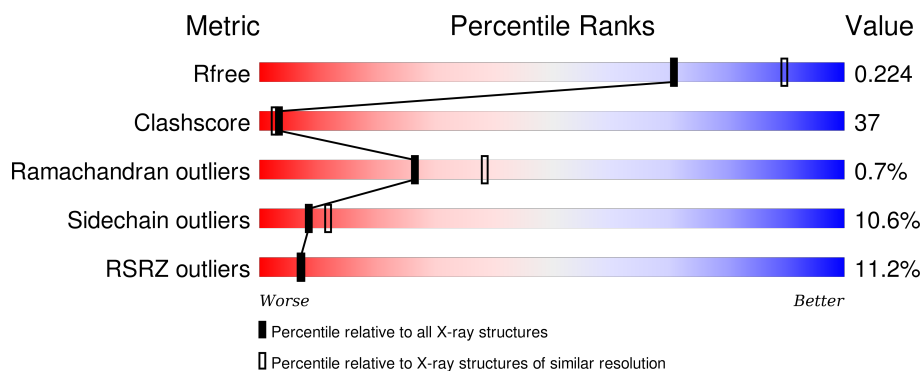
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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>59%</div> <div>31%</div> <div>6%</div> <div>..</div> </div>
1	B	605	<div> <div>15%</div> <div>46%</div> <div>43%</div> <div>8%</div> <div>..</div> </div>

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9933 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.

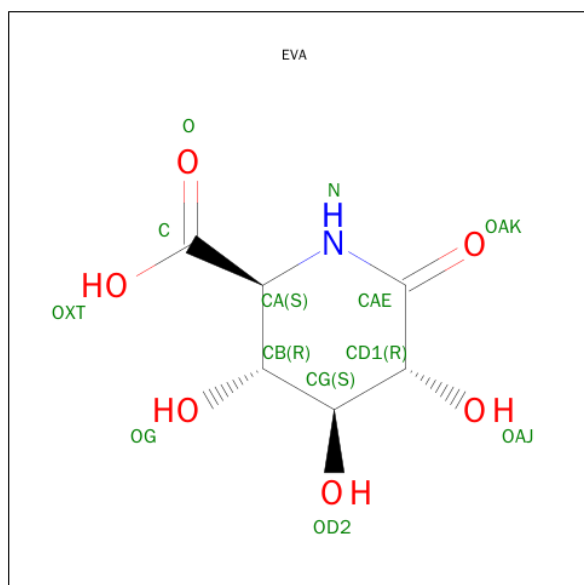
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total 4776	C 3032	N 825	O 897	S 22	0	0	0
1	B	596	Total 4776	C 3032	N 825	O 897	S 22	0	0	0

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 (2S,3R,4S,5R)-3,4,5-TRIHYDROXY-6-OXOPIPERIDINE-2-CARBOXYLIC ACID (three-letter code: EVA) (formula: C<sub>6</sub>H<sub>9</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 13	C 6	N 1	O 6	0	0
2	B	1	Total 13	C 6	N 1	O 6	0	0

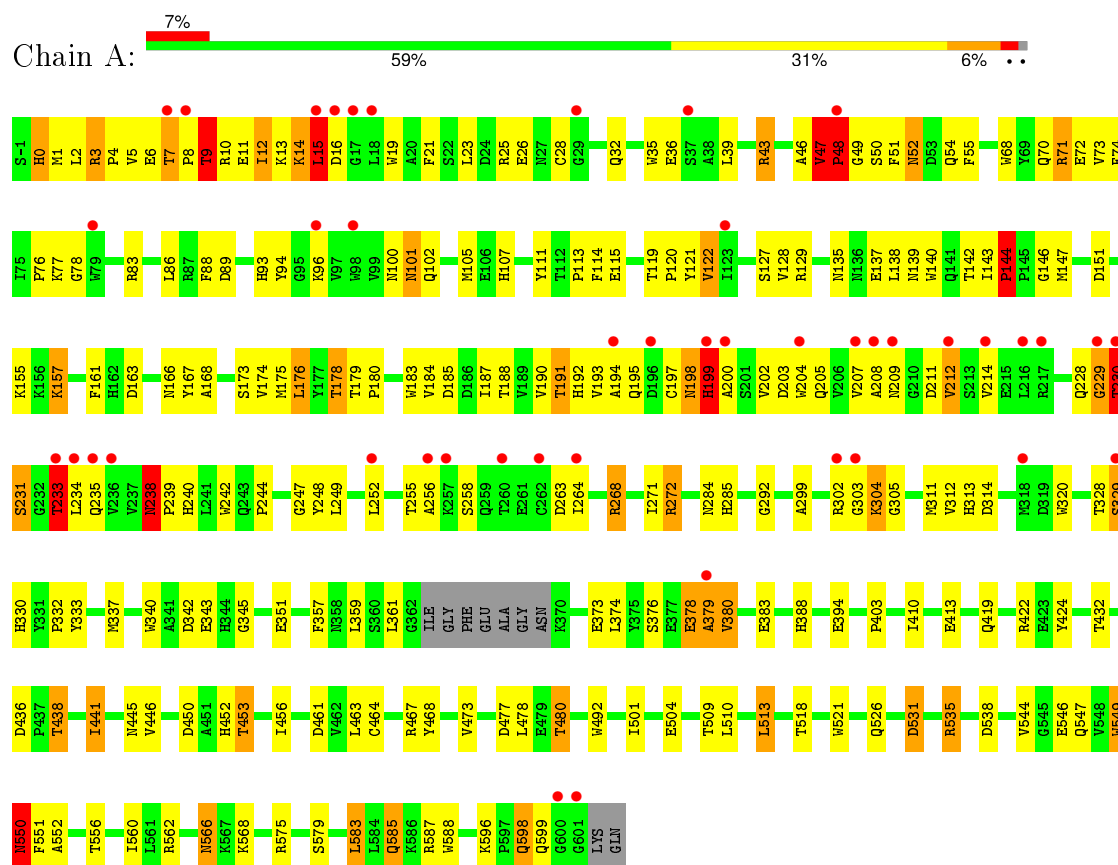
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total 244	O 244	0	0
3	B	111	Total 111	O 111	0	0

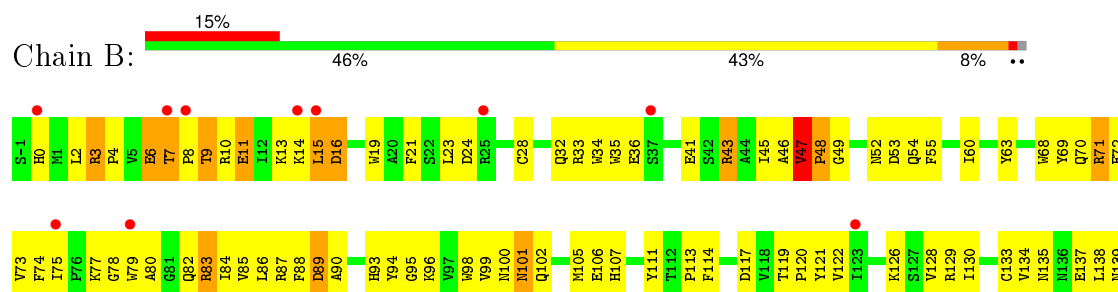
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	167.65Å 76.97Å 125.47Å 90.00° 124.98° 90.00°	Depositor
Resolution (Å)	29.57 – 2.39 47.79 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.57-2.39) 98.2 (47.79-2.39)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.33 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.205 , 0.237 0.206 , 0.224	Depositor DCC
$R_{free}$ test set	2603 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 51009 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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

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

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	0.65	3/4904 (0.1%)	0.91	26/6673 (0.4%)
1	B	0.49	0/4904	0.85	22/6673 (0.3%)
All	All	0.57	3/9808 (0.0%)	0.88	48/13346 (0.4%)

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	7
1	B	0	6
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	TYR	CD2-CE2	-6.67	1.29	1.39
1	A	468	TYR	CD1-CE1	-5.42	1.31	1.39
1	A	468	TYR	CE1-CZ	-5.22	1.31	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	SER	N-CA-CB	-14.31	89.04	110.50
1	B	80	ALA	CB-CA-C	-11.67	92.59	110.10
1	B	599	GLN	N-CA-CB	-10.65	91.43	110.60
1	B	358	ASN	N-CA-CB	-10.25	92.15	110.60
1	A	229	GLY	N-CA-C	-9.35	89.72	113.10
1	A	379	ALA	N-CA-C	8.89	135.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	VAL	N-CA-C	-8.57	87.87	111.00
1	A	14	LYS	CB-CA-C	-8.38	93.64	110.40
1	A	231	SER	CB-CA-C	8.00	125.31	110.10
1	A	233	THR	N-CA-CB	7.52	124.58	110.30
1	A	562	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	456	ILE	CB-CA-C	-7.08	97.44	111.60
1	A	379	ALA	CB-CA-C	-7.04	99.54	110.10
1	A	230	THR	CB-CA-C	6.96	130.38	111.60
1	A	329	SER	CB-CA-C	6.92	123.25	110.10
1	B	214	VAL	N-CA-C	6.82	129.42	111.00
1	A	329	SER	N-CA-C	-6.75	92.79	111.00
1	A	583	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	233	THR	CB-CA-C	-6.55	93.91	111.60
1	A	15	LEU	N-CA-C	-6.51	93.43	111.00
1	B	16	ASP	N-CA-C	-6.44	93.62	111.00
1	B	302	ARG	N-CA-C	-6.37	93.80	111.00
1	B	583	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	380	VAL	N-CA-CB	6.27	125.30	111.50
1	B	598	GLN	N-CA-C	-6.23	94.18	111.00
1	A	562	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	357	PHE	CB-CA-C	5.79	121.99	110.40
1	B	550	ASN	N-CA-C	5.79	126.64	111.00
1	A	228	GLN	N-CA-C	-5.79	95.38	111.00
1	A	199	HIS	N-CA-C	5.78	126.60	111.00
1	B	522	SER	N-CA-CB	5.76	119.14	110.50
1	A	48	PRO	N-CA-C	-5.71	97.27	112.10
1	B	177	TYR	CA-CB-CG	5.68	124.19	113.40
1	B	80	ALA	N-CA-C	5.61	126.14	111.00
1	A	378	GLU	CB-CA-C	5.60	121.59	110.40
1	B	6	GLU	CB-CA-C	-5.59	99.22	110.40
1	B	215	GLU	N-CA-C	5.51	125.89	111.00
1	B	599	GLN	N-CA-C	-5.51	96.12	111.00
1	A	550	ASN	N-CA-CB	5.44	120.40	110.60
1	B	200	ALA	N-CA-CB	-5.42	102.52	110.10
1	B	329	SER	CB-CA-C	5.39	120.34	110.10
1	B	457	SER	N-CA-CB	5.38	118.57	110.50
1	B	163	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	9	THR	N-CA-CB	-5.27	100.28	110.30
1	B	6	GLU	N-CA-C	5.26	125.21	111.00
1	A	144	PRO	N-CA-C	-5.25	98.46	112.10
1	A	329	SER	N-CA-CB	5.12	118.18	110.50
1	A	208	ALA	CB-CA-C	5.12	117.78	110.10

