



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID : 2B5N  
Title : Crystal Structure of the DDB1 BPB Domain  
Authors : Li, T.; Chen, X.; Garbutt, K.C.; Zhou, P.; Zheng, N.  
Deposited on : 2005-09-28  
Resolution : 2.80 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

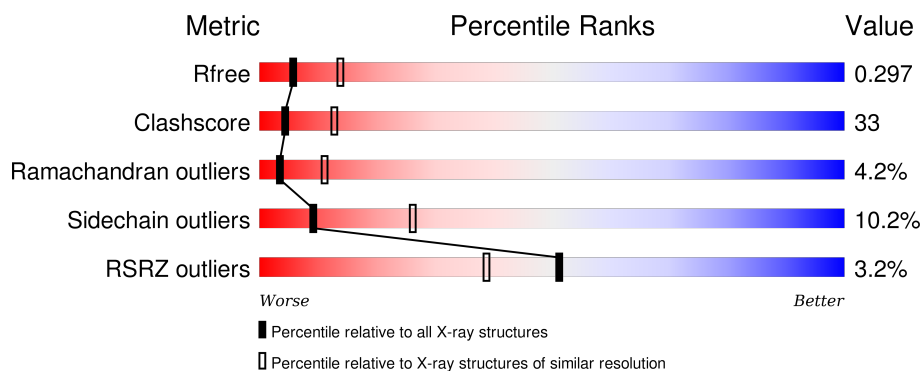
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

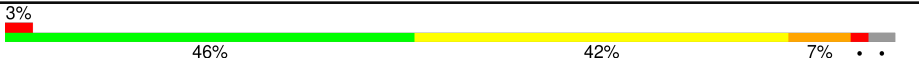



The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	323	
1	B	323	
1	C	323	
1	D	323	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IPA	B	1001	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9893 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 damage-specific DNA binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2421	1535	407	466	13			
1	B	321	Total	C	N	O	S	0	0	0
			2486	1570	422	480	14			
1	C	320	Total	C	N	O	S	0	0	0
			2478	1564	421	479	14			
1	D	320	Total	C	N	O	S	0	0	0
			2482	1568	421	479	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	GLY	-	CLONING ARTIFACT	GB 13435359
A	388	SER	-	CLONING ARTIFACT	GB 13435359
A	389	HIS	-	CLONING ARTIFACT	GB 13435359
A	390	MET	-	INITIATING METHIONINE	GB 13435359
B	387	GLY	-	CLONING ARTIFACT	GB 13435359
B	388	SER	-	CLONING ARTIFACT	GB 13435359
B	389	HIS	-	CLONING ARTIFACT	GB 13435359
B	390	MET	-	INITIATING METHIONINE	GB 13435359
C	387	GLY	-	CLONING ARTIFACT	GB 13435359
C	388	SER	-	CLONING ARTIFACT	GB 13435359
C	389	HIS	-	CLONING ARTIFACT	GB 13435359
C	390	MET	-	INITIATING METHIONINE	GB 13435359
D	387	GLY	-	CLONING ARTIFACT	GB 13435359
D	388	SER	-	CLONING ARTIFACT	GB 13435359
D	389	HIS	-	CLONING ARTIFACT	GB 13435359
D	390	MET	-	INITIATING METHIONINE	GB 13435359

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	3	1		

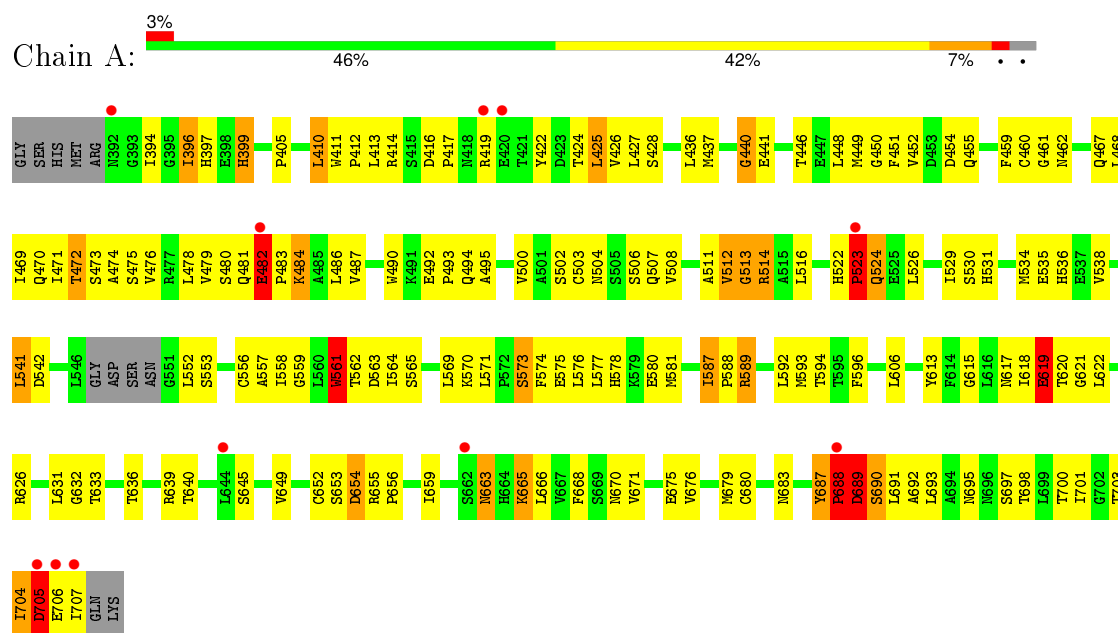
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	6	Total	O	0	0
			6	6		
3	C	6	Total	O	0	0
			6	6		
3	D	6	Total	O	0	0
			6	6		

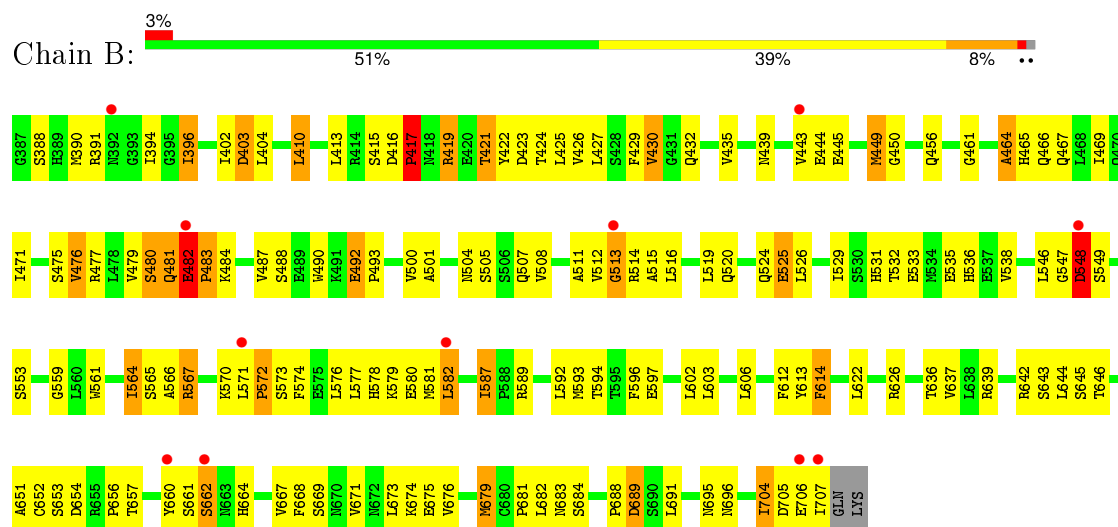
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

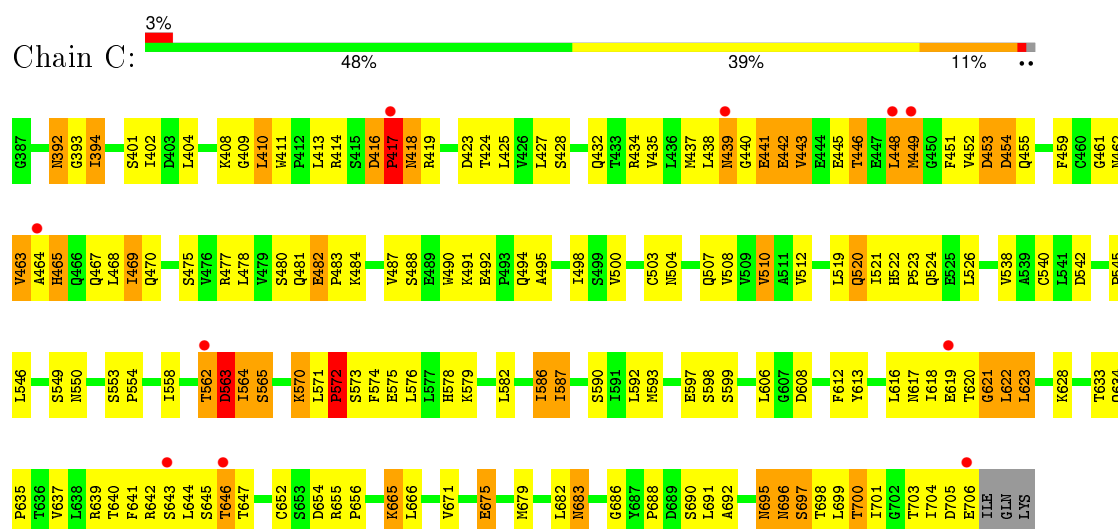
- Molecule 1: damage-specific DNA binding protein 1



