



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:44 pm GMT

PDB ID : 1IVO  
Title : Crystal Structure of the Complex of Human Epidermal Growth Factor and Receptor Extracellular Domains.  
Authors : Ogiso, H.; Ishitani, R.; Nureki, O.; Fukai, S.; Yamanaka, M.; Kim, J.H.; Saito, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2002-03-28  
Resolution : 3.30 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

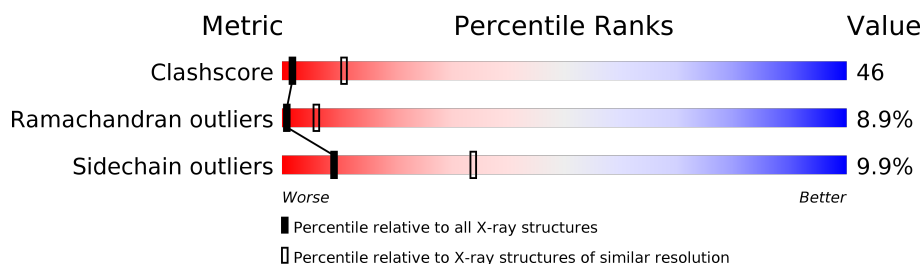
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	
2	C	53	
2	D	53	

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
3	NAG	A	1328	-	-	X	-
3	NAG	B	1328	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8892 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.

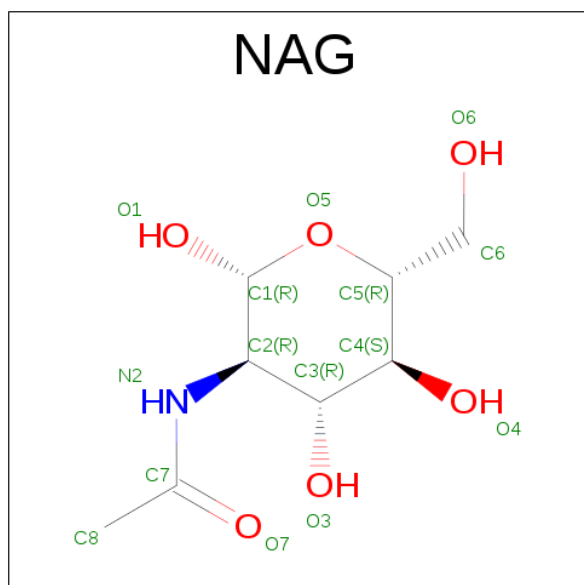
- Molecule 1 is a protein called Epidermal Growth Factor Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	111	0	0
			3956	2446	706	760	44			
1	B	510	Total	C	N	O	S	62	0	0
			3947	2441	705	757	44			

- Molecule 2 is a protein called Epidermal growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	47	Total	C	N	O	S	0	0	0
			385	244	63	71	7			
2	D	47	Total	C	N	O	S	0	0	0
			385	244	63	71	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is water.

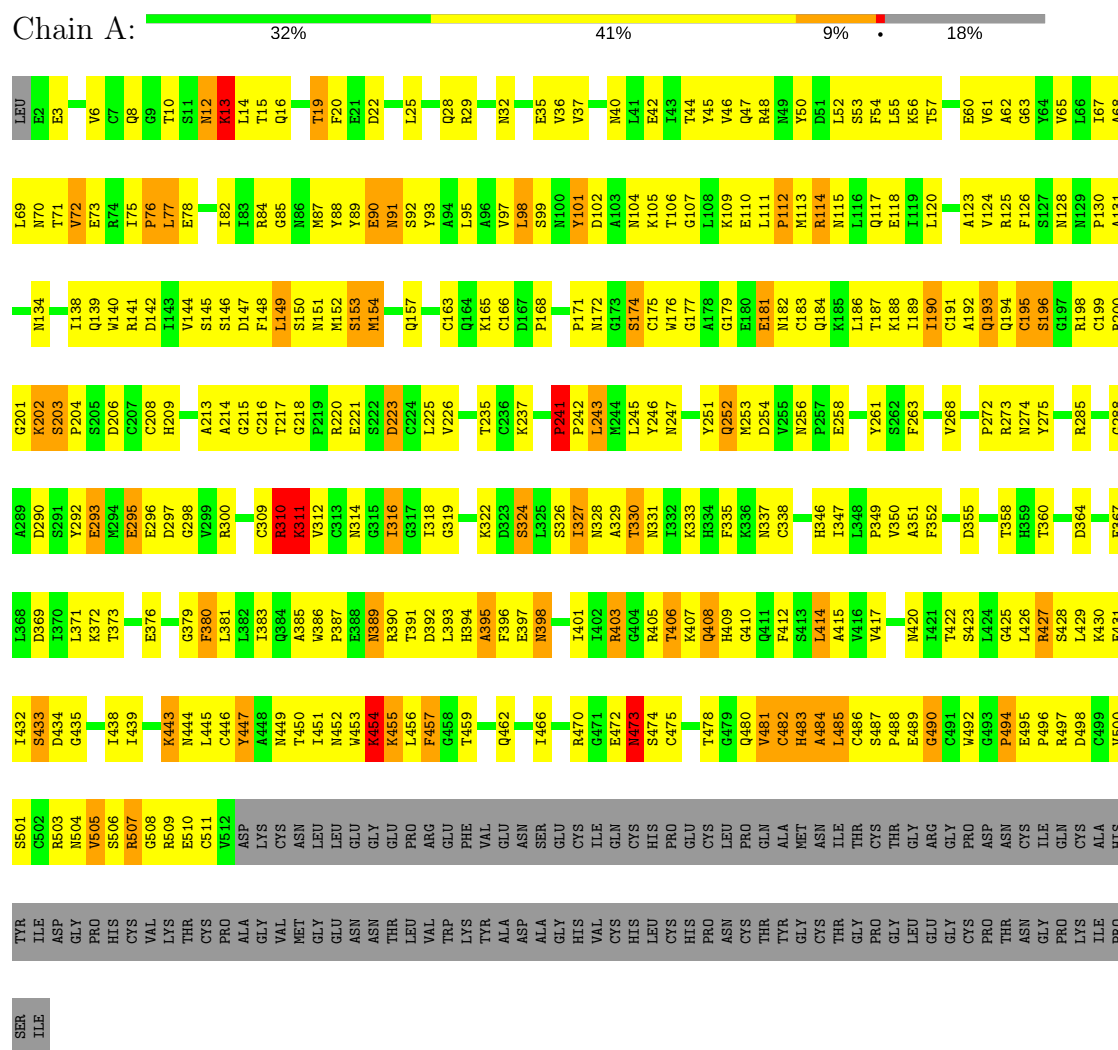
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		
5	C	6	Total	O	0	0
			6	6		
5	D	6	Total	O	0	0
			6	6		

### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: Epidermal Growth Factor Receptor



#### • Molecule 1: Epidermal Growth Factor Receptor





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.16 Å   220.16 Å   113.12 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	98.0 (10.00-3.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.255 , 0.326	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP



## 5 Model quality [i](#)

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

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

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	0.33	0/4027	0.67	1/5438 (0.0%)
1	B	0.34	0/4018	0.67	1/5426 (0.0%)
2	C	0.36	0/396	0.64	0/536
2	D	0.35	0/396	0.63	0/536
All	All	0.34	0/8837	0.67	2/11936 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	CYS	CA-CB-SG	-5.07	104.87	114.00
1	B	240	CYS	CA-CB-SG	-5.06	104.90	114.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	3843	342	0
1	B	3947	0	3843	397	0
2	C	385	0	344	22	0
2	D	385	0	344	42	0
3	A	70	0	65	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	39	21	0
4	A	28	0	25	4	0
5	A	35	0	0	2	0
5	B	32	0	0	5	0
5	C	6	0	0	1	0
5	D	6	0	0	2	0
All	All	8892	0	8503	788	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 46.