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ILE	Mainchain,Peptide
1	A	198	ASN	Peptide
1	A	238	ASN	Peptide
1	A	47	VAL	Peptide
1	A	549	TRP	Mainchain,Peptide
1	B	176	LEU	Peptide
1	B	238	ASN	Peptide
1	B	47	VAL	Mainchain,Peptide
1	B	549	TRP	Peptide
1	B	564	GLY	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	4776	0	4557	309	0
1	B	4776	0	4558	408	0
2	A	13	0	8	2	0
2	B	13	0	8	3	0
3	A	244	0	0	15	0
3	B	111	0	0	19	0
All	All	9933	0	9131	696	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 37.

All (696) 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:7:THR:CG2	1:A:8:PRO:HD3	1.44	1.47
1:B:7:THR:HB	1:B:8:PRO:CD	1.29	1.43
1:A:183:TRP:CZ3	1:A:185:ASP:HB3	1.63	1.34
1:B:7:THR:CB	1:B:8:PRO:CD	2.00	1.23
1:B:456:ILE:O	1:B:456:ILE:CG2	1.86	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:THR:CB	1:B:8:PRO:HD3	1.68	1.18
1:B:357:PHE:O	1:B:374:LEU:HD11	1.44	1.17
1:A:3:ARG:HH11	1:A:3:ARG:HG2	1.01	1.14
1:A:7:THR:HB	1:A:8:PRO:CD	1.78	1.14
1:B:212:VAL:HB	1:B:255:THR:O	1.48	1.14
1:A:598:GLN:HG2	1:A:598:GLN:O	1.43	1.13
1:B:436:ASP:OD1	1:B:438:THR:HG22	1.50	1.11
1:A:205:GLN:HE21	1:A:207:VAL:HG23	1.11	1.11
1:A:183:TRP:CZ3	1:A:185:ASP:CB	2.31	1.11
1:B:509:THR:HG21	1:B:526:GLN:HB2	1.35	1.09
1:A:184:VAL:HG13	1:A:205:GLN:HE22	1.16	1.08
1:B:214:VAL:O	1:B:214:VAL:CG1	2.00	1.08
1:A:15:LEU:HD12	1:A:173:SER:HA	1.17	1.08
1:A:212:VAL:HG13	1:A:230:THR:HG23	1.34	1.07
1:A:205:GLN:HE21	1:A:207:VAL:CG2	1.68	1.07
1:B:100:ASN:HA	1:B:129:ARG:NH2	1.69	1.07
1:A:7:THR:CB	1:A:8:PRO:CD	2.30	1.06
1:A:183:TRP:CE3	1:A:185:ASP:HB3	1.90	1.05
1:A:7:THR:CG2	1:A:8:PRO:CD	2.33	1.05
1:B:212:VAL:HG13	1:B:230:THR:OG1	1.55	1.05
1:A:7:THR:HG22	1:A:8:PRO:CD	1.85	1.04
1:A:7:THR:HB	1:A:8:PRO:HD2	1.33	1.04
1:B:193:VAL:O	1:B:285:HIS:NE2	1.90	1.03
1:B:240:HIS:CE1	1:B:248:TYR:CG	2.45	1.03
1:B:564:GLY:HA3	1:B:567:LYS:NZ	1.74	1.02
1:B:456:ILE:HG23	1:B:456:ILE:O	1.23	1.01
1:B:183:TRP:CZ3	1:B:185:ASP:HB3	1.97	1.00
1:B:7:THR:CB	1:B:8:PRO:HD2	1.89	1.00
1:A:77:LYS:NZ	1:B:8:PRO:O	1.95	0.99
1:B:598:GLN:C	1:B:600:GLY:H	1.61	0.99
1:A:203:ASP:OD1	1:A:233:THR:O	1.78	0.99
1:A:7:THR:HG22	1:A:8:PRO:HD3	1.01	0.99
1:B:8:PRO:HB2	3:B:675:HOH:O	1.62	0.99
1:A:203:ASP:OD1	1:A:233:THR:OG1	1.79	0.98
1:B:68:TRP:HZ3	1:B:98:TRP:CZ3	1.80	0.98
1:A:212:VAL:N	1:A:230:THR:OG1	1.95	0.97
1:B:6:GLU:HG2	1:B:11:GLU:OE2	1.63	0.96
1:B:240:HIS:HE1	1:B:248:TYR:CG	1.82	0.96
1:B:9:THR:HG22	1:B:178:THR:O	1.66	0.95
1:B:179:THR:CG2	1:B:183:TRP:CD1	2.50	0.94
1:A:212:VAL:H	1:A:230:THR:CG2	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HG2	1:B:35:TRP:CZ2	2.01	0.94
1:B:214:VAL:O	1:B:214:VAL:HG13	1.67	0.94
1:A:272:ARG:HA	1:A:284:ASN:HD21	1.33	0.94
1:B:7:THR:OG1	1:B:8:PRO:HD2	1.68	0.93
1:A:357:PHE:O	1:A:374:LEU:HD21	1.69	0.93
1:B:218:ASP:OD1	1:B:248:TYR:OH	1.86	0.93
1:A:119:THR:HB	1:A:120:PRO:HD3	1.50	0.93
1:B:85:VAL:O	1:B:177:TYR:HB3	1.69	0.92
1:B:513:LEU:HD13	1:B:521:TRP:O	1.67	0.92
1:A:7:THR:CB	1:A:8:PRO:HD3	1.94	0.92
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.34	0.91
1:A:3:ARG:HH11	1:A:3:ARG:CG	1.82	0.91
1:B:196:ASP:O	1:B:239:PRO:HG3	1.68	0.91
1:A:477:ASP:OD1	1:A:480:THR:HG23	1.71	0.90
1:A:14:LYS:HZ3	1:A:86:LEU:HD13	1.37	0.90
1:B:218:ASP:HB3	1:B:222:GLN:HG3	1.53	0.90
1:B:598:GLN:HB3	1:B:600:GLY:O	1.71	0.90
1:A:292:GLY:O	1:A:547:GLN:HA	1.71	0.89
1:A:191:THR:HG21	1:A:272:ARG:H	1.37	0.89
1:A:139:ASN:O	1:A:142:THR:HG22	1.71	0.89
1:A:183:TRP:HZ3	1:A:185:ASP:CB	1.76	0.89
1:B:179:THR:HG21	1:B:183:TRP:CD1	2.10	0.87
1:A:513:LEU:HD12	1:A:521:TRP:O	1.74	0.87
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.40	0.87
1:A:192:HIS:O	1:A:199:HIS:HB3	1.73	0.87
1:A:46:ALA:H	1:A:54:GLN:HE22	1.20	0.86
1:A:14:LYS:HD2	1:A:176:LEU:HD22	1.56	0.86
1:A:43:ARG:HD2	1:A:55:PHE:CE1	2.11	0.86
1:A:140:TRP:CE3	1:A:379:ALA:O	2.29	0.86
1:B:212:VAL:HG13	1:B:230:THR:CB	2.07	0.85
1:A:598:GLN:CG	1:A:598:GLN:O	2.25	0.85
1:B:240:HIS:CE1	1:B:248:TYR:CD1	2.65	0.85
1:B:357:PHE:O	1:B:374:LEU:CD1	2.24	0.84
1:B:46:ALA:H	1:B:54:GLN:HE22	1.23	0.84
1:A:15:LEU:CD1	1:A:173:SER:HA	2.04	0.84
1:A:3:ARG:NH1	1:A:3:ARG:HG2	1.82	0.84
1:A:198:ASN:O	1:A:199:HIS:HB2	1.76	0.84
1:B:240:HIS:O	1:B:240:HIS:ND1	2.09	0.84
1:B:200:ALA:HA	1:B:235:GLN:O	1.78	0.83
1:B:122:VAL:HG23	1:B:128:VAL:HG11	1.59	0.83
1:A:599:GLN:O	1:A:599:GLN:HG2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:CD1	1:B:521:TRP:O	2.26	0.83
1:A:15:LEU:HD13	1:A:173:SER:OG	1.78	0.82
1:A:14:LYS:NZ	1:A:86:LEU:HD13	1.92	0.82
1:A:105:MET:SD	3:A:844:HOH:O	2.36	0.82
1:A:52:ASN:HD21	1:A:168:ALA:H	1.26	0.82
1:A:36:GLU:HA	1:A:101:ASN:ND2	1.95	0.82
1:B:214:VAL:O	1:B:214:VAL:HG12	1.78	0.81
1:B:199:HIS:ND1	1:B:200:ALA:N	2.28	0.81
1:A:247:GLY:O	1:A:249:LEU:HD12	1.80	0.81
1:B:192:HIS:O	1:B:199:HIS:HB3	1.81	0.81
1:B:68:TRP:CZ3	1:B:98:TRP:CZ3	2.69	0.81
1:A:15:LEU:HD12	1:A:173:SER:CA	2.07	0.80
1:B:598:GLN:C	1:B:600:GLY:N	2.32	0.80
1:B:198:ASN:HB2	1:B:237:VAL:C	2.02	0.80
1:B:7:THR:HB	1:B:8:PRO:HD2	1.48	0.80
1:B:422:ARG:NH2	1:B:458:ASP:OD2	2.15	0.80
1:A:513:LEU:CD1	1:A:521:TRP:O	2.29	0.80
1:A:212:VAL:H	1:A:230:THR:CB	1.95	0.79
1:B:295:ARG:O	1:B:329:SER:HB2	1.84	0.78
1:B:179:THR:HG21	1:B:183:TRP:CG	2.18	0.78
1:A:212:VAL:CG1	1:A:230:THR:HG23	2.14	0.78
1:B:550:ASN:HD22	1:B:552:ALA:H	1.29	0.78
1:B:0:HIS:CD2	1:B:186:ASP:OD2	2.37	0.78
1:B:432:THR:HB	1:B:441:ILE:HD11	1.64	0.78
1:A:214:VAL:HG13	1:A:252:LEU:HD11	1.64	0.78
1:A:163:ASP:O	1:A:556:THR:HG22	1.83	0.78
1:A:579:SER:HB3	3:A:766:HOH:O	1.82	0.78
1:A:598:GLN:O	1:A:599:GLN:HB3	1.84	0.78
1:B:212:VAL:CG1	1:B:230:THR:OG1	2.32	0.77
1:B:179:THR:HG22	1:B:183:TRP:CD1	2.20	0.77
1:A:202:VAL:HG12	1:A:234:LEU:HD21	1.64	0.77
1:A:9:THR:HG22	1:A:178:THR:O	1.84	0.77
1:B:75:ILE:HG13	1:B:122:VAL:HG22	1.65	0.77
1:A:142:THR:HG23	1:A:144:PRO:O	1.84	0.77
1:B:335:GLU:H	1:B:335:GLU:CD	1.84	0.77
1:A:93:HIS:HE1	1:A:166:ASN:OD1	1.67	0.77
1:A:191:THR:HG21	1:A:272:ARG:N	1.99	0.77
1:B:564:GLY:HA3	1:B:567:LYS:HZ1	1.48	0.76
1:A:205:GLN:NE2	1:A:207:VAL:HG23	1.96	0.76
1:A:212:VAL:HG13	1:A:230:THR:CG2	2.13	0.76
1:B:172:ARG:NH2	1:B:333:TYR:C	2.39	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PRO:O	3:A:800:HOH:O	2.04	0.76
1:B:68:TRP:CZ3	1:B:98:TRP:CH2	2.74	0.75
1:B:15:LEU:C	1:B:15:LEU:HD23	2.06	0.75
1:A:184:VAL:HG13	1:A:205:GLN:NE2	1.99	0.75
1:A:3:ARG:HD2	1:A:4:PRO:HD2	1.68	0.75
1:A:212:VAL:H	1:A:230:THR:HG21	1.51	0.75
1:A:14:LYS:NZ	1:A:86:LEU:CD1	2.49	0.75
1:B:183:TRP:CZ3	1:B:185:ASP:CB	2.70	0.75
1:B:551:PHE:HE2	1:B:575:ARG:HH11	1.32	0.74
1:B:292:GLY:O	1:B:547:GLN:HA	1.88	0.74
1:A:477:ASP:OD1	1:A:480:THR:CG2	2.36	0.74
1:A:14:LYS:HZ3	1:A:86:LEU:CD1	2.00	0.73
1:B:469:TYR:O	1:B:529:TRP:CZ3	2.41	0.73
1:B:204:TRP:CD1	1:B:231:SER:O	2.41	0.73
1:B:420:GLY:O	1:B:423:GLU:HG3	1.87	0.73
1:A:205:GLN:HG2	1:A:212:VAL:HG21	1.71	0.73
1:B:328:THR:O	1:B:351:GLU:HB3	1.89	0.73
1:B:172:ARG:HH21	1:B:333:TYR:C	1.92	0.72
1:B:71:ARG:HH11	1:B:71:ARG:CG	2.02	0.72
1:B:7:THR:HB	1:B:8:PRO:HD3	0.73	0.72
1:B:467:ARG:HG2	1:B:469:TYR:CE1	2.24	0.72
1:A:311:MET:HE3	1:A:337:MET:HA	1.69	0.72
1:B:205:GLN:HG2	1:B:206:VAL:N	2.03	0.72
1:B:432:THR:CG2	1:B:441:ILE:HD11	2.18	0.72
1:B:432:THR:HB	1:B:441:ILE:CD1	2.19	0.72
1:B:220:ASP:HB2	1:B:222:GLN:HG2	1.70	0.72
1:B:105:MET:HE2	1:B:114:PHE:HD1	1.55	0.72
1:B:179:THR:HG22	1:B:183:TRP:HD1	1.55	0.72
1:B:539:ARG:HA	1:B:599:GLN:HG3	1.70	0.71
1:B:272:ARG:HA	1:B:284:ASN:HD21	1.55	0.71
1:A:8:PRO:HA	1:B:77:LYS:HZ3	1.56	0.71
1:A:107:HIS:HE1	1:A:394:GLU:OE1	1.74	0.71
1:B:432:THR:CB	1:B:441:ILE:HD11	2.21	0.71
1:B:247:GLY:O	1:B:249:LEU:HD12	1.91	0.71
1:B:212:VAL:CB	1:B:255:THR:O	2.34	0.71
1:B:425:PHE:HB2	1:B:456:ILE:HD11	1.71	0.70
1:B:101:ASN:N	1:B:101:ASN:HD22	1.88	0.70
1:B:7:THR:OG1	1:B:8:PRO:CD	2.32	0.70
1:A:14:LYS:HA	1:A:71:ARG:HH21	1.57	0.70
