



# Full wwPDB X-ray Structure Validation Report i

Sep 13, 2023 – 10:28 pm BST

PDB ID : 8BMX  
Title : Bacteroides thetaiotaomicron B12 TonB dependent transporter in complex with a surface lipoprotein  
Authors : Abellon-Ruiz, J.; Jana, K.; Silale, A.; Basle, A.; Kleinekathofer, U.; van den Berg, B.  
Deposited on : 2022-11-11  
Resolution : 3.72 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  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see references ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

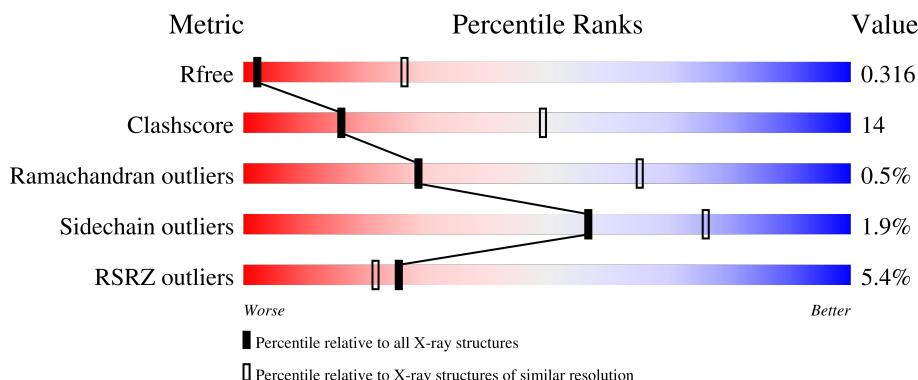
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.72 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))
$R_{free}$	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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.



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Mol	Chain	Length	Quality of chain			
2	F	366	9%	66%	25%	• 8%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 23366 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 Putative TonB-linked outer membrane receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	633	5078	3239	860	960	19	0	0	0
1	A	628	5038	3213	853	953	19	0	0	0
1	B	627	5021	3200	851	951	19	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	693	HIS	-	expression tag	UNP Q8A6D1
C	694	HIS	-	expression tag	UNP Q8A6D1
C	695	HIS	-	expression tag	UNP Q8A6D1
C	696	HIS	-	expression tag	UNP Q8A6D1
C	697	HIS	-	expression tag	UNP Q8A6D1
C	698	HIS	-	expression tag	UNP Q8A6D1
A	693	HIS	-	expression tag	UNP Q8A6D1
A	694	HIS	-	expression tag	UNP Q8A6D1
A	695	HIS	-	expression tag	UNP Q8A6D1
A	696	HIS	-	expression tag	UNP Q8A6D1
A	697	HIS	-	expression tag	UNP Q8A6D1
A	698	HIS	-	expression tag	UNP Q8A6D1
B	693	HIS	-	expression tag	UNP Q8A6D1
B	694	HIS	-	expression tag	UNP Q8A6D1
B	695	HIS	-	expression tag	UNP Q8A6D1
B	696	HIS	-	expression tag	UNP Q8A6D1
B	697	HIS	-	expression tag	UNP Q8A6D1
B	698	HIS	-	expression tag	UNP Q8A6D1