All (788) 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:243:LEU:HA	1:B:256:ASN:HB3	1.34	1.09
1:A:174:SER:HB3	1:A:184:GLN:HB3	1.39	1.02
1:A:481:VAL:HG12	1:A:482:CYS:H	1.24	0.99
1:B:328:ASN:H	3:B:1328:NAG:H82	1.27	0.97
1:A:331:ASN:HB2	3:A:1328:NAG:HN2	1.29	0.96
1:A:439:ILE:HB	1:A:466:ILE:HG22	1.48	0.94
1:B:328:ASN:H	3:B:1328:NAG:C8	1.81	0.93
1:B:416:VAL:HG23	1:B:439:ILE:HG23	1.50	0.93
1:B:442:ASN:HB2	1:B:469:ASN:HD22	1.35	0.92
1:B:295:GLU:HB3	1:B:300:ARG:HD2	1.50	0.91
1:B:366:GLN:HA	1:B:366:GLN:HE21	1.34	0.91
1:B:349:PRO:HG3	1:B:385:ALA:HB2	1.53	0.90
1:B:327:ILE:HA	3:B:1328:NAG:H83	1.53	0.90
1:A:190:ILE:HD13	1:A:202:LYS:HA	1.52	0.90
1:B:391:THR:HB	1:B:422:THR:HG22	1.54	0.89
1:B:6:VAL:HG12	1:B:36:VAL:HB	1.54	0.89
1:B:243:LEU:CA	1:B:256:ASN:HB3	2.02	0.89
1:B:485:LEU:H	1:B:485:LEU:HD12	1.37	0.88
1:B:4:LYS:HD3	1:B:4:LYS:H	1.36	0.88
1:A:46:VAL:HG11	1:A:52:LEU:HD11	1.56	0.88
1:B:390:ARG:HB2	1:B:390:ARG:HH11	1.36	0.88
1:A:186:LEU:HD12	1:A:186:LEU:H	1.39	0.87
1:B:99:SER:HA	1:B:128:ASN:O	1.76	0.86
1:B:123:ALA:HB1	1:B:152:MET:HB3	1.59	0.85
1:B:432:ILE:HB	1:B:457:PHE:HB3	1.57	0.85
1:B:196:SER:HB3	1:B:210:ASN:HB3	1.56	0.84
1:B:78:GLU:HA	1:B:112:PRO:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLU:HG2	1:B:112:PRO:HB2	1.60	0.83
1:B:303:LYS:HA	1:B:303:LYS:HE2	1.62	0.81
1:A:123:ALA:HB1	1:A:152:MET:HB3	1.63	0.81
1:A:139:GLN:H	1:A:184:GLN:HE22	1.26	0.79
1:B:390:ARG:HB2	1:B:390:ARG:NH1	1.96	0.79
1:B:439:ILE:HB	1:B:466:ILE:HG23	1.64	0.79
1:A:245:LEU:HD13	1:A:256:ASN:HB2	1.64	0.79
1:B:442:ASN:HB2	1:B:469:ASN:ND2	1.97	0.79
1:B:47:GLN:HA	1:B:47:GLN:HE21	1.48	0.78
1:B:480:GLN:HG3	1:B:481:VAL:H	1.48	0.78
1:A:84:ARG:HD3	1:A:120:LEU:HD12	1.64	0.78
2:D:15:LEU:HD21	2:D:41:ARG:NH2	1.99	0.77
1:A:450:THR:O	1:A:490:GLY:HA3	1.83	0.76
1:A:475:CYS:SG	1:A:480:GLN:HB2	2.24	0.76
1:B:124:VAL:H	1:B:152:MET:HE3	1.49	0.76
1:B:366:GLN:HA	1:B:366:GLN:NE2	2.00	0.76
1:B:371:LEU:HB2	1:B:395:ALA:HB1	1.67	0.76
1:B:135:VAL:HA	1:B:138:ILE:HD13	1.67	0.76
1:B:328:ASN:OD1	3:B:1328:NAG:H2	1.86	0.76
1:A:139:GLN:N	1:A:184:GLN:HE22	1.83	0.76
1:B:510:GLU:OE1	1:B:512:VAL:HG13	1.86	0.76
1:A:401:ILE:HG12	1:A:431:GLU:HB3	1.68	0.76
1:A:215:GLY:H	1:A:225:LEU:HD12	1.50	0.75
1:B:218:GLY:H	1:B:223:ASP:HB3	1.51	0.75
1:A:203:SER:H	1:A:204:PRO:HD2	1.51	0.75
1:A:215:GLY:N	1:A:225:LEU:HD12	2.01	0.75
1:A:115:ASN:O	1:A:117:GLN:HG3	1.87	0.75
1:A:82:ILE:HD11	1:A:120:LEU:HG	1.68	0.75
1:B:101:TYR:HB3	1:B:130:PRO:HD2	1.69	0.75
1:A:485:LEU:H	1:A:485:LEU:CD2	2.00	0.74
1:A:485:LEU:H	1:A:485:LEU:HD23	1.52	0.73
1:B:297:ASP:HB2	1:B:299:VAL:HG22	1.70	0.73
1:B:88:TYR:HD2	1:B:92:SER:H	1.34	0.73
1:A:300:ARG:HH21	1:A:403:ARG:NH2	1.87	0.73
1:B:69:LEU:HD11	2:D:26:LEU:HD11	1.69	0.73
1:B:4:LYS:HD3	1:B:4:LYS:N	2.03	0.73
1:A:295:GLU:HB3	1:A:300:ARG:HG2	1.71	0.73
2:D:19:VAL:HG22	2:D:32:ASN:HB3	1.70	0.73
1:B:271:CYS:SG	1:B:277:VAL:HG22	2.29	0.72
1:A:275:TYR:CD2	1:A:405:ARG:HD3	2.25	0.72
1:A:470:ARG:HH11	1:A:470:ARG:HG2	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:O	1:A:56:LYS:HG3	1.89	0.72
1:A:16:GLN:HB2	1:A:45:TYR:CE1	2.24	0.72
1:A:408:GLN:HA	1:A:408:GLN:HE21	1.55	0.72
1:A:46:VAL:HG12	1:A:72:VAL:HB	1.70	0.72
1:A:148:PHE:C	1:A:150:SER:H	1.93	0.71
1:A:331:ASN:HB2	3:A:1328:NAG:N2	2.02	0.71
1:A:432:ILE:HB	1:A:457:PHE:HB3	1.71	0.71
1:A:138:ILE:HG12	1:A:176:TRP:CE2	2.26	0.71
1:B:16:GLN:HB2	1:B:45:TYR:CE1	2.26	0.71
1:A:201:GLY:HA3	1:A:204:PRO:HG2	1.72	0.71
1:B:245:LEU:HG	1:B:257:PRO:HD3	1.73	0.71
1:A:203:SER:N	1:A:204:PRO:HD2	2.06	0.70
1:B:124:VAL:HB	1:B:154:MET:HE1	1.72	0.70
1:B:463:LYS:HB3	1:B:463:LYS:NZ	2.05	0.70
1:B:62:ALA:O	1:B:84:ARG:HB2	1.90	0.70
1:B:318:ILE:HD12	1:B:319:GLY:H	1.56	0.70
1:A:330:THR:HB	3:A:1328:NAG:H2	1.73	0.70
1:B:41:LEU:HD23	1:B:65:VAL:HG22	1.73	0.70
1:B:349:PRO:CG	1:B:385:ALA:HB2	2.21	0.70
1:A:25:LEU:O	1:A:29:ARG:HG3	1.92	0.70
1:B:109:LYS:HA	1:B:131:ALA:O	1.90	0.70
1:B:257:PRO:HG2	1:B:258:GLU:H	1.57	0.70
1:B:505:VAL:O	1:B:507:ARG:HG3	1.91	0.70
2:C:8:LEU:O	2:C:11:ASP:HB3	1.92	0.69
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.58	0.69
1:B:123:ALA:HB1	1:B:152:MET:CB	2.23	0.69
1:A:478:THR:HB	1:A:480:GLN:HG3	1.75	0.69
1:B:442:ASN:HD22	1:B:469:ASN:HD21	1.40	0.69
1:A:62:ALA:O	1:A:84:ARG:HB2	1.93	0.69
2:D:49:TRP:CE3	2:D:49:TRP:HA	2.27	0.69
1:B:243:LEU:HA	1:B:256:ASN:CB	2.20	0.68
1:A:47:GLN:HB2	1:A:50:TYR:CE1	2.29	0.68
1:A:102:ASP:HB2	1:A:106:THR:O	1.94	0.68
1:A:93:TYR:HA	1:A:123:ALA:O	1.93	0.68
1:A:165:LYS:HG3	1:A:166:CYS:H	1.59	0.68
1:B:459:THR:HB	1:B:462:GLN:HE21	1.59	0.67
1:B:46:VAL:HG11	1:B:52:LEU:HD21	1.74	0.67
1:A:446:CYS:C	1:A:447:TYR:HD1	1.97	0.67
1:B:134:ASN:HB3	1:B:175:CYS:O	1.92	0.67
1:B:454:LYS:H	1:B:454:LYS:HD3	1.60	0.67
4:A:1420:NAG:H4	4:A:2420:NAG:N2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:THR:HB	1:A:422:THR:HG22	1.76	0.67
1:B:347:ILE:HB	1:B:383:ILE:HG23	1.76	0.66
1:A:447:TYR:OH	1:A:494:PRO:HG3	1.95	0.66
1:A:99:SER:HA	1:A:128:ASN:O	1.95	0.66
1:A:142:ASP:OD2	1:A:188:LYS:HB3	1.96	0.66
1:A:89:TYR:CE2	1:A:90:GLU:HG2	2.31	0.66
1:B:32:ASN:O	1:B:33:ASN:HB2	1.94	0.66
1:B:115:ASN:O	1:B:117:GLN:HG3	1.96	0.66
1:A:412:PHE:HE1	2:C:48:LYS:HB3	1.61	0.65
1:B:436:ASP:CG	1:B:463:LYS:HG2	2.17	0.65
1:A:446:CYS:C	1:A:447:TYR:CD1	2.70	0.65
1:A:506:SER:HB2	1:A:511:CYS:SG	2.36	0.65
1:B:403:ARG:O	1:B:433:SER:HB2	1.95	0.65
1:B:485:LEU:HD22	1:B:496:PRO:HG3	1.79	0.65
2:D:49:TRP:HE3	2:D:49:TRP:HA	1.59	0.65
1:A:125:ARG:HH11	1:A:125:ARG:HG2	1.61	0.65
1:A:235:THR:OG1	1:A:237:LYS:HE2	1.97	0.65
1:A:489:GLU:OE2	1:A:501:SER:HB2	1.97	0.65
1:B:84:ARG:HG3	1:B:84:ARG:HH11	1.62	0.65
1:A:216:CYS:SG	1:A:218:GLY:O	2.55	0.65
1:A:201:GLY:C	1:A:203:SER:H	2.00	0.65
1:B:45:TYR:HE2	1:B:69:LEU:HD23	1.62	0.64
1:B:232:ASP:CB	1:B:237:LYS:HD2	2.27	0.64
1:B:4:LYS:CD	1:B:4:LYS:H	2.07	0.64
1:A:75:ILE:O	1:A:112:PRO:HD2	1.97	0.64
1:A:423:SER:HA	1:A:445:LEU:CD1	2.27	0.64
1:A:174:SER:CB	1:A:184:GLN:HB3	2.22	0.64
1:A:78:GLU:HA	1:A:112:PRO:O	1.98	0.64
1:B:408:GLN:C	1:B:410:GLY:H	2.00	0.64
1:B:444:ASN:H	1:B:444:ASN:ND2	1.96	0.63
1:A:386:TRP:CZ2	1:A:393:LEU:HA	2.34	0.63
1:A:76:PRO:O	1:A:78:GLU:N	2.29	0.63
1:B:40:ASN:ND2	1:B:64:TYR:H	1.96	0.63
1:B:459:THR:HB	1:B:462:GLN:NE2	2.13	0.63
2:C:7:PRO:HD3	2:C:29:TYR:CE2	2.34	0.63
1:B:14:LEU:HD21	2:D:26:LEU:CD1	2.29	0.63
1:B:331:ASN:HB2	3:B:1328:NAG:O3	1.98	0.63
1:A:349:PRO:HD2	5:C:57:HOH:O	1.98	0.62
1:A:84:ARG:HD3	1:A:120:LEU:CD1	2.30	0.62
1:A:138:ILE:HG23	1:A:184:GLN:NE2	2.15	0.62
1:A:47:GLN:HA	1:A:71:THR:OG1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLU:HA	1:B:456:LEU:O	1.99	0.62
1:B:480:GLN:HG3	1:B:481:VAL:N	2.14	0.62
1:A:481:VAL:HG12	1:A:482:CYS:N	2.05	0.62
1:B:218:GLY:N	1:B:223:ASP:HB3	2.15	0.62
1:A:112:PRO:O	1:A:114:ARG:HD2	1.99	0.62
1:B:93:TYR:HA	1:B:123:ALA:O	2.00	0.62
1:A:174:SER:HB3	1:A:184:GLN:HE21	1.65	0.62
1:A:364:ASP:HB3	1:A:367:GLU:HG2	1.82	0.61
1:B:152:MET:HG3	1:B:152:MET:O	1.98	0.61
1:B:339:THR:HG22	1:B:373:THR:O	1.99	0.61
1:B:190:ILE:HG22	1:B:190:ILE:O	2.00	0.61
1:A:444:ASN:HA	1:A:470:ARG:HD3	1.81	0.61
1:A:360:THR:HG21	3:A:1328:NAG:H62	1.82	0.60
1:B:328:ASN:N	3:B:1328:NAG:H82	2.09	0.60
1:B:303:LYS:HD3	1:B:304:LYS:H	1.65	0.60
1:A:149:LEU:HA	1:A:152:MET:HG2	1.84	0.60
1:B:331:ASN:HB2	3:B:1328:NAG:O7	2.00	0.60
1:B:368:LEU:O	1:B:395:ALA:HB2	2.01	0.60
1:B:421:ILE:HG13	1:B:445:LEU:HD13	1.83	0.60
1:A:438:ILE:HD13	2:C:47:LEU:HD22	1.82	0.60
1:B:29:ARG:HD2	2:D:49:TRP:CZ2	2.35	0.60
1:A:316:ILE:HD11	1:A:327:ILE:HG13	1.83	0.60
1:A:472:GLU:C	1:A:474:SER:H	2.05	0.60
1:A:16:GLN:HB2	1:A:45:TYR:HE1	1.62	0.60
2:D:23:ILE:O	2:D:23:ILE:HG22	2.01	0.60
1:B:328:ASN:O	3:B:1328:NAG:H82	2.00	0.60
1:A:310:ARG:C	1:A:311:LYS:HD3	2.23	0.60
1:B:187:THR:HB	1:B:199:CYS:O	2.02	0.59
1:B:47:GLN:HA	1:B:47:GLN:NE2	2.16	0.59
1:A:138:ILE:HG12	1:A:176:TRP:NE1	2.16	0.59
1:A:198:ARG:O	1:A:208:CYS:HB2	2.02	0.59
1:B:130:PRO:O	1:B:131:ALA:HB3	2.01	0.59
1:B:186:LEU:H	1:B:186:LEU:CD2	2.15	0.59
1:A:275:TYR:HD2	1:A:405:ARG:HD3	1.68	0.59
1:B:209:HIS:CE1	1:B:211:GLN:HB2	2.37	0.59
1:A:355:ASP:OD2	1:A:358:THR:HG23	2.01	0.59
1:A:352:PHE:HE2	1:A:387:PRO:HG3	1.66	0.59
1:A:455:LYS:HD3	1:A:456:LEU:N	2.17	0.59
1:A:466:ILE:O	1:A:466:ILE:HD12	2.02	0.59
1:B:352:PHE:HE2	1:B:363:LEU:HD23	1.67	0.59
1:A:118:GLU:HG2	1:A:213:ALA:HB1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:LEU:O	2:C:28:LYS:HG2	2.01	0.59
1:A:187:THR:HA	1:A:190:ILE:HD11	1.85	0.59
1:A:457:PHE:HD2	1:A:457:PHE:O	1.86	0.59
1:A:403:ARG:CG	1:A:403:ARG:HH11	2.15	0.59