1:B:598:GLN:O	1:B:600:GLY:N	2.25	0.69
1:B:463:LEU:HD21	1:B:492:TRP:CE3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLY:HA2	1:B:305:GLY:HA3	1.74	0.69
1:B:300:ASP:O	3:B:634:HOH:O	2.09	0.69
1:A:183:TRP:HZ3	1:A:185:ASP:HB2	1.54	0.69
1:A:13:LYS:HG2	1:A:15:LEU:HB3	1.73	0.69
1:A:211:ASP:HA	1:A:230:THR:HG21	1.73	0.69
1:A:538:ASP:HB3	1:A:599:GLN:HA	1.74	0.69
1:A:202:VAL:HG12	1:A:234:LEU:CD2	2.21	0.69
1:A:26:GLU:HB2	1:A:28:CYS:SG	2.32	0.69
1:B:203:ASP:OD1	1:B:233:THR:OG1	2.07	0.69
1:B:163:ASP:O	3:B:652:HOH:O	2.10	0.69
1:B:6:GLU:CG	1:B:11:GLU:OE2	2.39	0.69
1:A:328:THR:O	1:A:351:GLU:HB3	1.93	0.69
1:A:139:ASN:H	1:A:142:THR:CG2	2.06	0.69
1:B:196:ASP:HB3	1:B:241:LEU:HD11	1.73	0.68
1:A:436:ASP:OD1	1:A:438:THR:CG2	2.41	0.68
1:A:212:VAL:HA	1:A:255:THR:O	1.92	0.68
1:A:15:LEU:HG	1:A:48:PRO:HD3	1.75	0.68
1:A:36:GLU:C	1:A:129:ARG:HH21	1.97	0.68
1:B:15:LEU:HG	1:B:48:PRO:HD3	1.75	0.68
1:B:19:TRP:CD1	1:B:47:VAL:HG13	2.29	0.68
1:A:200:ALA:HA	1:A:235:GLN:O	1.93	0.68
1:A:311:MET:CE	1:A:340:TRP:HB2	2.24	0.68
1:A:378:GLU:O	3:A:619:HOH:O	2.12	0.68
1:B:205:GLN:HE22	1:B:212:VAL:HG21	1.59	0.67
1:B:179:THR:HG23	1:B:183:TRP:HB3	1.75	0.67
1:B:447:MET:HG2	1:B:467:ARG:HG3	1.76	0.67
1:A:450:ASP:OD2	1:A:453:THR:HG23	1.94	0.67
1:B:89:ASP:OD1	1:B:173:SER:O	2.13	0.67
1:B:445:ASN:ND2	1:B:467:ARG:HH22	1.92	0.67
1:A:205:GLN:NE2	1:A:207:VAL:CG2	2.51	0.66
1:A:138:LEU:HA	1:A:142:THR:HG21	1.76	0.66
1:B:242:TRP:CD1	1:B:270:GLY:HA3	2.31	0.66
1:A:477:ASP:CG	1:A:480:THR:HG23	2.15	0.66
1:B:0:HIS:HD2	1:B:186:ASP:OD2	1.77	0.66
1:A:240:HIS:HB2	1:A:248:TYR:CD2	2.31	0.66
1:B:90:ALA:HB3	1:B:172:ARG:HD3	1.77	0.66
1:B:0:HIS:HB3	1:B:186:ASP:OD2	1.95	0.66
1:B:96:LYS:HD3	1:B:98:TRP:CZ2	2.31	0.66
1:B:138:LEU:HD22	1:B:142:THR:HG21	1.76	0.65
1:B:355:VAL:HG23	1:B:412:ASN:HD22	1.60	0.65
1:A:8:PRO:HA	1:B:77:LYS:NZ	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:HIS:O	1:B:392:ILE:HG13	1.96	0.65
1:B:126:LYS:HA	3:B:704:HOH:O	1.96	0.65
1:B:564:GLY:HA3	1:B:567:LYS:HZ3	1.57	0.65
1:B:101:ASN:ND2	1:B:129:ARG:HH22	1.95	0.65
1:A:450:ASP:OD2	1:A:453:THR:CG2	2.45	0.65
1:B:392:ILE:HG21	1:B:410:ILE:HD11	1.79	0.65
1:B:75:ILE:HG13	1:B:122:VAL:CG2	2.27	0.65
1:B:179:THR:CG2	1:B:183:TRP:CG	2.79	0.64
1:B:204:TRP:HD1	1:B:231:SER:O	1.79	0.64
1:B:240:HIS:CE1	1:B:248:TYR:CD2	2.84	0.64
1:A:244:PRO:O	1:A:345:GLY:O	2.15	0.64
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.80	0.63
1:A:35:TRP:HD1	1:A:101:ASN:HA	1.62	0.63
1:B:509:THR:HG21	1:B:526:GLN:CB	2.22	0.63
1:A:550:ASN:HD22	1:A:552:ALA:H	1.44	0.63
1:B:187:ILE:HG22	1:B:188:THR:N	2.14	0.63
1:A:83:ARG:CB	1:A:179:THR:HG22	2.29	0.63
1:B:283:ILE:HG12	1:B:288:PHE:HB2	1.81	0.63
1:B:71:ARG:NH1	1:B:72:GLU:O	2.32	0.62
1:B:14:LYS:HD3	1:B:73:VAL:HG11	1.81	0.62
1:B:311:MET:CE	1:B:340:TRP:HB2	2.28	0.62
1:B:68:TRP:HZ3	1:B:98:TRP:CH2	2.09	0.62
1:A:357:PHE:O	1:A:374:LEU:HD11	1.99	0.62
1:B:240:HIS:HE1	1:B:248:TYR:CB	2.11	0.62
1:B:15:LEU:HD23	1:B:15:LEU:O	2.00	0.62
1:A:139:ASN:H	1:A:142:THR:HG22	1.63	0.62
1:B:111:TYR:HB2	1:B:332:PRO:HD2	1.81	0.62
1:B:52:ASN:HD21	1:B:168:ALA:H	1.47	0.62
1:B:14:LYS:NZ	1:B:130:ILE:HG13	2.15	0.62
1:B:172:ARG:HD2	3:B:627:HOH:O	2.00	0.62
1:A:357:PHE:O	1:A:374:LEU:CD2	2.47	0.61
1:A:36:GLU:C	1:A:129:ARG:NH2	2.54	0.61
1:B:243:GLN:NE2	1:B:284:ASN:OD1	2.33	0.61
1:B:189:VAL:H	1:B:401:ASN:HD21	1.48	0.61
1:B:311:MET:HE3	1:B:337:MET:HA	1.81	0.61
1:B:551:PHE:HE2	1:B:575:ARG:NH1	1.98	0.61
1:B:102:GLN:HG2	1:B:121:TYR:CD1	2.35	0.61
1:B:15:LEU:HD12	1:B:173:SER:CB	2.30	0.61
1:A:111:TYR:HB2	1:A:332:PRO:HD2	1.82	0.61
1:B:101:ASN:ND2	1:B:129:ARG:NH2	2.49	0.61
1:B:93:HIS:HE1	1:B:166:ASN:OD1	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:NE	1:B:117:ASP:HB2	2.15	0.61
1:A:135:ASN:HD21	1:A:137:GLU:HB2	1.65	0.61
1:A:207:VAL:CG1	1:A:256:ALA:HB1	2.31	0.60
1:A:26:GLU:OE1	1:A:26:GLU:HA	2.01	0.60
1:B:405:VAL:HG11	1:B:408:TRP:CZ3	2.37	0.60
1:B:529:TRP:CD1	1:B:529:TRP:C	2.74	0.60
1:A:452:HIS:HE1	3:A:743:HOH:O	1.83	0.60
1:A:43:ARG:NH1	3:A:781:HOH:O	2.34	0.60
1:A:52:ASN:H	1:A:52:ASN:HD22	1.48	0.60
1:A:155:LYS:HD3	3:A:835:HOH:O	2.01	0.60
1:A:138:LEU:CA	1:A:142:THR:HG21	2.32	0.60
1:B:163:ASP:HB3	3:B:665:HOH:O	2.00	0.60
1:B:295:ARG:O	1:B:333:TYR:OH	2.19	0.59
1:B:33:ARG:CG	1:B:35:TRP:CZ2	2.82	0.59
1:B:138:LEU:HD22	1:B:142:THR:CG2	2.30	0.59
1:A:105:MET:HE1	1:A:115:GLU:N	2.18	0.59
1:B:568:LYS:NZ	2:B:604:EVA:OXT	2.34	0.59
1:A:122:VAL:HG23	1:A:128:VAL:HG11	1.84	0.59
1:B:151:ASP:OD1	1:B:155:LYS:N	2.35	0.59
1:B:24:ASP:O	1:B:63:TYR:OH	2.21	0.59
1:A:441:ILE:HG22	1:A:461:ASP:OD2	2.03	0.58
1:A:15:LEU:CD1	1:A:173:SER:OG	2.51	0.58
1:A:413:GLU:OE2	2:A:604:EVA:OAK	2.21	0.58
1:B:389:LEU:HA	1:B:392:ILE:HD12	1.86	0.58
1:A:35:TRP:CD1	1:A:101:ASN:HA	2.38	0.58
1:B:240:HIS:HB3	1:B:250:TYR:OH	2.03	0.58
1:A:6:GLU:HG2	1:A:10:ARG:HA	1.86	0.58
1:B:101:ASN:HD22	1:B:129:ARG:NH2	2.01	0.58
1:A:193:VAL:HA	1:A:199:HIS:CB	2.34	0.58
1:B:276:VAL:CG1	1:B:499:PRO:HG3	2.34	0.58
1:B:83:ARG:N	1:B:179:THR:O	2.31	0.57
1:A:83:ARG:HB2	1:A:179:THR:HG22	1.86	0.57
1:B:183:TRP:CH2	1:B:185:ASP:HB3	2.39	0.57
1:B:494:GLU:HG2	1:B:495:LYS:H	1.68	0.57
1:B:399:ASP:HA	1:B:402:HIS:HD2	1.69	0.57
1:B:33:ARG:HB3	1:B:36:GLU:HG3	1.85	0.57
1:B:83:ARG:HE	1:B:117:ASP:HB2	1.69	0.57
1:B:509:THR:CG2	1:B:526:GLN:HB2	2.22	0.57
1:B:276:VAL:HG13	1:B:499:PRO:HG3	1.85	0.57
1:B:111:TYR:CB	1:B:332:PRO:HD2	2.34	0.57
1:B:83:ARG:CG	1:B:83:ARG:HH11	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:VAL:HG11	1:A:256:ALA:HB1	1.87	0.57
1:B:23:LEU:HD11	1:B:60:ILE:HG12	1.86	0.57
1:B:438:THR:HG23	1:B:439:ARG:HG3	1.87	0.57
1:B:328:THR:HA	1:B:333:TYR:CZ	2.40	0.57
1:A:312:VAL:HG11	1:B:54:GLN:HE21	1.69	0.57
1:B:164:PHE:N	3:B:665:HOH:O	2.38	0.57
1:B:212:VAL:HG13	1:B:230:THR:HB	1.83	0.56
1:B:11:GLU:CD	1:B:11:GLU:N	2.58	0.56
1:A:6:GLU:O	1:A:7:THR:OG1	2.19	0.56
1:B:100:ASN:CA	1:B:129:ARG:NH2	2.59	0.56
1:B:85:VAL:HB	1:B:177:TYR:CD2	2.41	0.56
1:B:462:VAL:HG22	1:B:499:PRO:HG2	1.86	0.56
1:A:436:ASP:OD1	1:A:438:THR:HG23	2.04	0.56
1:B:377:GLU:H	1:B:377:GLU:CD	2.07	0.56
1:B:138:LEU:CD2	1:B:142:THR:HG21	2.35	0.56
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.12	0.56
1:A:83:ARG:HH11	1:A:179:THR:HG21	1.71	0.56
1:A:7:THR:HG21	1:A:8:PRO:HD3	1.71	0.56
1:B:15:LEU:HD12	1:B:173:SER:HB2	1.88	0.56
1:B:179:THR:CG2	1:B:183:TRP:CB	2.83	0.56
1:B:596:LYS:HG2	1:B:597:PRO:O	2.06	0.56
1:A:212:VAL:N	1:A:230:THR:CG2	2.61	0.56
1:B:425:PHE:HB2	1:B:456:ILE:CD1	2.35	0.56
1:B:213:SER:O	1:B:227:GLY:O	2.24	0.56
1:A:272:ARG:CA	1:A:284:ASN:HD21	2.13	0.56
1:A:140:TRP:CD2	1:A:379:ALA:O	2.58	0.56
1:B:144:PRO:HD3	3:B:615:HOH:O	2.06	0.56
1:A:199:HIS:ND1	1:A:200:ALA:N	2.52	0.55
1:A:205:GLN:HE21	1:A:207:VAL:HG22	1.64	0.55
1:A:550:ASN:ND2	1:A:551:PHE:N	2.55	0.55
1:B:151:ASP:OD1	1:B:154:GLY:N	2.39	0.55
1:A:101:ASN:HD21	1:A:129:ARG:NH2	2.05	0.55
1:B:550:ASN:O	1:B:569:GLY:HA2	2.06	0.55
1:B:330:HIS:N	1:B:330:HIS:CD2	2.73	0.55
1:B:122:VAL:HG23	1:B:128:VAL:CG1	2.34	0.55
1:B:207:VAL:CG1	1:B:256:ALA:HB1	2.37	0.55
1:B:88:PHE:O	1:B:113:PRO:HA	2.07	0.55
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.57	0.54
1:B:247:GLY:O	1:B:249:LEU:CD1	2.55	0.54
1:B:179:THR:HG23	1:B:183:TRP:CB	2.38	0.54
1:A:193:VAL:HA	1:A:199:HIS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:O	1:B:374:LEU:HD21	2.07	0.54
1:B:207:VAL:HG13	1:B:256:ALA:HB1	1.90	0.54
1:B:14:LYS:HZ1	1:B:130:ILE:HG13	1.73	0.54
1:A:445:ASN:HD21	1:A:467:ARG:HH22	1.55	0.54
1:A:157:LYS:HB2	3:A:814:HOH:O	2.08	0.54
1:A:180:PRO:HG2	1:A:263:ASP:HB2	1.88	0.54
1:A:14:LYS:O	1:A:174:VAL:HG22	2.07	0.54
1:A:28:CYS:HB3	1:A:32:GLN:NE2	2.21	0.54
1:B:563:VAL:HG23	1:B:564:GLY:N	2.22	0.54
1:A:272:ARG:HA	1:A:284:ASN:ND2	2.14	0.54
1:B:192:HIS:HE1	1:B:202:VAL:HG13	1.72	0.54