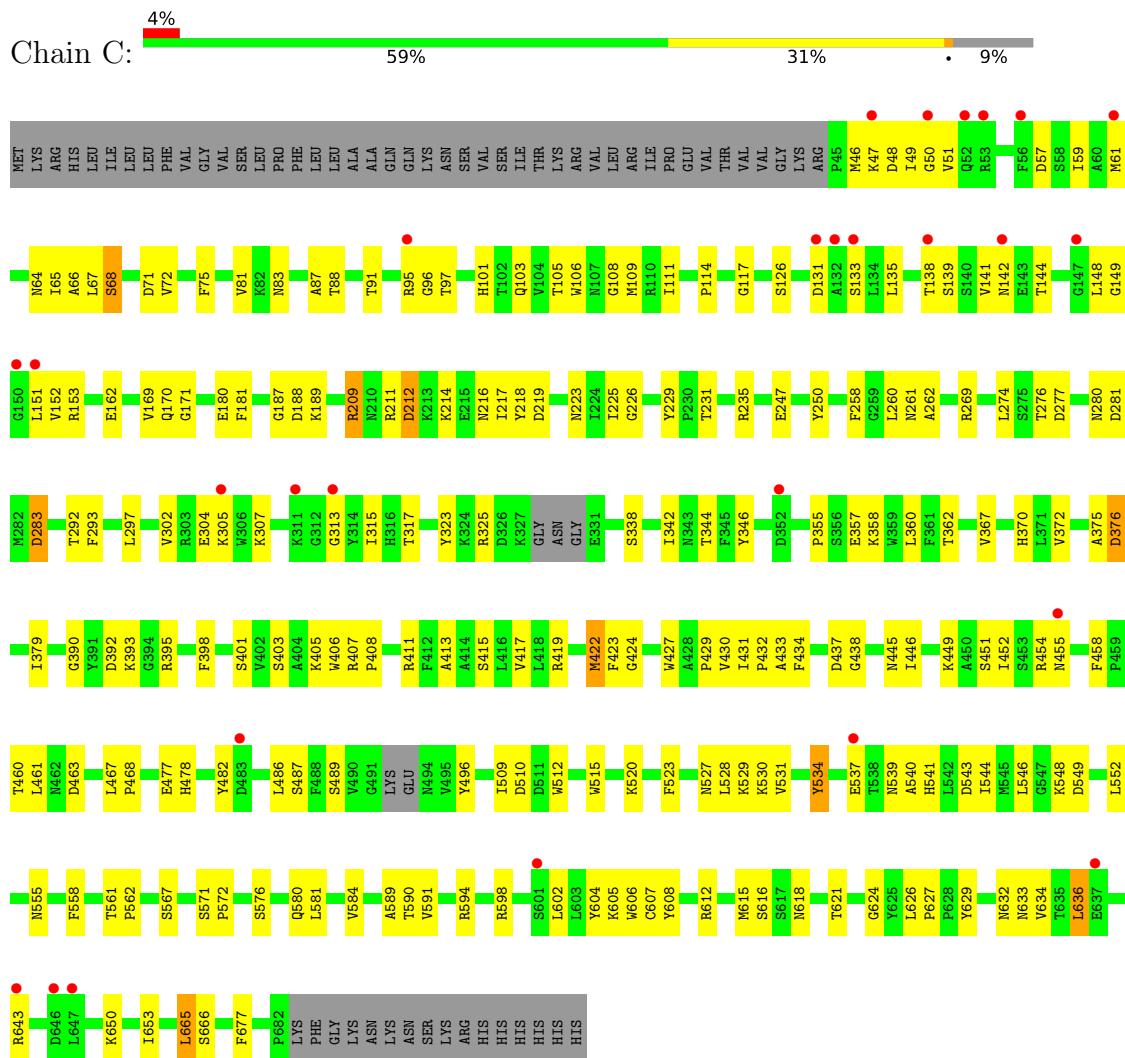
- Molecule 2 is a protein called YncE family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	335	Total	C	N	O	S	0	0	0
			2743	1769	434	526	14			
2	E	335	Total	C	N	O	S	0	0	0
			2743	1769	434	526	14			
2	F	335	Total	C	N	O	S	0	0	0
			2743	1769	434	526	14			