1:A:371:LEU:O	1:A:373:THR:N	2.36	0.59
1:A:398:ASN:N	1:A:398:ASN:HD22	2.01	0.59
1:B:292:TYR:O	1:B:302:CYS:HB2	2.02	0.59
1:B:56:LYS:HE3	1:B:78:GLU:OE1	2.03	0.59
1:B:125:ARG:HA	1:B:153:SER:O	2.03	0.59
2:D:48:LYS:O	2:D:49:TRP:CD2	2.55	0.59
1:A:216:CYS:HB2	1:A:223:ASP:O	2.03	0.58
1:A:189:ILE:C	1:A:191:CYS:H	2.04	0.58
1:B:139:GLN:HG3	1:B:184:GLN:HE22	1.68	0.58
1:A:186:LEU:H	1:A:186:LEU:CD1	2.14	0.58
1:A:293:GLU:OE1	1:A:300:ARG:HD3	2.04	0.58
1:A:446:CYS:SG	1:A:470:ARG:HG2	2.42	0.58
1:B:93:TYR:CE2	1:B:125:ARG:HB2	2.38	0.58
1:A:414:LEU:HD23	1:A:415:ALA:N	2.19	0.58
1:B:4:LYS:HE3	1:B:231:ARG:NH1	2.19	0.58
1:A:44:THR:HG22	1:A:68:ALA:O	2.03	0.58
1:B:14:LEU:HD21	2:D:26:LEU:HD12	1.85	0.58
1:A:139:GLN:HE22	1:A:172:ASN:HB2	1.68	0.58
1:B:444:ASN:H	1:B:444:ASN:HD22	1.52	0.58
1:B:47:GLN:CA	1:B:47:GLN:HE21	2.17	0.58
1:A:290:ASP:HA	1:A:309:CYS:SG	2.43	0.58
1:A:70:ASN:HB3	1:A:72:VAL:HG12	1.84	0.58
1:A:76:PRO:C	1:A:78:GLU:H	2.07	0.58
1:B:270:LYS:HG2	1:B:271:CYS:N	2.17	0.58
1:B:422:THR:HA	1:B:444:ASN:O	2.04	0.58
1:B:180:GLU:HB2	1:B:182:ASN:OD1	2.03	0.58
1:B:341:ILE:O	1:B:378:THR:HG23	2.04	0.58
1:B:295:GLU:HB3	1:B:300:ARG:HA	1.85	0.57
1:B:25:LEU:O	1:B:29:ARG:HG3	2.04	0.57
1:B:463:LYS:HZ3	1:B:463:LYS:HB3	1.69	0.57
1:B:28:GLN:HG3	1:B:54:PHE:CE2	2.39	0.57
1:A:130:PRO:HA	1:A:157:GLN:NE2	2.19	0.57
1:B:144:VAL:HG12	1:B:145:SER:N	2.19	0.57
1:B:438:ILE:HG13	1:B:465:LYS:O	2.04	0.57
2:D:45:ARG:O	2:D:47:LEU:N	2.37	0.57
1:B:421:ILE:HG13	1:B:445:LEU:CD1	2.34	0.57
1:B:472:GLU:N	5:B:1339:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG12	1:A:36:VAL:HB	1.86	0.57
1:A:97:VAL:O	1:A:98:LEU:HD23	2.04	0.57
1:B:216:CYS:HA	1:B:225:LEU:HD13	1.86	0.57
1:B:295:GLU:CB	1:B:300:ARG:HA	2.33	0.57
1:B:7:CYS:HB2	1:B:30:MET:CE	2.34	0.57
1:B:215:GLY:CA	1:B:225:LEU:HD22	2.34	0.57
1:B:16:GLN:HB2	1:B:45:TYR:CD1	2.40	0.57
1:B:74:ARG:NH1	1:B:112:PRO:HG2	2.20	0.57
1:B:119:ILE:O	1:B:119:ILE:HG22	2.05	0.57
1:B:367:GLU:O	1:B:370:ILE:HB	2.04	0.57
1:B:69:LEU:CD1	2:D:26:LEU:HD11	2.35	0.57
1:A:453:TRP:O	1:A:455:LYS:N	2.38	0.57
1:A:509:ARG:HD2	1:A:509:ARG:N	2.20	0.57
1:B:225:LEU:O	1:B:226:VAL:HG13	2.05	0.57
1:B:41:LEU:HB3	1:B:65:VAL:HG22	1.85	0.57
1:A:82:ILE:HD11	1:A:120:LEU:CG	2.36	0.56
1:A:68:ALA:HA	1:A:98:LEU:O	2.05	0.56
1:B:44:THR:HG22	1:B:68:ALA:O	2.05	0.56
1:A:190:ILE:HD12	1:A:199:CYS:SG	2.45	0.56
1:A:335:PHE:HA	1:A:338:CYS:SG	2.46	0.56
1:A:371:LEU:C	1:A:373:THR:H	2.09	0.56
1:A:453:TRP:C	1:A:455:LYS:H	2.08	0.56
1:B:47:GLN:HA	1:B:71:THR:OG1	2.04	0.56
1:A:148:PHE:O	1:A:150:SER:N	2.38	0.56
1:A:295:GLU:HA	1:A:300:ARG:HA	1.87	0.56
1:B:216:CYS:HB2	1:B:223:ASP:O	2.04	0.56
1:A:426:LEU:O	1:A:428:SER:N	2.37	0.56
1:B:443:LYS:HG3	1:B:444:ASN:H	1.70	0.56
1:A:144:VAL:HG12	1:A:145:SER:N	2.21	0.56
1:B:401:ILE:HG13	1:B:431:GLU:HB3	1.87	0.56
1:B:198:ARG:O	1:B:208:CYS:HB2	2.06	0.56
1:B:393:LEU:HB2	1:B:424:LEU:O	2.06	0.56
1:B:483:HIS:O	1:B:484:ALA:HB2	2.05	0.56
1:A:124:VAL:HG13	1:A:154:MET:SD	2.46	0.55
1:A:84:ARG:HG3	1:A:84:ARG:HH11	1.72	0.55
1:B:140:TRP:O	1:B:142:ASP:N	2.39	0.55
1:B:296:GLU:C	1:B:298:GLY:H	2.09	0.55
1:B:436:ASP:OD2	1:B:463:LYS:HG2	2.06	0.55
1:B:484:ALA:HB3	1:B:485:LEU:HD12	1.88	0.55
1:B:7:CYS:HB2	1:B:30:MET:HE1	1.87	0.55
1:A:310:ARG:N	1:A:310:ARG:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG11	1:A:52:LEU:CD1	2.32	0.55
1:B:243:LEU:C	1:B:256:ASN:HB3	2.27	0.55
1:A:35:GLU:HG2	1:A:57:THR:HG22	1.89	0.55
1:B:352:PHE:CZ	1:B:387:PRO:HD3	2.41	0.55
1:A:331:ASN:CB	3:A:1328:NAG:HN2	2.13	0.55
2:D:45:ARG:HG3	2:D:45:ARG:HH11	1.71	0.55
1:A:175:CYS:HA	1:A:183:CYS:HA	1.88	0.55
1:A:429:LEU:HD21	1:A:432:ILE:HD11	1.88	0.55
1:A:487:SER:HB2	1:A:488:PRO:CD	2.36	0.55
1:A:487:SER:HB2	1:A:488:PRO:HD2	1.88	0.55
1:B:459:THR:N	1:B:462:GLN:HE21	2.04	0.55
1:A:380:PHE:C	1:A:380:PHE:CD1	2.80	0.55
1:A:444:ASN:HA	1:A:470:ARG:CD	2.37	0.55
1:B:126:PHE:CD1	1:B:154:MET:HE2	2.42	0.55
1:B:386:TRP:HB3	1:B:419:LEU:HD12	1.89	0.55
1:B:416:VAL:CG2	1:B:439:ILE:HG23	2.31	0.55
1:A:417:VAL:HG11	2:C:47:LEU:CD2	2.37	0.55
1:A:186:LEU:HD12	1:A:186:LEU:N	2.15	0.54
1:B:196:SER:HB3	1:B:210:ASN:CB	2.35	0.54
1:A:350:VAL:CG2	1:A:355:ASP:HB2	2.37	0.54
1:B:29:ARG:NH1	2:D:49:TRP:NE1	2.54	0.54
1:B:442:ASN:HB3	1:B:445:LEU:HB2	1.89	0.54
1:B:442:ASN:HD22	1:B:469:ASN:ND2	2.05	0.54
1:A:36:VAL:HG22	1:A:60:GLU:CG	2.37	0.54
1:A:148:PHE:C	1:A:150:SER:N	2.61	0.54
1:A:76:PRO:O	1:A:78:GLU:HG2	2.07	0.54
1:B:140:TRP:O	1:B:143:ILE:N	2.41	0.54
1:A:300:ARG:NH2	1:A:403:ARG:NH2	2.55	0.54
1:B:140:TRP:C	1:B:142:ASP:N	2.60	0.54
1:B:114:ARG:HA	1:B:176:TRP:CD1	2.43	0.54
1:A:371:LEU:HB2	1:A:395:ALA:HB1	1.89	0.54
1:A:446:CYS:O	1:A:447:TYR:HD1	1.91	0.54
1:A:251:TYR:O	1:A:252:GLN:NE2	2.41	0.54
1:A:454:LYS:HD3	1:A:454:LYS:O	2.07	0.54
1:B:432:ILE:O	1:B:457:PHE:HB2	2.08	0.54
1:B:464:THR:HG23	1:B:464:THR:O	2.08	0.54
1:B:95:LEU:HB3	1:B:124:VAL:HG13	1.90	0.54
1:A:507:ARG:HD2	1:A:507:ARG:C	2.28	0.53
1:B:295:GLU:HB2	1:B:299:VAL:O	2.07	0.53
1:B:74:ARG:HH12	1:B:112:PRO:HG2	1.74	0.53
2:D:8:LEU:HA	2:D:11:ASP:OD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:SER:O	2:D:11:ASP:N	2.41	0.53
1:A:423:SER:HA	1:A:445:LEU:HD13	1.91	0.53
1:B:480:GLN:O	1:B:481:VAL:O	2.26	0.53
1:B:417:VAL:O	1:B:419:LEU:HD22	2.08	0.53
1:A:104:ASN:O	1:A:105:LYS:HB2	2.08	0.53
1:A:473:ASN:HD22	1:A:473:ASN:N	2.05	0.53
1:B:507:ARG:HA	1:B:510:GLU:O	2.09	0.53
1:A:394:HIS:O	1:A:397:GLU:HG3	2.08	0.53
1:B:124:VAL:HB	1:B:154:MET:CE	2.37	0.53
1:B:15:THR:HG23	2:D:31:CYS:O	2.09	0.53
1:B:242:PRO:O	1:B:257:PRO:HD2	2.08	0.53
1:A:92:SER:O	1:A:123:ALA:HB3	2.08	0.53
1:B:329:ALA:HB2	1:B:363:LEU:HA	1.90	0.53
1:B:352:PHE:CE1	1:B:387:PRO:HD3	2.44	0.53
1:B:385:ALA:O	1:B:386:TRP:HB2	2.09	0.53
1:A:125:ARG:HG2	1:A:125:ARG:NH1	2.21	0.52
1:B:352:PHE:CE2	1:B:363:LEU:HD23	2.44	0.52
1:B:47:GLN:NE2	1:B:71:THR:OG1	2.42	0.52
1:A:110:GLU:OE1	1:A:110:GLU:HA	2.08	0.52
1:B:453:TRP:O	1:B:455:LYS:N	2.43	0.52
1:A:213:ALA:O	1:A:214:ALA:HB3	2.10	0.52
1:B:26:SER:O	1:B:28:GLN:N	2.43	0.52
1:B:432:ILE:O	1:B:457:PHE:CB	2.58	0.52
1:B:232:ASP:OD2	1:B:237:LYS:HD2	2.08	0.52
1:A:45:TYR:CE2	1:A:69:LEU:HD12	2.45	0.52
1:B:114:ARG:HH11	1:B:182:ASN:ND2	2.08	0.52
1:B:358:THR:HG21	3:B:1328:NAG:O6	2.09	0.52
1:B:190:ILE:O	1:B:199:CYS:SG	2.68	0.52
1:A:352:PHE:CE2	1:A:387:PRO:HG3	2.45	0.52
1:B:186:LEU:HG	1:B:190:ILE:HG13	1.92	0.52
1:B:311:LYS:HD2	1:B:311:LYS:O	2.10	0.52
1:B:491:CYS:HA	1:B:500:VAL:HG23	1.92	0.52
1:A:408:GLN:C	1:A:410:GLY:N	2.62	0.51
1:A:89:TYR:O	1:A:91:ASN:N	2.44	0.51
1:A:97:VAL:C	1:A:98:LEU:HD23	2.30	0.51
1:B:215:GLY:N	1:B:225:LEU:HD22	2.25	0.51
1:B:30:MET:HG2	1:B:31:PHE:CE1	2.44	0.51
1:B:443:LYS:O	1:B:470:ARG:HA	2.10	0.51
1:A:101:TYR:HB3	1:A:130:PRO:HD2	1.91	0.51
1:A:409:HIS:CE1	2:C:38:ILE:HD11	2.45	0.51
1:B:293:GLU:HA	1:B:302:CYS:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:TYR:CE2	1:B:69:LEU:HD23	2.43	0.51
2:C:19:VAL:HG22	2:C:32:ASN:HB3	1.91	0.51
1:A:489:GLU:O	1:A:490:GLY:O	2.29	0.51
1:B:91:ASN:O	1:B:92:SER:OG	2.20	0.51
1:A:311:LYS:HD3	1:A:311:LYS:N	2.25	0.51
1:B:186:LEU:H	1:B:186:LEU:HD23	1.76	0.51
1:A:251:TYR:C	1:A:252:GLN:HE21	2.14	0.51
1:B:408:GLN:C	1:B:410:GLY:N	2.63	0.51
1:B:4:LYS:HE3	1:B:231:ARG:HH12	1.74	0.51
1:B:324:SER:HA	3:B:1328:NAG:H5	1.92	0.51
1:B:508:GLY:O	1:B:509:ARG:HB2	2.10	0.51
1:B:333:LYS:HE3	1:B:334:HIS:HE1	1.74	0.51
1:B:508:GLY:O	1:B:509:ARG:HD2	2.11	0.51
1:B:75:ILE:HG22	1:B:77:LEU:HG	1.91	0.51
1:A:201:GLY:O	1:A:203:SER:N	2.44	0.51
1:B:232:ASP:HB2	1:B:237:LYS:HD2	1.92	0.51
1:B:138:ILE:HG23	1:B:184:GLN:OE1	2.11	0.50
1:B:247:ASN:HD22	1:B:247:ASN:C	2.14	0.50
1:A:130:PRO:O	1:A:131:ALA:HB3	2.10	0.50
1:A:497:ARG:HG3	1:A:498:ASP:OD2	2.11	0.50
1:B:220:ARG:HG3	1:B:221:GLU:H	1.76	0.50
1:B:417:VAL:HA	1:B:440:SER:O	2.10	0.50
1:B:4:LYS:HG3	1:B:36:VAL:HG21	1.93	0.50
1:B:41:LEU:HD23	1:B:65:VAL:CG2	2.40	0.50
2:D:6:CYS:SG	2:D:29:TYR:HD2	2.35	0.50
1:A:333:LYS:HG2	5:A:2441:HOH:O	2.10	0.50
1:B:181:GLU:C	1:B:183:CYS:H	2.14	0.50
2:D:7:PRO:C	2:D:9:SER:N	2.63	0.50
1:B:485:LEU:N	1:B:485:LEU:HD12	2.16	0.50
1:B:28:GLN:HA	1:B:54:PHE:CZ	2.46	0.50
1:A:187:THR:HB	1:A:199:CYS:O	2.11	0.50
1:A:403:ARG:CG	1:A:403:ARG:NH1	2.73	0.50
1:A:65:VAL:HB	1:A:95:LEU:HD13	1.92	0.50
1:B:319:GLY:C	1:B:321:PHE:H	2.14	0.50
1:B:28:GLN:O	1:B:32:ASN:HB2	2.12	0.50
1:A:451:ILE:HG22	1:A:451:ILE:O	2.11	0.50
1:A:114:ARG:H	1:A:114:ARG:CD	2.25	0.50
4:A:1420:NAG:H4	4:A:2420:NAG:HN2	1.77	0.50
1:A:109:LYS:NZ	1:A:163:CYS:HB3	2.26	0.50
1:A:394:HIS:HA	1:A:397:GLU:HG3	1.93	0.50