1:B:432:THR:HG21	1:B:441:ILE:HD11	1.88	0.54
1:A:566:ASN:HD22	1:A:568:LYS:H	1.54	0.54
1:A:0:HIS:N	1:A:0:HIS:CD2	2.76	0.54
1:B:493:GLN:O	1:B:496:LEU:O	2.26	0.54
1:B:494:GLU:HG2	1:B:495:LYS:N	2.23	0.54
1:A:78:GLY:HA3	1:B:78:GLY:HA3	1.89	0.54
1:A:50:SER:HB2	1:A:303:GLY:H	1.73	0.54
1:B:193:VAL:HG11	1:B:284:ASN:HD21	1.73	0.53
1:A:191:THR:HG21	1:A:271:ILE:HA	1.90	0.53
1:B:191:THR:HG21	1:B:272:ARG:H	1.73	0.53
1:B:191:THR:HG21	1:B:271:ILE:HA	1.90	0.53
1:B:218:ASP:CB	1:B:222:GLN:HE21	2.21	0.53
1:A:513:LEU:HD13	1:A:521:TRP:O	2.08	0.53
1:B:85:VAL:HB	1:B:177:TYR:CG	2.44	0.53
1:A:52:ASN:H	1:A:52:ASN:ND2	2.07	0.53
1:B:425:PHE:CB	1:B:456:ILE:HD11	2.37	0.53
1:A:445:ASN:ND2	1:A:467:ARG:HH12	2.05	0.53
1:B:10:ARG:CZ	1:B:79:TRP:HE1	2.22	0.53
1:B:480:THR:O	1:B:484:VAL:HG23	2.08	0.53
1:A:13:LYS:HB3	1:B:13:LYS:HZ1	1.74	0.53
1:B:163:ASP:CB	3:B:665:HOH:O	2.57	0.53
1:A:13:LYS:HZ2	1:B:15:LEU:HD22	1.74	0.53
1:B:83:ARG:NH2	1:B:117:ASP:HB2	2.23	0.53
1:B:494:GLU:CG	1:B:495:LYS:N	2.71	0.53
1:B:96:LYS:HD3	1:B:98:TRP:HZ2	1.73	0.53
1:A:238:ASN:N	3:A:810:HOH:O	2.42	0.52
1:A:135:ASN:ND2	1:A:137:GLU:H	2.07	0.52
1:A:376:SER:O	1:A:380:VAL:O	2.27	0.52
1:A:6:GLU:HG3	1:A:11:GLU:OE2	2.09	0.52
1:B:272:ARG:HA	1:B:284:ASN:ND2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:THR:OG1	1:A:233:THR:O	2.24	0.52
1:A:212:VAL:N	1:A:230:THR:HG21	2.22	0.52
1:B:496:LEU:HB3	3:B:690:HOH:O	2.08	0.52
1:B:426:ALA:HA	1:B:459:LEU:CD1	2.39	0.52
1:A:193:VAL:HG22	1:A:285:HIS:NE2	2.25	0.52
1:A:214:VAL:HG13	1:A:252:LEU:CD1	2.37	0.52
1:B:408:TRP:HE1	1:B:436:ASP:HB3	1.74	0.52
1:B:28:CYS:O	1:B:32:GLN:HG3	2.10	0.52
1:A:198:ASN:O	1:A:199:HIS:CB	2.54	0.52
1:A:566:ASN:ND2	1:A:568:LYS:H	2.08	0.52
1:B:10:ARG:NH1	1:B:79:TRP:HE1	2.07	0.52
1:B:433:ARG:NH1	1:B:461:ASP:OD1	2.43	0.52
1:B:10:ARG:H	1:B:178:THR:HG22	1.75	0.51
1:B:119:THR:HB	1:B:120:PRO:HD3	1.92	0.51
1:A:311:MET:HE1	1:A:340:TRP:HB2	1.90	0.51
1:A:538:ASP:OD2	1:A:587:ARG:NH2	2.41	0.51
1:B:183:TRP:HE3	1:B:183:TRP:C	2.14	0.51
1:B:504:GLU:OE1	2:B:604:EVA:CAE	2.59	0.51
1:A:10:ARG:HH21	1:B:77:LYS:HD2	1.76	0.51
1:A:184:VAL:HG22	1:A:207:VAL:HG22	1.93	0.51
1:A:212:VAL:HG22	1:A:230:THR:HA	1.92	0.51
1:B:43:ARG:HD2	1:B:55:PHE:CE1	2.45	0.51
1:B:325:SER:HA	1:B:347:VAL:O	2.10	0.51
1:A:195:GLN:OE1	1:A:195:GLN:N	2.44	0.51
1:B:83:ARG:CZ	1:B:117:ASP:HB2	2.41	0.51
1:A:14:LYS:HZ1	1:A:86:LEU:HD11	1.75	0.51
1:A:36:GLU:O	1:A:129:ARG:NH2	2.44	0.51
1:B:163:ASP:C	3:B:665:HOH:O	2.49	0.51
1:B:3:ARG:NH1	1:B:335:GLU:HG2	2.26	0.51
1:B:445:ASN:ND2	1:B:467:ARG:NH2	2.58	0.51
1:A:122:VAL:CG2	1:A:128:VAL:HG11	2.40	0.51
1:A:147:MET:HE3	1:A:161:PHE:CZ	2.45	0.51
1:A:83:ARG:HB3	1:A:179:THR:HG22	1.93	0.50
1:B:68:TRP:CH2	1:B:98:TRP:CH2	2.99	0.50
1:A:73:VAL:O	1:A:127:SER:HA	2.11	0.50
1:B:311:MET:HE1	1:B:340:TRP:HB2	1.93	0.50
1:B:95:GLY:HA2	1:B:133:CYS:O	2.10	0.50
1:B:144:PRO:HG3	3:B:615:HOH:O	2.11	0.50
1:B:373:GLU:O	1:B:376:SER:HB3	2.10	0.50
1:B:289:TYR:HA	1:B:544:VAL:O	2.10	0.50
1:A:36:GLU:HA	1:A:101:ASN:HD21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD13	1:B:176:LEU:HD13	1.93	0.50
1:A:314:ASP:OD1	1:A:575:ARG:HD2	2.12	0.50
1:A:83:ARG:NH1	1:A:183:TRP:CD2	2.79	0.50
1:A:74:PHE:CE2	1:B:6:GLU:O	2.64	0.50
1:B:10:ARG:NH1	1:B:79:TRP:NE1	2.59	0.50
1:B:554:PHE:HE2	3:B:665:HOH:O	1.93	0.50
1:A:203:ASP:OD2	1:A:233:THR:HG23	2.11	0.49
1:A:535:ARG:HH11	1:A:535:ARG:HG2	1.77	0.49
1:B:212:VAL:HG21	1:B:214:VAL:HG23	1.94	0.49
1:B:183:TRP:CE3	1:B:183:TRP:C	2.85	0.49
1:A:445:ASN:HD22	1:A:467:ARG:HH12	1.58	0.49
1:A:167:TYR:CD1	1:A:303:GLY:HA3	2.47	0.49
1:A:299:ALA:O	1:A:302:ARG:O	2.30	0.49
1:A:207:VAL:CG1	1:A:256:ALA:CB	2.90	0.49
1:A:3:ARG:CG	1:A:3:ARG:NH1	2.52	0.49
1:A:13:LYS:NZ	1:B:15:LEU:CD2	2.75	0.49
1:B:101:ASN:ND2	1:B:101:ASN:N	2.59	0.49
1:B:191:THR:HG21	1:B:272:ARG:N	2.27	0.49
1:A:303:GLY:O	1:A:304:LYS:HG2	2.12	0.49
1:A:83:ARG:HD3	1:A:179:THR:CG2	2.43	0.49
1:A:546:GLU:OE1	1:A:587:ARG:HD3	2.12	0.49
1:B:83:ARG:NH1	1:B:83:ARG:CG	2.72	0.49
1:B:467:ARG:HD3	1:B:469:TYR:HE1	1.77	0.49
1:A:203:ASP:OD1	1:A:233:THR:CB	2.59	0.49
1:A:214:VAL:CG1	1:A:252:LEU:HD11	2.37	0.49
1:B:279:GLU:OE2	1:B:493:GLN:HG3	2.13	0.49
1:A:8:PRO:HG2	1:A:264:ILE:HB	1.95	0.49
1:A:179:THR:HG23	1:A:180:PRO:O	2.13	0.49
1:A:13:LYS:NZ	1:B:15:LEU:HD22	2.28	0.49
1:B:351:GLU:HG2	1:B:352:THR:O	2.12	0.49
1:A:139:ASN:HA	1:A:146:GLY:O	2.13	0.49
1:B:71:ARG:CG	1:B:71:ARG:NH1	2.68	0.49
1:B:15:LEU:CD2	1:B:15:LEU:C	2.78	0.49
1:B:283:ILE:HG12	1:B:288:PHE:CB	2.43	0.49
1:A:531:ASP:OD1	1:A:583:LEU:HD21	2.13	0.49
1:B:4:PRO:HG3	1:B:177:TYR:CE2	2.48	0.48
1:A:101:ASN:HD21	1:A:129:ARG:HH22	1.61	0.48
1:B:551:PHE:CE2	1:B:575:ARG:NH1	2.77	0.48
1:B:292:GLY:HA3	1:B:325:SER:O	2.12	0.48
1:B:469:TYR:O	1:B:529:TRP:CH2	2.65	0.48
1:B:193:VAL:HG13	1:B:273:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:N	1:B:401:ASN:HD21	2.12	0.48
1:B:240:HIS:HE1	1:B:248:TYR:CD1	2.18	0.48
1:A:93:HIS:HD2	3:A:708:HOH:O	1.96	0.48
1:B:218:ASP:OD2	1:B:222:GLN:NE2	2.46	0.48
1:B:242:TRP:HD1	1:B:270:GLY:HA3	1.76	0.48
1:B:538:ASP:HA	3:B:671:HOH:O	2.13	0.48
1:B:160:TYR:OH	1:B:557:SER:HB3	2.14	0.48
1:B:244:PRO:HG2	1:B:593:PHE:HE1	1.78	0.48
1:B:564:GLY:CA	1:B:567:LYS:HZ3	2.26	0.48
1:B:187:ILE:CG2	1:B:188:THR:N	2.77	0.48
1:B:155:LYS:NZ	3:B:702:HOH:O	2.39	0.48
1:A:410:ILE:HD11	1:A:432:THR:HG21	1.96	0.48
1:A:49:GLY:HA2	1:A:305:GLY:HA3	1.94	0.48
1:A:183:TRP:CZ3	1:A:185:ASP:CG	2.85	0.48
1:A:187:ILE:HG12	1:A:205:GLN:OE1	2.14	0.48
1:A:330:HIS:HD2	1:A:351:GLU:OE1	1.96	0.48
1:A:207:VAL:HG11	1:A:256:ALA:CB	2.44	0.47
1:B:179:THR:CG2	1:B:183:TRP:HB3	2.40	0.47
1:A:585:GLN:HG2	3:A:830:HOH:O	2.13	0.47
1:B:212:VAL:CG2	1:B:214:VAL:HG23	2.43	0.47
1:B:172:ARG:NH2	1:B:334:ALA:N	2.62	0.47
1:B:33:ARG:HA	1:B:35:TRP:CZ3	2.49	0.47
1:B:139:ASN:HA	1:B:146:GLY:O	2.14	0.47
1:B:100:ASN:HA	1:B:129:ARG:HH22	1.70	0.47
1:A:268:ARG:HH22	1:A:343:GLU:HB2	1.78	0.47
1:A:256:ALA:HB3	1:A:263:ASP:HB3	1.97	0.47
1:B:350:ASP:OD2	1:B:399:ASP:OD2	2.33	0.47
1:B:502:ILE:N	1:B:502:ILE:HD12	2.29	0.47
1:A:205:GLN:NE2	1:A:207:VAL:HG22	2.27	0.47
1:A:12:ILE:HG22	1:A:14:LYS:HG3	1.96	0.47
1:B:34:TRP:CE3	1:B:68:TRP:CD1	3.03	0.47
1:A:138:LEU:HB3	1:A:142:THR:HG21	1.97	0.47
1:B:19:TRP:CE2	1:B:71:ARG:HD2	2.50	0.47
1:B:198:ASN:OD1	1:B:198:ASN:O	2.32	0.47
1:B:538:ASP:HB3	1:B:599:GLN:HA	1.97	0.47
1:A:320:TRP:CE2	1:A:585:GLN:NE2	2.83	0.47
1:A:19:TRP:CD1	1:A:47:VAL:HG13	2.49	0.47
1:B:471:TRP:CZ2	1:B:508:ASP:HB2	2.49	0.47
1:B:105:MET:CE	1:B:114:PHE:HD1	2.24	0.47
1:B:498:GLN:HG2	1:B:499:PRO:HD2	1.97	0.47
1:B:396:ILE:O	1:B:400:LYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:VAL:C	1:B:568:LYS:HG2	2.34	0.47
1:B:89:ASP:HB2	1:B:172:ARG:HB3	1.97	0.47
1:B:183:TRP:CZ3	1:B:185:ASP:CG	2.88	0.47
1:A:100:ASN:ND2	1:A:129:ARG:HB3	2.29	0.47
1:A:163:ASP:O	1:A:556:THR:CG2	2.60	0.47
1:B:21:PHE:HB2	1:B:45:ILE:CG2	2.44	0.47
1:A:7:THR:HA	1:B:74:PHE:CE1	2.51	0.46
1:A:599:GLN:O	1:A:599:GLN:CG	2.52	0.46
1:B:242:TRP:CZ2	1:B:345:GLY:HA2	2.50	0.46
1:A:6:GLU:CG	1:A:11:GLU:OE2	2.63	0.46
1:A:6:GLU:HA	1:A:9:THR:O	2.15	0.46
1:B:513:LEU:HD12	1:B:521:TRP:O	2.10	0.46
1:B:456:ILE:HD13	1:B:459:LEU:HG	1.97	0.46
1:B:205:GLN:CG	1:B:206:VAL:N	2.74	0.46
1:B:14:LYS:HB2	1:B:174:VAL:HG22	1.98	0.46
1:A:202:VAL:HG12	1:A:234:LEU:CG	2.44	0.46
1:A:328:THR:HB	1:A:333:TYR:CD2	2.51	0.46
1:B:487:LYS:O	1:B:487:LYS:HD3	2.15	0.46
1:B:84:ILE:HA	1:B:177:TYR:O	2.14	0.46
1:A:190:VAL:HB	1:A:202:VAL:HG22	1.96	0.46
1:A:509:THR:OG1	1:A:526:GLN:HB2	2.16	0.46
1:B:11:GLU:CD	1:B:11:GLU:H	2.19	0.46
1:A:249:LEU:HD11	1:A:342:ASP:O	2.15	0.46
1:A:330:HIS:HE1	2:A:604:EVA:OD2	1.98	0.46
1:A:7:THR:HG23	1:B:74:PHE:CZ	2.51	0.46
1:B:70:GLN:NE2	1:B:129:ARG:HD2	2.30	0.46
1:B:563:VAL:CG2	1:B:564:GLY:N	2.78	0.46
1:A:83:ARG:HB2	1:A:179:THR:CG2	2.45	0.46
1:B:207:VAL:CG2	1:B:230:THR:OG1	2.64	0.46