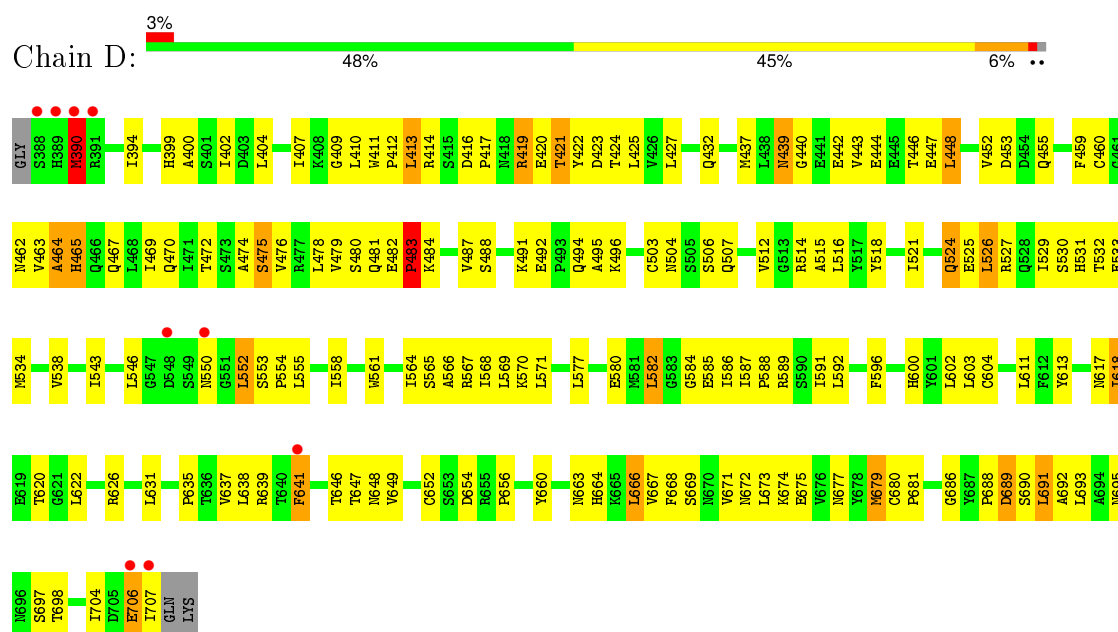
- Molecule 1: damage-specific DNA binding protein 1



- Molecule 1: damage-specific DNA binding protein 1



- Molecule 1: damage-specific DNA binding protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.54 Å   73.75 Å   136.78 Å 90.00°   111.73°   90.00°	Depositor
Resolution (Å)	48.80 – 2.80 48.77 – 2.54	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.80-2.80) 98.9 (48.77-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.75 (at 2.54 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236   ,   0.296 0.248   ,   0.297	Depositor DCC
$R_{free}$ test set	2385 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 1.4	EDS
Estimated twinning fraction	0.164 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 62244 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: IPA

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	0.43	0/2467	0.87	10/3354 (0.3%)
1	B	0.38	0/2534	0.81	4/3444 (0.1%)
1	C	0.37	0/2526	0.98	11/3433 (0.3%)
1	D	0.32	0/2530	0.73	0/3439
All	All	0.38	0/10057	0.85	25/13670 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	571	LEU	C-N-CD	-20.05	76.49	120.60
1	C	442	GLU	N-CA-C	-16.93	65.29	111.00
1	C	571	LEU	C-N-CA	13.74	179.69	122.00
1	C	442	GLU	CB-CA-C	12.23	134.87	110.40
1	B	417	PRO	CA-N-CD	-11.36	95.60	111.50
1	A	705	ASP	CB-CA-C	11.09	132.58	110.40
1	A	689	ASP	N-CA-C	-10.39	82.95	111.00
1	C	417	PRO	N-CA-C	-9.98	86.15	112.10
1	C	416	ASP	N-CA-C	8.68	134.44	111.00
1	C	443	VAL	N-CA-C	-8.64	87.66	111.00
1	A	689	ASP	CB-CA-C	-7.94	94.51	110.40
1	A	531	HIS	CB-CA-C	-7.83	94.74	110.40
1	A	688	PRO	CA-N-CD	-7.49	101.01	111.50
1	B	417	PRO	N-CA-C	7.41	131.36	112.10
1	A	688	PRO	N-CA-C	7.07	130.48	112.10
1	B	482	GLU	C-N-CD	6.37	141.78	128.40
1	C	572	PRO	CA-N-CD	-5.85	103.30	111.50
1	C	453	ASP	N-CA-C	-5.59	95.92	111.00
1	C	644	LEU	N-CA-C	-5.45	96.29	111.00
1	A	449	MET	N-CA-C	5.23	125.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	ILE	C-N-CA	-5.23	108.63	121.70
1	C	623	LEU	CA-CB-CG	-5.23	103.28	115.30
1	A	615	GLY	N-CA-C	-5.11	100.32	113.10
1	B	421	THR	N-CA-C	-5.04	97.38	111.00
1	A	596	PHE	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2421	0	2421	154	0
1	B	2486	0	2477	144	1
1	C	2478	0	2466	177	1
1	D	2482	0	2474	175	1
2	B	4	0	8	2	0
3	A	4	0	0	0	0
3	B	6	0	0	2	1
3	C	6	0	0	0	0
3	D	6	0	0	3	0
All	All	9893	0	9846	646	2

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 33.