1:B:241:PRO:CB	1:B:259:GLY:HA2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:ARG:HH11	2:C:45:ARG:HG2	1.77	0.50
1:A:220:ARG:HG3	1:A:220:ARG:HH11	1.77	0.50
1:A:326:SER:OG	1:A:351:ALA:HB2	2.12	0.50
1:B:417:VAL:HG12	1:B:440:SER:H	1.77	0.50
1:B:459:THR:CB	1:B:462:GLN:HE21	2.23	0.50
1:B:494:PRO:HG2	1:B:495:GLU:H	1.77	0.50
2:D:22:TYR:OH	2:D:27:ASP:HA	2.11	0.50
1:B:111:LEU:HG	1:B:113:MET:HG3	1.94	0.49
1:B:297:ASP:C	1:B:299:VAL:H	2.15	0.49
2:D:15:LEU:HD21	2:D:41:ARG:HH21	1.76	0.49
2:C:49:TRP:HA	2:C:49:TRP:CE3	2.47	0.49
1:A:329:ALA:O	1:A:330:THR:C	2.51	0.49
1:A:485:LEU:HB2	5:A:2443:HOH:O	2.12	0.49
1:B:399:LEU:HD21	1:B:402:ILE:HD11	1.95	0.49
1:A:134:ASN:HB3	1:A:175:CYS:O	2.12	0.49
1:A:481:VAL:HG12	1:A:483:HIS:H	1.78	0.49
1:B:451:ILE:O	1:B:452:ASN:C	2.50	0.49
1:B:92:SER:O	1:B:123:ALA:HB3	2.13	0.49
1:B:134:ASN:O	1:B:136:GLU:N	2.45	0.49
1:B:485:LEU:CD1	1:B:485:LEU:H	2.05	0.49
1:A:153:SER:O	1:A:154:MET:HB3	2.12	0.49
1:A:327:ILE:HA	3:A:1328:NAG:H81	1.95	0.49
1:B:256:ASN:HB2	1:B:259:GLY:HA3	1.94	0.49
1:B:325:LEU:O	1:B:348:LEU:HD12	2.12	0.49
1:B:350:VAL:CG2	1:B:355:ASP:HB2	2.42	0.49
1:B:339:THR:HA	1:B:374:VAL:HA	1.95	0.49
2:D:9:SER:C	2:D:11:ASP:H	2.15	0.49
1:A:201:GLY:C	1:A:203:SER:N	2.66	0.49
1:B:149:LEU:HD12	1:B:150:SER:H	1.77	0.49
1:A:73:GLU:HA	1:A:107:GLY:O	2.13	0.49
1:B:46:VAL:HG23	1:B:70:ASN:OD1	2.12	0.49
1:A:203:SER:N	1:A:204:PRO:CD	2.76	0.49
1:A:485:LEU:HD23	1:A:485:LEU:N	2.25	0.49
1:B:138:ILE:HD11	1:B:175:CYS:C	2.33	0.49
1:A:16:GLN:HE22	1:A:20:PHE:HE2	1.61	0.49
1:A:13:LYS:HB3	1:A:42:GLU:OE2	2.12	0.49
1:B:243:LEU:O	1:B:256:ASN:N	2.45	0.49
2:D:6:CYS:HB3	2:D:10:HIS:HB2	1.95	0.49
1:A:300:ARG:HH21	1:A:403:ARG:HH21	1.59	0.48
1:B:444:ASN:HD22	1:B:444:ASN:N	2.09	0.48
1:B:84:ARG:CG	1:B:84:ARG:HH11	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:PRO:HB2	2:D:9:SER:HB3	1.95	0.48
1:A:181:GLU:C	1:A:183:CYS:H	2.17	0.48
1:A:296:GLU:O	1:A:298:GLY:N	2.42	0.48
1:B:20:PHE:H	1:B:20:PHE:HD1	1.61	0.48
2:D:6:CYS:SG	2:D:29:TYR:CD2	3.06	0.48
1:B:102:ASP:O	1:B:105:LYS:N	2.45	0.48
1:B:368:LEU:O	1:B:395:ALA:CB	2.61	0.48
1:B:453:TRP:CD1	1:B:453:TRP:N	2.81	0.48
1:B:293:GLU:HA	1:B:302:CYS:HB3	1.96	0.48
1:B:485:LEU:CD2	1:B:496:PRO:HG3	2.42	0.48
1:B:67:ILE:O	1:B:97:VAL:HA	2.13	0.48
1:B:328:ASN:N	3:B:1328:NAG:C8	2.65	0.48
1:B:199:CYS:SG	1:B:201:GLY:O	2.72	0.48
1:B:371:LEU:O	1:B:395:ALA:O	2.31	0.48
2:D:48:LYS:O	2:D:49:TRP:CG	2.66	0.48
1:A:151:ASN:OD1	1:A:151:ASN:O	2.31	0.48
1:A:394:HIS:O	1:A:396:PHE:N	2.47	0.48
1:B:69:LEU:N	1:B:69:LEU:CD1	2.77	0.48
2:D:49:TRP:CB	5:D:57:HOH:O	2.62	0.48
1:A:28:GLN:HA	1:A:54:PHE:CZ	2.49	0.48
1:B:380:PHE:CB	1:B:413:SER:HA	2.44	0.48
1:B:439:ILE:O	1:B:466:ILE:HA	2.14	0.48
1:B:467:ILE:HG22	1:B:468:SER:N	2.28	0.48
1:B:510:GLU:HG3	1:B:512:VAL:HG22	1.95	0.48
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.13	0.48
1:A:67:ILE:HG22	1:A:67:ILE:O	2.14	0.48
1:B:209:HIS:ND1	1:B:211:GLN:HB2	2.28	0.48
1:B:390:ARG:HH11	1:B:390:ARG:CB	2.17	0.48
1:B:453:TRP:HA	1:B:456:LEU:HD23	1.96	0.48
1:B:447:TYR:CE2	1:B:480:GLN:O	2.66	0.48
1:A:142:ASP:CG	1:A:188:LYS:HB3	2.34	0.48
1:A:72:VAL:HG22	1:A:73:GLU:N	2.28	0.48
1:A:62:ALA:HA	1:A:84:ARG:HB2	1.96	0.48
2:C:15:LEU:HD23	2:C:15:LEU:N	2.28	0.48
1:A:242:PRO:O	1:A:256:ASN:HB3	2.14	0.47
1:B:346:HIS:HE2	1:B:380:PHE:HZ	1.61	0.47
1:B:38:LEU:O	1:B:62:ALA:HB3	2.14	0.47
1:A:508:GLY:C	1:A:510:GLU:H	2.17	0.47
1:A:47:GLN:HB2	1:A:50:TYR:CD1	2.48	0.47
1:B:446:CYS:C	1:B:447:TYR:CD1	2.87	0.47
1:B:453:TRP:O	1:B:456:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HD11	2:D:26:LEU:CD1	2.43	0.47
1:A:473:ASN:ND2	1:A:473:ASN:N	2.62	0.47
1:A:62:ALA:O	1:A:85:GLY:N	2.47	0.47
1:B:140:TRP:C	1:B:142:ASP:H	2.18	0.47
1:B:394:HIS:ND1	1:B:395:ALA:N	2.62	0.47
1:B:78:GLU:O	1:B:115:ASN:HB2	2.14	0.47
1:B:12:ASN:HD22	1:B:12:ASN:C	2.17	0.47
1:B:324:SER:HB3	3:B:1328:NAG:H3	1.96	0.47
1:B:386:TRP:CZ2	1:B:393:LEU:HA	2.49	0.47
1:A:138:ILE:HA	1:A:184:GLN:NE2	2.30	0.47
1:A:243:LEU:N	1:A:243:LEU:CD1	2.77	0.47
1:A:403:ARG:O	1:A:433:SER:HB2	2.14	0.47
1:B:510:GLU:CD	1:B:512:VAL:HG13	2.35	0.47
1:A:199:CYS:HA	1:A:208:CYS:H	1.79	0.47
1:A:483:HIS:O	1:A:484:ALA:HB2	2.14	0.47
1:B:58:ILE:HG22	1:B:80:LEU:HD13	1.97	0.47
1:A:56:LYS:HG2	1:A:76:PRO:HB3	1.97	0.47
1:B:296:GLU:O	1:B:298:GLY:N	2.45	0.47
1:B:330:THR:HG22	1:B:331:ASN:ND2	2.30	0.47
1:B:64:TYR:HB2	1:B:94:ALA:O	2.14	0.47
1:A:420:ASN:OD1	4:A:1420:NAG:H2	2.15	0.47
1:A:114:ARG:HG3	1:A:182:ASN:OD1	2.15	0.47
1:A:397:GLU:C	1:A:398:ASN:HD22	2.18	0.47
1:A:432:ILE:O	1:A:432:ILE:HG22	2.15	0.47
1:A:450:THR:O	1:A:490:GLY:CA	2.61	0.47
1:B:303:LYS:CD	1:B:304:LYS:H	2.28	0.47
1:B:412:PHE:HA	1:B:436:ASP:O	2.14	0.47
1:B:416:VAL:O	1:B:439:ILE:HA	2.15	0.47
1:A:45:TYR:HE2	1:A:69:LEU:HD12	1.79	0.47
1:B:443:LYS:HG3	1:B:444:ASN:N	2.29	0.47
1:A:252:GLN:HE21	1:A:252:GLN:CA	2.28	0.46
1:A:347:ILE:HD11	1:A:396:PHE:HZ	1.80	0.46
1:A:422:THR:HA	1:A:444:ASN:O	2.14	0.46
1:A:451:ILE:CG2	1:A:451:ILE:O	2.62	0.46
1:B:315:GLY:O	1:B:318:ILE:HG22	2.15	0.46
1:B:432:ILE:N	1:B:456:LEU:O	2.48	0.46
1:B:504:ASN:C	1:B:506:SER:H	2.19	0.46
2:D:22:TYR:CE2	2:D:24:GLU:HA	2.50	0.46
1:A:174:SER:HB3	1:A:184:GLN:NE2	2.30	0.46
1:A:371:LEU:C	1:A:373:THR:N	2.67	0.46
1:A:472:GLU:C	1:A:474:SER:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:CYS:O	1:A:485:LEU:HD23	2.15	0.46
3:B:1032:NAG:O3	3:B:1032:NAG:H83	2.16	0.46
1:B:310:ARG:HH11	1:B:310:ARG:HG2	1.80	0.46
2:D:38:ILE:HG12	2:D:39:GLY:N	2.31	0.46
1:A:213:ALA:HB3	1:A:226:VAL:HG23	1.97	0.46
1:A:82:ILE:HA	1:A:118:GLU:O	2.15	0.46
1:A:87:MET:O	1:A:88:TYR:HD2	1.98	0.46
1:A:350:VAL:HG21	1:A:355:ASP:HB2	1.96	0.46
1:A:389:ASN:O	1:A:390:ARG:HD3	2.15	0.46
1:A:466:ILE:CD1	1:A:466:ILE:O	2.61	0.46
1:A:65:VAL:HB	1:A:95:LEU:CD1	2.46	0.46
1:B:189:ILE:HG13	1:B:190:ILE:HG12	1.97	0.46
1:B:213:ALA:O	1:B:214:ALA:HB3	2.15	0.46
1:B:303:LYS:CA	1:B:303:LYS:HE2	2.40	0.46
1:B:324:SER:CB	3:B:1328:NAG:H3	2.46	0.46
2:C:13:TYR:CE2	2:C:41:ARG:HG2	2.51	0.46
1:B:202:LYS:HD3	1:B:202:LYS:C	2.35	0.46
1:B:464:THR:HG22	5:B:1346:HOH:O	2.15	0.46
2:C:9:SER:C	2:C:11:ASP:H	2.18	0.46
1:A:125:ARG:HA	1:A:153:SER:O	2.16	0.46
1:A:12:ASN:O	1:A:15:THR:HB	2.16	0.46
1:A:174:SER:HB3	1:A:184:GLN:CB	2.27	0.46
1:A:408:GLN:C	1:A:410:GLY:H	2.19	0.46
1:B:328:ASN:H	3:B:1328:NAG:H83	1.72	0.46
2:D:7:PRO:HD3	2:D:29:TYR:CZ	2.51	0.46
1:A:478:THR:CB	1:A:480:GLN:HG3	2.44	0.46
1:B:126:PHE:HD1	1:B:154:MET:HE2	1.81	0.46
1:B:363:LEU:O	1:B:365:PRO:HD3	2.16	0.46
1:B:346:HIS:HD2	1:B:382:LEU:HB3	1.80	0.46
1:B:453:TRP:C	1:B:455:LYS:N	2.68	0.46
1:A:379:GLY:CA	1:A:406:THR:HG23	2.45	0.46
1:B:104:ASN:O	1:B:106:THR:HG23	2.16	0.46
1:B:213:ALA:HB3	1:B:226:VAL:HG23	1.98	0.46
1:B:12:ASN:OD1	2:D:38:ILE:HG13	2.16	0.46
1:B:82:ILE:HG12	1:B:83:ILE:N	2.29	0.45
2:C:50:TRP:N	2:C:50:TRP:CD1	2.84	0.45
1:A:324:SER:HB3	3:A:1328:NAG:H5	1.98	0.45
1:B:318:ILE:CD1	1:B:319:GLY:H	2.27	0.45
2:C:24:GLU:N	2:C:24:GLU:CD	2.70	0.45
1:A:310:ARG:H	1:A:310:ARG:HD2	1.82	0.45
1:A:28:GLN:O	1:A:32:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:NH2	1:B:251:TYR:CE2	2.84	0.45
1:B:339:THR:HA	1:B:373:THR:O	2.17	0.45
1:B:69:LEU:HD12	1:B:69:LEU:N	2.32	0.45
1:A:391:THR:HB	1:A:422:THR:H	1.82	0.45
1:A:453:TRP:C	1:A:455:LYS:N	2.70	0.45
1:B:149:LEU:HD12	1:B:150:SER:N	2.31	0.45
1:B:295:GLU:CB	1:B:300:ARG:HD2	2.36	0.45
1:B:311:LYS:HD2	1:B:311:LYS:C	2.36	0.45
1:B:285:ARG:HD3	1:B:405:ARG:HB3	1.97	0.45
1:A:426:LEU:C	1:A:428:SER:H	2.20	0.45
1:A:431:GLU:HA	1:A:456:LEU:O	2.16	0.45
1:B:272:PRO:O	1:B:274:ASN:N	2.49	0.45
1:A:192:ALA:O	1:A:193:GLN:C	2.55	0.45
1:A:443:LYS:O	1:A:470:ARG:HA	2.17	0.45
1:B:124:VAL:HB	1:B:152:MET:CE	2.47	0.45
1:A:10:THR:O	1:A:40:ASN:HB2	2.17	0.45
1:A:497:ARG:HB3	1:A:510:GLU:HB3	1.99	0.45
1:B:494:PRO:HG2	1:B:495:GLU:N	2.32	0.45
1:B:40:ASN:ND2	1:B:63:GLY:HA3	2.32	0.45
1:B:55:LEU:HB3	1:B:77:LEU:CD2	2.47	0.45
1:B:117:GLN:HA	1:B:143:ILE:HD12	1.99	0.45
1:B:446:CYS:SG	1:B:470:ARG:HG2	2.57	0.45
1:B:473:ASN:O	1:B:476:LYS:HD3	2.17	0.45
1:B:333:LYS:HE3	1:B:334:HIS:CE1	2.51	0.45
1:B:333:LYS:C	1:B:335:PHE:H	2.19	0.45
1:A:379:GLY:HA2	1:A:406:THR:HG23	1.98	0.45
1:A:432:ILE:O	1:A:457:PHE:HB2	2.17	0.45
1:B:129:ASN:C	1:B:157:GLN:HE22	2.20	0.45
1:A:451:ILE:HB	1:A:453:TRP:CE2	2.52	0.44
1:A:189:ILE:C	1:A:191:CYS:N	2.70	0.44
1:B:327:ILE:CA	3:B:1328:NAG:H83	2.36	0.44
1:B:29:ARG:NH1	2:D:49:TRP:HE1	2.14	0.44
1:B:376:GLU:HB2	1:B:401:ILE:CG2	2.48	0.44
1:A:504:ASN:O	1:A:505:VAL:C	2.55	0.44
1:B:149:LEU:O	1:B:152:MET:HG2	2.17	0.44
1:B:454:LYS:N	1:B:454:LYS:HD3	2.31	0.44
1:B:324:SER:OG	3:B:1328:NAG:H3	2.18	0.44