1:B:192:HIS:HE1	1:B:202:VAL:CG1	2.28	0.46
1:B:198:ASN:HB3	1:B:238:ASN:HA	1.98	0.46
1:B:504:GLU:HG2	1:B:549:TRP:CE3	2.51	0.46
1:A:188:THR:HB	1:A:204:TRP:HE3	1.81	0.46
1:B:167:TYR:HB2	1:B:304:LYS:HD2	1.97	0.46
1:A:7:THR:HA	1:B:74:PHE:CZ	2.50	0.46
1:B:167:TYR:HB2	1:B:304:LYS:CD	2.46	0.46
1:B:193:VAL:HG11	1:B:284:ASN:ND2	2.31	0.45
1:B:192:HIS:CE1	1:B:202:VAL:HG13	2.50	0.45
1:A:342:ASP:CG	1:A:403:PRO:HD2	2.36	0.45
1:B:107:HIS:HD2	3:B:668:HOH:O	1.97	0.45
1:B:10:ARG:HB2	1:B:79:TRP:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:O	1:B:16:ASP:C	2.54	0.45
1:B:183:TRP:CE3	1:B:183:TRP:O	2.69	0.45
1:A:191:THR:HG23	1:A:271:ILE:HG23	1.98	0.45
1:A:249:LEU:HD22	1:A:268:ARG:NH2	2.30	0.45
1:B:467:ARG:HG2	1:B:469:TYR:CD1	2.51	0.45
1:B:529:TRP:CD1	1:B:530:LEU:N	2.85	0.45
1:B:94:TYR:O	1:B:134:VAL:HA	2.16	0.45
1:B:355:VAL:CG2	1:B:412:ASN:HD22	2.27	0.45
1:A:16:ASP:OD2	1:B:13:LYS:NZ	2.47	0.45
1:B:172:ARG:HH21	1:B:334:ALA:N	2.14	0.45
1:B:183:TRP:HZ3	1:B:185:ASP:CG	2.20	0.45
1:A:151:ASP:CG	3:A:835:HOH:O	2.55	0.45
1:B:117:ASP:OD2	1:B:119:THR:OG1	2.22	0.45
1:B:75:ILE:HD11	1:B:128:VAL:HG22	1.98	0.45
1:B:96:LYS:HE3	1:B:106:GLU:OE2	2.16	0.45
1:A:73:VAL:HG22	1:A:74:PHE:N	2.32	0.45
1:B:396:ILE:HD11	1:B:432:THR:HG23	1.99	0.45
1:B:489:LEU:O	1:B:492:TRP:HB2	2.17	0.45
1:A:8:PRO:O	1:B:77:LYS:NZ	2.50	0.45
1:B:34:TRP:CZ3	1:B:68:TRP:CD1	3.05	0.45
1:A:242:TRP:CZ2	1:A:345:GLY:HA2	2.52	0.44
1:B:376:SER:OG	1:B:378:GLU:HG2	2.16	0.44
1:A:86:LEU:HD12	1:A:175:MET:O	2.17	0.44
1:A:102:GLN:HG2	1:A:121:TYR:CD1	2.52	0.44
1:A:36:GLU:CA	1:A:129:ARG:HH21	2.30	0.44
1:A:50:SER:OG	1:A:303:GLY:HA3	2.17	0.44
1:B:433:ARG:NH2	1:B:461:ASP:OD1	2.50	0.44
1:A:463:LEU:HD21	1:A:492:TRP:CD2	2.53	0.44
1:A:119:THR:HB	1:A:120:PRO:CD	2.33	0.44
1:B:142:THR:HG22	1:B:144:PRO:O	2.17	0.44
1:A:167:TYR:CZ	1:A:303:GLY:HA2	2.52	0.44
1:B:184:VAL:HG21	1:B:254:VAL:HG12	2.00	0.44
1:B:374:LEU:HD23	1:B:375:TYR:CE2	2.53	0.44
1:A:596:LYS:HE3	3:A:782:HOH:O	2.16	0.44
1:B:0:HIS:CG	1:B:186:ASP:OD2	2.70	0.44
1:A:504:GLU:HG2	1:A:549:TRP:CE3	2.53	0.44
1:A:212:VAL:HG13	1:A:230:THR:CB	2.47	0.44
1:B:205:GLN:NE2	1:B:212:VAL:HG21	2.29	0.44
1:A:14:LYS:HZ1	1:A:86:LEU:CD1	2.25	0.44
1:B:83:ARG:HH21	1:B:117:ASP:HB2	1.81	0.44
1:A:445:ASN:ND2	1:A:467:ARG:HH22	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:O	1:A:376:SER:HB2	2.17	0.44
1:B:69:TYR:CD1	1:B:170:ILE:HD12	2.53	0.44
1:A:138:LEU:CB	1:A:142:THR:HG21	2.47	0.44
1:A:43:ARG:HD2	1:A:55:PHE:CD1	2.52	0.44
1:B:242:TRP:CE3	1:B:242:TRP:C	2.91	0.43
1:B:288:PHE:HE2	1:B:290:PHE:HA	1.82	0.43
1:B:52:ASN:ND2	1:B:168:ALA:H	2.14	0.43
1:A:88:PHE:O	1:A:113:PRO:HA	2.18	0.43
1:B:302:ARG:HB3	1:B:302:ARG:CZ	2.47	0.43
1:A:13:LYS:HE3	1:A:15:LEU:HD22	2.00	0.43
1:B:236:VAL:O	1:B:237:VAL:HG23	2.19	0.43
1:A:77:LYS:H	1:B:10:ARG:HE	1.66	0.43
1:B:198:ASN:CB	1:B:237:VAL:C	2.80	0.43
1:A:111:TYR:CB	1:A:332:PRO:HD2	2.46	0.43
1:B:276:VAL:HG13	1:B:280:GLN:O	2.18	0.43
1:A:464:CYS:HA	1:A:501:ILE:O	2.18	0.43
1:B:2:LEU:O	1:B:87:ARG:NH1	2.52	0.43
1:B:537:PHE:CD1	1:B:546:GLU:HG2	2.54	0.43
1:B:422:ARG:HH22	1:B:458:ASP:CG	2.16	0.43
1:B:85:VAL:O	1:B:177:TYR:CB	2.54	0.43
1:A:422:ARG:HA	1:A:456:ILE:CD1	2.49	0.43
1:A:76:PRO:HA	1:B:10:ARG:CD	2.49	0.43
1:A:193:VAL:HG22	1:A:285:HIS:HE2	1.83	0.43
1:A:229:GLY:O	1:A:231:SER:N	2.52	0.43
1:B:328:THR:HA	1:B:333:TYR:CE1	2.54	0.43
1:B:218:ASP:OD1	1:B:219:ALA:N	2.47	0.43
1:B:426:ALA:HA	1:B:459:LEU:HD13	2.01	0.43
1:B:213:SER:HB3	1:B:255:THR:OG1	2.19	0.43
1:A:13:LYS:O	1:A:174:VAL:O	2.37	0.43
1:A:238:ASN:HB2	3:A:810:HOH:O	2.19	0.43
1:A:147:MET:HE3	1:A:161:PHE:HZ	1.84	0.43
1:A:188:THR:HB	1:A:204:TRP:CE3	2.54	0.43
1:A:361:LEU:HA	1:A:361:LEU:HD23	1.79	0.43
1:A:77:LYS:CE	1:B:8:PRO:O	2.67	0.43
1:A:15:LEU:CD1	1:A:173:SER:CA	2.82	0.43
1:A:204:TRP:HA	1:A:231:SER:O	2.19	0.43
1:B:207:VAL:HG13	1:B:256:ALA:CB	2.49	0.43
1:B:531:ASP:O	1:B:535:ARG:HD3	2.17	0.43
1:B:193:VAL:O	1:B:193:VAL:HG22	2.18	0.42
1:B:290:PHE:HB2	1:B:545:GLY:HA3	1.99	0.42
1:B:99:VAL:HG22	1:B:130:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HA	1:B:35:TRP:CE3	2.55	0.42
1:A:357:PHE:O	1:A:374:LEU:CD1	2.66	0.42
1:A:23:LEU:HD12	1:A:25:ARG:NH1	2.34	0.42
1:A:14:LYS:HD2	1:A:176:LEU:CD2	2.38	0.42
1:A:200:ALA:HB1	1:A:234:LEU:CD2	2.50	0.42
1:A:388:HIS:HD2	1:A:424:TYR:OH	2.02	0.42
1:B:595:GLU:HB3	3:B:676:HOH:O	2.19	0.42
1:B:426:ALA:HB3	1:B:427:PRO:HD3	2.00	0.42
1:B:83:ARG:HB3	1:B:179:THR:HG22	2.02	0.42
1:B:529:TRP:HD1	1:B:530:LEU:N	2.18	0.42
1:A:240:HIS:HB2	1:A:248:TYR:CE2	2.54	0.42
1:A:14:LYS:NZ	1:A:86:LEU:HD11	2.28	0.42
1:B:240:HIS:C	1:B:240:HIS:ND1	2.73	0.42
1:B:552:ALA:HA	1:B:571:PHE:O	2.19	0.42
1:B:447:MET:CG	1:B:467:ARG:HG3	2.48	0.42
1:A:566:ASN:HD21	1:A:568:LYS:HB2	1.84	0.42
1:B:0:HIS:CB	1:B:186:ASP:OD2	2.63	0.41
1:B:242:TRP:O	1:B:242:TRP:HE3	2.03	0.41
1:A:77:LYS:H	1:B:10:ARG:NE	2.18	0.41
1:B:14:LYS:O	1:B:16:ASP:O	2.37	0.41
1:B:272:ARG:HH21	1:B:403:PRO:HA	1.85	0.41
1:B:467:ARG:HD3	1:B:469:TYR:CE1	2.55	0.41
1:B:279:GLU:OE2	1:B:493:GLN:CG	2.67	0.41
1:B:43:ARG:HD3	3:B:616:HOH:O	2.20	0.41
1:A:51:PHE:C	1:A:51:PHE:CD1	2.93	0.41
1:A:207:VAL:HG13	1:A:256:ALA:HB1	2.02	0.41
1:A:199:HIS:CG	1:A:200:ALA:H	2.33	0.41
1:B:21:PHE:HB2	1:B:45:ILE:HG21	2.02	0.41
1:B:35:TRP:CE3	1:B:98:TRP:CZ2	3.08	0.41
1:A:193:VAL:C	1:A:199:HIS:HD2	2.23	0.41
1:A:93:HIS:CE1	1:A:166:ASN:OD1	2.58	0.41
1:A:13:LYS:O	1:A:14:LYS:HB2	2.19	0.41
1:B:15:LEU:CD1	1:B:173:SER:OG	2.68	0.41
1:B:11:GLU:OE2	1:B:11:GLU:N	2.54	0.41
1:B:200:ALA:CA	1:B:235:GLN:O	2.59	0.41
1:B:135:ASN:HD21	1:B:137:GLU:HB2	1.85	0.41
1:B:190:VAL:O	1:B:201:SER:HA	2.21	0.41
1:A:89:ASP:OD2	1:A:173:SER:HB2	2.20	0.41
1:A:192:HIS:HE1	1:A:202:VAL:HG13	1.86	0.41
1:B:10:ARG:CZ	1:B:79:TRP:NE1	2.83	0.41
1:A:194:ALA:HB2	1:A:199:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASN:HD22	1:A:551:PHE:N	2.19	0.41
1:B:497:HIS:N	3:B:690:HOH:O	2.53	0.41
1:B:94:TYR:HB3	1:B:135:ASN:HB3	2.02	0.41
1:A:21:PHE:HA	1:A:68:TRP:O	2.20	0.41
1:B:35:TRP:CD1	1:B:101:ASN:HA	2.55	0.41
1:B:237:VAL:CG1	1:B:238:ASN:N	2.83	0.41
1:A:39:LEU:N	1:A:70:GLN:OE1	2.50	0.41
1:B:386:GLN:O	1:B:390:GLN:N	2.43	0.41
1:B:10:ARG:HB2	1:B:79:TRP:NE1	2.36	0.41
1:B:7:THR:HG1	1:B:8:PRO:CD	2.31	0.41
1:B:3:ARG:O	1:B:265:TYR:OH	2.29	0.41
1:B:242:TRP:C	1:B:242:TRP:HE3	2.25	0.41
1:B:568:LYS:CE	2:B:604:EVA:OXT	2.69	0.41
1:A:566:ASN:HD22	1:A:566:ASN:C	2.24	0.41
1:A:303:GLY:O	1:A:304:LYS:CG	2.68	0.41
1:A:2:LEU:HA	1:A:2:LEU:HD23	1.85	0.41
1:A:313:HIS:HD2	1:B:53:ASP:O	2.04	0.41
1:B:259:GLN:H	1:B:259:GLN:HG3	1.58	0.41
1:A:587:ARG:HG2	1:A:588:TRP:CD1	2.55	0.41
1:A:105:MET:HE2	1:A:105:MET:HB2	1.68	0.41
1:A:330:HIS:CD2	1:A:330:HIS:N	2.85	0.41
1:A:550:ASN:ND2	1:A:552:ALA:H	2.15	0.41
1:A:361:LEU:HD21	1:A:446:VAL:HG21	2.03	0.41
1:B:7:THR:HG1	1:B:8:PRO:N	2.19	0.40
1:B:183:TRP:HZ3	1:B:185:ASP:CB	2.30	0.40
1:A:73:VAL:HG22	1:A:74:PHE:H	1.86	0.40
1:A:247:GLY:O	1:A:249:LEU:CD1	2.62	0.40
1:A:151:ASP:OD2	3:A:835:HOH:O	2.22	0.40
1:B:422:ARG:HA	1:B:456:ILE:HG12	2.03	0.40
1:B:35:TRP:HD1	1:B:101:ASN:HA	1.85	0.40
1:B:83:ARG:O	1:B:179:THR:N	2.51	0.40
1:A:105:MET:HE2	1:A:114:PHE:HD1	1.86	0.40
1:B:35:TRP:HB3	1:B:98:TRP:CE3	2.56	0.40
1:A:94:TYR:OH	1:A:96:LYS:HE3	2.21	0.40
1:A:72:GLU:HA	1:A:128:VAL:O	2.22	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	592/605 (98%)	568 (96%)	19 (3%)	5 (1%)	24	35
1	B	592/605 (98%)	566 (96%)	23 (4%)	3 (0%)	34	48
All	All	1184/1210 (98%)	1134 (96%)	42 (4%)	8 (1%)	26	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	B	7	THR
1	B	48	PRO
1	A	304	LYS
1	A	48	PRO
1	A	144	PRO
1	A	238	ASN
1	B	266	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	506/513 (99%)	459 (91%)	47 (9%)	11	16
1	B	506/513 (99%)	446 (88%)	60 (12%)	6	8
All	All	1012/1026 (99%)	905 (89%)	107 (11%)	8	12