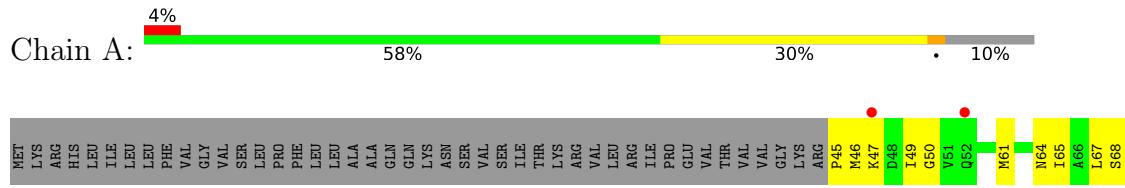
### 3 Residue-property plots

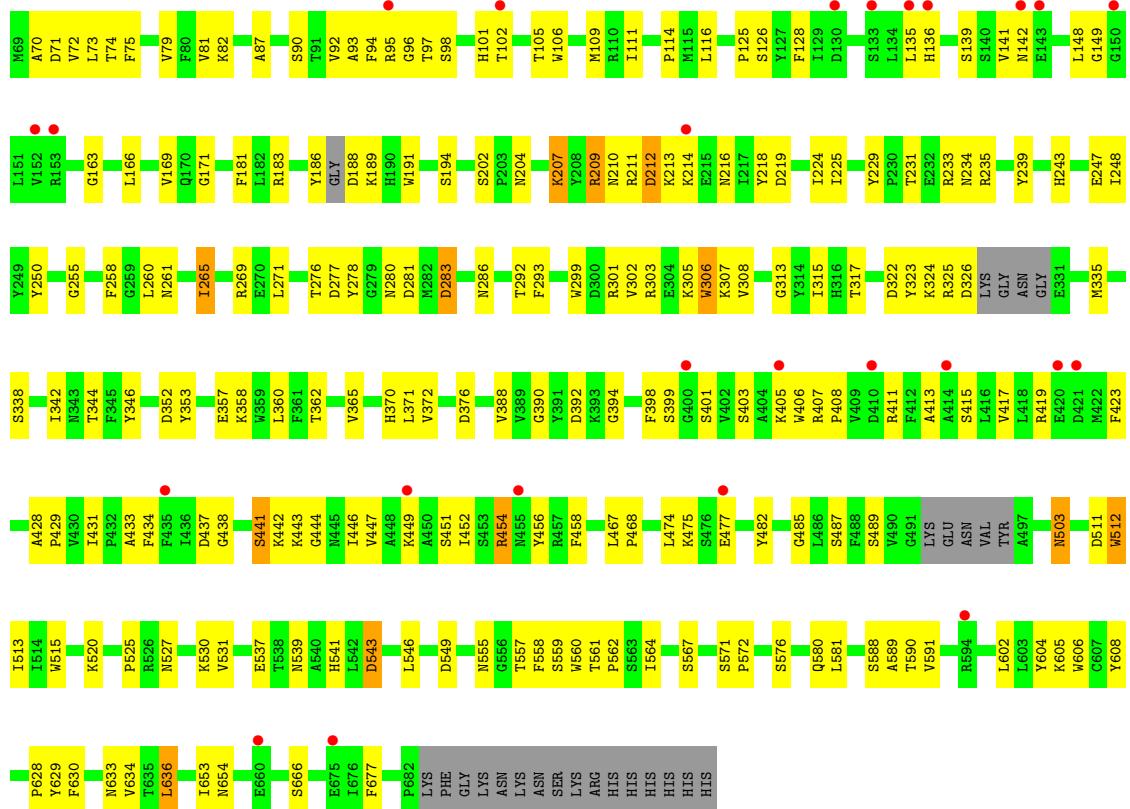
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Molecule 1: Putative TonB-linked outer membrane receptor

