



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 AM GMT

PDB ID : 3ABG  
Title : X-ray Crystal Analysis of Bilirubin Oxidase from Myrothecium verrucaria at 2.3 angstrom Resolution using a Twin Crystal  
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Deposited on : 2009-12-10  
Resolution : 2.30 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

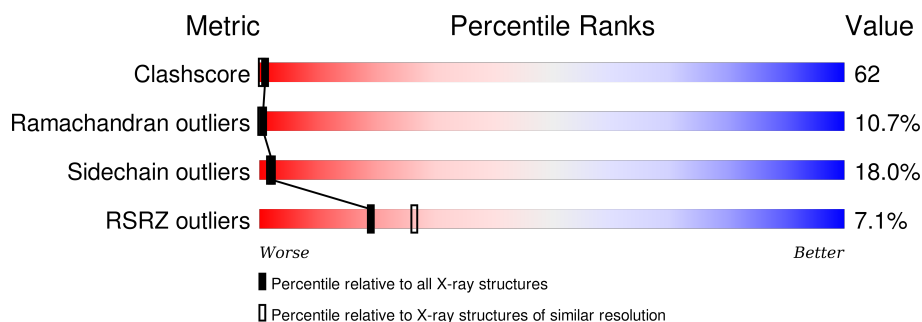
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	534	
1	B	534	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CU	A	702	-	-	-	X
4	CU	B	701	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8616 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 Bilirubin oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	1	0
			4045	2587	686	759	13			
1	B	518	Total	C	N	O	S	0	1	0
			4112	2628	698	773	13			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cu	0	0
			4	4		
4	A	4	Total	Cu	0	0
			4	4		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

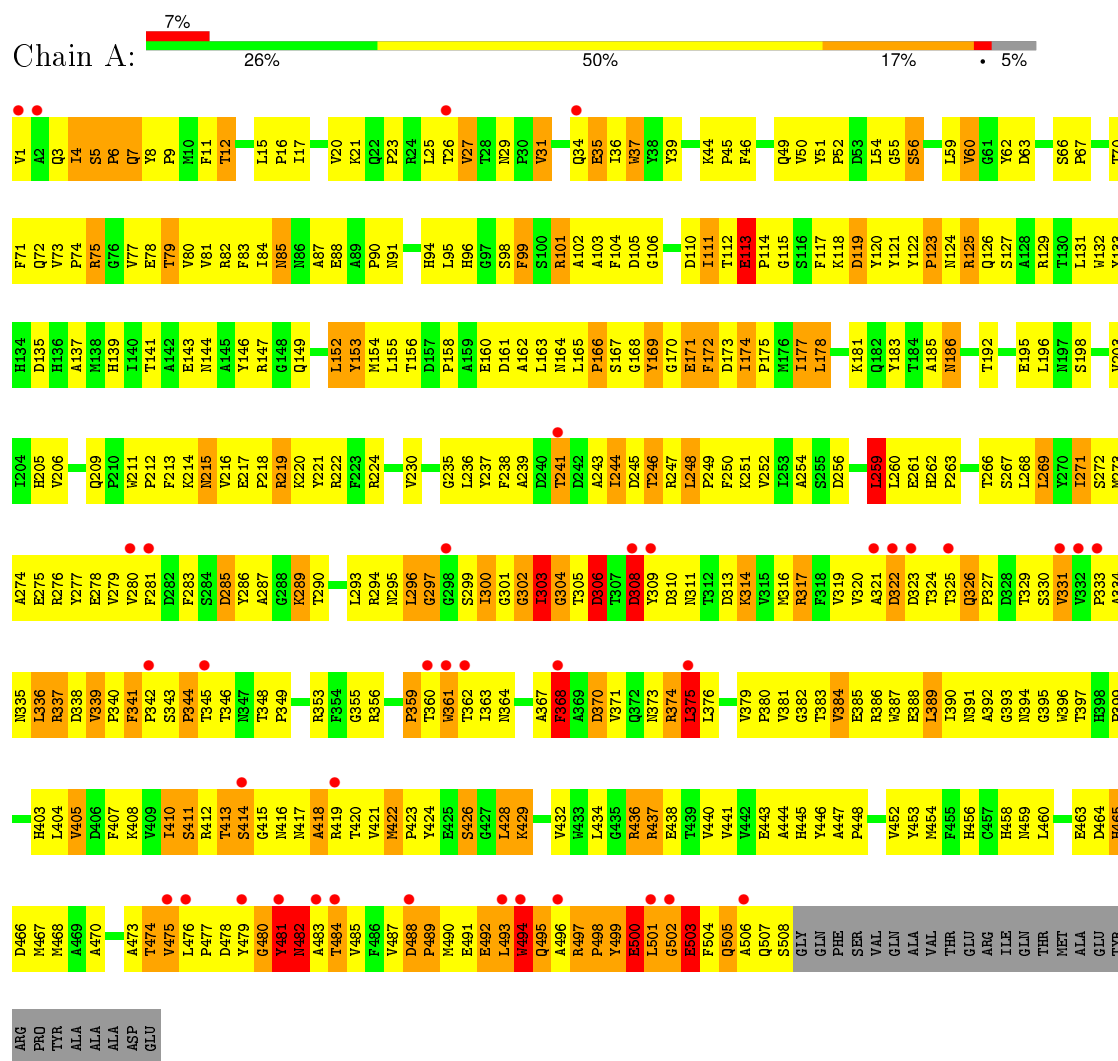
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total 147	O 147	0	0
6	B	170	Total 170	O 170	0	0

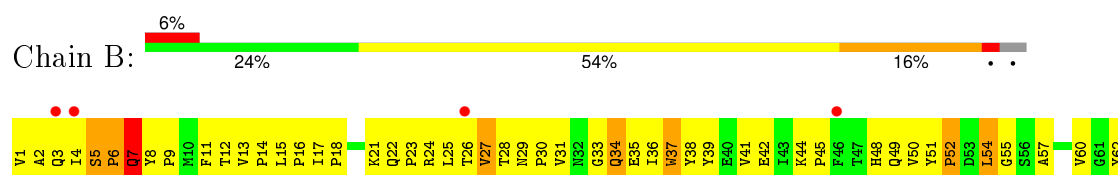
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: Bilirubin oxidase



#### • Molecule 1: Bilirubin oxidase



ALA	I461	T397	P333	S272	P210	A128	D63
GLU		H398	A334	R273	R211	R129	G64
TYR	D464	P399	N335	A274	E275	T130	M65
ARG	H465	I400	L336	E276	R213	L131	S66
PRO	D466	H401	R337	R276	R214	W132	P67
TYR	M467	I402	D338	Y277	R215		
ALA	M468	H403	V339	E278	R216	A137	T70
ALA	M469	L404	P340	V279	W138	F71	
ALA	A470	V405	F341	V280	H139	Q72	
ASP		D406	P342	F281	Y146		
GLU	A473	F407	S343	D282	R147		
	T474	M408	P344	F283			
	V475	V409	T345	S284			
		I410	T346	D285	L152		
	D478	S411	N347	Y286	Y153		
	Y479	R412	T348	A287	M154		
	G480	T413	P349	G288	L155		
	Y481	S414	R350	K289	T225		
	M482	G415		T290	L226		
	A483	M416	G355	T291	D227		
	T484	N417	R356	I291	D157		
	V485	A418	T357		P158		
	F486	R419	G358	R294	A159		
	V487	T420	P359	N295	D161		
	D488	V421	T360	L296	A162		
	P489	M422	W361	G297	L163		
	M490	P423	T362	G298	N164		
	E491	Y424	I363	S299	L165		
	E492	E425	N364	T300	P166		
	L493	S426	G365	G301	S167		
	M494	G427	V366	G302	G168		
	Q495	L428	A367	I303	Y169		
	A496	K429	F368	G304	G170		
	R497	D430	A369	T305	E171		
	P498	V431	D370	D306	F172		
	Y499	V432	V371	T307	D173		
	E500		Q372	D308	I174		
	L501	R436	N373	Y309	P175		
	G502	R437	R374	D310	M176		
	E503		L375	N311	I177		
	F504	V440	L376	T312			
	M505	V441	A377	D313	Q182		
	A506	V442	N378	K314	E109		
	Q507	E443	V379	V315	D110		
	S508	A444	P380	N316	T112		
	G509	H445	V381	R317	E113		
	F510	Y446	G382	F318	P114		
	F511	A447	T383	V319	T191		
	S512	P448	V384	V320	T192		
	M513		P385	A321	G193		
	Q514	G451	R386	D322	E194		
	A515	V452	W387	P323	E195		
	V516	Y453	E388	T324	D119		
	T517	M454	L389	T325	L196		
	E518	F455		Q326	M197		
	ARG	H456	A392	P327	S198		
	ILE	C457		D328	Y121		
	GLN	N458	G393	T329	Y122		
	THR	N459	N394	S330	P123		
	MET	L460	G395	V331	N124		
			W396	V332	R125		
					S127		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.74Å 139.74Å 135.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.56 – 2.30 48.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (33.56-2.30) 96.7 (48.65-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.203 , 0.263 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 76.9	EDS
Estimated twinning fraction	0.487 for h,-h-k,-l 0.469 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.487 for h,-h-k,-l	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 66357 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: BMA, NDG, NAG, CU

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	0.37	0/4175	0.66	0/5712
1	B	0.37	0/4243	0.65	0/5805
All	All	0.37	0/8418	0.65	0/11517

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	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ASP	Peptide
1	A	304	GLY	Peptide
1	A	465	HIS	Peptide
1	A	484	THR	Peptide
1	B	119	ASP	Peptide
1	B	304	GLY	Peptide
1	B	465	HIS	Peptide
1	B	484	THR	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	4045	0	3842	505	0
1	B	4112	0	3897	502	0
2	A	39	0	34	1	0
2	B	39	0	34	4	0
3	A	28	0	25	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	B	28	0	25	2	0
6	A	147	0	0	23	0
6	B	170	0	0	29	0
All	All	8616	0	7857	1004	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 62.