1:B:352:PHE:HE1	1:B:386:TRP:HA	1.83	0.44
1:A:381:LEU:HD11	1:A:383:ILE:HD11	1.98	0.44
1:A:391:THR:O	1:A:392:ASP:HB2	2.16	0.44
1:A:12:ASN:HB3	2:C:39:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG22	1:A:60:GLU:HG3	1.99	0.44
1:B:21:GLU:HG2	1:B:25:LEU:HD23	2.00	0.44
1:B:507:ARG:HB2	1:B:508:GLY:H	1.52	0.44
1:A:145:SER:O	1:A:147:ASP:N	2.51	0.44
1:A:71:THR:O	1:A:72:VAL:C	2.56	0.44
1:B:295:GLU:HG3	1:B:295:GLU:O	2.17	0.44
1:B:310:ARG:N	1:B:310:ARG:HD2	2.32	0.44
1:B:487:SER:HB3	1:B:488:PRO:HD2	1.99	0.44
2:D:39:GLY:HA3	2:D:43:GLN:OE1	2.18	0.44
1:A:111:LEU:HD21	1:A:113:MET:HE1	1.99	0.44
1:A:126:PHE:H	1:A:154:MET:HB3	1.83	0.44
1:A:385:ALA:O	1:A:386:TRP:HB2	2.17	0.44
1:B:109:LYS:NZ	1:B:163:CYS:HB3	2.32	0.44
1:A:200:ARG:HD3	1:A:216:CYS:O	2.18	0.44
1:B:181:GLU:O	1:B:183:CYS:N	2.50	0.44
1:B:257:PRO:CG	1:B:258:GLU:H	2.21	0.44
1:B:391:THR:HB	1:B:422:THR:CG2	2.37	0.44
1:B:444:ASN:ND2	1:B:444:ASN:N	2.59	0.44
1:A:324:SER:HB3	3:A:1328:NAG:H3	2.00	0.43
1:A:263:PHE:HE1	1:A:275:TYR:CE1	2.36	0.43
1:B:125:ARG:HH11	1:B:125:ARG:HG3	1.83	0.43
1:B:438:ILE:O	1:B:438:ILE:HG23	2.17	0.43
1:A:35:GLU:HA	1:A:57:THR:O	2.18	0.43
1:A:52:LEU:O	1:A:76:PRO:HG2	2.18	0.43
1:B:203:SER:HB3	1:B:206:ASP:CG	2.39	0.43
1:B:319:GLY:C	1:B:321:PHE:N	2.72	0.43
2:C:16:HIS:HD2	2:C:42:CYS:O	2.01	0.43
2:C:46:ASP:CG	2:C:49:TRP:CD1	2.92	0.43
1:A:430:LYS:CG	1:A:430:LYS:O	2.65	0.43
1:B:180:GLU:O	1:B:181:GLU:C	2.56	0.43
1:B:41:LEU:HD13	1:B:58:ILE:CD1	2.48	0.43
1:B:90:GLU:O	1:B:91:ASN:HB2	2.17	0.43
1:A:134:ASN:ND2	1:A:177:GLY:HA2	2.33	0.43
1:A:408:GLN:HA	1:A:408:GLN:NE2	2.28	0.43
1:A:45:TYR:HE2	1:A:69:LEU:CD1	2.31	0.43
1:B:4:LYS:HB3	5:B:1332:HOH:O	2.18	0.43
1:A:140:TRP:C	1:A:142:ASP:N	2.70	0.43
1:A:216:CYS:SG	1:A:216:CYS:O	2.76	0.43
1:A:209:HIS:CD2	1:A:221:GLU:HB2	2.53	0.43
1:A:438:ILE:O	1:A:438:ILE:HG23	2.18	0.43
1:B:134:ASN:C	1:B:136:GLU:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:C	1:B:28:GLN:N	2.72	0.43
1:B:78:GLU:HG2	1:B:112:PRO:CB	2.41	0.43
1:A:391:THR:CB	1:A:422:THR:HG22	2.46	0.43
1:B:411:GLN:OE1	2:D:48:LYS:HE3	2.19	0.43
1:A:19:THR:O	1:A:20:PHE:C	2.57	0.43
1:B:15:THR:CG2	1:B:16:GLN:N	2.81	0.43
1:B:25:LEU:HD22	1:B:25:LEU:H	1.84	0.43
1:A:503:ARG:O	1:A:504:ASN:HB2	2.19	0.43
1:A:508:GLY:C	1:A:510:GLU:N	2.71	0.43
1:A:37:VAL:CG2	1:A:61:VAL:HG22	2.49	0.43
1:B:124:VAL:N	1:B:152:MET:HE3	2.23	0.43
1:A:246:TYR:HA	1:A:253:MET:SD	2.58	0.43
1:A:470:ARG:HH11	1:A:470:ARG:CG	2.26	0.43
1:A:478:THR:C	1:A:480:GLN:H	2.21	0.43
1:B:439:ILE:HG22	1:B:442:ASN:ND2	2.34	0.43
2:D:43:GLN:N	2:D:43:GLN:OE1	2.45	0.43
1:A:97:VAL:HG21	1:A:126:PHE:CE2	2.53	0.43
1:A:314:ASN:HB3	1:A:318:ILE:CG2	2.49	0.43
1:A:67:ILE:O	1:A:97:VAL:HA	2.19	0.43
1:B:331:ASN:O	3:B:1328:NAG:H81	2.18	0.43
1:B:424:LEU:HD13	1:B:492:TRP:CZ3	2.54	0.43
2:C:46:ASP:CG	2:C:49:TRP:HD1	2.23	0.43
1:B:29:ARG:HB3	2:D:49:TRP:CH2	2.54	0.43
1:B:487:SER:HB3	1:B:488:PRO:CD	2.49	0.42
1:A:241:PRO:CB	1:A:258:GLU:O	2.67	0.42
1:B:380:PHE:HB2	1:B:413:SER:HA	2.00	0.42
1:B:438:ILE:HG21	2:D:47:LEU:HD22	2.00	0.42
3:A:1337:NAG:O3	3:A:1337:NAG:C7	2.66	0.42
1:A:478:THR:HG21	1:A:480:GLN:HE21	1.84	0.42
1:B:201:GLY:HA3	1:B:206:ASP:HB3	2.00	0.42
2:C:43:GLN:OE1	2:C:43:GLN:N	2.46	0.42
1:A:76:PRO:C	1:A:78:GLU:N	2.69	0.42
1:B:118:GLU:HG3	1:B:119:ILE:N	2.34	0.42
1:B:328:ASN:OD1	3:B:1328:NAG:C2	2.60	0.42
1:A:101:TYR:O	1:A:101:TYR:HD1	2.03	0.42
1:A:218:GLY:H	1:A:223:ASP:HB2	1.85	0.42
1:A:425:GLY:C	1:A:427:ARG:H	2.23	0.42
1:B:32:ASN:O	1:B:33:ASN:CB	2.65	0.42
1:A:126:PHE:HB2	1:A:154:MET:HB2	2.01	0.42
1:B:442:ASN:CB	1:B:469:ASN:HD22	2.19	0.42
1:B:87:MET:C	1:B:88:TYR:HD1	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LYS:HG3	1:A:333:LYS:H	1.67	0.42
1:A:495:GLU:HA	1:A:496:PRO:HD3	1.84	0.42
1:B:124:VAL:HG21	1:B:140:TRP:CE3	2.55	0.42
1:A:78:GLU:HB3	1:A:112:PRO:HB2	2.02	0.42
1:A:194:GLN:O	1:A:194:GLN:HG3	2.20	0.42
1:A:243:LEU:HD12	1:A:243:LEU:N	2.35	0.42
1:A:478:THR:C	1:A:480:GLN:N	2.74	0.42
1:A:489:GLU:HB3	1:A:500:VAL:CG1	2.50	0.42
1:A:62:ALA:HA	1:A:84:ARG:HG3	2.02	0.42
1:B:152:MET:O	1:B:152:MET:CG	2.67	0.42
1:B:274:ASN:OD1	1:B:275:TYR:HD2	2.03	0.42
1:A:109:LYS:HG3	1:A:131:ALA:O	2.19	0.42
1:A:114:ARG:HD2	1:A:114:ARG:H	1.84	0.42
1:A:478:THR:HG22	1:A:478:THR:O	2.20	0.42
3:B:1151:NAG:H3	3:B:1151:NAG:H82	2.02	0.42
1:B:82:ILE:HD11	1:B:120:LEU:HD12	2.00	0.42
1:B:130:PRO:O	1:B:131:ALA:CB	2.66	0.42
1:B:463:LYS:CB	1:B:463:LYS:NZ	2.79	0.42
1:A:55:LEU:HB3	1:A:77:LEU:HD23	2.01	0.41
1:B:331:ASN:CB	3:B:1328:NAG:O7	2.67	0.41
1:B:430:LYS:HE3	5:B:1338:HOH:O	2.20	0.41
1:B:5:LYS:HD3	5:B:1341:HOH:O	2.20	0.41
1:A:29:ARG:HB3	2:C:49:TRP:CZ2	2.55	0.41
1:A:394:HIS:C	1:A:396:PHE:N	2.74	0.41
1:A:487:SER:OG	1:A:501:SER:HB3	2.20	0.41
1:A:497:ARG:HA	1:A:510:GLU:HA	2.01	0.41
1:B:192:ALA:CB	1:B:204:PRO:HA	2.50	0.41
1:B:82:ILE:HD12	1:B:213:ALA:CB	2.49	0.41
2:D:34:VAL:HG12	2:D:35:VAL:N	2.35	0.41
1:A:434:ASP:OD2	1:A:435:GLY:N	2.46	0.41
1:B:215:GLY:C	1:B:225:LEU:HD22	2.40	0.41
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.85	0.41
1:A:247:ASN:HB2	1:A:254:ASP:OD2	2.20	0.41
1:A:430:LYS:O	1:A:430:LYS:HG3	2.21	0.41
1:A:48:ARG:HH11	1:A:48:ARG:HG2	1.85	0.41
1:B:97:VAL:HG12	1:B:100:ASN:HD22	1.85	0.41
1:B:418:SER:HA	1:B:441:GLY:O	2.21	0.41
1:B:475:CYS:HB3	1:B:480:GLN:HB2	2.02	0.41
1:A:139:GLN:HG2	1:A:174:SER:OG	2.21	0.41
1:A:272:PRO:O	1:A:274:ASN:N	2.53	0.41
1:A:312:VAL:O	1:A:312:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:OE1	1:A:403:ARG:NH1	2.50	0.41
1:A:472:GLU:O	1:A:474:SER:N	2.54	0.41
1:A:478:THR:CG2	1:A:480:GLN:HG3	2.50	0.41
1:B:314:ASN:O	1:B:342:SER:O	2.38	0.41
1:B:369:ASP:O	1:B:372:LYS:HB2	2.20	0.41
1:B:393:LEU:HD12	1:B:424:LEU:HA	2.02	0.41
2:C:37:TYR:CD2	2:C:45:ARG:HA	2.55	0.41
1:A:144:VAL:CG1	1:A:145:SER:N	2.84	0.41
1:A:13:LYS:O	1:A:15:THR:N	2.54	0.41
1:A:19:THR:H	1:A:22:ASP:HB2	1.85	0.41
4:A:1420:NAG:C4	4:A:2420:NAG:N2	2.81	0.41
1:A:46:VAL:CG1	1:A:72:VAL:HB	2.46	0.41
1:B:209:HIS:C	1:B:211:GLN:H	2.24	0.41
1:B:82:ILE:HD11	1:B:120:LEU:CD1	2.51	0.41
2:D:49:TRP:HB2	5:D:57:HOH:O	2.19	0.41
1:A:102:ASP:C	1:A:104:ASN:N	2.71	0.41
1:A:446:CYS:O	1:A:447:TYR:CD1	2.73	0.41
1:B:144:VAL:CG1	1:B:145:SER:N	2.83	0.41
1:B:349:PRO:CD	1:B:385:ALA:HB2	2.50	0.41
1:A:138:ILE:HD11	1:A:175:CYS:C	2.40	0.41
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.86	0.41
1:A:380:PHE:HB3	1:A:406:THR:O	2.20	0.41
1:A:44:THR:O	1:A:45:TYR:HB2	2.21	0.41
1:A:457:PHE:HB2	1:A:462:GLN:HE22	1.85	0.41
1:B:319:GLY:O	1:B:321:PHE:N	2.54	0.41
1:B:376:GLU:CB	1:B:401:ILE:HG22	2.50	0.41
1:B:447:TYR:HE2	1:B:480:GLN:O	2.03	0.41
1:A:68:ALA:O	1:A:69:LEU:HB2	2.21	0.41
1:A:453:TRP:CE3	1:A:456:LEU:HD23	2.56	0.41
1:A:454:LYS:HE3	1:A:454:LYS:HA	2.02	0.41
1:A:46:VAL:HG21	1:A:52:LEU:HD11	2.03	0.41
1:B:247:ASN:ND2	1:B:247:ASN:C	2.74	0.41
1:B:296:GLU:C	1:B:298:GLY:N	2.73	0.41
1:A:89:TYR:O	1:A:90:GLU:C	2.59	0.40
1:B:102:ASP:HB2	1:B:106:THR:O	2.21	0.40
1:B:135:VAL:HG12	1:B:156:PHE:CE2	2.56	0.40
1:B:21:GLU:O	1:B:24:PHE:N	2.53	0.40
1:B:366:GLN:CA	1:B:366:GLN:HE21	2.18	0.40
1:B:459:THR:N	1:B:462:GLN:NE2	2.68	0.40
1:B:75:ILE:HA	1:B:76:PRO:HD3	1.83	0.40
1:B:138:ILE:HG12	1:B:176:TRP:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:HG2	1:B:258:GLU:N	2.32	0.40
1:B:453:TRP:C	1:B:455:LYS:H	2.25	0.40
1:B:493:GLY:HA3	1:B:498:ASP:OD1	2.21	0.40
1:B:74:ARG:O	1:B:76:PRO:HD3	2.21	0.40
1:A:195:CYS:O	1:A:196:SER:C	2.59	0.40
1:A:261:TYR:HB2	1:A:268:VAL:HG23	2.02	0.40
1:A:427:ARG:HA	1:A:492:TRP:CD1	2.57	0.40
1:A:85:GLY:C	1:A:87:MET:H	2.23	0.40
1:B:129:ASN:C	1:B:157:GLN:NE2	2.75	0.40
1:B:380:PHE:CE1	1:B:408:GLN:HG2	2.56	0.40
1:B:447:TYR:O	1:B:450:THR:OG1	2.35	0.40
1:B:55:LEU:HB3	1:B:77:LEU:HD23	2.03	0.40
2:D:45:ARG:HG3	2:D:45:ARG:NH1	2.36	0.40
1:A:451:ILE:O	1:A:452:ASN:C	2.60	0.40
1:B:310:ARG:HB3	1:B:311:LYS:H	1.71	0.40
1:B:451:ILE:HG22	1:B:451:ILE:O	2.20	0.40
1:B:483:HIS:O	1:B:484:ALA:CB	2.68	0.40
1:A:394:HIS:O	1:A:397:GLU:N	2.55	0.40
1:A:65:VAL:O	1:A:95:LEU:HD12	2.21	0.40
1:B:263:PHE:CE1	1:B:272:PRO:HG2	2.56	0.40
1:B:318:ILE:CG1	1:B:319:GLY:N	2.84	0.40
1:B:68:ALA:HB1	1:B:69:LEU:HD13	2.04	0.40
1:B:69:LEU:HD21	2:D:23:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	509/622 (82%)	368 (72%)	93 (18%)	48 (9%)	<b>1</b> <b>5</b>
1	B	508/622 (82%)	369 (73%)	98 (19%)	41 (8%)	<b>1</b> <b>7</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	45/53 (85%)	35 (78%)	9 (20%)	1 (2%)	8	37
2	D	45/53 (85%)	31 (69%)	6 (13%)	8 (18%)	0	1
All	All	1107/1350 (82%)	803 (72%)	206 (19%)	98 (9%)	1	6