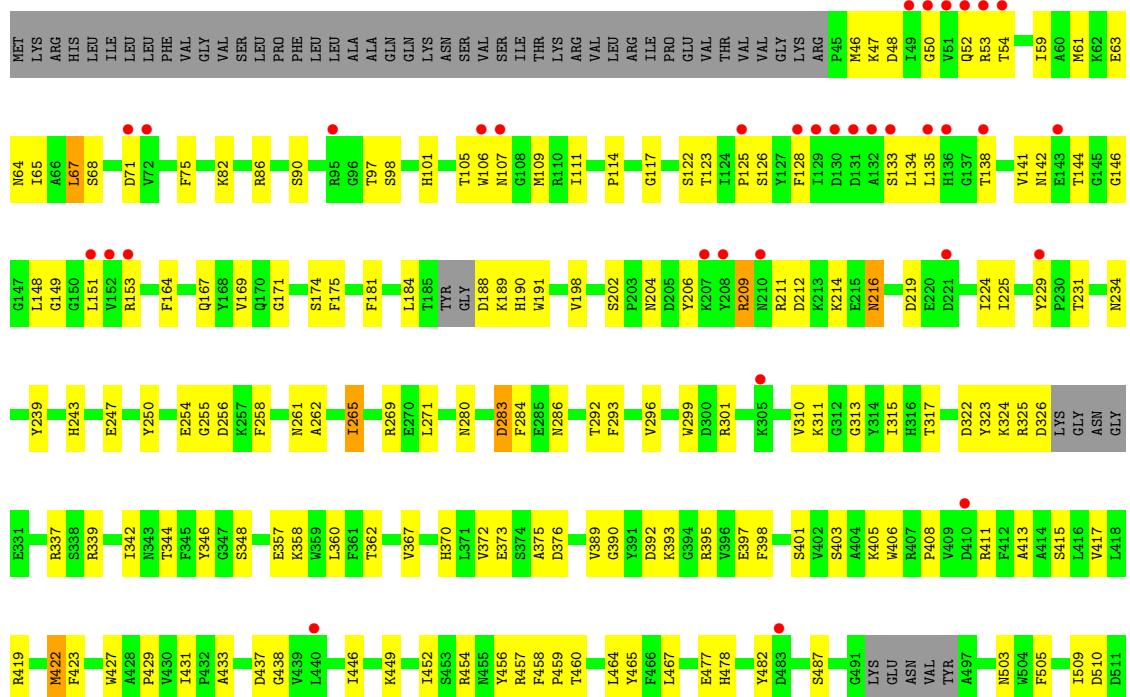


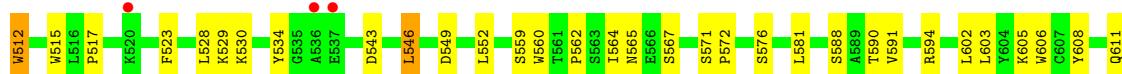
- Molecule 1: Putative TonB-linked outer membrane receptor





- Molecule 1: Putative TonB-linked outer membrane receptor

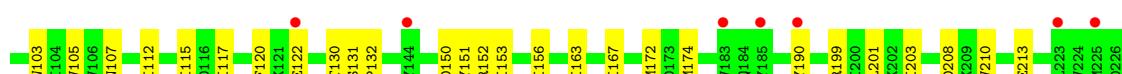




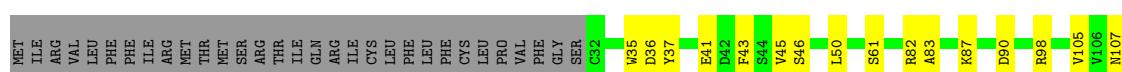
- Molecule 2: YncE family protein

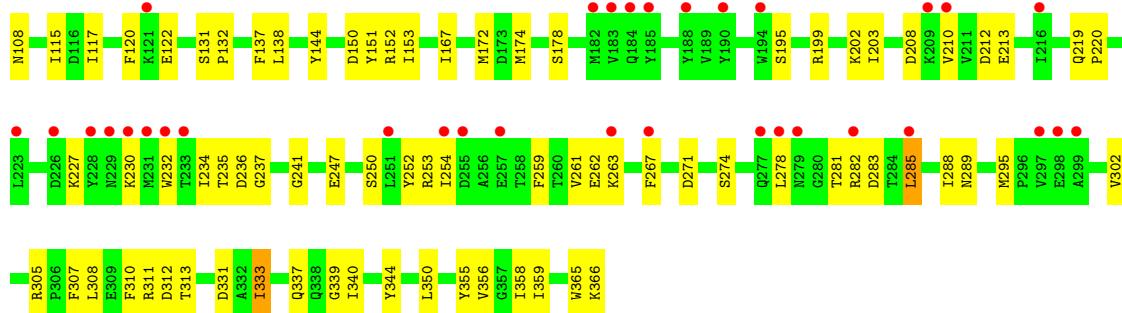


- Molecule 2: YncE family protein



- Molecule 2: YncE family protein





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	280.25 Å    154.30 Å    107.51 Å 90.00°    106.96°    90.00°	Depositor
Resolution (Å)	72.06 – 3.72 76.33 – 3.72	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.06-3.72) 99.2 (76.33-3.72)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.32 (at 3.67 Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
$R$ , $R_{free}$	0.253 , 0.318 0.252 , 0.316	Depositor DCC
$R_{free}$ test set	2232 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	23366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [\(i\)](#)