All (646) 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:D:465:HIS:N	3:D:16:HOH:O	1.64	1.25
1:A:683:ASN:OD1	1:A:688:PRO:O	1.61	1.17
1:A:417:PRO:HG3	1:A:481:GLN:HG2	1.25	1.16
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.22	1.15
1:A:689:ASP:O	1:A:689:ASP:OD2	1.65	1.15
1:B:561:TRP:O	2:B:1001:IPA:H12	1.48	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:LEU:HB2	1:C:451:PHE:HB2	1.28	1.14
1:A:689:ASP:O	1:A:689:ASP:CG	1.86	1.10
1:D:446:THR:HG22	1:D:447:GLU:H	1.16	1.09
1:A:695:ASN:HD22	1:A:698:THR:HB	1.05	1.09
1:B:419:ARG:NH1	1:B:423:ASP:HB3	1.71	1.06
1:A:482:GLU:HB2	1:A:483:PRO:CD	1.91	1.01
1:D:679:MET:HE3	1:D:680:CYS:HA	1.39	1.01
1:B:507:GLN:NE2	1:B:553:SER:H	1.60	1.00
1:B:419:ARG:HH11	1:B:423:ASP:HB3	1.21	1.00
1:C:394:ILE:HD11	1:C:671:VAL:HG22	1.40	0.99
1:A:695:ASN:ND2	1:A:698:THR:HB	1.82	0.94
1:B:481:GLN:HE21	1:B:481:GLN:HA	1.33	0.93
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.51	0.93
1:A:707:ILE:H	1:A:707:ILE:HD12	1.32	0.92
1:D:589:ARG:HD3	1:D:635:PRO:HB3	1.51	0.91
1:C:414:ARG:H	1:C:462:ASN:HD21	1.18	0.90
1:A:472:THR:HG22	1:A:474:ALA:H	1.34	0.89
1:A:553:SER:O	1:A:571:LEU:HD12	1.73	0.89
1:A:472:THR:CG2	1:A:474:ALA:H	1.89	0.85
1:A:589:ARG:HB3	1:A:589:ARG:HH11	1.42	0.84
1:A:417:PRO:CG	1:A:481:GLN:HG2	2.08	0.83
1:A:516:LEU:HD21	1:A:538:VAL:HG21	1.59	0.83
1:C:704:ILE:CD1	1:C:706:GLU:HB2	2.08	0.83
1:C:564:ILE:HG22	1:C:582:LEU:HB2	1.61	0.83
1:A:504:ASN:HD21	1:A:507:GLN:HE21	1.23	0.83
1:D:679:MET:HE3	1:D:680:CYS:CA	2.08	0.82
1:C:448:LEU:H	1:C:448:LEU:HD23	1.45	0.82
1:C:587:ILE:H	1:C:587:ILE:HD13	1.43	0.82
1:D:463:VAL:CG1	1:D:521:ILE:HG21	2.09	0.81
1:D:467:GLN:HE22	1:D:524:GLN:H	1.28	0.81
1:D:618:ILE:HD13	1:D:618:ILE:H	1.44	0.81
1:C:504:ASN:HD21	1:C:545:PRO:HG3	1.45	0.81
1:C:448:LEU:HD23	1:C:448:LEU:N	1.97	0.80
1:C:435:VAL:HG21	1:C:448:LEU:HB3	1.62	0.80
1:B:579:LYS:HE2	1:B:581:MET:HE3	1.63	0.80
1:A:663:ASN:HD22	1:A:665:LYS:HE3	1.46	0.79
1:C:704:ILE:HD11	1:C:706:GLU:HB2	1.63	0.79
1:D:446:THR:HG22	1:D:447:GLU:N	1.97	0.78
1:C:695:ASN:HD22	1:C:695:ASN:C	1.87	0.78
1:D:504:ASN:ND2	1:D:507:GLN:HB2	1.99	0.78
1:D:654:ASP:HA	1:D:675:GLU:HG2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ARG:H	1:D:462:ASN:HD21	1.28	0.77
1:D:631:LEU:O	1:D:631:LEU:HD12	1.85	0.77
1:C:704:ILE:HG13	1:C:706:GLU:H	1.46	0.77
1:B:644:LEU:HD13	1:B:706:GLU:OE1	1.85	0.77
1:A:589:ARG:NH1	1:A:589:ARG:HB3	1.98	0.77
1:A:690:SER:C	1:A:691:LEU:HD12	2.04	0.77
1:A:564:ILE:HG22	1:A:564:ILE:O	1.85	0.76
1:C:582:LEU:HD23	1:C:606:LEU:HD21	1.67	0.76
1:A:471:ILE:HG23	1:A:476:VAL:HG22	1.68	0.76
1:D:482:GLU:HB3	1:D:483:PRO:HD2	1.68	0.76
1:D:641:PHE:CZ	1:D:679:MET:SD	2.79	0.76
1:C:564:ILE:HG22	1:C:564:ILE:O	1.85	0.76
1:C:695:ASN:HD22	1:C:697:SER:H	1.32	0.76
1:C:642:ARG:HH21	1:C:646:THR:HA	1.50	0.75
1:A:472:THR:HG23	1:A:473:SER:N	2.03	0.74
1:D:402:ILE:HD11	1:D:443:VAL:HG21	1.68	0.74
1:B:480:SER:OG	1:B:483:PRO:O	2.05	0.74
1:C:410:LEU:HB3	1:C:427:LEU:CD2	2.18	0.74
1:C:563:ASP:OD1	1:C:565:SER:HB3	1.88	0.74
1:A:414:ARG:H	1:A:462:ASN:HD21	1.35	0.74
1:D:487:VAL:HG11	1:D:524:GLN:HG3	1.69	0.73
1:D:463:VAL:HG13	1:D:521:ILE:HG21	1.68	0.73
1:B:413:LEU:HB3	1:B:424:THR:HB	1.71	0.73
1:B:403:ASP:C	1:B:404:LEU:HD22	2.09	0.73
1:A:437:MET:HB2	1:A:446:THR:CG2	2.19	0.72
1:C:586:ILE:H	1:C:586:ILE:HD13	1.54	0.72
1:C:572:PRO:HD2	1:C:573:SER:H	1.54	0.72
1:D:482:GLU:O	1:D:483:PRO:C	2.28	0.72
1:B:481:GLN:HE21	1:B:481:GLN:CA	2.01	0.71
1:D:586:ILE:H	1:D:586:ILE:HD12	1.55	0.71
1:B:507:GLN:NE2	1:B:553:SER:N	2.38	0.71
1:D:600:HIS:CD2	1:D:618:ILE:HD12	2.26	0.71
1:B:573:SER:O	1:B:574:PHE:HB2	1.90	0.70
1:C:695:ASN:ND2	1:C:698:THR:H	1.89	0.70
1:B:416:ASP:O	1:B:419:ARG:HG2	1.91	0.70
1:C:656:PRO:HB2	1:C:671:VAL:HB	1.73	0.70
1:A:483:PRO:O	1:A:484:LYS:HB2	1.89	0.70
1:C:448:LEU:HB2	1:C:451:PHE:CB	2.17	0.70
1:A:707:ILE:N	1:A:707:ILE:HD12	2.06	0.69
1:A:450:GLY:HA3	1:A:479:VAL:CG2	2.22	0.69
1:B:507:GLN:HE22	1:B:553:SER:H	1.36	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ASN:ND2	1:D:620:THR:H	1.88	0.69
1:B:579:LYS:HE2	1:B:581:MET:CE	2.22	0.69
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.73	0.69
1:C:695:ASN:ND2	1:C:697:SER:H	1.90	0.69
1:A:663:ASN:HB2	1:A:665:LYS:HE3	1.73	0.69
1:C:642:ARG:HG2	1:C:646:THR:O	1.93	0.69
1:C:414:ARG:N	1:C:462:ASN:HD21	1.91	0.69
1:B:644:LEU:H	1:B:644:LEU:HD23	1.58	0.69
1:D:641:PHE:CZ	1:D:691:LEU:HD22	2.29	0.68
1:C:467:GLN:HE22	1:C:524:GLN:H	1.41	0.68
1:D:440:GLY:O	1:D:686:GLY:HA3	1.93	0.68
1:D:446:THR:O	1:D:447:GLU:HG3	1.92	0.68
1:C:634:GLN:HG2	1:C:654:ASP:OD2	1.93	0.68
1:D:437:MET:HB2	1:D:446:THR:OG1	1.94	0.68
1:D:394:ILE:HD13	1:D:669:SER:HB3	1.76	0.68
1:D:564:ILE:O	1:D:564:ILE:HG22	1.93	0.67
1:B:662:SER:HB2	1:B:667:VAL:CG2	2.25	0.67
1:D:617:ASN:HD21	1:D:620:THR:HG23	1.60	0.67
1:B:524:GLN:O	3:B:9:HOH:O	2.12	0.67
1:D:514:ARG:HD3	1:D:534:MET:O	1.95	0.67
1:B:546:LEU:HD11	1:B:593:MET:HB3	1.77	0.67
1:A:679:MET:CE	1:A:691:LEU:HD23	2.25	0.67
1:B:532:THR:HG22	1:B:533:GLU:H	1.60	0.67
1:B:532:THR:HG22	1:B:533:GLU:N	2.10	0.67
1:D:478:LEU:HD22	1:D:526:LEU:HD13	1.76	0.67
1:D:618:ILE:H	1:D:618:ILE:CD1	2.06	0.67
1:B:419:ARG:HH11	1:B:423:ASP:CB	2.01	0.66
1:B:419:ARG:NH1	1:B:423:ASP:CB	2.55	0.66
1:A:507:GLN:HE22	1:A:553:SER:H	1.42	0.66
1:C:639:ARG:HG2	1:C:639:ARG:HH11	1.60	0.66
1:D:646:THR:HG22	1:D:647:THR:N	2.10	0.66
1:D:413:LEU:HB3	1:D:424:THR:HB	1.76	0.66
1:D:414:ARG:HD3	1:D:420:GLU:O	1.95	0.66
1:C:448:LEU:HD12	1:C:451:PHE:HB3	1.78	0.66
1:D:467:GLN:NE2	1:D:524:GLN:H	1.94	0.66
1:A:450:GLY:HA3	1:A:479:VAL:HG21	1.76	0.66
1:A:536:HIS:CD2	1:A:563:ASP:HB2	2.31	0.65
1:C:459:PHE:CD2	1:C:503:CYS:HB3	2.30	0.65
1:B:482:GLU:O	1:B:483:PRO:C	2.23	0.65
1:C:654:ASP:OD1	1:C:655:ARG:HG3	1.96	0.65
1:B:662:SER:HB2	1:B:667:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:VAL:H	1:D:470:GLN:HE22	1.44	0.65
1:B:492:GLU:HG3	1:B:512:VAL:HG21	1.77	0.65
1:D:416:ASP:HB3	1:D:419:ARG:HB2	1.78	0.65
1:D:407:ILE:HG21	1:D:410:LEU:HD21	1.79	0.65
1:C:449:MET:N	1:C:449:MET:SD	2.66	0.65
1:C:440:GLY:O	1:C:442:GLU:O	2.14	0.65
1:B:482:GLU:O	1:B:484:LYS:N	2.29	0.65
1:A:452:VAL:H	1:A:470:GLN:HE22	1.43	0.65
1:B:390:MET:O	1:B:391:ARG:HG3	1.97	0.64
1:D:463:VAL:CG1	1:D:464:ALA:N	2.60	0.64
1:A:704:ILE:C	1:A:705:ASP:O	2.34	0.64
1:A:707:ILE:H	1:A:707:ILE:CD1	2.09	0.64
1:B:704:ILE:H	1:B:704:ILE:HD13	1.63	0.64
1:D:414:ARG:HG2	1:D:421:THR:O	1.98	0.64
1:A:437:MET:HB2	1:A:446:THR:HG23	1.79	0.64
1:A:663:ASN:HD22	1:A:665:LYS:CE	2.10	0.64
1:A:472:THR:CG2	1:A:473:SER:N	2.61	0.64
1:C:587:ILE:H	1:C:587:ILE:CD1	2.10	0.64
1:D:518:TYR:HB3	1:D:530:SER:HB2	1.79	0.64
1:A:690:SER:HA	1:A:703:THR:HG22	1.80	0.64
1:B:507:GLN:HE22	1:B:553:SER:N	1.94	0.64
1:D:476:VAL:HG12	1:D:526:LEU:HD21	1.81	0.64
1:C:461:GLY:O	1:C:469:ILE:HD12	1.96	0.64
1:D:679:MET:HA	1:D:692:ALA:O	1.98	0.63
1:C:619:GLU:HG3	1:C:620:THR:HG23	1.80	0.63
1:C:512:VAL:HG23	1:C:512:VAL:O	1.99	0.63
1:C:480:SER:HB2	1:C:487:VAL:HG11	1.79	0.63
1:D:474:ALA:O	1:D:475:SER:HB3	1.98	0.63
1:D:648:ASN:HD22	1:D:660:TYR:HB3	1.63	0.63
1:A:416:ASP:OD2	1:A:419:ARG:N	2.32	0.62