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	LEU
1	A	146	SER
1	A	171	PRO
1	A	203	SER
1	A	310	ARG
1	A	311	LYS
1	A	427	ARG
1	A	433	SER
1	A	490	GLY
1	B	13	LYS
1	B	14	LEU
1	B	171	PRO
1	B	273	ARG
1	B	292	TYR
1	B	309	CYS
1	B	477	ALA
1	B	481	VAL
1	B	484	ALA
1	B	505	VAL
2	D	10	HIS
2	D	46	ASP
2	D	49	TRP
1	A	90	GLU
1	A	91	ASN
1	A	149	LEU
1	A	193	GLN
1	A	196	SER
1	A	202	LYS
1	A	273	ARG
1	A	288	GLY
1	A	372	LYS
1	A	389	ASN
1	A	443	LYS

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Mol	Chain	Res	Type
1	A	454	LYS
1	A	484	ALA
1	A	505	VAL
1	B	27	LEU
1	B	180	GLU
1	B	257	PRO
1	B	289	ALA
1	B	454	LYS
2	C	47	LEU
2	D	48	LYS
1	A	77	LEU
1	A	174	SER
1	A	241	PRO
1	A	297	ASP
1	A	316	ILE
1	A	330	THR
1	A	395	ALA
1	A	486	CYS
1	B	99	SER
1	B	135	VAL
1	B	141	ARG
1	B	182	ASN
1	B	241	PRO
1	B	297	ASP
1	B	306	GLU
1	B	320	GLU
1	B	336	LYS
1	B	449	ASN
1	B	502	CYS
2	D	7	PRO
2	D	9	SER
2	D	17	ASP
1	A	63	GLY
1	A	154	MET
1	A	322	LYS
1	A	449	ASN
1	A	473	ASN
1	A	482	CYS
1	A	483	HIS
1	B	91	ASN
1	B	147	ASP
1	B	165	LYS