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

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	0.27	0/5176	0.58	1/7013 (0.0%)
1	B	0.27	0/5158	0.58	2/6989 (0.0%)
1	C	0.27	0/5218	0.58	0/7071
2	D	0.31	0/2820	0.69	0/3836
2	E	0.29	0/2820	0.68	0/3836
2	F	0.28	0/2820	0.68	2/3836 (0.1%)
All	All	0.28	0/24012	0.62	5/32581 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	265	ILE	CG1-CB-CG2	-7.07	95.84	111.40
1	B	603	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	265	ILE	CG1-CB-CG2	-5.08	100.22	111.40
2	F	285	LEU	CA-CB-CG	5.08	126.99	115.30
2	F	278	LEU	CA-CB-CG	5.07	126.97	115.30

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	5038	0	4827	166	0
1	B	5021	0	4806	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5078	0	4868	174	0
2	D	2743	0	2601	73	0
2	E	2743	0	2601	57	0
2	F	2743	0	2601	67	0
All	All	23366	0	22304	660	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 14.

All (660) 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:C:219:ASP:HB3	1:C:225:ILE:HD11	1.44	0.99
1:C:235:ARG:HG2	1:C:281:ASP:HB2	1.56	0.87
1:A:442:LYS:H	1:A:442:LYS:HD2	1.40	0.83
1:C:247:GLU:HB3	1:C:261:ASN:HB3	1.62	0.81
1:B:362:THR:HG1	1:B:403:SER:HG	1.29	0.81
1:C:280:ASN:HB3	1:C:283:ASP:HB2	1.62	0.81
1:C:59:ILE:HD13	1:C:594:ARG:HH12	1.46	0.81
1:A:219:ASP:HB3	1:A:225:ILE:HD11	1.62	0.80
1:C:496:TYR:HB2	1:C:544:ILE:HG22	1.63	0.80
1:B:123:THR:HG22	1:B:269:ARG:HH12	1.47	0.78
1:C:401:SER:HB3	1:C:419:ARG:HG2	1.66	0.78
1:B:219:ASP:HB3	1:B:225:ILE:HD11	1.65	0.78
1:C:419:ARG:HB2	1:C:431:ILE:HG23	1.67	0.77
1:C:114:PRO:HG3	1:C:370:HIS:CG	2.20	0.76
1:B:59:ILE:HD13	1:B:594:ARG:HH12	1.50	0.76
2:D:230:LYS:NZ	2:D:262:GLU:OE1	2.17	0.76
2:E:230:LYS:NZ	2:E:262:GLU:OE1	2.19	0.76
1:B:313:GLY:H	1:B:346:TYR:HB3	1.51	0.75
1:C:209:ARG:HG3	1:C:231:THR:HG22	1.69	0.74
1:B:133:SER:HB2	1:B:153:ARG:HD3	1.70	0.73
1:A:82:LYS:O	1:A:90:SER:HA	1.88	0.73
1:B:209:ARG:HG3	1:B:231:THR:HG22	1.70	0.72
1:A:171:GLY:HA3	1:A:677:PHE:HD1	1.53	0.72
2:E:277:GLN:NE2	2:E:318:LEU:O	2.21	0.72
1:A:477:GLU:HG2	1:A:512:TRP:HA	1.71	0.72
1:B:125:PRO:HD3	1:B:243:HIS:CD2	2.25	0.72
2:E:308:LEU:HD21	2:E:344:TYR:CE2	2.25	0.72
2:F:230:LYS:NZ	2:F:262:GLU:OE1	2.23	0.72