1:A:440:GLY:O	1:A:441:GLU:HB2	1.99	0.62
1:D:586:ILE:N	1:D:586:ILE:HD12	2.14	0.62
1:C:413:LEU:HD13	1:C:461:GLY:HA2	1.82	0.62
1:A:482:GLU:CD	1:A:482:GLU:H	2.02	0.62
1:D:390:MET:HG2	1:D:667:VAL:HG11	1.82	0.62
1:B:481:GLN:NE2	1:B:481:GLN:HA	2.11	0.62
1:D:641:PHE:HD2	1:D:681:PRO:HG3	1.65	0.62
1:C:504:ASN:HB3	1:C:507:GLN:H	1.65	0.62
1:A:578:HIS:CD2	1:A:622:LEU:HD12	2.35	0.61
1:B:548:ASP:N	1:B:548:ASP:OD2	2.33	0.61
1:C:642:ARG:HE	1:C:646:THR:HA	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:VAL:HB	1:C:519:LEU:HB2	1.82	0.61
1:D:504:ASN:HD22	1:D:507:GLN:HB2	1.65	0.61
1:A:455:GLN:HA	1:A:455:GLN:HE21	1.65	0.61
1:C:494:GLN:O	1:C:495:ALA:HB3	2.00	0.61
1:C:482:GLU:HB2	1:C:483:PRO:CD	2.31	0.61
1:D:679:MET:HB2	1:D:693:LEU:HD23	1.81	0.61
1:C:482:GLU:CB	1:C:483:PRO:CD	2.78	0.61
1:D:617:ASN:HD22	1:D:620:THR:H	1.49	0.61
1:D:409:GLY:O	1:D:410:LEU:HD23	2.01	0.61
1:C:463:VAL:HG11	1:C:521:ILE:CD1	2.31	0.61
1:B:654:ASP:O	1:B:656:PRO:HD3	2.01	0.61
1:C:538:VAL:HG22	1:C:558:ILE:HD11	1.83	0.61
1:C:475:SER:HB2	1:C:490:TRP:O	2.01	0.61
1:A:654:ASP:OD2	1:A:654:ASP:N	2.32	0.60
1:C:665:LYS:HA	1:C:665:LYS:HE3	1.83	0.60
1:D:618:ILE:HD13	1:D:618:ILE:N	2.12	0.60
1:B:520:GLN:HG3	1:B:529:ILE:HG13	1.84	0.60
1:B:444:GLU:HG2	1:B:445:GLU:N	2.16	0.60
1:D:626:ARG:HG2	1:D:626:ARG:HH11	1.65	0.60
1:A:504:ASN:HD21	1:A:507:GLN:NE2	1.98	0.60
1:C:586:ILE:H	1:C:586:ILE:CD1	2.14	0.60
1:B:582:LEU:CD2	1:B:614:PHE:HZ	2.15	0.60
1:C:410:LEU:HB3	1:C:427:LEU:HD23	1.83	0.60
1:B:516:LEU:HD11	1:B:538:VAL:HG21	1.83	0.60
1:B:507:GLN:HE22	1:B:553:SER:HB3	1.66	0.59
1:C:416:ASP:OD2	1:C:418:ASN:HA	2.02	0.59
1:A:573:SER:O	1:A:574:PHE:HB2	2.02	0.59
1:B:564:ILE:HD12	1:B:564:ILE:N	2.17	0.59
1:C:410:LEU:HB3	1:C:427:LEU:HD21	1.85	0.59
1:D:463:VAL:HG13	1:D:464:ALA:H	1.66	0.59
1:A:480:SER:O	1:A:484:LYS:HA	2.03	0.59
1:C:570:LYS:HB2	1:C:575:GLU:HG2	1.83	0.59
1:C:394:ILE:HD13	1:C:394:ILE:H	1.68	0.59
1:A:472:THR:HG22	1:A:474:ALA:N	2.13	0.59
1:C:592:LEU:HD21	1:C:640:THR:HG23	1.85	0.59
1:D:518:TYR:CE2	1:D:529:ILE:HD11	2.38	0.59
1:A:478:LEU:O	1:A:486:LEU:HD12	2.03	0.58
1:D:617:ASN:ND2	1:D:620:THR:HG23	2.18	0.58
1:D:613:TYR:CE1	1:D:666:LEU:HD21	2.38	0.58
1:C:417:PRO:HD2	1:C:419:ARG:HG2	1.84	0.58
1:A:472:THR:HG23	1:A:473:SER:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HG22	1:A:454:ASP:OD1	2.04	0.58
1:A:578:HIS:HD2	1:A:622:LEU:HD12	1.68	0.58
1:B:682:LEU:HD13	1:B:683:ASN:N	2.19	0.58
1:B:413:LEU:CD1	1:B:461:GLY:HA2	2.34	0.58
1:C:394:ILE:HD13	1:C:671:VAL:HA	1.85	0.57
1:D:463:VAL:HG11	1:D:521:ILE:HG21	1.87	0.57
1:A:513:GLY:O	1:A:514:ARG:HB2	2.04	0.57
1:C:564:ILE:HD12	1:C:564:ILE:H	1.68	0.57
1:A:494:GLN:O	1:A:495:ALA:HB3	2.04	0.57
1:D:532:THR:HG22	1:D:533:GLU:N	2.19	0.57
1:C:449:MET:HG2	1:C:484:LYS:HG2	1.86	0.57
1:C:482:GLU:HB3	1:C:483:PRO:HD3	1.85	0.57
1:A:639:ARG:NH1	1:A:679:MET:O	2.37	0.57
1:B:580:GLU:HG2	1:B:614:PHE:CE2	2.40	0.57
1:A:472:THR:HG22	1:A:475:SER:H	1.69	0.57
1:C:642:ARG:NH2	1:C:646:THR:HA	2.17	0.57
1:A:414:ARG:N	1:A:462:ASN:HD21	2.03	0.57
1:A:617:ASN:ND2	1:A:620:THR:OG1	2.38	0.57
1:C:448:LEU:CD2	1:C:448:LEU:N	2.67	0.57
1:D:564:ILE:HD12	1:D:585:GLU:N	2.20	0.57
1:A:437:MET:HB2	1:A:446:THR:HG21	1.85	0.57
1:A:413:LEU:HD21	1:A:461:GLY:HA2	1.87	0.57
1:A:412:PRO:HG3	1:A:680:CYS:SG	2.44	0.57
1:D:467:GLN:HE22	1:D:524:GLN:N	2.02	0.56
1:D:402:ILE:CD1	1:D:443:VAL:HG21	2.33	0.56
1:C:459:PHE:CE2	1:C:503:CYS:HB3	2.40	0.56
1:D:666:LEU:N	1:D:666:LEU:HD23	2.21	0.56
1:A:558:ILE:HG22	1:A:559:GLY:N	2.20	0.56
1:C:392:ASN:CG	1:C:393:GLY:H	2.08	0.56
1:D:394:ILE:HG21	1:D:704:ILE:HD11	1.88	0.56
1:D:506:SER:C	1:D:521:ILE:HD12	2.26	0.56
1:C:549:SER:O	1:C:550:ASN:HB3	2.05	0.56
1:C:414:ARG:H	1:C:462:ASN:ND2	1.97	0.56
1:D:512:VAL:HB	1:D:515:ALA:HB3	1.86	0.56
1:D:487:VAL:HG11	1:D:524:GLN:HA	1.88	0.56
1:C:482:GLU:CB	1:C:483:PRO:HD3	2.36	0.56
1:B:425:LEU:CD2	1:B:427:LEU:HD11	2.35	0.56
1:A:481:GLN:O	1:A:484:LYS:HG2	2.06	0.56
1:C:639:ARG:NH1	1:C:639:ARG:HG2	2.21	0.56
1:B:417:PRO:HD3	1:B:481:GLN:OE1	2.05	0.56
1:A:690:SER:O	1:A:691:LEU:HD12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:LEU:HA	1:B:626:ARG:HH22	1.70	0.56
1:D:463:VAL:HG13	1:D:464:ALA:N	2.21	0.55
1:B:516:LEU:CD1	1:B:538:VAL:HG21	2.36	0.55
1:C:452:VAL:H	1:C:470:GLN:HE22	1.55	0.55
1:A:578:HIS:CE1	1:A:580:GLU:HG2	2.41	0.55
1:B:475:SER:HB2	1:B:490:TRP:O	2.06	0.55
1:D:617:ASN:ND2	1:D:620:THR:N	2.54	0.55
1:C:578:HIS:ND1	1:C:622:LEU:HD13	2.21	0.55
1:D:568:ILE:O	1:D:569:LEU:HD23	2.07	0.55
1:B:654:ASP:C	1:B:656:PRO:HD3	2.27	0.55
1:A:570:LYS:O	1:A:574:PHE:N	2.36	0.55
1:C:480:SER:HB2	1:C:487:VAL:CG1	2.36	0.55
1:D:472:THR:HG23	1:D:475:SER:H	1.70	0.55
1:C:695:ASN:HD21	1:C:698:THR:N	2.05	0.55
1:C:634:GLN:HB2	1:C:635:PRO:CD	2.37	0.55
1:B:520:GLN:HG3	1:B:529:ILE:CG1	2.37	0.55
1:B:570:LYS:HG3	1:B:572:PRO:HD2	1.88	0.55
1:C:438:LEU:O	1:C:439:ASN:C	2.45	0.55
1:B:504:ASN:HD21	1:B:507:GLN:HE21	1.55	0.54
1:B:492:GLU:HG2	1:B:493:PRO:HD2	1.89	0.54
1:B:592:LEU:HD23	1:B:603:LEU:HD12	1.89	0.54
1:D:674:LYS:HG2	1:D:675:GLU:H	1.71	0.54
1:B:642:ARG:HG2	1:B:646:THR:O	2.07	0.54
1:C:617:ASN:HD21	1:C:619:GLU:HG3	1.71	0.54
1:A:502:SER:HB3	1:A:541:LEU:HD23	1.89	0.54
1:B:596:PHE:HB3	1:B:661:SER:HB2	1.88	0.54
1:B:508:VAL:HB	1:B:519:LEU:HB2	1.90	0.54
1:A:663:ASN:ND2	1:A:665:LYS:HE3	2.20	0.54
1:C:437:MET:HB2	1:C:446:THR:HG21	1.89	0.54
1:C:392:ASN:ND2	1:C:393:GLY:N	2.56	0.54
1:C:564:ILE:CG2	1:C:582:LEU:HB2	2.36	0.54
1:B:507:GLN:HE22	1:B:553:SER:CB	2.21	0.53
1:C:705:ASP:O	1:C:706:GLU:C	2.46	0.53
1:D:688:PRO:O	1:D:689:ASP:C	2.46	0.53
1:C:546:LEU:HD11	1:C:593:MET:HB3	1.90	0.53
1:A:665:LYS:O	1:A:665:LYS:HD2	2.08	0.53
1:A:397:HIS:HD2	1:A:705:ASP:OD1	1.91	0.53
1:C:582:LEU:CD2	1:C:606:LEU:HD21	2.36	0.53
1:A:564:ILE:CG2	1:A:564:ILE:O	2.57	0.53
1:B:513:GLY:O	1:B:514:ARG:CB	2.57	0.53
1:D:446:THR:CG2	1:D:447:GLU:H	1.99	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ILE:N	1:C:587:ILE:HD13	2.16	0.53
1:D:417:PRO:HG3	1:D:481:GLN:HB3	1.91	0.53
1:C:434:ARG:HD2	1:C:445:GLU:OE1	2.09	0.53
1:C:401:SER:C	1:C:402:ILE:HD12	2.28	0.52
1:C:655:ARG:HH11	1:C:655:ARG:HG2	1.74	0.52
1:D:414:ARG:N	1:D:462:ASN:HD21	2.02	0.52
1:C:562:THR:O	1:C:563:ASP:HB3	2.09	0.52
1:C:578:HIS:CE1	1:C:623:LEU:H	2.27	0.52
1:D:587:ILE:HG22	1:D:588:PRO:O	2.09	0.52
1:C:700:THR:O	1:C:701:ILE:HD13	2.10	0.52
1:B:476:VAL:HG22	1:B:526:LEU:HD13	1.92	0.52
1:B:566:ALA:CB	1:B:582:LEU:HD21	2.40	0.52
1:B:582:LEU:HD23	1:B:614:PHE:HZ	1.74	0.52
1:D:554:PRO:HD2	1:D:555:LEU:HD13	1.92	0.52
1:A:500:VAL:HB	1:A:511:ALA:HB3	1.91	0.52
1:A:460:CYS:HA	1:A:469:ILE:O	2.10	0.52
1:B:636:THR:HG21	1:B:651:ALA:HB1	1.91	0.52
1:A:450:GLY:HA3	1:A:479:VAL:HG22	1.92	0.52
1:A:413:LEU:CD2	1:A:461:GLY:HA2	2.40	0.52
1:B:410:LEU:N	1:B:410:LEU:HD23	2.24	0.52
1:A:542:ASP:OD2	1:A:592:LEU:HD12	2.10	0.51
1:A:578:HIS:HE1	1:A:580:GLU:HG2	1.74	0.51
1:C:542:ASP:OD1	1:C:592:LEU:HD12	2.10	0.51
1:A:475:SER:HB2	1:A:490:TRP:O	2.10	0.51
1:B:467:GLN:HB2	3:B:2:HOH:O	2.09	0.51
1:B:511:ALA:HA	1:B:515:ALA:O	2.11	0.51
1:C:695:ASN:ND2	1:C:698:THR:N	2.57	0.51
1:A:522:HIS:HB3	1:A:523:PRO:CD	2.40	0.51