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Mol	Chain	Res	Type
1	B	193	GLN
1	B	488	PRO
1	B	507	ARG
2	D	47	LEU
1	A	76	PRO
1	A	112	PRO
1	A	168	PRO
1	A	179	GLY
1	A	190	ILE
1	A	481	VAL
1	B	334	HIS
1	A	494	PRO
1	B	494	PRO
1	A	72	VAL
1	A	319	GLY
1	B	387	PRO
1	B	487	SER
1	B	76	PRO
1	B	288	GLY
1	B	308	PRO
1	B	63	GLY
1	B	354	GLY

### 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	449/543 (83%)	408 (91%)	41 (9%)	11	38
1	B	448/543 (82%)	402 (90%)	46 (10%)	8	32
2	C	41/47 (87%)	37 (90%)	4 (10%)	9	34
2	D	41/47 (87%)	35 (85%)	6 (15%)	3	18
All	All	979/1180 (83%)	882 (90%)	97 (10%)	9	34

All (97) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	8	GLN
1	A	12	ASN
1	A	13	LYS
1	A	19	THR
1	A	98	LEU
1	A	101	TYR
1	A	114	ARG
1	A	153	SER
1	A	181	GLU
1	A	206	ASP
1	A	217	THR
1	A	223	ASP
1	A	241	PRO
1	A	243	LEU
1	A	252	GLN
1	A	292	TYR
1	A	293	GLU
1	A	295	GLU
1	A	310	ARG
1	A	311	LYS
1	A	324	SER
1	A	327	ILE
1	A	328	ASN
1	A	337	ASN
1	A	346	HIS
1	A	369	ASP
1	A	380	PHE
1	A	398	ASN
1	A	403	ARG
1	A	406	THR
1	A	407	LYS
1	A	408	GLN
1	A	414	LEU
1	A	447	TYR
1	A	454	LYS
1	A	455	LYS
1	A	457	PHE
1	A	459	THR
1	A	473	ASN
1	A	485	LEU
1	A	507	ARG
1	B	4	LYS
1	B	12	ASN