1:C:520:LYS:NZ	2:D:273:PRO:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ASN:HB3	1:C:67:LEU:HG	1.71	0.69
1:C:142:ASN:HB3	1:C:417:VAL:HG11	1.73	0.69
2:E:253:ARG:HD2	2:E:263:LYS:HD2	1.72	0.69
1:C:666:SER:HB2	2:D:61:SER:HB2	1.73	0.69
1:B:358:LYS:HE2	1:B:408:PRO:HA	1.75	0.69
1:A:61:MET:O	1:A:126:SER:OG	2.10	0.68
1:B:608:TYR:HA	1:B:629:TYR:O	1.93	0.68
1:B:64:ASN:OD1	1:B:65:ILE:N	2.25	0.68
2:F:153:ILE:HB	2:F:167:ILE:HB	1.75	0.67
2:F:253:ARG:HD2	2:F:263:LYS:HD2	1.77	0.67
1:B:47:LYS:HA	1:B:405:LYS:HE2	1.75	0.67
1:B:315:ILE:HG12	1:B:344:THR:HB	1.75	0.67
1:C:64:ASN:OD1	1:C:65:ILE:N	2.28	0.67
1:C:362:THR:OG1	1:C:403:SER:OG	2.11	0.67
1:B:666:SER:HB2	2:F:61:SER:HB2	1.77	0.67
1:B:680:ILE:HG22	1:B:682:PRO:HD3	1.75	0.67
1:A:211:ARG:HB3	2:E:37:TYR:HB3	1.76	0.67
2:E:153:ILE:HB	2:E:167:ILE:HB	1.76	0.66
1:C:101:HIS:HB3	1:C:148:LEU:HB2	1.78	0.66
2:D:153:ILE:HB	2:D:167:ILE:HB	1.78	0.66
1:C:250:TYR:HB3	1:C:258:PHE:HB2	1.76	0.66
1:C:171:GLY:HA3	1:C:677:PHE:HD1	1.61	0.65
2:E:253:ARG:HB3	2:E:263:LYS:HB2	1.78	0.65
1:C:211:ARG:HG2	2:D:37:TYR:HD2	1.61	0.65
1:C:262:ALA:HB1	1:C:293:PHE:HE2	1.62	0.65
1:A:666:SER:HB2	2:E:61:SER:HB2	1.79	0.65
1:C:61:MET:O	1:C:126:SER:OG	2.13	0.65
2:D:311:ARG:NH1	2:D:344:TYR:OH	2.29	0.65
1:C:615:MET:HG2	2:D:337:GLN:HA	1.79	0.65
1:A:358:LYS:HE2	1:A:408:PRO:HA	1.78	0.65
2:E:61:SER:O	2:E:87:LYS:HE2	1.97	0.64
2:E:105:VAL:HG13	2:E:132:PRO:HB2	1.79	0.64
1:C:211:ARG:HB3	2:D:37:TYR:HB3	1.80	0.64
1:C:75:PHE:HB3	1:C:605:LYS:HD2	1.78	0.64
1:C:405:LYS:HD3	1:C:415:SER:HB2	1.79	0.64
1:B:478:HIS:HB3	1:B:510:ASP:HB2	1.80	0.64
1:C:530:LYS:H	1:C:567:SER:HB3	1.63	0.63
1:A:96:GLY:N	1:A:561:THR:OG1	2.31	0.63
2:F:35:TRP:HD1	2:F:36:ASP:H	1.47	0.63
1:B:114:PRO:HG3	1:B:370:HIS:CG	2.34	0.63
1:B:477:GLU:HG2	1:B:512:TRP:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:TYR:HB3	1:B:258:PHE:HB2	1.81	0.63
1:A:419:ARG:HB2	1:A:431:ILE:HG23	1.81	0.62
1:C:276:THR:OG1	2:D:61:SER:OG	2.15	0.62
1:A:247:GLU:HB3	1:A:261:ASN:HB3	1.79	0.62
1:B:395:ARG:NH2	1:B:397:GLU:OE2	2.31	0.62
1:C:106:TRP:HB3	1:C:111:ILE:HD11	1.81	0.62
2:D:234:ILE:HD11	2:D:267:PHE:HE2	1.64	0.62
1:A:64:ASN:OD1	1:A:65:ILE:N	2.32	0.62
1:A:303:ARG:HG3	1:A:305:LYS:HB2	1.81	0.62
1:A:602:LEU:HD12	1:A:636:LEU:HB3	1.80	0.62
1:A:250:TYR:HB3	1:A:258:PHE:HB2	1.82	0.62