All (1004) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:GLN:HB3	5:B:611:NAG:H62	1.23	1.14
1:A:317:ARG:HH11	1:A:317:ARG:HG2	1.02	1.14
1:A:17:ILE:HG21	1:A:172:PHE:HA	1.32	1.12
1:A:247:ARG:HD3	1:A:267:SER:HB3	1.15	1.11
1:B:158:PRO:HA	1:B:161:ASP:HB3	1.31	1.11
1:A:301:GLY:HA3	1:A:436[B]:ARG:H	1.13	1.11
1:A:301:GLY:HA3	1:A:436[A]:ARG:H	1.13	1.10
1:B:17:ILE:HG21	1:B:172:PHE:HA	1.36	1.04
1:A:101:ARG:HD2	1:A:101:ARG:H	1.25	1.01
1:B:505:GLN:HG3	1:B:511:PHE:HB2	1.41	1.00
1:A:37:TRP:HE3	1:A:77:VAL:HG21	1.26	0.99
1:B:29:ASN:HB2	1:B:78:GLU:HG2	1.44	0.99
1:B:220:LYS:HG3	1:B:329:THR:HG22	1.48	0.95
1:A:412:ARG:HG2	1:A:414:SER:HB3	1.47	0.95
1:A:496:ALA:HB3	1:A:497:ARG:HB2	1.47	0.95
1:A:158:PRO:HA	1:A:161:ASP:HB3	1.47	0.95
1:A:404:LEU:HD11	1:A:448:PRO:HB2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:PRO:C	1:A:342:PRO:HD3	1.87	0.94
1:B:374:ARG:HE	1:B:374:ARG:HA	1.33	0.94
1:B:419:ARG:O	1:B:420:THR:HG23	1.69	0.91
1:B:23:PRO:HG3	1:B:37:TRP:HE1	1.33	0.91
1:B:356:ARG:HE	1:B:394:ASN:HB2	1.35	0.91
1:A:356:ARG:HG2	1:A:392:ALA:HB3	1.52	0.90
1:B:247:ARG:HD3	1:B:267:SER:HB3	1.53	0.90
1:B:494:TRP:HH2	1:B:499:TYR:HD2	1.20	0.89
1:A:95:LEU:HD12	1:A:98:SER:HB2	1.55	0.89
1:B:497:ARG:HG2	1:B:497:ARG:O	1.72	0.89
1:B:300:ILE:HG23	1:B:301:GLY:H	1.37	0.89
1:B:504:PHE:HE2	1:B:511:PHE:HA	1.35	0.89
1:A:70:THR:HG23	1:A:152:LEU:HB3	1.56	0.88
1:A:496:ALA:HB3	1:A:497:ARG:HD2	1.55	0.88
1:A:507:GLN:HG3	1:A:508:SER:H	1.38	0.88
1:B:494:TRP:HE3	1:B:494:TRP:H	1.20	0.88
1:A:29:ASN:HD22	1:A:497:ARG:HH21	1.22	0.88
1:B:254:ALA:HB2	1:B:259:LEU:HD12	1.55	0.87
1:A:164:ASN:HB3	1:A:331:VAL:HB	1.55	0.87
1:A:297:GLY:HA2	1:A:303:ILE:O	1.75	0.86
1:A:337:ARG:HD3	1:A:338:ASP:O	1.76	0.86
1:A:317:ARG:NH1	1:A:317:ARG:HG2	1.83	0.85
1:A:247:ARG:HD3	1:A:267:SER:CB	2.05	0.85
1:B:412:ARG:HG2	1:B:414:SER:OG	1.77	0.83
1:B:101:ARG:HD2	1:B:101:ARG:H	1.41	0.83
1:B:223:PHE:HE1	1:B:318:PHE:CZ	1.96	0.83
1:B:494:TRP:HH2	1:B:499:TYR:CD2	1.96	0.82
1:A:247:ARG:CD	1:A:267:SER:HB3	2.04	0.82
1:A:117:PHE:O	1:A:118:LYS:HD2	1.80	0.82
1:B:27:VAL:HG23	1:B:36:ILE:O	1.80	0.82
1:B:494:TRP:CH2	1:B:499:TYR:HD2	1.98	0.82
1:A:492:GLU:O	6:A:641:HOH:O	1.96	0.82
1:A:6:PRO:HG2	1:A:311:ASN:HB2	1.62	0.81
1:A:99:PHE:HD2	1:A:448:PRO:HB3	1.46	0.80
1:A:39:TYR:HB2	1:A:81:VAL:HG22	1.63	0.80
1:A:496:ALA:CB	1:A:497:ARG:HB2	2.10	0.80
1:A:173:ASP:O	1:A:174:ILE:HB	1.81	0.80
1:B:121:TYR:OH	1:B:497:ARG:HD2	1.81	0.80
1:A:497:ARG:N	1:A:498:PRO:HD3	1.96	0.80
1:A:15:LEU:HD23	1:A:174:ILE:HD11	1.63	0.80
1:B:186:ASN:ND2	6:B:560:HOH:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PRO:HA	1:A:474:THR:HG22	1.65	0.79
1:B:371:VAL:CG2	1:B:468:MET:HB3	2.12	0.79
1:A:37:TRP:CE3	1:A:77:VAL:HG21	2.15	0.79
1:B:95:LEU:HD12	1:B:98:SER:HB2	1.65	0.79
1:B:341:PHE:N	1:B:342:PRO:HD3	1.97	0.79
1:A:72:GLN:HG2	1:A:154:MET:HE2	1.65	0.78
1:B:356:ARG:NE	1:B:394:ASN:HB2	1.97	0.78
1:B:326:GLN:N	1:B:327:PRO:HD3	1.99	0.78
1:A:101:ARG:HD2	1:A:101:ARG:N	1.99	0.78
1:A:23:PRO:HG2	1:A:37:TRP:HE1	1.50	0.77
1:B:25:LEU:CD1	1:B:501:LEU:HB2	2.15	0.77
1:A:110:ASP:HB2	1:A:489:PRO:CG	2.15	0.77
1:B:8:TYR:CD2	1:B:9:PRO:HD2	2.20	0.77
1:A:317:ARG:HH11	1:A:317:ARG:CG	1.88	0.77
1:A:373:ASN:O	1:A:374:ARG:NH2	2.17	0.77
1:B:219:ARG:HB2	1:B:329:THR:HG23	1.67	0.76
1:B:504:PHE:CE2	1:B:511:PHE:HA	2.21	0.76
1:A:445:HIS:CE1	1:A:447:ALA:HB2	2.19	0.76
1:B:340:PRO:C	1:B:342:PRO:HD3	2.05	0.76
1:B:37:TRP:CE3	1:B:77:VAL:HG21	2.20	0.76
1:B:247:ARG:HG2	1:B:248:LEU:N	1.98	0.76
1:B:412:ARG:H	1:B:420:THR:HB	1.51	0.76
1:A:217:GLU:OE1	1:A:324:THR:HG22	1.85	0.75
1:B:494:TRP:CE2	1:B:498:PRO:HA	2.21	0.75
1:B:15:LEU:HD12	1:B:16:PRO:HD2	1.67	0.75
1:A:371:VAL:CG2	1:A:468:MET:HB3	2.17	0.75
1:B:507:GLN:HG3	1:B:508:SER:H	1.51	0.75
1:B:371:VAL:HG22	1:B:468:MET:HB3	1.68	0.75
1:A:261:GLU:H	1:A:261:GLU:CD	1.89	0.75
1:A:481:TYR:HE1	1:A:495:GLN:HE22	1.31	0.75
1:A:216:VAL:HG13	1:A:221:TYR:CE1	2.22	0.75
1:B:300:ILE:HG23	1:B:301:GLY:N	2.01	0.75
1:A:396:TRP:CD1	1:A:436[A]:ARG:NH2	2.55	0.74
1:A:493:LEU:HD12	1:A:494:TRP:CD1	2.22	0.74
1:A:496:ALA:CA	1:A:497:ARG:HB2	2.17	0.74
1:A:342:PRO:O	1:A:344:PRO:HD3	1.88	0.74
1:A:252:VAL:HG11	1:A:424:TYR:HB3	1.69	0.74
1:B:311:ASN:HD22	1:B:314:LYS:NZ	1.85	0.74
1:A:72:GLN:HE22	1:A:170:GLY:HA2	1.52	0.74
1:B:157:ASP:HB3	1:B:160:GLU:HG2	1.68	0.73
1:B:424:TYR:OH	6:B:691:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:ND2	1:A:497:ARG:HH21	1.84	0.73
1:A:94:HIS:O	1:A:133:TYR:HA	1.87	0.73
1:A:74:PRO:O	1:A:77:VAL:HG12	1.88	0.73
1:A:139:HIS:HD2	1:A:464:ASP:O	1.72	0.73
1:A:361:TRP:HZ3	1:A:363:ILE:HD12	1.52	0.73
1:A:423:PRO:O	1:A:426:SER:HB2	1.88	0.73
1:B:13:VAL:HG12	6:B:670:HOH:O	1.89	0.72
1:B:370:ASP:CB	1:B:466:ASP:HB3	2.18	0.72
1:A:456:HIS:HB3	1:A:468:MET:HG3	1.71	0.72
1:B:116:SER:HB3	1:B:513:VAL:HG21	1.71	0.72
1:B:247:ARG:HG2	1:B:248:LEU:H	1.53	0.72
1:B:409:VAL:HA	1:B:442:VAL:HG12	1.70	0.72
1:B:490:MET:O	1:B:492:GLU:HA	1.89	0.72
1:B:29:ASN:CB	1:B:78:GLU:HG2	2.20	0.72
1:B:15:LEU:HD23	1:B:174:ILE:CD1	2.20	0.72
1:B:177:ILE:HG13	1:B:177:ILE:O	1.90	0.72
1:A:110:ASP:HB2	1:A:489:PRO:HG2	1.70	0.72
1:A:79:THR:HB	1:A:124:ASN:HD21	1.52	0.72
1:B:158:PRO:CA	1:B:161:ASP:HB3	2.15	0.71
1:A:75:ARG:HG2	1:A:125:ARG:HA	1.72	0.71
1:A:27:VAL:HG21	1:A:501:LEU:HD22	1.73	0.71
1:B:164:ASN:HB3	1:B:331:VAL:HB	1.73	0.71
1:B:183:TYR:OH	1:B:205:HIS:HE1	1.74	0.70
1:A:326:GLN:N	1:A:327:PRO:HD3	2.06	0.70
1:A:289:LYS:HE3	1:A:289:LYS:HA	1.71	0.70
1:A:415:GLY:O	1:A:420:THR:HA	1.90	0.70
1:A:85:ASN:HB3	1:A:113:GLU:O	1.90	0.70
1:B:512:SER:O	1:B:513:VAL:HG13	1.92	0.69
1:B:176:MET:HG3	1:B:223:PHE:HB3	1.72	0.69
1:B:86:ASN:HB3	6:B:647:HOH:O	1.92	0.69
1:A:381:VAL:HG22	1:A:473:ALA:HB1	1.74	0.69
1:B:95:LEU:HD12	1:B:98:SER:CB	2.23	0.69
1:B:407:PHE:HB3	1:B:444:ALA:HB2	1.75	0.69
1:B:261:GLU:H	1:B:261:GLU:CD	1.96	0.69
1:A:301:GLY:H	1:A:436[B]:ARG:HG3	1.57	0.69
1:B:494:TRP:CZ2	1:B:498:PRO:HA	2.28	0.69
1:B:72:GLN:NE2	1:B:170:GLY:HA2	2.06	0.69
1:A:252:VAL:HG11	1:A:424:TYR:CB	2.21	0.69
1:B:358:GLY:O	1:B:361:TRP:HB2	1.93	0.69
1:B:375:LEU:HG	1:B:376:LEU:N	2.08	0.68
1:B:356:ARG:CG	1:B:392:ALA:HB3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASN:H	1:A:186:ASN:ND2	1.91	0.68
1:B:302:GLY:O	1:B:303:ILE:HG23	1.92	0.68
1:A:496:ALA:HB3	1:A:497:ARG:CB	2.22	0.68
1:A:497:ARG:H	1:A:498:PRO:HD3	1.58	0.68
1:A:343:SER:HB3	6:A:614:HOH:O	1.94	0.68
1:A:254:ALA:HB2	1:A:259:LEU:HD12	1.75	0.68
1:B:238:PHE:HB3	1:B:291:ILE:CG2	2.24	0.68
1:B:254:ALA:HB3	1:B:278:GLU:HG3	1.74	0.68
1:A:393:GLY:O	1:A:436[A]:ARG:NH2	2.27	0.68
1:A:31:VAL:HG21	1:A:35:GLU:HG3	1.76	0.68
1:B:407:PHE:CE1	1:B:429:LYS:HB2	2.29	0.68
1:A:396:TRP:HD1	1:A:436[A]:ARG:NH2	1.92	0.68
1:A:196:LEU:HD21	1:A:362:THR:O	1.92	0.68
1:A:71:PHE:HB2	1:A:153:TYR:HA	1.75	0.68
1:A:168:GLY:O	1:A:173:ASP:HB2	1.94	0.67
1:B:401:HIS:HB2	1:B:431:VAL:HG22	1.76	0.67
1:B:374:ARG:CA	1:B:374:ARG:HE	2.06	0.67
1:B:246:THR:O	1:B:247:ARG:HB3	1.95	0.67
1:A:371:VAL:HG21	1:A:468:MET:HB3	1.76	0.67
1:B:247:ARG:CD	1:B:267:SER:HB3	2.25	0.67
1:B:269:LEU:HA	6:B:691:HOH:O	1.94	0.67
1:B:79:THR:HB	1:B:124:ASN:HD21	1.58	0.67
1:A:418:ALA:O	1:A:419:ARG:HD2	1.95	0.67
1:A:237:TYR:CZ	1:A:294:ARG:HB2	2.30	0.66
1:B:79:THR:CB	1:B:124:ASN:HD21	2.09	0.66
1:B:370:ASP:HB2	1:B:466:ASP:HB3	1.75	0.66
1:B:355:GLY:O	1:B:356:ARG:HB2	1.94	0.66
1:A:186:ASN:H	1:A:186:ASN:HD22	1.43	0.66
1:B:386:ARG:HD2	1:B:410:ILE:HD12	1.77	0.66
1:A:237:TYR:HE1	1:A:239:ALA:HB3	1.60	0.66
1:B:499:TYR:HB2	1:B:501:LEU:CD1	2.25	0.66
1:A:113:GLU:C	1:A:115:GLY:H	1.99	0.66
1:A:23:PRO:HG2	1:A:37:TRP:NE1	2.11	0.66
1:A:237:TYR:CE1	1:A:239:ALA:HB3	2.31	0.66
1:B:374:ARG:NH2	6:B:643:HOH:O	2.24	0.66
1:B:311:ASN:HD22	1:B:314:LYS:HZ3	1.42	0.66
1:B:421:VAL:HG13	1:B:425:GLU:OE1	1.96	0.66
1:B:82:ARG:NH2	1:B:513:VAL:HB	2.12	0.65
1:B:485:VAL:HG11	1:B:495:GLN:HG2	1.77	0.65
1:B:252:VAL:HG11	1:B:424:TYR:HB3	1.78	0.65
1:A:209:GLN:HG3	1:A:212:PRO:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:HB2	1:A:78:GLU:HG2	1.79	0.65
1:A:15:LEU:CD2	1:A:174:ILE:HD11	2.26	0.65
1:B:158:PRO:HD2	6:B:698:HOH:O	1.96	0.65
1:B:513:VAL:HG23	1:B:514:GLN:H	1.62	0.65
1:B:49:GLN:OE1	1:B:49:GLN:N	2.28	0.65
1:A:493:LEU:O	1:A:494:TRP:HB2	1.97	0.65
1:A:337:ARG:HH11	1:A:339:VAL:HG12	1.60	0.65
1:A:341:PHE:N	1:A:342:PRO:HD3	2.12	0.65
1:A:380:PRO:HA	1:A:474:THR:CG2	2.27	0.65
1:A:123:PRO:O	1:A:125:ARG:HD3	1.97	0.65
1:A:393:GLY:HA2	1:A:437:ARG:H	1.63	0.64
1:A:96:HIS:HB3	1:A:132:TRP:CD1	2.32	0.64
1:B:474:THR:HG23	1:B:475:VAL:H	1.61	0.64
1:A:205:HIS:HA	1:A:209:GLN:O	1.96	0.64
1:A:496:ALA:H	1:A:497:ARG:HB2	1.61	0.64
1:A:34:GLN:C	1:A:35:GLU:HG2	2.17	0.64
1:A:343:SER:O	6:A:683:HOH:O	2.15	0.64
1:A:296:LEU:HD11	1:A:305:THR:O	1.97	0.64
1:B:494:TRP:N	1:B:494:TRP:HE3	1.94	0.64
1:A:326:GLN:N	1:A:327:PRO:CD	2.60	0.64
1:B:407:PHE:HE1	1:B:432:VAL:HG13	1.63	0.64
1:A:364:ASN:HB3	1:A:467:MET:CE	2.28	0.64
1:A:15:LEU:HD12	1:A:16:PRO:HD2	1.78	0.64
1:A:496:ALA:N	1:A:497:ARG:HB2	2.12	0.64
1:B:484:THR:O	1:B:484:THR:HG22	1.97	0.64
1:B:34:GLN:NE2	1:B:499:TYR:O	2.31	0.64
1:B:325:THR:HG22	1:B:327:PRO:CD	2.28	0.64
1:B:2:ALA:O	1:B:3:GLN:HG2	1.98	0.64
1:A:290:THR:O	1:A:290:THR:HG23	1.97	0.64
1:A:474:THR:HG23	1:A:475:VAL:N	2.12	0.63
1:A:341:PHE:CG	1:A:408:LYS:HD2	2.34	0.63
1:A:62:TYR:O	1:A:63:ASP:HB2	1.97	0.63
1:A:364:ASN:HB3	1:A:467:MET:HE2	1.80	0.63
1:B:302:GLY:C	1:B:303:ILE:HG12	2.18	0.63
1:A:247:ARG:O	1:A:248:LEU:HD13	1.99	0.63
1:B:216:VAL:C	1:B:321:ALA:HB2	2.19	0.63
1:A:412:ARG:H	1:A:420:THR:HB	1.64	0.63
1:A:95:LEU:HD12	1:A:98:SER:CB	2.26	0.63
1:A:286:TYR:O	1:A:320:VAL:HG21	1.99	0.63
1:A:237:TYR:HB3	1:A:268:LEU:HD12	1.80	0.63
1:A:496:ALA:HB3	1:A:497:ARG:CD	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:O	1:A:36:ILE:HG13	1.99	0.63
1:B:486:PHE:O	1:B:487:VAL:HG23	1.98	0.63
2:B:601:NAG:H62	2:B:602:NAG:N2	2.13	0.63
1:B:505:GLN:NE2	6:B:571:HOH:O	2.30	0.63
1:A:410:ILE:HG12	1:A:441:VAL:HG13	1.80	0.62
1:B:494:TRP:NE1	1:B:498:PRO:HA	2.13	0.62
1:B:405:VAL:HG21	1:B:444:ALA:HB1	1.79	0.62
1:B:36:ILE:HD11	1:B:497:ARG:HD3	1.79	0.62
1:B:241:THR:O	1:B:289:LYS:HG3	1.99	0.62
1:B:82:ARG:HH22	1:B:513:VAL:HB	1.64	0.62
1:A:29:ASN:CG	1:A:78:GLU:HG2	2.19	0.62
1:B:373:ASN:O	1:B:374:ARG:NH2	2.32	0.62
1:A:412:ARG:HG2	1:A:414:SER:CB	2.26	0.62
1:A:161:ASP:HB2	6:A:635:HOH:O	2.00	0.62
1:B:484:THR:HB	2:B:602:NAG:O7	2.00	0.62
1:B:60:VAL:HG12	1:B:147:ARG:HB3	1.80	0.62
1:A:29:ASN:HB2	1:A:78:GLU:H	1.65	0.62
1:A:403:HIS:O	1:A:404:LEU:HB3	2.00	0.62
1:B:94:HIS:CE1	1:B:403:HIS:CE1	2.88	0.62
1:B:494:TRP:CH2	1:B:499:TYR:CD2	2.81	0.62
1:B:494:TRP:NE1	1:B:497:ARG:O	2.32	0.62
1:A:301:GLY:CA	1:A:436[A]:ARG:H	2.02	0.61
1:A:339:VAL:HG21	1:A:341:PHE:CZ	2.35	0.61
1:A:23:PRO:HG3	1:A:39:TYR:CZ	2.34	0.61
1:B:37:TRP:HE3	1:B:77:VAL:HG21	1.63	0.61
1:B:405:VAL:CG2	1:B:444:ALA:HB1	2.30	0.61
1:B:113:GLU:CB	1:B:114:PRO:CD	2.78	0.61