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Mol	Chain	Res	Type
1	B	13	LYS
1	B	14	LEU
1	B	30	MET
1	B	47	GLN
1	B	57	THR
1	B	128	ASN
1	B	139	GLN
1	B	149	LEU
1	B	163	CYS
1	B	186	LEU
1	B	202	LYS
1	B	219	PRO
1	B	221	GLU
1	B	226	VAL
1	B	240	CYS
1	B	241	PRO
1	B	247	ASN
1	B	249	THR
1	B	253	MET
1	B	285	ARG
1	B	290	ASP
1	B	292	TYR
1	B	303	LYS
1	B	304	LYS
1	B	305	CYS
1	B	310	ARG
1	B	311	LYS
1	B	358	THR
1	B	366	GLN
1	B	378	THR
1	B	389	ASN
1	B	390	ARG
1	B	408	GLN
1	B	416	VAL
1	B	437	VAL
1	B	444	ASN
1	B	449	ASN
1	B	454	LYS
1	B	457	PHE
1	B	463	LYS
1	B	485	LEU
1	B	507	ARG

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Mol	Chain	Res	Type
1	B	509	ARG
1	B	512	VAL
2	C	13	TYR
2	C	15	LEU
2	C	24	GLU
2	C	50	TRP
2	D	5	GLU
2	D	19	VAL
2	D	28	LYS
2	D	32	ASN
2	D	49	TRP
2	D	50	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	129	ASN
1	A	134	ASN
1	A	139	GLN
1	A	157	GLN
1	A	184	GLN
1	A	252	GLN
1	A	314	ASN
1	A	398	ASN
1	A	408	GLN
1	A	409	HIS
1	A	473	ASN
1	A	480	GLN
1	B	16	GLN
1	B	23	HIS
1	B	28	GLN
1	B	40	ASN
1	B	47	GLN
1	B	79	ASN
1	B	128	ASN
1	B	139	GLN
1	B	157	GLN
1	B	193	GLN
1	B	334	HIS
1	B	366	GLN
1	B	389	ASN

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Mol	Chain	Res	Type
1	B	398	ASN
1	B	444	ASN
1	B	449	ASN
1	B	452	ASN
1	B	462	GLN
1	B	469	ASN
2	C	16	HIS
2	D	32	ASN

### 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 ⓘ

2 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	$\# Z  > 2$
4	NAG	A	1420	1,4	14,14,15	0.63	0	15,19,21	1.17	1 (6%)
4	NAG	A	2420	4	14,14,15	0.67	0	15,19,21	0.68	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
4	NAG	A	1420	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2420	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1420	NAG	C4-C3-C2	3.13	115.60	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1420	NAG	4	0
4	A	2420	NAG	3	0

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
3	NAG	A	1032	1	14,14,15	0.58	0	15,19,21	0.67	0
3	NAG	A	1151	1	14,14,15	0.59	0	15,19,21	0.86	0
3	NAG	A	1172	1	14,14,15	0.59	0	15,19,21	0.71	0
3	NAG	A	1328	1	14,14,15	0.81	1 (7%)	15,19,21	1.00	1 (6%)
3	NAG	A	1337	1	14,14,15	0.54	0	15,19,21	0.58	0
3	NAG	B	1032	1	14,14,15	0.47	0	15,19,21	0.86	1 (6%)
3	NAG	B	1151	1	14,14,15	0.61	0	15,19,21	0.62	0
3	NAG	B	1328	1	14,14,15	0.74	0	15,19,21	1.00	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
3	NAG	A	1032	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1172	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1328	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1337	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1032	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1151	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1328	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1328	NAG	C1-C2	2.48	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1328	NAG	C3-C4-C5	-2.67	105.51	110.22
3	B	1032	NAG	C2-N2-C7	-2.22	119.70	122.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1172	NAG	C8-C7-N2-C2
3	A	1328	NAG	O7-C7-N2-C2
3	A	1172	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1328	NAG	8	0
3	A	1337	NAG	1	0
3	B	1032	NAG	1	0
3	B	1151	NAG	1	0
3	B	1328	NAG	19	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.