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MET
1	A	3	ARG
1	A	5	VAL
1	A	9	THR
1	A	12	ILE
1	A	15	LEU
1	A	43	ARG
1	A	47	VAL
1	A	52	ASN
1	A	71	ARG
1	A	101	ASN
1	A	122	VAL
1	A	157	LYS
1	A	176	LEU
1	A	178	THR
1	A	191	THR
1	A	197	CYS
1	A	199	HIS
1	A	209	ASN
1	A	212	VAL
1	A	230	THR
1	A	233	THR
1	A	258	SER
1	A	268	ARG
1	A	272	ARG
1	A	329	SER
1	A	359	LEU
1	A	383	GLU
1	A	419	GLN
1	A	438	THR
1	A	441	ILE
1	A	453	THR
1	A	473	VAL
1	A	478	LEU
1	A	480	THR
1	A	510	LEU
1	A	513	LEU
1	A	518	THR
1	A	531	ASP
1	A	535	ARG
1	A	544	VAL
1	A	550	ASN

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Mol	Chain	Res	Type
1	A	560	ILE
1	A	566	ASN
1	A	585	GLN
1	A	598	GLN
1	B	3	ARG
1	B	9	THR
1	B	11	GLU
1	B	15	LEU
1	B	41	GLU
1	B	43	ARG
1	B	47	VAL
1	B	71	ARG
1	B	82	GLN
1	B	83	ARG
1	B	89	ASP
1	B	101	ASN
1	B	141	GLN
1	B	142	THR
1	B	148	VAL
1	B	157	LYS
1	B	172	ARG
1	B	174	VAL
1	B	176	LEU
1	B	177	TYR
1	B	178	THR
1	B	179	THR
1	B	186	ASP
1	B	193	VAL
1	B	196	ASP
1	B	197	CYS
1	B	201	SER
1	B	202	VAL
1	B	207	VAL
1	B	209	ASN
1	B	222	GLN
1	B	234	LEU
1	B	237	VAL
1	B	238	ASN
1	B	242	TRP
1	B	246	GLU
1	B	257	LYS
1	B	259	GLN