1:B:113:GLU:HB3	1:B:114:PRO:CD	2.31	0.61
1:A:169:TYR:CD2	1:A:170:GLY:N	2.69	0.61
1:A:220:LYS:HG3	1:A:329:THR:HG22	1.81	0.61
1:A:252:VAL:HA	1:A:279:VAL:HG12	1.82	0.61
1:A:305:THR:HG23	6:A:626:HOH:O	2.00	0.61
1:B:510:GLN:HA	1:B:510:GLN:HE21	1.65	0.61
1:B:412:ARG:H	1:B:420:THR:CB	2.11	0.61
1:A:311:ASN:HD22	1:A:314:LYS:HE2	1.63	0.61
1:A:374:ARG:HB3	6:A:643:HOH:O	1.99	0.61
1:A:289:LYS:CE	1:A:289:LYS:HA	2.29	0.61
1:A:72:GLN:NE2	1:A:170:GLY:HA2	2.15	0.61
1:B:512:SER:C	1:B:513:VAL:HG22	2.21	0.61
1:B:254:ALA:HB3	1:B:278:GLU:CG	2.30	0.61
1:B:309:TYR:O	1:B:310:ASP:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:VAL:HG11	1:B:62:TYR:HB3	1.82	0.61
1:B:342:PRO:O	1:B:344:PRO:HD3	2.01	0.61
1:A:504:PHE:O	1:A:505:GLN:CD	2.39	0.61
1:B:409:VAL:HG12	6:B:550:HOH:O	1.99	0.61
1:B:367:ALA:O	1:B:368:PHE:CB	2.49	0.61
1:A:135:ASP:HB2	1:A:149:GLN:HE21	1.66	0.61
1:B:183:TYR:OH	1:B:205:HIS:CE1	2.53	0.61
1:A:302:GLY:C	1:A:303:ILE:HG12	2.20	0.61
1:B:412:ARG:HG2	1:B:414:SER:HG	1.63	0.60
1:A:99:PHE:HB2	1:A:404:LEU:HD12	1.82	0.60
1:B:49:GLN:HB2	1:B:55:GLY:HA2	1.83	0.60
1:A:482:ASN:N	1:A:482:ASN:ND2	2.48	0.60
1:A:500:GLU:HA	1:A:500:GLU:OE2	2.00	0.60
1:B:201:GLY:O	1:B:232:ARG:NH1	2.34	0.60
1:B:517:THR:HG22	1:B:518:GLU:N	2.16	0.60
1:A:306:ASP:C	1:A:308:ASP:N	2.53	0.60
1:B:501:LEU:HD12	6:B:705:HOH:O	2.01	0.60
1:B:356:ARG:HG2	1:B:392:ALA:HB3	1.83	0.60
1:A:211:TRP:CZ2	1:A:311:ASN:O	2.55	0.60
1:A:91:ASN:OD1	1:A:112:THR:HB	2.00	0.60
1:A:36:ILE:HD13	1:A:121:TYR:HE1	1.67	0.60
1:A:413:THR:O	1:A:413:THR:HG22	2.01	0.60
1:A:99:PHE:CD2	1:A:448:PRO:HB3	2.32	0.60
1:B:495:GLN:HA	1:B:495:GLN:NE2	2.16	0.60
1:A:329:THR:O	1:A:329:THR:HG22	2.01	0.60
1:B:165:LEU:O	1:B:167:SER:N	2.34	0.60
1:B:126:GLN:HB3	1:B:129:ARG:NH2	2.17	0.60
1:B:158:PRO:HA	1:B:161:ASP:CB	2.21	0.59
1:B:169:TYR:C	1:B:171:GLU:N	2.55	0.59
1:A:371:VAL:HG22	1:A:468:MET:HB3	1.83	0.59
1:A:143:GLU:OE2	1:A:192:THR:HG23	2.02	0.59
1:B:123:PRO:O	1:B:125:ARG:HD3	2.02	0.59
1:B:25:LEU:HD11	1:B:501:LEU:HB2	1.84	0.59
1:B:474:THR:CG2	1:B:475:VAL:N	2.65	0.59
1:B:116:SER:CB	1:B:513:VAL:HG21	2.31	0.59
1:B:356:ARG:HG3	1:B:392:ALA:HB3	1.84	0.59
1:A:507:GLN:HG3	1:A:508:SER:N	2.14	0.59
1:A:196:LEU:HD22	1:A:362:THR:HB	1.85	0.59
1:A:302:GLY:O	1:A:303:ILE:HG23	2.03	0.59
1:B:29:ASN:HB2	1:B:78:GLU:CG	2.24	0.59
1:B:456:HIS:HB3	1:B:468:MET:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:HD2	1:A:316:MET:HB3	1.84	0.59
1:A:396:TRP:HD1	1:A:436[A]:ARG:HH21	1.50	0.59
1:A:481:TYR:HE1	1:A:495:GLN:NE2	2.00	0.59
1:B:419:ARG:O	1:B:420:THR:CG2	2.47	0.59
1:A:135:ASP:HB2	1:A:149:GLN:NE2	2.17	0.59
1:B:113:GLU:C	1:B:115:GLY:H	2.05	0.59
1:B:253:ILE:HG13	1:B:278:GLU:HB2	1.83	0.59
1:B:171:GLU:O	1:B:175:PRO:HD3	2.02	0.58
1:A:349:PRO:HA	1:A:386:ARG:O	2.03	0.58
1:A:482:ASN:N	1:A:482:ASN:HD22	2.01	0.58
1:A:484:THR:HG22	1:A:484:THR:O	2.03	0.58
1:B:121:TYR:OH	1:B:497:ARG:CD	2.51	0.58
1:B:373:ASN:O	1:B:374:ARG:CZ	2.50	0.58
1:A:370:ASP:OD1	1:A:370:ASP:N	2.36	0.58
1:B:400:ILE:HD13	1:B:457:CYS:HA	1.85	0.58
1:A:4:ILE:CD1	1:A:4:ILE:N	2.66	0.58
1:B:23:PRO:HG3	1:B:37:TRP:NE1	2.14	0.58
1:B:474:THR:HG23	1:B:475:VAL:N	2.19	0.58
1:A:311:ASN:ND2	1:A:314:LYS:HE2	2.19	0.58
1:A:23:PRO:HG3	1:A:39:TYR:CE1	2.39	0.58
1:B:96:HIS:HB3	1:B:132:TRP:CD1	2.38	0.58
1:A:296:LEU:CD1	1:A:305:THR:H	2.16	0.58
1:A:165:LEU:O	1:A:166:PRO:C	2.41	0.58
1:B:216:VAL:HG11	1:B:283:PHE:CE2	2.39	0.58
1:A:221:TYR:HB2	1:A:281:PHE:HB2	1.86	0.58
1:B:14:PRO:HA	1:B:213:PHE:O	2.02	0.58
1:A:169:TYR:C	1:A:171:GLU:H	2.07	0.58
1:B:223:PHE:CE1	1:B:318:PHE:CZ	2.87	0.58
1:B:412:ARG:HG2	1:B:414:SER:CB	2.33	0.58
1:B:371:VAL:HG21	1:B:468:MET:HB3	1.84	0.58
1:B:507:GLN:HG3	1:B:508:SER:N	2.19	0.58
1:B:7:GLN:O	1:B:51:TYR:CE1	2.57	0.58
1:A:101:ARG:HB2	1:A:104:PHE:HD2	1.69	0.57
1:B:219:ARG:CB	1:B:329:THR:HG23	2.33	0.57
1:A:481:TYR:CE1	1:A:495:GLN:NE2	2.71	0.57
1:A:341:PHE:HB2	1:A:408:LYS:HD2	1.84	0.57
1:B:404:LEU:HD11	1:B:448:PRO:HB2	1.85	0.57
1:B:264:ALA:HB1	1:B:423:PRO:HB2	1.86	0.57
1:B:171:GLU:OE1	1:B:171:GLU:HA	2.03	0.57
1:B:31:VAL:CG2	6:B:689:HOH:O	2.51	0.57
1:B:412:ARG:O	1:B:420:THR:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASP:C	1:B:284:SER:H	2.07	0.57
1:B:325:THR:C	1:B:327:PRO:HD3	2.25	0.57
1:B:268:LEU:HD21	1:B:270:TYR:CE1	2.39	0.57
1:B:273:MET:O	1:B:274:ALA:HB3	2.03	0.57
1:B:329:THR:HG22	1:B:329:THR:O	2.04	0.57
1:B:261:GLU:OE2	1:B:426:SER:HB3	2.04	0.57
1:B:412:ARG:N	1:B:420:THR:HB	2.20	0.57
1:B:29:ASN:O	1:B:31:VAL:N	2.36	0.57
1:A:27:VAL:HG23	1:A:36:ILE:O	2.04	0.57
1:A:230:VAL:HG13	1:A:460:LEU:HB2	1.86	0.57
1:A:392:ALA:HA	1:A:437:ARG:HD3	1.86	0.56
1:B:82:ARG:HH21	1:B:513:VAL:HG12	1.70	0.56
1:B:494:TRP:HZ2	1:B:499:TYR:N	2.03	0.56
1:B:217:GLU:CB	1:B:219:ARG:HG2	2.35	0.56
1:B:321:ALA:O	1:B:322:ASP:CB	2.53	0.56
1:B:445:HIS:CE1	1:B:447:ALA:HB2	2.40	0.56
1:A:83:PHE:N	1:A:119:ASP:OD1	2.36	0.56
1:A:169:TYR:C	1:A:171:GLU:N	2.58	0.56
1:B:247:ARG:HD3	1:B:267:SER:CB	2.30	0.56
1:B:260:LEU:O	1:B:337:ARG:HG3	2.05	0.56
1:A:211:TRP:HZ2	1:A:311:ASN:O	1.88	0.56
1:B:422:MET:HB2	1:B:425:GLU:HG3	1.86	0.56
1:A:110:ASP:CG	1:A:118:LYS:HG2	2.26	0.56
1:A:383:THR:O	1:A:446:TYR:HD2	1.88	0.56
1:B:364:ASN:ND2	6:B:614:HOH:O	2.35	0.56
1:A:256:ASP:HB2	1:A:429:LYS:HA	1.86	0.56
1:A:237:TYR:CE1	1:A:294:ARG:HB2	2.40	0.56
1:A:29:ASN:CB	1:A:78:GLU:HG2	2.34	0.56
1:A:447:ALA:N	1:A:448:PRO:CD	2.69	0.56
1:B:26:THR:O	1:B:27:VAL:HG13	2.06	0.56
1:A:17:ILE:CG2	1:A:172:PHE:HA	2.22	0.55
1:A:494:TRP:O	1:A:495:GLN:HB2	2.06	0.55
1:B:252:VAL:HG11	1:B:424:TYR:CB	2.36	0.55
1:A:504:PHE:HA	6:A:675:HOH:O	2.07	0.55
1:A:126:GLN:HB3	1:A:129:ARG:NH2	2.21	0.55
1:A:317:ARG:NH1	1:A:317:ARG:CG	2.58	0.55
1:A:279:VAL:O	1:A:279:VAL:HG23	2.05	0.55
1:A:386:ARG:HG2	1:A:443:GLU:HG3	1.88	0.55
1:A:452:VAL:HG23	1:A:487:VAL:HG23	1.87	0.55
1:B:164:ASN:HB3	1:B:331:VAL:CB	2.35	0.55
1:A:111:ILE:HG23	1:A:112:THR:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:OG1	1:B:28:THR:HG21	2.07	0.55
1:A:506:ALA:HB2	1:B:49:GLN:OE1	2.06	0.55
1:A:163:LEU:HD13	1:A:165:LEU:HD21	1.87	0.55
1:B:407:PHE:CE1	1:B:432:VAL:HG13	2.42	0.55
1:B:72:GLN:HE22	1:B:170:GLY:HA2	1.70	0.55
1:A:120:TYR:N	1:A:120:TYR:CD1	2.74	0.55
1:B:306:ASP:C	1:B:308:ASP:H	2.09	0.55
1:A:163:LEU:HB3	1:A:165:LEU:HG	1.88	0.55
1:A:16:PRO:O	1:A:17:ILE:HD13	2.06	0.55
1:A:236:LEU:HB3	1:A:293:LEU:HD11	1.89	0.55
1:A:263:PRO:HG2	1:A:333:PRO:HB2	1.87	0.55
1:B:500:GLU:N	1:B:501:LEU:HD13	2.21	0.55
1:A:387:TRP:O	1:A:441:VAL:HG23	2.07	0.55
1:A:384:VAL:HA	1:A:444:ALA:O	2.07	0.55
1:A:313:ASP:OD1	1:A:314:LYS:HG2	2.06	0.55
1:A:480:GLY:O	1:A:482:ASN:N	2.41	0.55
1:A:49:GLN:HB3	1:B:506:ALA:HB2	1.89	0.55
1:B:417:ASN:O	1:B:418:ALA:HB3	2.07	0.55
1:A:251:LYS:O	1:A:279:VAL:HA	2.07	0.54
1:B:36:ILE:HG23	1:B:78:GLU:HB2	1.88	0.54
1:A:367:ALA:O	1:A:368:PHE:CB	2.55	0.54
1:A:133:TYR:HE2	1:A:152:LEU:O	1.89	0.54
1:A:490:MET:HG2	1:A:491:GLU:H	1.71	0.54
1:B:262:HIS:CE1	1:B:335:ASN:HD21	2.25	0.54
1:B:311:ASN:HA	1:B:314:LYS:HZ3	1.73	0.54
1:B:269:LEU:HD11	1:B:277:TYR:CD2	2.42	0.54
1:A:178:LEU:HD23	1:A:206:VAL:HG22	1.89	0.54
1:B:310:ASP:HB3	1:B:312:THR:H	1.72	0.54
1:B:271:ILE:HD11	1:B:275:GLU:O	2.07	0.54
1:A:263:PRO:HD3	1:A:336:LEU:HG	1.88	0.54
1:A:481:TYR:CE1	1:A:495:GLN:OE1	2.61	0.54
1:B:410:ILE:HB	1:B:441:VAL:HG13	1.89	0.54
1:B:75:ARG:HG3	1:B:125:ARG:HA	1.89	0.54
1:B:339:VAL:HG21	1:B:341:PHE:CZ	2.43	0.54
1:A:177:ILE:O	1:A:177:ILE:HG13	2.07	0.54
1:B:6:PRO:HG2	1:B:311:ASN:HB2	1.88	0.54
1:B:105:ASP:CG	1:B:403:HIS:HD1	2.10	0.54
1:A:375:LEU:HG	1:A:376:LEU:N	2.22	0.54
1:A:220:LYS:HA	1:A:281:PHE:O	2.08	0.54
1:B:27:VAL:HB	1:B:36:ILE:N	2.23	0.54
1:A:36:ILE:HD13	1:A:121:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:TYR:HB2	1:B:501:LEU:HD11	1.89	0.53
1:B:34:GLN:HE22	1:B:500:GLU:HG2	1.74	0.53
1:B:216:VAL:O	1:B:320:VAL:HA	2.09	0.53
1:B:412:ARG:HG3	1:B:440:VAL:HG22	1.89	0.53
1:B:326:GLN:N	1:B:327:PRO:CD	2.69	0.53
1:A:456:HIS:HB3	1:A:468:MET:HA	1.89	0.53
1:A:271:ILE:HD11	1:A:275:GLU:O	2.07	0.53
1:B:217:GLU:C	1:B:219:ARG:H	2.12	0.53
1:A:111:ILE:HD11	1:A:137:ALA:HB1	1.90	0.53
1:A:4:ILE:HD12	1:A:4:ILE:N	2.23	0.53
1:B:202:ASP:OD2	1:B:203:VAL:HG23	2.08	0.53
1:A:87:ALA:C	1:A:88:GLU:HG3	2.29	0.53
1:A:215:ASN:HA	1:A:319:VAL:O	2.08	0.53
1:B:487:VAL:O	1:B:490:MET:HG3	2.08	0.53
1:B:94:HIS:NE2	1:B:96:HIS:HA	2.23	0.53
1:A:375:LEU:O	1:A:376:LEU:HD23	2.08	0.53
1:B:383:THR:HG22	1:B:384:VAL:N	2.23	0.53
1:B:92:SER:HB2	1:B:110:ASP:O	2.08	0.53
1:B:475:VAL:HG22	6:B:584:HOH:O	2.08	0.53
1:A:386:ARG:HD2	1:A:410:ILE:HD11	1.91	0.53
1:A:16:PRO:HG2	1:A:209:GLN:HB2	1.90	0.53
1:B:494:TRP:N	1:B:494:TRP:CE3	2.71	0.53
1:B:217:GLU:O	1:B:283:PHE:HB2	2.09	0.53
1:B:478:ASP:CG	1:B:479:TYR:H	2.12	0.53
1:B:83:PHE:N	1:B:119:ASP:OD1	2.42	0.53
1:B:152:LEU:HD13	1:B:153:TYR:H	1.73	0.53
1:A:237:TYR:CD1	1:A:237:TYR:C	2.82	0.53
1:B:15:LEU:HD12	1:B:16:PRO:CD	2.36	0.53
1:A:475:VAL:HB	2:A:601:NAG:H61	1.90	0.53
1:A:102:ALA:HB3	1:A:488:ASP:H	1.72	0.53
1:A:341:PHE:HB3	1:A:428:LEU:HD11	1.91	0.53
1:B:259:LEU:O	1:B:337:ARG:HD2	2.09	0.53
1:A:112:THR:HG22	1:A:113:GLU:O	2.08	0.53
1:A:51:TYR:HB3	1:A:54:LEU:HD13	1.89	0.53
1:B:417:ASN:O	1:B:418:ALA:CB	2.56	0.53
1:A:79:THR:CB	1:A:124:ASN:HD21	2.22	0.53
1:B:329:THR:O	1:B:330:SER:HB2	2.09	0.53
1:B:382:GLY:O	1:B:445:HIS:CE1	2.62	0.53
1:A:417:ASN:O	1:A:418:ALA:HB2	2.09	0.53
1:A:478:ASP:O	1:A:479:TYR:C	2.46	0.53
1:B:174:ILE:O	1:B:174:ILE:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASP:HB3	1:B:466:ASP:HB3	1.91	0.52
1:A:216:VAL:HG13	1:A:221:TYR:HE1	1.74	0.52
1:A:375:LEU:HB2	1:A:470:ALA:HB3	1.91	0.52
1:A:412:ARG:O	1:A:414:SER:N	2.41	0.52
1:A:311:ASN:HD22	1:A:314:LYS:CE	2.23	0.52
1:A:55:GLY:O	1:A:56:SER:HB3	2.10	0.52
1:B:17:ILE:CG2	1:B:172:PHE:HA	2.25	0.52
1:A:25:LEU:HD13	1:A:501:LEU:HB2	1.91	0.52
1:A:247:ARG:HG2	1:A:248:LEU:H	1.74	0.52
1:B:131:LEU:HD11	1:B:155:LEU:HB2	1.91	0.52
1:A:374:ARG:HE	1:A:374:ARG:CA	2.23	0.52
1:A:301:GLY:CA	1:A:436[B]:ARG:H	2.02	0.52
1:A:101:ARG:HB2	1:A:104:PHE:CD2	2.45	0.52
1:A:80:VAL:HG22	1:A:121:TYR:CD1	2.45	0.52
1:B:507:GLN:CG	1:B:508:SER:H	2.18	0.52
1:A:168:GLY:O	1:A:169:TYR:O	2.28	0.52
1:B:216:VAL:O	1:B:321:ALA:N	2.43	0.52
1:B:373:ASN:O	1:B:374:ARG:NE	2.43	0.52
1:A:324:THR:CG2	1:A:325:THR:N	2.73	0.52
1:B:409:VAL:HG11	1:B:425:GLU:HB3	1.91	0.52
1:B:160:GLU:C	1:B:162:ALA:H	2.13	0.51
1:B:104:PHE:CE2	1:B:121:TYR:HB3	2.46	0.51
1:B:217:GLU:HB3	1:B:219:ARG:HG2	1.92	0.51
1:A:110:ASP:OD2	1:A:118:LYS:HG2	2.10	0.51
1:B:411:SER:HB2	1:B:441:VAL:HG12	1.91	0.51
1:B:113:GLU:C	1:B:115:GLY:N	2.63	0.51
1:A:302:GLY:O	1:A:303:ILE:HG12	2.11	0.51
1:B:15:LEU:HD23	1:B:174:ILE:HD11	1.92	0.51
1:B:517:THR:CG2	1:B:518:GLU:N	2.73	0.51
1:A:127:SER:HB3	6:A:608:HOH:O	2.10	0.51
1:B:196:LEU:HD22	1:B:362:THR:HG22	1.93	0.51
1:A:59:LEU:HD22	1:A:147:ARG:O	2.11	0.51
1:B:31:VAL:HG23	6:B:689:HOH:O	2.11	0.51