1:B:597:GLU:HG3	1:B:661:SER:OG	2.11	0.51
1:A:632:GLY:HA3	1:A:654:ASP:OD2	2.10	0.51
1:B:492:GLU:HG2	1:B:493:PRO:CD	2.41	0.51
1:D:459:PHE:CD1	1:D:460:CYS:N	2.79	0.51
1:A:535:GLU:H	1:A:535:GLU:CD	2.14	0.51
1:D:600:HIS:HD2	1:D:618:ILE:HD12	1.71	0.51
1:D:483:PRO:O	1:D:484:LYS:C	2.49	0.51
1:C:554:PRO:O	1:C:570:LYS:HD2	2.11	0.51
1:D:591:ILE:HG13	1:D:603:LEU:O	2.11	0.51
1:D:584:GLY:O	1:D:585:GLU:HB2	2.11	0.50
1:A:619:GLU:OE1	1:A:619:GLU:HA	2.11	0.50
1:D:641:PHE:CE2	1:D:679:MET:SD	3.04	0.50
1:A:655:ARG:HB3	1:B:391:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:O	1:A:701:ILE:HA	2.12	0.50
1:C:469:ILE:H	1:C:469:ILE:HD12	1.75	0.50
1:D:639:ARG:HB3	1:D:679:MET:HE1	1.94	0.50
1:A:577:LEU:O	1:A:578:HIS:HB2	2.11	0.50
1:C:419:ARG:HH11	1:C:423:ASP:HB3	1.75	0.50
1:B:476:VAL:HG22	1:B:526:LEU:CD1	2.41	0.50
1:C:608:ASP:C	1:C:608:ASP:OD2	2.48	0.50
1:B:695:ASN:CG	1:B:696:ASN:N	2.64	0.50
1:A:507:GLN:NE2	1:A:553:SER:H	2.07	0.50
1:D:555:LEU:N	1:D:555:LEU:HD12	2.26	0.50
1:D:565:SER:HA	1:D:580:GLU:O	2.10	0.50
1:D:641:PHE:CD2	1:D:681:PRO:HG3	2.44	0.50
1:A:562:THR:O	1:A:564:ILE:HG13	2.10	0.50
1:B:507:GLN:HE22	1:B:553:SER:CA	2.24	0.50
1:C:441:GLU:CD	1:C:441:GLU:N	2.63	0.50
1:D:564:ILE:HD12	1:D:585:GLU:H	1.77	0.49
1:B:653:SER:O	1:B:675:GLU:HG3	2.12	0.49
1:A:410:LEU:HA	1:A:426:VAL:O	2.12	0.49
1:B:422:TYR:O	1:B:684:SER:HB3	2.12	0.49
1:A:437:MET:HE2	1:C:628:LYS:HD3	1.95	0.49
1:D:564:ILE:HD13	1:D:586:ILE:O	2.11	0.49
1:C:655:ARG:NH1	1:C:655:ARG:HG2	2.28	0.49
1:D:646:THR:CG2	1:D:647:THR:N	2.75	0.49
1:C:692:ALA:HA	1:C:701:ILE:HD13	1.93	0.49
1:C:564:ILE:N	1:C:564:ILE:HD12	2.26	0.49
1:C:572:PRO:HD2	1:C:573:SER:N	2.26	0.49
1:C:654:ASP:HA	1:C:675:GLU:HB3	1.94	0.49
1:C:408:LYS:HB2	1:C:428:SER:OG	2.12	0.49
1:A:440:GLY:O	1:A:441:GLU:CB	2.61	0.49
1:C:500:VAL:HG11	1:C:540:CYS:HA	1.93	0.49
1:D:448:LEU:HD23	1:D:448:LEU:H	1.77	0.49
1:B:689:ASP:N	1:B:689:ASP:OD1	2.46	0.49
1:D:463:VAL:HG21	1:D:469:ILE:HB	1.95	0.49
1:C:695:ASN:ND2	1:C:695:ASN:C	2.61	0.49
1:C:441:GLU:HG3	1:C:686:GLY:HA3	1.94	0.49
1:A:507:GLN:HE22	1:A:553:SER:N	2.11	0.49
1:B:706:GLU:O	1:B:707:ILE:HB	2.13	0.49
1:B:582:LEU:HD23	1:B:614:PHE:CZ	2.48	0.49
1:B:419:ARG:NE	1:B:421:THR:HB	2.28	0.48
1:B:417:PRO:HG2	1:B:481:GLN:HB3	1.94	0.48
1:C:573:SER:O	1:C:574:PHE:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:660:TYR:O	1:D:666:LEU:HA	2.12	0.48
1:C:613:TYR:CD1	1:C:666:LEU:HD12	2.48	0.48
1:A:541:LEU:O	1:A:541:LEU:HD23	2.13	0.48
1:B:636:THR:HG22	1:B:637:VAL:N	2.28	0.48
1:D:672:ASN:O	1:D:673:LEU:HG	2.13	0.48
1:B:679:MET:HE1	1:B:681:PRO:HD3	1.94	0.48
1:D:656:PRO:HB2	1:D:671:VAL:HB	1.95	0.48
1:D:410:LEU:HD22	1:D:427:LEU:CD2	2.43	0.48
1:C:492:GLU:HG3	1:C:512:VAL:HG21	1.96	0.48
1:A:670:ASN:ND2	1:B:391:ARG:HB2	2.27	0.48
1:C:642:ARG:HH21	1:C:646:THR:CA	2.23	0.48
1:B:413:LEU:HD12	1:B:461:GLY:HA2	1.93	0.48
1:A:396:ILE:O	1:A:396:ILE:HG22	2.14	0.48
1:D:646:THR:HG22	1:D:647:THR:H	1.78	0.48
1:D:472:THR:HG23	1:D:475:SER:N	2.29	0.48
1:D:558:ILE:HG23	1:D:567:ARG:HG3	1.96	0.48
1:A:425:LEU:HD12	1:A:427:LEU:HD21	1.95	0.48
1:D:492:GLU:OE1	1:D:496:LYS:HD2	2.12	0.48
1:B:394:ILE:HG12	1:B:660:TYR:OH	2.14	0.48
1:A:467:GLN:NE2	1:A:487:VAL:HG21	2.29	0.47
1:D:667:VAL:HG12	1:D:668:PHE:N	2.29	0.47
1:C:613:TYR:CE1	1:C:666:LEU:HD12	2.49	0.47
1:C:498:ILE:HG23	1:C:510:VAL:HG22	1.96	0.47
1:B:480:SER:HB3	1:B:487:VAL:HG11	1.97	0.47
1:A:563:ASP:OD1	1:A:565:SER:HB3	2.15	0.47
1:D:666:LEU:N	1:D:666:LEU:CD2	2.78	0.47
1:A:424:THR:HG22	1:A:425:LEU:N	2.30	0.47
1:D:602:LEU:C	1:D:602:LEU:HD13	2.33	0.47
1:B:576:LEU:HD13	1:B:576:LEU:C	2.33	0.47
1:A:561:TRP:HB3	1:A:562:THR:H	1.61	0.47
1:C:392:ASN:ND2	1:C:393:GLY:H	2.12	0.47
1:C:634:GLN:HB2	1:C:635:PRO:HD2	1.96	0.47
1:B:488:SER:OG	1:B:525:GLU:HA	2.14	0.47
1:C:413:LEU:HB3	1:C:424:THR:HB	1.96	0.47
1:B:547:GLY:O	1:B:549:SER:N	2.41	0.47
1:C:425:LEU:CD1	1:C:427:LEU:HG	2.44	0.47
1:C:413:LEU:CD1	1:C:461:GLY:HA2	2.45	0.47
1:A:541:LEU:HA	1:A:557:ALA:O	2.15	0.47
1:D:423:ASP:C	1:D:423:ASP:OD2	2.52	0.47
1:A:405:PRO:HA	1:A:697:SER:HA	1.97	0.47
1:D:464:ALA:C	3:D:16:HOH:O	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:ASN:ND2	1:D:660:TYR:HB3	2.28	0.47
1:B:410:LEU:HA	1:B:426:VAL:O	2.15	0.47
1:B:606:LEU:HD11	1:B:612:PHE:HE1	1.80	0.47
1:C:481:GLN:O	1:C:482:GLU:O	2.32	0.47
1:B:425:LEU:HD23	1:B:427:LEU:HD11	1.97	0.47
1:A:588:PRO:HA	1:A:606:LEU:HD23	1.96	0.47
1:B:582:LEU:CD2	1:B:614:PHE:CZ	2.96	0.46
1:C:641:PHE:CD2	1:C:679:MET:HE3	2.50	0.46
1:B:652:CYS:HB3	1:B:676:VAL:O	2.15	0.46
1:B:587:ILE:H	1:B:587:ILE:HD13	1.81	0.46
1:D:402:ILE:O	1:D:698:THR:HG23	2.16	0.46
1:D:617:ASN:ND2	1:D:620:THR:OG1	2.48	0.46
1:A:558:ILE:HD12	1:A:569:LEU:HD11	1.95	0.46
1:B:602:LEU:O	1:B:613:TYR:HA	2.15	0.46
1:C:475:SER:HB3	1:C:491:LYS:HG2	1.98	0.46
1:D:412:PRO:HB3	1:D:422:TYR:CD1	2.50	0.46
1:C:642:ARG:NE	1:C:646:THR:HA	2.29	0.46
1:D:577:LEU:HD22	1:D:620:THR:O	2.16	0.46
1:A:617:ASN:O	1:A:621:GLY:N	2.44	0.46
1:C:480:SER:O	1:C:484:LYS:HA	2.15	0.46
1:A:679:MET:HE3	1:A:691:LEU:HD23	1.98	0.46
1:D:553:SER:HA	1:D:554:PRO:HD3	1.79	0.46
1:D:459:PHE:CG	1:D:460:CYS:N	2.83	0.46
1:C:453:ASP:O	1:C:455:GLN:N	2.49	0.46
1:A:679:MET:C	1:A:679:MET:SD	2.94	0.46
1:C:418:ASN:HD22	1:C:418:ASN:HA	1.38	0.46
1:C:616:LEU:HD11	1:C:621:GLY:HA2	1.98	0.46
1:D:604:CYS:O	1:D:611:LEU:HD12	2.16	0.46
1:A:570:LYS:HG2	1:A:577:LEU:HD21	1.96	0.46
1:D:564:ILE:CD1	1:D:585:GLU:N	2.79	0.46
1:D:626:ARG:HG2	1:D:626:ARG:NH1	2.30	0.46
1:B:566:ALA:HB3	1:B:582:LEU:HD21	1.98	0.46
1:C:576:LEU:HD21	1:C:579:LYS:HB2	1.98	0.46
1:B:535:GLU:CD	1:B:567:ARG:HH22	2.19	0.46
1:A:413:LEU:HD21	1:A:461:GLY:CA	2.46	0.46
1:B:578:HIS:HD2	1:B:622:LEU:HD12	1.81	0.46
1:D:538:VAL:HG13	1:D:558:ILE:HD11	1.98	0.46
1:A:455:GLN:NE2	1:A:455:GLN:HA	2.29	0.46
1:A:652:CYS:HB3	1:A:676:VAL:O	2.16	0.46
1:B:443:VAL:O	1:B:443:VAL:HG12	2.15	0.46
1:C:467:GLN:NE2	1:C:524:GLN:H	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:GLN:O	1:B:525:GLU:HB3	2.15	0.45
1:C:437:MET:HB2	1:C:446:THR:CG2	2.46	0.45
1:D:416:ASP:O	1:D:417:PRO:C	2.54	0.45
1:C:459:PHE:CD2	1:C:503:CYS:CB	2.98	0.45
1:A:593:MET:O	1:A:594:THR:HG23	2.16	0.45
1:A:613:TYR:CE1	1:A:666:LEU:HD22	2.51	0.45
1:A:631:LEU:HD11	1:A:668:PHE:HD2	1.81	0.45
1:C:478:LEU:HB2	1:C:488:SER:HB3	1.98	0.45
1:C:597:GLU:C	1:C:599:SER:H	2.20	0.45
1:B:587:ILE:CG2	2:B:1001:IPA:H33	2.46	0.45
1:C:586:ILE:HD13	1:C:586:ILE:N	2.25	0.45
1:A:571:LEU:HA	1:A:571:LEU:HD23	1.62	0.45
1:B:662:SER:HB2	1:B:667:VAL:HG23	1.97	0.45
1:B:656:PRO:HB2	1:B:671:VAL:HB	1.98	0.45
1:C:549:SER:O	1:C:550:ASN:CB	2.63	0.45
1:C:618:ILE:O	1:C:618:ILE:HG22	2.16	0.45
1:C:482:GLU:O	1:C:484:LYS:N	2.49	0.45
1:A:472:THR:HG23	1:A:474:ALA:H	1.78	0.45
1:D:546:LEU:HD23	1:D:600:HIS:HB3	1.98	0.45
1:B:516:LEU:O	1:B:531:HIS:HA	2.17	0.45
1:A:653:SER:C	1:A:655:ARG:N	2.70	0.45
1:D:410:LEU:HD22	1:D:427:LEU:HD23	1.99	0.45
1:A:704:ILE:O	1:A:705:ASP:O	2.35	0.45
1:B:426:VAL:C	1:B:427:LEU:HD12	2.36	0.45
1:D:538:VAL:HG13	1:D:558:ILE:HG13	1.99	0.45
1:B:481:GLN:NE2	1:B:481:GLN:CA	2.75	0.45
1:B:688:PRO:O	1:B:689:ASP:C	2.53	0.45
1:B:450:GLY:HA3	1:B:479:VAL:HG22	1.98	0.45