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Mol	Chain	Res	Type
1	B	273	SER
1	B	298	ASP
1	B	302	ARG
1	B	335	GLU
1	B	352	THR
1	B	359	LEU
1	B	372	LYS
1	B	453	THR
1	B	456	ILE
1	B	457	SER
1	B	459	LEU
1	B	467	ARG
1	B	478	LEU
1	B	487	LYS
1	B	503	THR
1	B	513	LEU
1	B	518	THR
1	B	529	TRP
1	B	531	ASP
1	B	535	ARG
1	B	541	SER
1	B	586	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	52	ASN
1	A	54	GLN
1	A	66	ASN
1	A	93	HIS
1	A	100	ASN
1	A	101	ASN
1	A	102	GLN
1	A	107	HIS
1	A	135	ASN
1	A	192	HIS
1	A	205	GLN
1	A	235	GLN
1	A	243	GLN
1	A	280	GLN
1	A	284	ASN

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Mol	Chain	Res	Type
1	A	313	HIS
1	A	330	HIS
1	A	388	HIS
1	A	401	ASN
1	A	445	ASN
1	A	550	ASN
1	A	566	ASN
1	A	599	GLN
1	B	0	HIS
1	B	52	ASN
1	B	54	GLN
1	B	66	ASN
1	B	93	HIS
1	B	101	ASN
1	B	107	HIS
1	B	135	ASN
1	B	181	ASN
1	B	192	HIS
1	B	195	GLN
1	B	205	GLN
1	B	209	ASN
1	B	222	GLN
1	B	235	GLN
1	B	238	ASN
1	B	243	GLN
1	B	284	ASN
1	B	313	HIS
1	B	330	HIS
1	B	385	GLN
1	B	401	ASN
1	B	412	ASN
1	B	445	ASN
1	B	498	GLN
1	B	534	HIS
1	B	550	ASN
1	B	585	GLN
1	B	598	GLN