1:A:456:HIS:CB	1:A:468:MET:HG3	2.39	0.51
1:B:424:TYR:CZ	6:B:691:HOH:O	2.54	0.51
1:B:379:VAL:HG11	1:B:446:TYR:CD2	2.46	0.51
1:B:356:ARG:NH1	1:B:394:ASN:OD1	2.44	0.51
1:A:324:THR:HG23	1:A:325:THR:N	2.26	0.51
1:B:456:HIS:HB3	1:B:468:MET:HG3	1.93	0.51
1:B:288:GLY:H	1:B:320:VAL:HG21	1.76	0.51
1:A:373:ASN:O	1:A:374:ARG:NE	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:CD1	1:A:320:VAL:HG22	2.46	0.51
1:A:103:ALA:HB2	1:A:488:ASP:O	2.10	0.51
1:A:297:GLY:HA2	1:A:303:ILE:C	2.31	0.51
1:B:116:SER:O	1:B:513:VAL:HG11	2.11	0.50
1:B:35:GLU:O	1:B:36:ILE:HG13	2.10	0.50
1:B:501:LEU:HD23	1:B:502:GLY:O	2.11	0.50
1:B:300:ILE:CG2	1:B:301:GLY:H	2.16	0.50
1:A:497:ARG:N	1:A:498:PRO:CD	2.72	0.50
1:B:310:ASP:HA	6:B:609:HOH:O	2.10	0.50
1:B:423:PRO:HG2	1:B:424:TYR:CD2	2.45	0.50
1:B:50:VAL:HG23	1:B:51:TYR:H	1.76	0.50
1:B:107:TRP:HB3	1:B:110:ASP:HB3	1.93	0.50
1:B:305:THR:HG23	6:B:697:HOH:O	2.09	0.50
1:B:480:GLY:O	1:B:482:ASN:N	2.44	0.50
1:A:174:ILE:O	1:A:174:ILE:HG23	2.10	0.50
1:A:219:ARG:HB2	1:A:329:THR:HG23	1.94	0.50
1:A:77:VAL:O	1:A:124:ASN:HB2	2.11	0.50
1:A:110:ASP:OD1	1:A:489:PRO:HB3	2.11	0.50
1:B:403:HIS:O	1:B:404:LEU:HB3	2.12	0.50
1:B:113:GLU:HB3	1:B:114:PRO:HD3	1.92	0.50
1:B:355:GLY:O	1:B:356:ARG:CB	2.59	0.50
1:A:296:LEU:HD13	1:A:305:THR:H	1.75	0.50
1:A:67:PRO:HG3	1:A:177:ILE:HD11	1.94	0.50
1:B:24:ARG:HH22	1:B:504:PHE:HA	1.77	0.50
1:B:350:ARG:HB2	1:B:387:TRP:CD1	2.47	0.50
1:A:196:LEU:HA	1:A:465:HIS:HD2	1.75	0.50
1:A:414:SER:HB2	1:A:438:GLU:HG2	1.93	0.50
1:A:420:THR:OG1	1:A:421:VAL:HG23	2.11	0.50
1:A:306:ASP:C	1:A:308:ASP:H	2.13	0.50
1:B:379:VAL:O	1:B:473:ALA:HA	2.11	0.50
1:B:146:TYR:CD2	1:B:192:THR:HG23	2.47	0.50
1:B:241:THR:HG23	1:B:248:LEU:HD21	1.93	0.50
1:B:216:VAL:CA	1:B:321:ALA:HB2	2.42	0.50
1:A:21:LYS:HG2	1:A:71:PHE:CZ	2.47	0.50
1:B:168:GLY:O	1:B:173:ASP:HB2	2.11	0.50
1:A:49:GLN:OE1	1:A:49:GLN:N	2.42	0.50
1:B:48:HIS:O	1:B:57:ALA:HB3	2.12	0.50
1:A:391:ASN:O	1:A:437:ARG:HA	2.11	0.50
1:A:493:LEU:HD12	1:A:494:TRP:HD1	1.75	0.50
1:A:374:ARG:HE	1:A:374:ARG:HA	1.77	0.50
1:A:127:SER:O	1:A:155:LEU:HD23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ILE:HG13	1:A:436[B]:ARG:HD3	1.94	0.49
1:B:84:ILE:HG23	1:B:514:GLN:NE2	2.26	0.49
1:B:370:ASP:N	1:B:370:ASP:OD1	2.41	0.49
1:B:451:GLY:HA2	1:B:487:VAL:CG2	2.42	0.49
1:B:302:GLY:O	1:B:303:ILE:HG12	2.12	0.49
1:A:452:VAL:HG23	1:A:487:VAL:CG2	2.42	0.49
1:A:45:PRO:HA	1:A:60:VAL:HA	1.94	0.49
1:A:164:ASN:O	1:A:330:SER:HB3	2.12	0.49
1:B:15:LEU:CD2	1:B:174:ILE:HD11	2.42	0.49
1:B:238:PHE:HB3	1:B:291:ILE:HG21	1.94	0.49
1:B:164:ASN:CB	1:B:331:VAL:HB	2.42	0.49
1:B:301:GLY:CA	1:B:397:THR:HG21	2.41	0.49
1:A:309:TYR:O	1:A:310:ASP:C	2.50	0.49
1:A:220:LYS:HG3	1:A:329:THR:CG2	2.43	0.49
1:B:116:SER:CA	1:B:513:VAL:HG21	2.42	0.49
1:B:375:LEU:CG	1:B:376:LEU:N	2.74	0.49
1:A:371:VAL:HG11	1:A:468:MET:HE2	1.93	0.49
1:B:386:ARG:HD3	1:B:443:GLU:OE2	2.12	0.49
1:A:218:PRO:HB3	1:A:287:ALA:HB2	1.94	0.49
1:A:386:ARG:HD2	1:A:410:ILE:CD1	2.42	0.49
1:A:252:VAL:HG11	1:A:424:TYR:HB2	1.95	0.49
1:B:25:LEU:HG	1:B:38:TYR:CD1	2.46	0.49
1:A:149:GLN:HG3	6:A:599:HOH:O	2.12	0.49
1:B:195:GLU:OE2	1:B:461:ILE:HG21	2.12	0.49
1:A:160:GLU:C	1:A:162:ALA:H	2.14	0.49
1:B:290:THR:O	1:B:290:THR:HG23	2.11	0.49
1:A:247:ARG:HG2	1:A:248:LEU:N	2.27	0.49
1:B:511:PHE:CG	1:B:512:SER:N	2.79	0.49
1:A:341:PHE:CB	1:A:408:LYS:HD2	2.43	0.49
1:B:268:LEU:O	6:B:691:HOH:O	2.20	0.49
1:A:283:PHE:HD1	1:A:320:VAL:HG22	1.78	0.49
1:A:407:PHE:HB3	1:A:444:ALA:HB2	1.94	0.49
1:B:111:ILE:HD11	1:B:137:ALA:CB	2.41	0.49
1:A:272:SER:OG	1:A:399:PRO:HG3	2.13	0.49
1:A:214:LYS:HG3	6:A:649:HOH:O	2.11	0.49
1:A:183:TYR:OH	1:A:205:HIS:CE1	2.66	0.49
1:B:92:SER:HB2	1:B:111:ILE:HD12	1.94	0.49
1:B:263:PRO:HG2	1:B:333:PRO:HB2	1.93	0.49
1:A:301:GLY:O	1:A:302:GLY:C	2.50	0.49
1:B:4:ILE:O	1:B:4:ILE:HG22	2.13	0.49
1:A:75:ARG:CG	1:A:125:ARG:HA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HD12	1:B:84:ILE:N	2.28	0.49
1:B:35:GLU:N	6:B:689:HOH:O	2.45	0.49
1:B:325:THR:HG22	1:B:327:PRO:HD3	1.94	0.49
1:A:90:PRO:HA	1:A:112:THR:O	2.12	0.49
1:B:49:GLN:O	1:B:49:GLN:CG	2.60	0.49
1:A:407:PHE:CE1	1:A:432:VAL:HG13	2.47	0.49
1:B:345:THR:HB	1:B:384:VAL:HG22	1.94	0.49
1:A:168:GLY:O	1:A:173:ASP:CB	2.61	0.49
1:A:49:GLN:O	1:A:49:GLN:CD	2.51	0.49
1:A:346:THR:HG22	1:A:386:ARG:NH1	2.28	0.48
1:B:247:ARG:O	1:B:248:LEU:HD13	2.13	0.48
1:A:421:VAL:HG12	1:A:422:MET:N	2.28	0.48
1:A:25:LEU:HD12	1:A:501:LEU:HD13	1.95	0.48
1:A:495:GLN:HA	3:A:611:NDG:H6C2	1.95	0.48
1:A:403:HIS:CE1	1:A:454:MET:HE3	2.48	0.48
1:A:477:PRO:HA	1:A:483:ALA:HB2	1.95	0.48
1:A:164:ASN:CB	1:A:331:VAL:HB	2.37	0.48
5:B:611:NAG:O3	5:B:612:NAG:N2	2.44	0.48
1:A:355:GLY:O	1:A:395:GLY:N	2.46	0.48
1:B:259:LEU:O	1:B:337:ARG:NH1	2.46	0.48
1:A:348:THR:HA	1:A:349:PRO:HD3	1.69	0.48
1:B:350:ARG:NH1	1:B:377:ALA:HB1	2.28	0.48
1:B:4:ILE:HD12	1:B:4:ILE:N	2.27	0.48
1:A:460:LEU:O	1:A:464:ASP:HB2	2.14	0.48
1:A:495:GLN:HB3	1:A:496:ALA:H	1.42	0.48
1:B:169:TYR:C	1:B:171:GLU:H	2.16	0.48
1:A:54:LEU:N	1:A:54:LEU:HD12	2.29	0.48
1:A:101:ARG:O	1:A:105:ASP:HB2	2.13	0.48
1:A:20:VAL:HG12	1:B:22:GLN:NE2	2.28	0.48
1:B:35:GLU:C	1:B:36:ILE:HG13	2.34	0.48
1:B:281:PHE:C	1:B:282:ASP:OD1	2.51	0.48
1:A:113:GLU:C	1:A:115:GLY:N	2.66	0.48
1:A:74:PRO:HA	1:A:156:THR:OG1	2.13	0.48
1:A:385:GLU:CD	6:A:668:HOH:O	2.51	0.48
1:B:491:GLU:OE1	1:B:491:GLU:O	2.32	0.48
1:A:300:ILE:HG13	1:A:436[B]:ARG:CD	2.44	0.48
1:B:27:VAL:HG12	1:B:35:GLU:HB3	1.96	0.48
1:A:493:LEU:HD23	1:A:493:LEU:H	1.78	0.48
1:A:6:PRO:HG2	1:A:311:ASN:CB	2.39	0.48
1:B:395:GLY:HA3	1:B:398:HIS:NE2	2.29	0.48
1:A:164:ASN:O	1:A:165:LEU:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:CG1	1:B:35:GLU:HB3	2.44	0.47
1:A:158:PRO:HA	1:A:161:ASP:CB	2.32	0.47
1:B:169:TYR:CD2	1:B:170:GLY:N	2.82	0.47
1:A:165:LEU:O	1:A:167:SER:N	2.47	0.47
1:B:514:GLN:O	1:B:515:ALA:O	2.32	0.47
1:B:238:PHE:CZ	1:B:281:PHE:HE1	2.31	0.47
1:B:239:ALA:O	1:B:241:THR:N	2.47	0.47
1:A:95:LEU:CD1	1:A:98:SER:HB2	2.36	0.47
1:B:300:ILE:CG2	1:B:301:GLY:N	2.72	0.47
1:B:96:HIS:CE1	1:B:401:HIS:CE1	3.02	0.47
1:B:367:ALA:O	1:B:368:PHE:HB2	2.14	0.47
1:B:51:TYR:HA	1:B:52:PRO:HD3	1.80	0.47
1:A:54:LEU:HD12	1:A:54:LEU:H	1.79	0.47
1:A:341:PHE:HD1	1:A:341:PHE:O	1.98	0.47
1:A:323:ASP:O	1:B:31:VAL:HG12	2.13	0.47
1:A:62:TYR:OH	6:A:595:HOH:O	2.19	0.47
1:A:385:GLU:HB2	1:A:446:TYR:HE2	1.80	0.47
1:A:181:LYS:NZ	6:A:583:HOH:O	2.41	0.47
1:B:216:VAL:HG11	1:B:283:PHE:CZ	2.50	0.47
1:A:5:SER:OG	6:A:632:HOH:O	2.20	0.47
1:B:4:ILE:HB	1:B:310:ASP:OD1	2.14	0.47
1:B:157:ASP:CB	1:B:160:GLU:HG2	2.40	0.47
1:B:409:VAL:O	1:B:409:VAL:HG13	2.15	0.47
1:A:296:LEU:HA	1:A:296:LEU:HD22	1.76	0.47
1:A:407:PHE:HE1	1:A:432:VAL:CG1	2.27	0.47
1:A:379:VAL:HG11	1:A:446:TYR:CG	2.49	0.47
1:A:254:ALA:HB3	1:A:278:GLU:HB2	1.95	0.47
1:B:60:VAL:O	1:B:60:VAL:HG13	2.14	0.47
1:B:296:LEU:HB3	6:B:565:HOH:O	2.15	0.47
1:A:269:LEU:HD11	1:A:277:TYR:HB2	1.96	0.47
1:B:36:ILE:CG2	1:B:37:TRP:N	2.78	0.47
1:B:316:MET:SD	1:B:318:PHE:CZ	3.08	0.47
1:A:158:PRO:CA	1:A:161:ASP:HB3	2.32	0.47
1:B:310:ASP:HB3	1:B:311:ASN:H	1.37	0.47
1:B:5:SER:HA	1:B:6:PRO:HD3	1.64	0.47
1:A:9:PRO:O	1:A:12:THR:HG22	2.14	0.47
1:B:21:LYS:HG2	1:B:71:PHE:CZ	2.50	0.47
1:A:39:TYR:HA	6:A:542:HOH:O	2.14	0.47
1:B:216:VAL:HG13	1:B:221:TYR:CE1	2.50	0.47
1:B:321:ALA:O	1:B:322:ASP:CG	2.53	0.47
1:B:374:ARG:O	1:B:375:LEU:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:VAL:HG21	1:A:444:ALA:HB1	1.97	0.47
1:A:54:LEU:HD23	1:A:185:ALA:O	2.15	0.47
1:B:495:GLN:O	1:B:496:ALA:C	2.53	0.47
1:A:27:VAL:HA	6:A:645:HOH:O	2.15	0.47
1:A:62:TYR:CD1	1:A:133:TYR:CE1	3.03	0.47
1:B:139:HIS:CD2	1:B:464:ASP:O	2.68	0.47
1:B:380:PRO:HB2	1:B:383:THR:OG1	2.15	0.47
1:A:170:GLY:O	1:A:171:GLU:C	2.53	0.46
1:A:203:VAL:O	1:A:205:HIS:CD2	2.69	0.46
1:A:302:GLY:H	1:A:436[B]:ARG:HE	1.63	0.46
1:A:496:ALA:CB	1:A:497:ARG:HD2	2.36	0.46
1:B:515:ALA:O	1:B:516:VAL:HG12	2.15	0.46
1:A:20:VAL:HG22	1:A:21:LYS:N	2.30	0.46
1:A:21:LYS:HG2	1:A:71:PHE:CE1	2.50	0.46
1:A:171:GLU:HB3	1:A:175:PRO:HG3	1.97	0.46
1:A:219:ARG:HH12	1:A:330:SER:N	2.14	0.46
1:A:379:VAL:HG11	1:A:446:TYR:CD2	2.50	0.46
1:A:349:PRO:CA	1:A:386:ARG:O	2.62	0.46
1:B:44:LYS:HA	1:B:45:PRO:HD3	1.69	0.46
1:B:101:ARG:CD	1:B:101:ARG:H	2.18	0.46
1:B:341:PHE:N	1:B:342:PRO:CD	2.73	0.46
1:A:254:ALA:HA	1:A:259:LEU:HA	1.96	0.46
1:B:44:LYS:HE3	1:B:64:GLY:HA3	1.96	0.46
1:A:502:GLY:O	1:A:503:GLU:CB	2.64	0.46
1:A:382:GLY:O	1:A:445:HIS:HE1	1.98	0.46
1:B:204:ILE:O	1:B:210:PRO:HA	2.15	0.46
1:A:238:PHE:CZ	1:A:281:PHE:CE1	3.03	0.46
1:A:110:ASP:OD1	1:A:118:LYS:HG2	2.16	0.46
1:B:54:LEU:HA	6:B:585:HOH:O	2.16	0.46
1:A:252:VAL:HG22	1:A:279:VAL:HG12	1.98	0.46
1:B:223:PHE:CD2	1:B:281:PHE:CE2	3.04	0.46
1:B:321:ALA:O	1:B:322:ASP:HB2	2.16	0.46
1:A:379:VAL:O	1:A:473:ALA:HA	2.16	0.46
1:A:169:TYR:CG	1:A:170:GLY:N	2.82	0.46
1:B:79:THR:HG22	1:B:122:TYR:HD2	1.80	0.46
1:B:78:GLU:C	1:B:124:ASN:HD22	2.19	0.46
1:B:79:THR:CG2	1:B:122:TYR:HD2	2.28	0.46
1:A:500:GLU:CA	1:A:500:GLU:OE2	2.64	0.46
1:B:395:GLY:O	1:B:398:HIS:CE1	2.69	0.46
1:A:146:TYR:O	1:A:181:LYS:HE2	2.15	0.46
1:A:73:VAL:HG11	1:A:124:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ARG:NE	1:B:374:ARG:HA	2.15	0.46
1:A:261:GLU:N	1:A:261:GLU:CD	2.66	0.46
1:A:506:ALA:CB	1:B:49:GLN:OE1	2.64	0.46
1:A:106:GLY:HA2	6:A:653:HOH:O	2.15	0.46
1:B:217:GLU:HB2	1:B:219:ARG:HG2	1.97	0.46
1:A:23:PRO:CG	1:A:37:TRP:HE1	2.25	0.45
1:B:78:GLU:C	1:B:124:ASN:ND2	2.70	0.45
1:B:412:ARG:CG	1:B:414:SER:OG	2.57	0.45
1:B:105:ASP:OD1	1:B:403:HIS:ND1	2.45	0.45
1:B:170:GLY:O	1:B:171:GLU:C	2.54	0.45
1:A:411:SER:OG	1:A:441:VAL:HG12	2.16	0.45
1:B:505:GLN:HE21	1:B:505:GLN:N	2.14	0.45
1:B:311:ASN:ND2	1:B:314:LYS:NZ	2.59	0.45
1:A:361:TRP:HZ3	1:A:363:ILE:CD1	2.24	0.45
1:B:174:ILE:HG12	1:B:223:PHE:CE1	2.52	0.45
1:B:263:PRO:HD3	1:B:336:LEU:HG	1.98	0.45
1:B:21:LYS:N	1:B:70:THR:O	2.45	0.45
1:B:436[A]:ARG:NH1	6:B:635:HOH:O	2.49	0.45
1:A:165:LEU:O	1:A:222:ARG:NH1	2.49	0.45
1:A:285:ASP:OD1	1:A:285:ASP:N	2.49	0.45
1:A:428:LEU:HA	1:A:428:LEU:HD12	1.80	0.45
1:A:386:ARG:CD	1:A:410:ILE:CD1	2.95	0.45
1:A:66:SER:HA	1:A:67:PRO:C	2.37	0.45
1:A:375:LEU:N	6:A:558:HOH:O	2.50	0.45
1:B:29:ASN:HB3	1:B:30:PRO:HD3	1.99	0.45
1:B:23:PRO:HB3	1:B:39:TYR:CZ	2.51	0.45
1:B:74:PRO:O	1:B:77:VAL:HG12	2.17	0.45
1:B:176:MET:HE2	1:B:225:PHE:CE2	2.51	0.45
1:B:281:PHE:CD2	1:B:281:PHE:N	2.84	0.45
1:B:405:VAL:HG23	1:B:445:HIS:O	2.17	0.45
1:B:7:GLN:HG2	1:B:51:TYR:HE1	1.81	0.45
1:A:160:GLU:C	1:A:162:ALA:N	2.69	0.45
1:B:503:GLU:OE1	1:B:503:GLU:N	2.49	0.45
1:B:221:TYR:HB3	1:B:223:PHE:HE2	1.82	0.45
1:A:99:PHE:H	1:A:99:PHE:HD1	1.63	0.45
1:B:229:ALA:O	1:B:273:MET:HG3	2.16	0.45
1:B:437:ARG:C	1:B:437:ARG:HD2	2.37	0.45
1:A:79:THR:HB	1:A:124:ASN:ND2	2.27	0.45
1:B:164:ASN:O	1:B:330:SER:HB3	2.17	0.45
1:A:493:LEU:HD12	1:A:498:PRO:HB3	1.99	0.45