1:C:432:GLN:NE2	1:C:454:ASP:HA	2.31	0.45
1:A:573:SER:HB2	1:A:575:GLU:HG3	1.99	0.45
1:C:562:THR:O	1:C:563:ASP:CB	2.64	0.45
1:C:463:VAL:HG11	1:C:521:ILE:HD13	1.98	0.45
1:D:492:GLU:HG3	1:D:512:VAL:HG11	1.99	0.45
1:D:453:ASP:OD1	1:D:453:ASP:C	2.55	0.45
1:B:416:ASP:OD2	1:B:416:ASP:C	2.55	0.45
1:B:614:PHE:N	1:B:614:PHE:CD1	2.84	0.45
1:D:592:LEU:HD22	1:D:638:LEU:HB2	1.97	0.45
1:C:612:PHE:CZ	1:C:628:LYS:HD2	2.52	0.44
1:D:532:THR:CG2	1:D:533:GLU:N	2.80	0.44
1:D:538:VAL:HG13	1:D:558:ILE:CG1	2.48	0.44
1:B:464:ALA:O	1:B:466:GLN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:SER:OG	1:A:703:THR:HG23	2.17	0.44
1:B:704:ILE:HG12	1:B:705:ASP:O	2.16	0.44
1:D:695:ASN:ND2	1:D:697:SER:H	2.15	0.44
1:B:424:THR:CG2	1:B:435:VAL:HG13	2.47	0.44
1:D:475:SER:HB3	1:D:491:LYS:HG2	1.99	0.44
1:D:516:LEU:O	1:D:531:HIS:HA	2.17	0.44
1:D:487:VAL:CG1	1:D:524:GLN:HG3	2.44	0.44
1:C:465:HIS:O	1:C:467:GLN:HG3	2.18	0.44
1:A:411:TRP:CE2	1:A:459:PHE:HA	2.52	0.44
1:B:500:VAL:HG12	1:B:501:ALA:N	2.33	0.44
1:A:512:VAL:O	1:A:514:ARG:N	2.51	0.44
1:C:553:SER:HA	1:C:554:PRO:HD3	1.76	0.44
1:A:468:LEU:O	1:A:478:LEU:HD12	2.17	0.44
1:B:507:GLN:NE2	1:B:553:SER:HB3	2.33	0.44
1:D:482:GLU:O	1:D:484:LYS:N	2.51	0.44
1:B:402:ILE:CG2	1:B:404:LEU:HD21	2.48	0.44
1:C:512:VAL:CG2	1:C:512:VAL:O	2.65	0.44
1:B:657:THR:HG23	1:B:669:SER:O	2.17	0.44
1:C:409:GLY:HA3	1:C:411:TRP:CH2	2.52	0.44
1:D:695:ASN:HD21	1:D:697:SER:HB2	1.82	0.44
1:D:424:THR:HG22	1:D:425:LEU:N	2.32	0.44
1:C:590:SER:CB	1:C:637:VAL:HA	2.48	0.44
1:A:514:ARG:NH1	1:A:536:HIS:HA	2.33	0.44
1:D:677:ASN:ND2	1:D:695:ASN:HA	2.33	0.44
1:C:637:VAL:HG22	1:C:652:CYS:HB2	1.99	0.44
1:C:683:ASN:ND2	1:C:688:PRO:HA	2.32	0.44
1:D:464:ALA:HB3	3:D:16:HOH:O	2.18	0.43
1:B:559:GLY:HA2	1:B:565:SER:O	2.18	0.43
1:D:706:GLU:O	1:D:707:ILE:C	2.55	0.43
1:A:556:CYS:HB2	1:A:571:LEU:HD21	1.99	0.43
1:D:448:LEU:H	1:D:448:LEU:CD2	2.30	0.43
1:C:478:LEU:HG	1:C:526:LEU:HD21	2.00	0.43
1:D:488:SER:HB2	1:D:524:GLN:O	2.17	0.43
1:D:660:TYR:O	1:D:667:VAL:N	2.47	0.43
1:A:455:GLN:CA	1:A:455:GLN:HE21	2.27	0.43
1:C:494:GLN:O	1:C:495:ALA:CB	2.65	0.43
1:C:665:LYS:HE3	1:C:666:LEU:H	1.84	0.43
1:C:520:GLN:HB3	1:C:522:HIS:CE1	2.54	0.43
1:D:494:GLN:O	1:D:495:ALA:HB3	2.18	0.43
1:D:690:SER:O	1:D:691:LEU:HD23	2.18	0.43
1:D:584:GLY:O	1:D:586:ILE:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:LEU:HD22	1:B:614:PHE:HZ	1.83	0.43
1:B:427:LEU:N	1:B:427:LEU:HD12	2.33	0.43
1:D:558:ILE:CG2	1:D:567:ARG:HG3	2.49	0.43
1:A:451:PHE:HD1	1:A:451:PHE:N	2.17	0.43
1:B:404:LEU:HD22	1:B:404:LEU:N	2.33	0.43
1:B:514:ARG:HG3	1:B:536:HIS:O	2.19	0.43
1:A:636:THR:HA	1:A:652:CYS:O	2.19	0.43
1:C:394:ILE:HD13	1:C:394:ILE:N	2.32	0.43
1:B:390:MET:C	1:B:391:ARG:HG3	2.38	0.43
1:A:451:PHE:CD1	1:A:451:PHE:N	2.85	0.43
1:B:532:THR:CG2	1:B:533:GLU:N	2.79	0.43
1:D:566:ALA:HB2	1:D:582:LEU:HD11	2.01	0.43
1:B:417:PRO:HG3	1:B:481:GLN:HG3	2.01	0.43
1:C:462:ASN:HA	1:C:468:LEU:HD23	2.01	0.43
1:A:589:ARG:CB	1:A:589:ARG:HH11	2.21	0.43
1:C:402:ILE:O	1:C:698:THR:HG23	2.19	0.43
1:A:394:ILE:HG23	1:A:704:ILE:HG23	2.01	0.43
1:D:459:PHE:C	1:D:459:PHE:CD1	2.92	0.43
1:B:403:ASP:O	1:B:404:LEU:HD22	2.19	0.43
1:A:446:THR:HG22	1:C:628:LYS:O	2.19	0.43
1:B:596:PHE:HB3	1:B:661:SER:CB	2.48	0.43
1:C:503:CYS:SG	1:C:508:VAL:HG22	2.59	0.42
1:B:565:SER:OG	1:B:567:ARG:HD3	2.19	0.42
1:A:587:ILE:HD13	1:A:587:ILE:N	2.34	0.42
1:B:587:ILE:H	1:B:587:ILE:CD1	2.32	0.42
1:A:471:ILE:HG12	1:A:476:VAL:HG13	2.00	0.42
1:D:417:PRO:HG3	1:D:481:GLN:CB	2.49	0.42
1:B:402:ILE:HG22	1:B:404:LEU:CD2	2.48	0.42
1:D:411:TRP:CE2	1:D:459:PHE:HA	2.54	0.42
1:D:596:PHE:HZ	1:D:649:VAL:HG23	1.84	0.42
1:A:480:SER:HB3	1:A:487:VAL:HG11	2.00	0.42
1:B:390:MET:O	1:B:391:ARG:CG	2.66	0.42
1:A:492:GLU:HG3	1:A:512:VAL:HG11	2.00	0.42
1:D:487:VAL:CG1	1:D:524:GLN:HA	2.48	0.42
1:C:683:ASN:HD22	1:C:688:PRO:HA	1.84	0.42
1:D:596:PHE:CZ	1:D:649:VAL:HG23	2.53	0.42
1:D:525:GLU:OE1	1:D:527:ARG:HD3	2.19	0.42
1:C:440:GLY:C	1:C:442:GLU:H	2.23	0.42
1:C:617:ASN:HD21	1:C:619:GLU:CG	2.31	0.42
1:C:590:SER:HB2	1:C:637:VAL:HA	2.02	0.42
1:D:637:VAL:HB	1:D:652:CYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:VAL:HG12	1:D:480:SER:N	2.34	0.42
1:D:641:PHE:HD2	1:D:641:PHE:HA	1.77	0.42
1:B:570:LYS:HE2	1:B:577:LEU:HD11	2.01	0.42
1:A:506:SER:HB2	1:A:552:LEU:HD23	2.02	0.42
1:D:503:CYS:HA	1:D:543:ILE:HD11	2.00	0.42
1:D:492:GLU:HB3	1:D:496:LYS:H	1.84	0.42
1:C:679:MET:CE	1:C:691:LEU:HD22	2.49	0.42
1:A:659:ILE:HD12	1:A:668:PHE:CE2	2.55	0.42
1:B:416:ASP:HB3	1:B:419:ARG:HD2	2.01	0.42
1:D:639:ARG:HB3	1:D:679:MET:CE	2.49	0.42
1:C:394:ILE:H	1:C:394:ILE:CD1	2.30	0.42
1:B:576:LEU:HD21	1:B:579:LYS:HB3	2.02	0.42
1:A:571:LEU:C	1:A:573:SER:H	2.23	0.42
1:A:692:ALA:HA	1:A:700:THR:O	2.20	0.42
1:D:399:HIS:O	1:D:400:ALA:HB2	2.20	0.42
1:A:536:HIS:HD2	1:A:563:ASP:HB2	1.83	0.42
1:B:396:ILE:HG21	1:B:673:LEU:HD11	2.02	0.42
1:C:448:LEU:HA	1:C:449:MET:HE1	2.02	0.41
1:A:523:PRO:HB3	1:A:524:GLN:NE2	2.35	0.41
1:B:429:PHE:O	1:B:430:VAL:C	2.59	0.41
1:C:616:LEU:CD1	1:C:621:GLY:HA2	2.50	0.41
1:A:565:SER:HA	1:A:580:GLU:O	2.20	0.41
1:B:512:VAL:O	1:B:513:GLY:C	2.58	0.41
1:A:649:VAL:HB	1:A:659:ILE:HB	2.01	0.41
1:C:522:HIS:HB3	1:C:523:PRO:CD	2.51	0.41
1:D:439:ASN:HA	1:D:439:ASN:HD22	1.61	0.41
1:C:698:THR:HG22	1:C:699:LEU:N	2.35	0.41
1:C:646:THR:O	1:C:647:THR:HG23	2.20	0.41
1:B:577:LEU:O	1:B:578:HIS:HB2	2.19	0.41
1:D:571:LEU:HD23	1:D:571:LEU:HA	1.70	0.41
1:D:695:ASN:OD1	1:D:698:THR:N	2.48	0.41
1:B:668:PHE:CD1	1:B:668:PHE:N	2.88	0.41
1:A:529:ILE:O	1:A:530:SER:HB3	2.21	0.41
1:A:619:GLU:OE1	1:A:619:GLU:CA	2.68	0.41
1:D:443:VAL:O	1:D:443:VAL:HG23	2.20	0.41
1:C:542:ASP:CG	1:C:592:LEU:HD12	2.41	0.41
1:C:679:MET:HE2	1:C:691:LEU:HD22	2.01	0.41
1:D:679:MET:CB	1:D:693:LEU:HD23	2.49	0.41
1:D:538:VAL:HG22	1:D:558:ILE:HD11	2.02	0.41
1:D:550:ASN:C	1:D:552:LEU:H	2.24	0.41
1:C:448:LEU:HA	1:C:449:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:MET:HB3	1:D:444:GLU:HB2	2.03	0.41
1:C:416:ASP:OD2	1:C:417:PRO:O	2.39	0.41
1:A:412:PRO:HB2	1:A:422:TYR:CE2	2.56	0.41
1:C:578:HIS:HD2	1:C:579:LYS:N	2.19	0.41
1:D:422:TYR:CD2	1:D:422:TYR:N	2.89	0.41
1:B:589:ARG:HB3	1:B:589:ARG:HE	1.54	0.41
1:A:399:HIS:HD2	1:A:687:TYR:HD2	1.68	0.41
1:D:411:TRP:HA	1:D:412:PRO:HD3	1.79	0.41
1:A:655:ARG:HA	1:A:656:PRO:HD3	1.92	0.40
1:A:516:LEU:HD23	1:A:534:MET:HG2	2.03	0.40
1:A:690:SER:HB3	1:A:691:LEU:H	1.73	0.40
1:D:555:LEU:CD1	1:D:555:LEU:N	2.84	0.40
1:C:482:GLU:O	1:C:483:PRO:C	2.57	0.40
1:C:586:ILE:HG12	1:C:606:LEU:HD13	2.04	0.40
1:C:392:ASN:CG	1:C:393:GLY:N	2.73	0.40
1:B:471:ILE:HG12	1:B:476:VAL:HB	2.02	0.40
1:A:503:CYS:SG	1:A:508:VAL:HG22	2.61	0.40
1:D:481:GLN:C	1:D:482:GLU:O	2.58	0.40
1:B:394:ILE:HD13	1:B:669:SER:HB3	2.04	0.40
1:B:429:PHE:O	1:B:456:GLN:HG3	2.22	0.40
1:C:643:SER:OG	1:C:704:ILE:HD11	2.22	0.40
1:D:419:ARG:HH11	1:D:419:ARG:HA	1.86	0.40
1:D:695:ASN:CG	1:D:698:THR:H	2.23	0.40
1:D:570:LYS:HD3	1:D:577:LEU:HD11	2.04	0.40
1:B:469:ILE:HG13	1:B:477:ARG:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:SER:O	1:D:524:GLN:O[2_544]	1.97	0.23
1:C:524:GLN:O	3:B:9:HOH:O[1_454]	2.08	0.12