### 5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EVA	A	604	-	9,13,13	0.62	0	10,19,19	1.53	1 (10%)
2	EVA	B	604	-	9,13,13	2.32	2 (22%)	10,19,19	1.95	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EVA	A	604	-	-	0/0/24/24	0/1/1/1
2	EVA	B	604	-	-	0/0/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	EVA	CA-N	2.84	1.48	1.46
2	B	604	EVA	CAE-N	5.95	1.43	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	604	EVA	OAK-CAE-N	-3.97	117.51	122.77
2	A	604	EVA	OAK-CAE-N	-3.63	117.96	122.77
2	B	604	EVA	OD2-CG-CD1	-2.48	105.01	109.49
2	B	604	EVA	CD1-CAE-N	2.36	123.53	118.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	EVA	2	0
2	B	604	EVA	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	596/605 (98%)	0.39	44 (7%) 17 17	19, 46, 107, 127	0
1	B	596/605 (98%)	0.91	90 (15%) 3 3	26, 87, 178, 207	0
All	All	1192/1210 (98%)	0.65	134 (11%) 7 7	19, 67, 152, 207	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	VAL	10.9
1	A	207	VAL	9.1
1	A	303	GLY	8.8
1	B	601	GLY	8.2
1	B	230	THR	7.8
1	B	204	TRP	7.7
1	B	545	GLY	7.1
1	B	8	PRO	7.1
1	B	600	GLY	6.8
1	B	282	LEU	6.6
1	A	199	HIS	6.4
1	B	213	SER	6.3
1	B	425	PHE	5.8
1	B	229	GLY	5.5
1	B	208	ALA	5.4
1	B	212	VAL	5.2
1	A	208	ALA	4.5
1	A	209	ASN	4.5
1	A	230	THR	4.5
1	A	204	TRP	4.4
1	B	357	PHE	4.4
1	A	256	ALA	4.3
1	A	15	LEU	4.2
1	B	214	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	205	GLN	4.0
1	B	239	PRO	3.8
1	B	209	ASN	3.8
1	B	196	ASP	3.8
1	B	7	THR	3.8
1	B	409	SER	3.8
1	B	190	VAL	3.8
1	B	252	LEU	3.7
1	A	8	PRO	3.7
1	B	216	LEU	3.6
1	A	302	ARG	3.6
1	B	265	TYR	3.5
1	B	260	THR	3.5
1	B	271	ILE	3.5
1	A	260	THR	3.5
1	B	79	TRP	3.5
1	A	7	THR	3.3
1	B	262	CYS	3.3
1	B	289	TYR	3.3
1	B	231	SER	3.3
1	B	311	MET	3.2
1	B	463	LEU	3.2
1	A	18	LEU	3.2
1	B	199	HIS	3.1
1	B	235	GLN	3.1
1	B	598	GLN	3.1
1	B	288	PHE	3.1
1	A	229	GLY	3.0
1	A	37	SER	3.0
1	B	537	PHE	3.0
1	B	410	ILE	3.0
1	B	465	LEU	3.0
1	A	17	GLY	2.9
1	A	235	GLN	2.9
1	B	152	GLU	2.9
1	B	597	PRO	2.9
1	A	212	VAL	2.9
1	B	277	LYS	2.9
1	B	261	GLU	2.9
1	A	98	TRP	2.9
1	A	29	GLY	2.9
1	B	153	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	379	ALA	2.8
1	A	214	VAL	2.7
1	B	587	ARG	2.7
1	B	309	VAL	2.7
1	B	211	ASP	2.6
1	A	123	ILE	2.6
1	A	16	ASP	2.6
1	A	236	VAL	2.6
1	B	380	VAL	2.6
1	B	266	PRO	2.6
1	B	0	HIS	2.6
1	B	274	VAL	2.6
1	B	264	ILE	2.5
1	A	233	THR	2.5
1	B	240	HIS	2.5
1	B	259	GLN	2.5
1	B	75	ILE	2.5
1	B	290	PHE	2.5
1	B	253	CYS	2.4
1	A	252	LEU	2.4
1	A	329	SER	2.4
1	A	257	LYS	2.4
1	B	591	MET	2.4
1	B	123	ILE	2.4
1	A	217	ARG	2.3
1	A	216	LEU	2.3
1	B	599	GLN	2.3
1	A	264	ILE	2.3
1	B	494	GLU	2.3
1	A	262	CYS	2.3
1	B	226	THR	2.3
1	B	201	SER	2.3
1	B	501	ILE	2.3
1	B	248	TYR	2.2
1	B	25	ARG	2.2
1	B	236	VAL	2.2
1	B	543	VAL	2.2
1	A	600	GLY	2.2
1	A	601	GLY	2.2
1	B	245	GLY	2.2
1	A	48	PRO	2.2
1	B	37	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	206	VAL	2.2
1	A	200	ALA	2.2
1	B	310	LEU	2.2
1	B	227	GLY	2.1
1	A	79	TRP	2.1
1	A	318	MET	2.1
1	B	256	ALA	2.1
1	B	596	LYS	2.1
1	B	15	LEU	2.1
1	B	588	TRP	2.1
1	A	379	ALA	2.1
1	B	187	ILE	2.1
1	A	194	ALA	2.1
1	B	198	ASN	2.1
1	B	149	ILE	2.1
1	B	456	ILE	2.1
1	B	250	TYR	2.1
1	A	234	LEU	2.0
1	B	241	LEU	2.0
1	A	96	LYS	2.0
1	A	196	ASP	2.0
1	B	14	LYS	2.0
1	B	595	GLU	2.0
1	B	540	VAL	2.0
1	B	563	VAL	2.0
1	B	219	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EVA	B	604	13/13	0.89	0.16	0.96	22,23,29,30	0
2	EVA	A	604	13/13	0.95	0.15	0.26	20,21,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.