1:A:119:ASP:HA	1:A:120:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PRO:O	1:B:458:HIS:N	2.50	0.45
1:A:300:ILE:HD12	1:A:300:ILE:HA	1.81	0.45
1:A:73:VAL:HG12	1:A:77:VAL:HG13	1.99	0.45
1:B:382:GLY:O	1:B:445:HIS:HE1	1.99	0.45
1:A:238:PHE:O	1:A:248:LEU:HB2	2.17	0.45
1:B:505:GLN:HE21	1:B:505:GLN:H	1.63	0.45
1:B:501:LEU:N	1:B:501:LEU:HD13	2.31	0.45
1:B:95:LEU:HD11	1:B:131:LEU:HD22	1.99	0.45
1:B:262:HIS:ND1	1:B:335:ASN:ND2	2.65	0.45
1:B:90:PRO:HA	1:B:112:THR:O	2.17	0.45
1:B:251:LYS:O	1:B:279:VAL:HA	2.17	0.44
1:A:295:ASN:N	1:A:313:ASP:O	2.46	0.44
1:B:345:THR:HB	1:B:384:VAL:HG13	1.99	0.44
1:A:459:ASN:C	1:A:459:ASN:OD1	2.56	0.44
1:B:218:PRO:HA	1:B:283:PHE:O	2.16	0.44
1:B:227:ASP:HB3	1:B:272:SER:O	2.17	0.44
1:A:84:ILE:HD12	1:A:84:ILE:H	1.81	0.44
1:A:389:LEU:N	1:A:440:VAL:O	2.43	0.44
1:B:177:ILE:O	1:B:177:ILE:CG1	2.64	0.44
1:B:296:LEU:CD1	1:B:305:THR:H	2.29	0.44
1:B:285:ASP:C	1:B:287:ALA:H	2.21	0.44
1:B:223:PHE:N	1:B:223:PHE:HD2	2.15	0.44
1:B:393:GLY:O	1:B:436[A]:ARG:NH2	2.50	0.44
1:A:279:VAL:O	1:A:281:PHE:CE2	2.71	0.44
1:B:75:ARG:HG2	1:B:76:GLY:N	2.33	0.44
1:B:85:ASN:HB3	1:B:113:GLU:O	2.18	0.44
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.85	0.44
1:B:381:VAL:HG22	1:B:473:ALA:HB1	1.99	0.44
1:B:191:THR:C	1:B:193:ASN:H	2.21	0.44
1:A:388:GLU:OE1	1:A:390:ILE:HD11	2.17	0.44
1:A:349:PRO:HB3	1:A:386:ARG:O	2.17	0.44
1:B:116:SER:HB2	1:B:117:PHE:HD1	1.82	0.44
1:A:380:PRO:O	1:A:383:THR:HB	2.17	0.44
1:B:171:GLU:HB3	1:B:175:PRO:HD3	1.99	0.44
1:B:34:GLN:O	1:B:35:GLU:HG2	2.18	0.44
1:B:223:PHE:CD2	1:B:223:PHE:N	2.85	0.44
1:A:412:ARG:H	1:A:420:THR:CB	2.28	0.44
1:B:253:ILE:O	1:B:259:LEU:HA	2.17	0.44
1:B:509:GLY:O	1:B:517:THR:HG21	2.18	0.44
1:B:345:THR:CB	1:B:384:VAL:HG13	2.48	0.44
1:A:273:MET:O	1:A:274:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:HG21	1:A:463:GLU:OE2	2.18	0.44
1:A:165:LEU:N	1:A:331:VAL:HG12	2.32	0.44
1:B:310:ASP:O	1:B:311:ASN:CG	2.56	0.44
1:A:499:TYR:O	1:A:500:GLU:HB2	2.18	0.44
1:A:453:TYR:O	1:A:470:ALA:HA	2.18	0.44
1:B:130:THR:OG1	1:B:224:ARG:HD3	2.17	0.44
1:B:167:SER:C	1:B:169:TYR:N	2.71	0.43
1:A:4:ILE:CD1	1:A:4:ILE:H	2.30	0.43
1:A:487:VAL:O	1:A:488:ASP:HB2	2.17	0.43
1:B:130:THR:HG23	1:B:152:LEU:HD11	2.00	0.43
1:B:54:LEU:N	1:B:54:LEU:CD1	2.81	0.43
1:A:249:PRO:O	1:A:250:PHE:CD1	2.71	0.43
1:B:117:PHE:O	1:B:118:LYS:HB2	2.18	0.43
1:B:36:ILE:HG22	1:B:37:TRP:N	2.33	0.43
1:A:29:ASN:O	1:A:31:VAL:N	2.51	0.43
1:B:491:GLU:HA	1:B:492:GLU:HA	1.76	0.43
1:A:85:ASN:HD22	1:A:85:ASN:C	2.22	0.43
1:B:366:VAL:O	1:B:367:ALA:C	2.56	0.43
1:A:490:MET:HE2	1:A:490:MET:HB3	1.80	0.43
1:A:209:GLN:CG	1:A:212:PRO:HG3	2.45	0.43
1:B:176:MET:SD	1:B:223:PHE:CD1	3.12	0.43
1:A:99:PHE:CD1	1:A:99:PHE:N	2.86	0.43
1:B:376:LEU:HB3	1:B:377:ALA:H	1.68	0.43
1:A:373:ASN:O	1:A:374:ARG:CZ	2.65	0.43
1:A:259:LEU:H	1:A:259:LEU:CD1	2.31	0.43
1:A:364:ASN:HB3	1:A:467:MET:HE3	1.98	0.43
1:A:308:ASP:N	1:A:308:ASP:OD1	2.51	0.43
1:A:485:VAL:O	1:A:490:MET:CE	2.65	0.43
1:B:182:GLN:HB3	1:B:190:VAL:HB	2.00	0.43
1:B:66:SER:HA	1:B:67:PRO:C	2.39	0.43
1:B:82:ARG:NH2	1:B:513:VAL:CB	2.79	0.43
1:B:497:ARG:HE	1:B:497:ARG:HB3	1.37	0.43
1:B:499:TYR:HD1	1:B:500:GLU:H	1.63	0.43
1:A:80:VAL:HG22	1:A:121:TYR:HD1	1.83	0.43
1:A:95:LEU:HD11	1:A:131:LEU:HD22	1.99	0.43
1:B:49:GLN:O	1:B:49:GLN:HG2	2.18	0.43
1:A:499:TYR:O	1:A:500:GLU:CB	2.66	0.43
1:A:306:ASP:O	1:A:308:ASP:N	2.51	0.43
1:A:127:SER:H	1:A:129:ARG:HH21	1.66	0.43
1:B:224:ARG:NH2	6:B:645:HOH:O	2.51	0.43
1:B:244:ILE:HG12	1:B:244:ILE:H	1.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:NH2	1:A:394:ASN:HB2	2.32	0.43
1:B:289:LYS:O	1:B:320:VAL:HG22	2.18	0.43
1:A:122:TYR:HA	1:A:123:PRO:HD3	1.77	0.43
1:B:412:ARG:O	1:B:414:SER:N	2.41	0.43
1:A:507:GLN:HB3	6:A:586:HOH:O	2.18	0.43
1:A:311:ASN:HD22	1:A:314:LYS:NZ	2.17	0.43
1:B:34:GLN:NE2	1:B:500:GLU:HG2	2.33	0.43
1:B:220:LYS:H	1:B:329:THR:HG23	1.83	0.43
1:A:131:LEU:H	1:A:131:LEU:HD12	1.84	0.43
1:B:339:VAL:HA	1:B:340:PRO:HD3	1.67	0.43
1:B:403:HIS:HB2	1:B:453:TYR:HB3	2.01	0.43
1:A:259:LEU:H	1:A:259:LEU:HD13	1.82	0.43
1:B:510:GLN:HA	1:B:510:GLN:NE2	2.31	0.43
1:A:135:ASP:CG	1:A:144:ASN:HD22	2.21	0.43
1:A:353:ARG:HG3	1:A:390:ILE:HB	2.00	0.43
1:A:251:LYS:HD3	1:A:333:PRO:HG2	2.00	0.43
1:A:356:ARG:NH1	1:A:394:ASN:HD22	2.17	0.43
1:B:280:VAL:C	1:B:281:PHE:CD2	2.92	0.43
1:A:496:ALA:H	1:A:497:ARG:CB	2.30	0.43
1:B:374:ARG:CA	1:B:374:ARG:NE	2.78	0.43
1:B:101:ARG:HD2	1:B:101:ARG:N	2.22	0.43
1:B:451:GLY:HA2	1:B:487:VAL:HG22	2.01	0.43
1:A:271:ILE:O	1:A:271:ILE:HG23	2.18	0.43
1:A:281:PHE:CD2	1:A:281:PHE:N	2.86	0.43
1:B:514:GLN:O	1:B:515:ALA:C	2.58	0.43
1:A:26:THR:O	1:A:27:VAL:HG13	2.18	0.43
1:B:346:THR:HG22	1:B:386:ARG:NH1	2.33	0.43
1:A:144:ASN:O	6:A:599:HOH:O	2.21	0.43
1:A:237:TYR:O	1:A:293:LEU:HA	2.19	0.43
1:B:515:ALA:O	1:B:516:VAL:CB	2.66	0.43
1:A:496:ALA:HB3	1:A:497:ARG:CG	2.49	0.43
2:B:601:NAG:H62	2:B:602:NAG:HN2	1.81	0.43
1:A:359:PRO:HB2	1:A:360:THR:H	1.64	0.43
1:A:183:TYR:OH	1:A:205:HIS:HE1	2.00	0.42
1:B:174:ILE:HG21	1:B:223:PHE:CE2	2.54	0.42
1:A:34:GLN:HG3	1:A:34:GLN:O	2.19	0.42
1:A:339:VAL:HA	1:A:340:PRO:HD3	1.75	0.42
1:B:236:LEU:O	1:B:268:LEU:HA	2.19	0.42
1:A:407:PHE:CE1	1:A:432:VAL:CG1	3.02	0.42
1:A:31:VAL:HG21	1:A:35:GLU:CG	2.48	0.42
1:B:419:ARG:HD2	1:B:419:ARG:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:PHE:CD2	1:B:317:ARG:HB2	2.54	0.42
1:A:329:THR:O	1:A:330:SER:HB2	2.20	0.42
1:A:356:ARG:CZ	1:A:394:ASN:HB2	2.48	0.42
1:B:221:TYR:HB2	1:B:281:PHE:HB2	2.01	0.42
1:B:163:LEU:HD22	1:B:331:VAL:HG11	2.01	0.42
1:A:5:SER:HA	1:A:6:PRO:HD3	1.58	0.42
1:B:349:PRO:HA	1:B:386:ARG:O	2.19	0.42
2:B:602:NAG:H62	2:B:603:BMA:C1	2.49	0.42
1:B:231:SER:HB3	1:B:459:ASN:HD21	1.84	0.42
1:A:23:PRO:CG	1:A:37:TRP:NE1	2.80	0.42
1:B:225:PHE:HE1	1:B:279:VAL:HG21	1.84	0.42
1:B:99:PHE:CD2	1:B:448:PRO:HB3	2.54	0.42
1:A:218:PRO:HA	1:A:283:PHE:HB3	2.01	0.42
1:B:273:MET:O	1:B:274:ALA:CB	2.67	0.42
1:B:154:MET:HE2	1:B:154:MET:HB2	1.90	0.42
1:A:11:PHE:CD2	1:A:317:ARG:HB2	2.53	0.42
1:A:239:ALA:HB1	1:A:245:ASP:HA	2.02	0.42
1:A:235:GLY:O	1:A:295:ASN:HA	2.19	0.42
1:B:297:GLY:HA2	1:B:303:ILE:O	2.19	0.42
1:A:504:PHE:O	1:A:504:PHE:CG	2.72	0.42
1:A:499:TYR:O	1:A:500:GLU:HG2	2.19	0.42
1:B:258:GLY:N	6:B:672:HOH:O	2.46	0.42
1:B:122:TYR:HA	1:B:123:PRO:HD3	1.68	0.42
1:B:34:GLN:HG3	1:B:34:GLN:O	2.20	0.42
1:B:28:THR:O	1:B:35:GLU:O	2.37	0.42
1:B:217:GLU:HA	1:B:218:PRO:HD3	1.87	0.42
1:B:412:ARG:C	1:B:414:SER:H	2.23	0.42
1:A:371:VAL:HG11	1:A:468:MET:CE	2.50	0.42
1:A:485:VAL:O	1:A:490:MET:HE3	2.19	0.42
1:B:295:ASN:OD1	1:B:296:LEU:N	2.52	0.42
1:A:243:ALA:O	1:A:244:ILE:O	2.38	0.42
1:B:347:ASN:HA	6:B:685:HOH:O	2.20	0.42
1:B:497:ARG:HA	1:B:498:PRO:HD3	1.73	0.42
1:A:99:PHE:HD1	1:A:99:PHE:N	2.17	0.42
1:B:42:GLU:HG2	6:B:647:HOH:O	2.18	0.42
1:A:51:TYR:HB2	1:A:54:LEU:HB2	2.00	0.42
1:A:167:SER:C	1:A:169:TYR:H	2.23	0.42
1:A:280:VAL:HG22	1:A:281:PHE:N	2.34	0.42
1:B:363:ILE:HG21	1:B:370:ASP:OD2	2.20	0.42
1:B:96:HIS:CG	1:B:132:TRP:HE1	2.37	0.42
1:A:3:GLN:NE2	1:A:306:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:HD2	1:A:46:PHE:CE2	2.55	0.42
1:A:72:GLN:HG2	1:A:154:MET:CE	2.42	0.42
1:B:512:SER:O	1:B:513:VAL:HG22	2.19	0.42
1:A:36:ILE:HG12	1:A:78:GLU:HB2	2.02	0.42
1:A:313:ASP:OD1	1:A:314:LYS:NZ	2.53	0.42
1:B:279:VAL:HG23	1:B:281:PHE:CE2	2.55	0.42
1:A:75:ARG:NH2	6:A:573:HOH:O	2.53	0.42
1:A:218:PRO:HA	1:A:283:PHE:O	2.20	0.42
1:B:240:ASP:O	1:B:290:THR:O	2.38	0.42
1:B:163:LEU:HD11	1:B:334:ALA:HB3	2.00	0.41
1:A:341:PHE:HD2	1:A:428:LEU:HD13	1.84	0.41
1:B:131:LEU:HD12	1:B:131:LEU:N	2.35	0.41
1:B:447:ALA:N	1:B:448:PRO:HD3	2.35	0.41
1:B:484:THR:O	1:B:484:THR:CG2	2.67	0.41
1:A:15:LEU:HD11	1:A:206:VAL:HG12	2.02	0.41
1:A:299:SER:O	1:A:300:ILE:HB	2.21	0.41
1:A:412:ARG:O	1:A:420:THR:HB	2.21	0.41
1:A:143:GLU:HA	1:A:143:GLU:OE2	2.19	0.41
1:B:306:ASP:C	1:B:308:ASP:N	2.73	0.41
1:A:8:TYR:CD2	1:A:9:PRO:HD2	2.55	0.41
1:B:108:ALA:HB1	1:B:138:MET:HB2	2.01	0.41
1:A:317:ARG:HD3	1:A:317:ARG:HA	1.72	0.41
1:A:219:ARG:HH11	1:A:329:THR:HA	1.85	0.41
1:B:174:ILE:HG12	1:B:223:PHE:CZ	2.55	0.41
1:B:412:ARG:O	1:B:420:THR:CG2	2.68	0.41
1:A:383:THR:HG22	1:A:385:GLU:HG2	2.02	0.41
1:B:111:ILE:HG23	1:B:112:THR:N	2.34	0.41
1:B:222:ARG:HD2	6:B:645:HOH:O	2.20	0.41
1:A:246:THR:O	1:A:247:ARG:HB3	2.21	0.41
1:A:219:ARG:NH2	1:A:330:SER:OG	2.46	0.41
1:B:515:ALA:O	1:B:516:VAL:HB	2.20	0.41
1:A:77:VAL:HG13	1:A:77:VAL:O	2.21	0.41
1:B:359:PRO:C	1:B:361:TRP:H	2.24	0.41
1:B:18:PRO:HB2	1:B:70:THR:OG1	2.20	0.41
1:B:237:TYR:CZ	1:B:294:ARG:HB2	2.55	0.41
1:B:166:PRO:HG2	1:B:221:TYR:O	2.20	0.41
1:B:375:LEU:HB2	1:B:470:ALA:HB3	2.02	0.41
1:A:12:THR:O	1:A:213:PHE:CD1	2.74	0.41
1:A:321:ALA:O	1:A:322:ASP:HB2	2.20	0.41
1:B:158:PRO:CD	6:B:698:HOH:O	2.63	0.41
1:B:214:LYS:HD2	1:B:216:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:TYR:CE1	1:A:495:GLN:CD	2.94	0.41
1:B:282:ASP:C	1:B:284:SER:N	2.73	0.41
1:A:373:ASN:C	1:A:374:ARG:HE	2.23	0.41
1:A:280:VAL:HG22	1:A:281:PHE:H	1.86	0.41
1:A:239:ALA:CB	1:A:247:ARG:H	2.34	0.41
1:A:94:HIS:NE2	1:A:96:HIS:HA	2.36	0.41
1:A:507:GLN:HB3	6:A:584:HOH:O	2.20	0.41
1:B:213:PHE:HB2	1:B:317:ARG:HB3	2.02	0.41
1:A:44:LYS:HA	1:A:45:PRO:HD3	1.65	0.41
1:A:489:PRO:O	1:A:489:PRO:HD2	2.21	0.41
1:B:82:ARG:O	1:B:84:ILE:HD12	2.21	0.40
1:B:500:GLU:C	1:B:501:LEU:HD13	2.41	0.40
1:B:219:ARG:NH2	1:B:330:SER:OG	2.54	0.40
1:B:160:GLU:C	1:B:162:ALA:N	2.74	0.40
1:A:85:ASN:CB	1:A:113:GLU:O	2.66	0.40
1:A:389:LEU:HB3	1:A:434:LEU:HD11	2.03	0.40
1:A:262:HIS:ND1	1:A:335:ASN:HB2	2.36	0.40
1:A:219:ARG:NH1	1:A:329:THR:HA	2.35	0.40
1:A:355:GLY:HA3	1:A:391:ASN:OD1	2.21	0.40
1:A:62:TYR:CD1	1:A:133:TYR:HE1	2.38	0.40
1:A:123:PRO:C	1:A:125:ARG:HD3	2.41	0.40
1:B:474:THR:HG23	1:B:475:VAL:HG12	2.03	0.40
1:B:475:VAL:HG13	1:B:475:VAL:O	2.22	0.40
1:A:415:GLY:HA3	1:A:420:THR:O	2.22	0.40
1:B:424:TYR:CE2	6:B:691:HOH:O	2.74	0.40
1:A:345:THR:N	6:A:683:HOH:O	2.54	0.40
1:A:488:ASP:O	1:A:490:MET:HB3	2.21	0.40
1:B:107:TRP:HD1	1:B:110:ASP:H	1.68	0.40
1:A:84:ILE:HD12	1:A:84:ILE:N	2.37	0.40
1:B:82:ARG:HH21	1:B:513:VAL:CG1	2.34	0.40
1:A:73:VAL:HG12	1:A:77:VAL:CG1	2.52	0.40
1:B:339:VAL:CG2	1:B:341:PHE:CZ	3.04	0.40
1:B:311:ASN:HA	1:B:311:ASN:HD22	1.76	0.40
1:A:506:ALA:HB2	1:B:49:GLN:NE2	2.36	0.40
1:A:211:TRP:CZ2	1:A:311:ASN:HB3	2.57	0.40
1:B:455:PHE:C	1:B:456:HIS:CD2	2.95	0.40
1:B:95:LEU:HD12	1:B:98:SER:HB3	2.01	0.40
1:B:4:ILE:CD1	1:B:4:ILE:N	2.84	0.40
1:A:213:PHE:HE2	1:A:215:ASN:OD1	2.05	0.40
1:A:8:TYR:HA	1:A:9:PRO:HD2	1.79	0.40
1:B:383:THR:CG2	1:B:384:VAL:N	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:MET:O	1:B:139:HIS:HB2	2.22	0.40
1:B:244:ILE:HG22	1:B:245:ASP:H	1.86	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	507/534 (95%)	349 (69%)	106 (21%)	52 (10%)	1	0
1	B	517/534 (97%)	365 (71%)	95 (18%)	57 (11%)	0	0
All	All	1024/1068 (96%)	714 (70%)	201 (20%)	109 (11%)	0	0