## 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	308/323 (95%)	253 (82%)	40 (13%)	15 (5%)	3	8
1	B	319/323 (99%)	271 (85%)	35 (11%)	13 (4%)	3	11
1	C	318/323 (98%)	267 (84%)	36 (11%)	15 (5%)	3	9
1	D	318/323 (98%)	260 (82%)	48 (15%)	10 (3%)	5	17
All	All	1263/1292 (98%)	1051 (83%)	159 (13%)	53 (4%)	3	11

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	GLU
1	A	514	ARG
1	A	561	TRP
1	A	645	SER
1	B	449	MET
1	B	464	ALA
1	B	465	HIS
1	B	482	GLU
1	B	548	ASP
1	B	662	SER
1	C	417	PRO
1	C	454	ASP
1	C	464	ALA
1	C	482	GLU
1	C	563	ASP
1	C	572	PRO
1	C	645	SER
1	D	464	ALA
1	D	483	PRO
1	D	664	HIS
1	A	513	GLY
1	A	573	SER
1	A	705	ASP
1	B	430	VAL
1	B	643	SER
1	C	439	ASN
1	C	465	HIS
1	C	646	THR
1	D	706	GLU
1	A	619	GLU

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Mol	Chain	Res	Type
1	B	645	SER
1	B	664	HIS
1	D	390	MET
1	D	465	HIS
1	D	582	LEU
1	C	696	ASN
1	D	432	GLN
1	D	689	ASP
1	A	484	LYS
1	A	493	PRO
1	A	523	PRO
1	A	663	ASN
1	B	564	ILE
1	C	562	THR
1	C	621	GLY
1	C	697	SER
1	D	475	SER
1	A	440	GLY
1	B	572	PRO
1	C	564	ILE
1	A	512	VAL
1	A	618	ILE
1	B	513	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	276/285 (97%)	244 (88%)	32 (12%)	7	20
1	B	283/285 (99%)	254 (90%)	29 (10%)	9	26
1	C	282/285 (99%)	249 (88%)	33 (12%)	7	20
1	D	283/285 (99%)	262 (93%)	21 (7%)	17	43
All	All	1124/1140 (99%)	1009 (90%)	115 (10%)	9	26