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	113	GLU
1	A	166	PRO
1	A	169	TYR
1	A	244	ILE
1	A	303	ILE
1	A	308	ASP
1	A	334	ALA
1	A	481	TYR
1	A	494	TRP
1	A	495	GLN
1	A	497	ARG
1	A	498	PRO
1	A	500	GLU
1	A	505	GLN
1	B	34	GLN

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Mol	Chain	Res	Type
1	B	113	GLU
1	B	118	LYS
1	B	240	ASP
1	B	244	ILE
1	B	300	ILE
1	B	303	ILE
1	B	322	ASP
1	B	356	ARG
1	B	375	LEU
1	B	420	THR
1	B	448	PRO
1	B	466	ASP
1	B	475	VAL
1	B	481	TYR
1	B	482	ASN
1	B	483	ALA
1	B	487	VAL
1	B	493	LEU
1	B	501	LEU
1	B	511	PHE
1	B	513	VAL
1	B	515	ALA
1	B	516	VAL
1	A	56	SER
1	A	304	GLY
1	A	359	PRO
1	A	375	LEU
1	A	413	THR
1	A	418	ALA
1	A	466	ASP
1	A	482	ASN
1	A	489	PRO
1	A	492	GLU
1	B	115	GLY
1	B	166	PRO
1	B	169	TYR
1	B	171	GLU
1	B	255	SER
1	B	359	PRO
1	B	368	PHE
1	B	418	ALA
1	B	499	TYR