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	ILE
1	A	399	HIS
1	A	410	LEU
1	A	425	LEU
1	A	428	SER
1	A	436	LEU
1	A	448	LEU
1	A	472	THR
1	A	482	GLU
1	A	523	PRO
1	A	524	GLN
1	A	526	LEU
1	A	541	LEU
1	A	561	TRP
1	A	576	LEU
1	A	581	MET
1	A	587	ILE
1	A	589	ARG
1	A	619	GLU
1	A	626	ARG
1	A	633	THR
1	A	640	THR
1	A	654	ASP
1	A	665	LYS
1	A	675	GLU
1	A	687	TYR
1	A	688	PRO
1	A	689	ASP
1	A	690	SER
1	A	693	LEU
1	A	705	ASP
1	A	706	GLU
1	B	396	ILE
1	B	403	ASP
1	B	410	LEU
1	B	415	SER
1	B	417	PRO
1	B	419	ARG
1	B	432	GLN
1	B	439	ASN
1	B	449	MET
1	B	476	VAL
1	B	480	SER

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Mol	Chain	Res	Type
1	B	481	GLN
1	B	483	PRO
1	B	492	GLU
1	B	505	SER
1	B	525	GLU
1	B	548	ASP
1	B	567	ARG
1	B	571	LEU
1	B	582	LEU
1	B	587	ILE
1	B	594	THR
1	B	614	PHE
1	B	639	ARG
1	B	674	LYS
1	B	679	MET
1	B	689	ASP
1	B	691	LEU
1	B	704	ILE
1	C	392	ASN
1	C	394	ILE
1	C	404	LEU
1	C	410	LEU
1	C	417	PRO
1	C	418	ASN
1	C	441	GLU
1	C	443	VAL
1	C	446	THR
1	C	448	LEU
1	C	449	MET
1	C	463	VAL
1	C	469	ILE
1	C	477	ARG
1	C	510	VAL
1	C	520	GLN
1	C	563	ASP
1	C	565	SER
1	C	570	LYS
1	C	586	ILE
1	C	587	ILE
1	C	598	SER
1	C	622	LEU
1	C	633	THR

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Mol	Chain	Res	Type
1	C	665	LYS
1	C	675	GLU
1	C	682	LEU
1	C	683	ASN
1	C	690	SER
1	C	695	ASN
1	C	696	ASN
1	C	700	THR
1	C	703	THR
1	D	390	MET
1	D	404	LEU
1	D	413	LEU
1	D	419	ARG
1	D	421	THR
1	D	439	ASN
1	D	442	GLU
1	D	448	LEU
1	D	455	GLN
1	D	483	PRO
1	D	524	GLN
1	D	526	LEU
1	D	552	LEU
1	D	561	TRP
1	D	618	ILE
1	D	622	LEU
1	D	641	PHE
1	D	663	ASN
1	D	666	LEU
1	D	679	MET
1	D	691	LEU

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

Mol	Chain	Res	Type
1	A	397	HIS
1	A	399	HIS
1	A	432	GLN
1	A	455	GLN
1	A	456	GLN
1	A	462	ASN
1	A	467	GLN
1	A	470	GLN

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Mol	Chain	Res	Type
1	A	507	GLN
1	A	520	GLN
1	A	524	GLN
1	A	578	HIS
1	A	617	ASN
1	A	648	ASN
1	A	663	ASN
1	A	664	HIS
1	A	670	ASN
1	A	683	ASN
1	A	695	ASN
1	B	439	ASN
1	B	455	GLN
1	B	481	GLN
1	B	507	GLN
1	B	578	HIS
1	B	672	ASN
1	B	677	ASN
1	C	392	ASN
1	C	418	ASN
1	C	462	ASN
1	C	466	GLN
1	C	467	GLN
1	C	470	GLN
1	C	520	GLN
1	C	522	HIS
1	C	550	ASN
1	C	617	ASN
1	C	634	GLN
1	C	683	ASN
1	C	695	ASN
1	C	696	ASN
1	D	439	ASN
1	D	462	ASN
1	D	467	GLN
1	D	470	GLN
1	D	504	ASN
1	D	520	GLN
1	D	524	GLN
1	D	528	GLN
1	D	550	ASN
1	D	617	ASN

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Mol	Chain	Res	Type
1	D	648	ASN
1	D	677	ASN
1	D	683	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	IPA	B	1001	-	3,3,3	0.29	0	3,3,3	1.69	1 (33%)

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	IPA	B	1001	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	1001	IPA	C3-C2-C1	-2.61	92.38	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	IPA	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	312/323 (96%)	-0.01	11 (3%)	48 35	10, 32, 77, 124	0
1	B	321/323 (99%)	-0.09	11 (3%)	49 36	6, 25, 77, 129	0
1	C	320/323 (99%)	0.10	10 (3%)	52 40	4, 27, 75, 130	0
1	D	320/323 (99%)	-0.00	9 (2%)	56 44	8, 30, 85, 141	0
All	All	1273/1292 (98%)	-0.00	41 (3%)	51 39	4, 28, 80, 141	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	388	SER	6.6
1	C	448	LEU	5.0
1	D	389	HIS	4.9
1	D	390	MET	4.8
1	A	705	ASP	4.2
1	D	391	ARG	4.2
1	A	706	GLU	4.1
1	C	439	ASN	3.9
1	B	660	TYR	3.8
1	C	417	PRO	3.5
1	B	707	ILE	3.5
1	B	482	GLU	3.3
1	C	646	THR	3.3
1	B	392	ASN	3.1
1	A	644	LEU	3.1
1	D	548	ASP	3.0
1	C	643	SER	2.8
1	C	464	ALA	2.8
1	B	443	VAL	2.6
1	A	523	PRO	2.5
1	B	571	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	420	GLU	2.5
1	D	707	ILE	2.5
1	D	706	GLU	2.4
1	A	688	PRO	2.4
1	B	662	SER	2.4
1	B	582	LEU	2.3
1	C	619	GLU	2.3
1	C	706	GLU	2.3
1	A	662	SER	2.3
1	A	707	ILE	2.2
1	A	482	GLU	2.2
1	B	706	GLU	2.1
1	A	419	ARG	2.1
1	C	449	MET	2.1
1	C	562	THR	2.1
1	D	641	PHE	2.1
1	D	550	ASN	2.1
1	B	513	GLY	2.1
1	A	392	ASN	2.1
1	B	548	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	IPA	B	1001	4/4	0.78	0.34	7.14	20,20,20,20	0

## 6.5 Other polymers

There are no such residues in this entry.