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Mol	Chain	Res	Type
1	A	6	PRO
1	A	171	GLU
1	A	174	ILE
1	A	368	PHE
1	A	437	ARG
1	A	488	ASP
1	B	6	PRO
1	B	78	GLU
1	B	107	TRP
1	B	334	ALA
1	B	478	ASP
1	B	488	ASP
1	A	153	TYR
1	A	241	THR
1	A	306	ASP
1	A	336	LEU
1	A	414	SER
1	A	502	GLY
1	A	503	GLU
1	B	33	GLY
1	B	110	ASP
1	B	297	GLY
1	B	304	GLY
1	B	336	LEU
1	A	52	PRO
1	A	322	ASP
1	A	341	PHE
1	A	475	VAL
1	A	480	GLY
1	B	7	GLN
1	B	286	TYR
1	B	309	TYR
1	B	311	ASN
1	B	447	ALA
1	B	505	GLN
1	A	259	LEU
1	B	341	PHE
1	A	31	VAL
1	A	60	VAL
1	A	326	GLN
1	B	249	PRO
1	A	114	PRO

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Mol	Chain	Res	Type
1	A	297	GLY
1	A	300	ILE
1	A	302	GLY
1	B	212	PRO
1	A	123	PRO
1	B	218	PRO
1	B	326	GLN
1	B	480	GLY
1	B	52	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/453 (96%)	356 (82%)	78 (18%)	2	2
1	B	440/453 (97%)	360 (82%)	80 (18%)	2	2
All	All	874/906 (96%)	716 (82%)	158 (18%)	2	2

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	4	ILE
1	A	5	SER
1	A	7	GLN
1	A	12	THR
1	A	27	VAL
1	A	35	GLU
1	A	37	TRP
1	A	50	VAL
1	A	75	ARG
1	A	79	THR
1	A	82	ARG
1	A	85	ASN
1	A	99	PHE

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Mol	Chain	Res	Type
1	A	101	ARG
1	A	111	ILE
1	A	113	GLU
1	A	125	ARG
1	A	152	LEU
1	A	172	PHE
1	A	177	ILE
1	A	178	LEU
1	A	186	ASN
1	A	195	GLU
1	A	198	SER
1	A	215	ASN
1	A	219	ARG
1	A	224	ARG
1	A	241	THR
1	A	246	THR
1	A	248	LEU
1	A	259	LEU
1	A	260	LEU
1	A	266	THR
1	A	269	LEU
1	A	271	ILE
1	A	276	ARG
1	A	285	ASP
1	A	289	LYS
1	A	296	LEU
1	A	303	ILE
1	A	306	ASP
1	A	308	ASP
1	A	314	LYS
1	A	317	ARG
1	A	331	VAL
1	A	337	ARG
1	A	339	VAL
1	A	344	PRO
1	A	361	TRP
1	A	368	PHE
1	A	370	ASP
1	A	374	ARG
1	A	375	LEU
1	A	384	VAL
1	A	389	LEU

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Mol	Chain	Res	Type
1	A	397	THR
1	A	405	VAL
1	A	410	ILE
1	A	411	SER
1	A	416	ASN
1	A	422	MET
1	A	426	SER
1	A	428	LEU
1	A	429	LYS
1	A	436[A]	ARG
1	A	436[B]	ARG
1	A	458	HIS
1	A	474	THR
1	A	476	LEU
1	A	481	TYR
1	A	482	ASN
1	A	493	LEU
1	A	494	TRP
1	A	499	TYR
1	A	500	GLU
1	A	501	LEU
1	A	503	GLU
1	B	1	VAL
1	B	5	SER
1	B	7	GLN
1	B	12	THR
1	B	27	VAL
1	B	37	TRP
1	B	54	LEU
1	B	82	ARG
1	B	85	ASN
1	B	99	PHE
1	B	100	SER
1	B	101	ARG
1	B	110	ASP
1	B	111	ILE
1	B	121	TYR
1	B	125	ARG
1	B	127	SER
1	B	152	LEU
1	B	171	GLU
1	B	172	PHE

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Mol	Chain	Res	Type
1	B	177	ILE
1	B	186	ASN
1	B	195	GLU
1	B	196	LEU
1	B	198	SER
1	B	215	ASN
1	B	242	ASP
1	B	244	ILE
1	B	245	ASP
1	B	248	LEU
1	B	260	LEU
1	B	266	THR
1	B	268	LEU
1	B	269	LEU
1	B	276	ARG
1	B	281	PHE
1	B	282	ASP
1	B	289	LYS
1	B	296	LEU
1	B	299	SER
1	B	303	ILE
1	B	305	THR
1	B	307	THR
1	B	320	VAL
1	B	337	ARG
1	B	339	VAL
1	B	341	PHE
1	B	348	THR
1	B	357	THR
1	B	360	THR
1	B	362	THR
1	B	368	PHE
1	B	370	ASP
1	B	371	VAL
1	B	374	ARG
1	B	375	LEU
1	B	384	VAL
1	B	389	LEU
1	B	405	VAL
1	B	406	ASP
1	B	416	ASN
1	B	417	ASN

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Mol	Chain	Res	Type
1	B	419	ARG
1	B	428	LEU
1	B	429	LYS
1	B	479	TYR
1	B	481	TYR
1	B	482	ASN
1	B	485	VAL
1	B	488	ASP
1	B	490	MET
1	B	491	GLU
1	B	494	TRP
1	B	497	ARG
1	B	500	GLU
1	B	501	LEU
1	B	503	GLU
1	B	505	GLN
1	B	510	GLN
1	B	513	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	72	GLN
1	A	85	ASN
1	A	124	ASN
1	A	139	HIS
1	A	149	GLN
1	A	186	ASN
1	A	205	HIS
1	A	311	ASN
1	A	347	ASN
1	A	351	GLN
1	A	364	ASN
1	A	394	ASN
1	A	417	ASN
1	A	445	HIS
1	A	495	GLN
1	B	7	GLN
1	B	29	ASN
1	B	34	GLN
1	B	72	GLN

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Mol	Chain	Res	Type
1	B	85	ASN
1	B	86	ASN
1	B	96	HIS
1	B	124	ASN
1	B	149	GLN
1	B	186	ASN
1	B	205	HIS
1	B	311	ASN
1	B	335	ASN
1	B	347	ASN
1	B	351	GLN
1	B	445	HIS
1	B	495	GLN
1	B	505	GLN
1	B	510	GLN
1	B	514	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

10 carbohydrates 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	NAG	A	601	1,2	14,14,15	0.52	0	15,19,21	0.85	0
2	NAG	A	602	2	14,14,15	0.56	0	15,19,21	1.35	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMA	A	603	2	11,11,12	0.53	0	14,15,17	1.90	3 (21%)
3	NDG	A	611	1,3	14,14,15	0.55	0	15,19,21	1.51	2 (13%)
3	NAG	A	612	3	14,14,15	0.44	0	15,19,21	1.93	3 (20%)
2	NAG	B	601	1,2	14,14,15	0.57	0	15,19,21	2.00	2 (13%)
2	NAG	B	602	2	14,14,15	0.37	0	15,19,21	3.10	5 (33%)
2	BMA	B	603	2	11,11,12	0.75	0	14,15,17	1.72	2 (14%)
5	NAG	B	611	1,5	14,14,15	0.38	0	15,19,21	1.26	3 (20%)
5	NAG	B	612	5	14,14,15	0.67	0	15,19,21	1.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	BMA	A	603	2	-	0/2/19/22	0/1/1/1
3	NDG	A	611	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	612	3	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	2	-	0/6/23/26	0/1/1/1
2	BMA	B	603	2	-	0/2/19/22	0/1/1/1
5	NAG	B	611	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	612	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NAG	C2-N2-C7	-5.97	115.37	123.04
2	A	603	BMA	C1-C2-C3	-4.70	103.98	109.54
3	A	612	NAG	C2-N2-C7	-4.67	117.04	123.04
2	B	602	NAG	C4-C3-C2	-4.13	104.81	111.23
2	A	602	NAG	C2-N2-C7	-3.90	118.03	123.04
2	A	603	BMA	C2-C3-C4	-2.99	105.96	111.04
3	A	612	NAG	C4-C3-C2	-2.94	106.66	111.23
2	A	602	NAG	C4-C3-C2	-2.39	107.52	111.23
2	A	603	BMA	O5-C1-C2	-2.32	107.10	110.86
2	B	602	NAG	C3-C4-C5	-2.15	106.46	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	611	NAG	O4-C4-C5	-2.11	103.64	109.24
5	B	611	NAG	C2-N2-C7	-2.06	120.39	123.04
5	B	611	NAG	C6-C5-C4	-2.04	107.98	113.02
3	A	611	NDG	O4-C4-C3	2.17	115.23	110.34
2	B	603	BMA	C2-C3-C4	2.45	115.20	111.04
2	B	601	NAG	O4-C4-C5	2.74	116.50	109.24
2	B	602	NAG	O4-C4-C5	3.42	118.30	109.24
3	A	611	NDG	C1-O-C5	3.47	116.65	112.25
3	A	612	NAG	C1-O5-C5	4.07	117.41	112.25
2	B	603	BMA	C1-C2-C3	5.42	115.96	109.54
2	B	601	NAG	C1-O5-C5	6.34	120.29	112.25
2	B	602	NAG	C1-O5-C5	8.20	122.66	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0
3	A	611	NDG	1	0
2	B	601	NAG	2	0
2	B	602	NAG	4	0
2	B	603	BMA	1	0
5	B	611	NAG	2	0
5	B	612	NAG	1	0

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	508/534 (95%)	0.27	39 (7%)	16 23	28, 48, 79, 125	0
1	B	518/534 (97%)	0.25	34 (6%)	22 29	28, 48, 81, 125	0
All	All	1026/1068 (96%)	0.26	73 (7%)	19 26	28, 48, 80, 125	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	LEU	10.4
1	A	342	PRO	8.3
1	B	322	ASP	7.7
1	B	416	ASN	6.7
1	A	476	LEU	6.6
1	B	494	TRP	6.5
1	B	484	THR	6.5
1	A	322	ASP	5.9
1	B	418	ALA	5.8
1	B	415	GLY	5.6
1	A	494	TRP	5.5
1	B	515	ALA	5.4
1	B	516	VAL	5.3
1	A	361	TRP	5.3
1	A	419	ARG	5.2
1	B	358	GLY	5.1
1	B	359	PRO	4.5
1	A	321	ALA	4.5
1	B	324	THR	4.4
1	B	361	TRP	4.3
1	A	360	THR	4.3
1	A	332	VAL	3.7
1	B	4	ILE	3.6
1	B	338	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	281	PHE	3.5
1	A	414	SER	3.5
1	A	496	ALA	3.5
1	B	342	PRO	3.3
1	A	241	THR	3.3
1	B	419	ARG	3.2
1	B	518	GLU	3.2
1	B	355	GLY	3.2
1	B	493	LEU	3.1
1	A	484	THR	3.0
1	B	3	GLN	3.0
1	B	481	TYR	3.0
1	A	345	THR	2.9
1	B	414	SER	2.9
1	A	2	ALA	2.9
1	B	300	ILE	2.8
1	A	309	TYR	2.8
1	A	479	TYR	2.8
1	B	46	PHE	2.7
1	B	26	THR	2.7
1	A	493	LEU	2.6
1	A	333	PRO	2.6
1	A	506	ALA	2.5
1	B	479	TYR	2.4
1	A	26	THR	2.4
1	A	362	THR	2.4
1	A	475	VAL	2.4
1	A	308	ASP	2.4
1	A	368	PHE	2.3
1	A	325	THR	2.3
1	A	323	ASP	2.3
1	B	495	GLN	2.2
1	B	323	ASP	2.2
1	A	298	GLY	2.2
1	B	298	GLY	2.2
1	A	1	VAL	2.1
1	A	280	VAL	2.1
1	B	169	TYR	2.1
1	A	502	GLY	2.1
1	A	481	TYR	2.1
1	A	331	VAL	2.1
1	B	501	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	483	ALA	2.1
1	B	506	ALA	2.1
1	A	375	LEU	2.1
1	A	488	ASP	2.1
1	A	34	GLN	2.0
1	B	174	ILE	2.0
1	B	165	LEU	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](#)

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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	601	14/15	0.94	0.12	-0.66	41,47,54,57	0
2	NAG	B	601	14/15	0.96	0.13	-0.67	33,43,55,57	0
5	NAG	B	611	14/15	0.87	0.16	-1.73	60,69,78,83	0
5	NAG	B	612	14/15	0.87	0.12	-	54,64,70,79	0
3	NDG	A	611	14/15	0.74	0.17	-	75,85,93,93	0
2	BMA	A	603	11/12	0.90	0.10	-	52,72,84,84	0
2	BMA	B	603	11/12	0.76	0.19	-	76,79,91,92	0
2	NAG	B	602	14/15	0.94	0.10	-	48,59,68,74	0
3	NAG	A	612	14/15	0.72	0.26	-	78,95,106,109	0
2	NAG	A	602	14/15	0.89	0.12	-	57,63,71,72	0

## 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
4	CU	A	702	1/1	1.00	0.15	4.38	43,43,43,43	0
4	CU	B	701	1/1	0.99	0.14	2.69	37,37,37,37	0
4	CU	A	701	1/1	0.99	0.14	1.83	35,35,35,35	0
4	CU	B	704	1/1	1.00	0.13	0.99	32,32,32,32	0
4	CU	B	702	1/1	0.99	0.12	0.67	36,36,36,36	0
4	CU	A	703	1/1	0.98	0.11	-0.44	43,43,43,43	0
4	CU	A	704	1/1	1.00	0.11	-1.27	34,34,34,34	0
4	CU	B	703	1/1	1.00	0.14	-	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.