2:F:115:ILE:HG22	2:F:122:GLU:HA	1.81	0.62
1:C:47:LYS:HA	1:C:405:LYS:HE2	1.82	0.62
1:A:442:LYS:H	1:A:442:LYS:CD	2.11	0.62
1:B:171:GLY:HA3	1:B:677:PHE:HD1	1.64	0.61
1:B:86:ARG:NH1	1:B:239:TYR:OH	2.33	0.61
2:F:105:VAL:HG13	2:F:132:PRO:HB2	1.82	0.61
2:F:253:ARG:HB3	2:F:263:LYS:HB2	1.80	0.61
1:B:64:ASN:HB3	1:B:67:LEU:HG	1.82	0.61
1:B:405:LYS:HD3	1:B:415:SER:HB2	1.83	0.61
2:E:234:ILE:HD11	2:E:267:PHE:HE2	1.66	0.61
2:D:253:ARG:HD2	2:D:263:LYS:HD2	1.82	0.61
1:C:274:LEU:HD13	2:D:59:GLN:HA	1.83	0.61
1:B:342:ILE:HD12	1:B:372:VAL:HG12	1.82	0.61
2:F:61:SER:O	2:F:87:LYS:HE2	2.01	0.60
1:C:608:TYR:HA	1:C:629:TYR:O	2.01	0.60
2:D:105:VAL:HG13	2:D:132:PRO:HB2	1.82	0.60
2:D:107:ASN:OD1	2:D:131:SER:OG	2.19	0.60
1:C:50:GLY:HA2	1:C:449:LYS:HB3	1.84	0.60
1:A:70:ALA:HB1	1:A:81:VAL:HG11	1.82	0.60
1:A:209:ARG:HG3	1:A:231:THR:HG22	1.83	0.60
1:B:142:ASN:HB3	1:B:417:VAL:HG11	1.82	0.60
1:C:342:ILE:HG22	1:C:372:VAL:HA	1.82	0.60
1:C:64:ASN:H	1:C:67:LEU:HD12	1.67	0.60
1:A:106:TRP:HB3	1:A:111:ILE:HD11	1.83	0.59
1:C:95:ARG:HE	1:C:537:GLU:HB3	1.66	0.59
1:A:64:ASN:HB3	1:A:67:LEU:HG	1.84	0.59
1:A:280:ASN:HB3	1:A:283:ASP:HB2	1.83	0.59
1:A:243:HIS:CE1	1:A:265:ILE:HD11	2.38	0.59
2:F:43:PHE:HE1	2:F:120:PHE:CD2	2.20	0.59
1:A:307:LYS:HD2	1:A:352:ASP:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:PHE:HD1	1:A:589:ALA:HB2	1.68	0.59
1:A:559:SER:OG	1:A:588:SER:OG	2.20	0.58
1:B:101:HIS:HB3	1:B:148:LEU:HB2	1.83	0.58
1:B:357:GLU:HG3	1:B:358:LYS:H	1.68	0.58
1:B:452:ILE:HG12	1:B:482:TYR:HB2	1.84	0.58
2:F:311:ARG:NH1	2:F:344:TYR:OH	2.36	0.58
1:C:423:PHE:HB2	1:C:458:PHE:CD2	2.38	0.58
1:B:271:LEU:HB3	1:B:286:ASN:HB3	1.85	0.58
1:A:357:GLU:HG3	1:A:358:LYS:H	1.69	0.58
1:B:65:ILE:HG12	1:B:169:VAL:HG21	1.84	0.58
1:C:612:ARG:NH2	1:C:627:PRO:O	2.35	0.58
1:B:280:ASN:HB3	1:B:283:ASP:HB2	1.85	0.58
2:E:76:GLU:OE1	2:E:82:ARG:NH1	2.32	0.58
1:A:313:GLY:H	1:A:346:TYR:HB3	1.68	0.58
1:A:401:SER:HB3	1:A:419:ARG:HG2	1.84	0.58
1:A:338:SER:HB2	1:A:376:ASP:HA	1.85	0.57
1:A:362:THR:OG1	1:A:403:SER:OG	2.16	0.57
2:D:283:ASP:OD1	2:D:283:ASP:N	2.37	0.57
1:C:171:GLY:HA3	1:C:677:PHE:CD1	2.40	0.57
1:A:73:LEU:HD12	1:A:92:VAL:HG11	1.86	0.57
1:A:114:PRO:HG3	1:A:370:HIS:CG	2.39	0.57
1:A:171:GLY:HA3	1:A:677:PHE:CD1	2.39	0.57
1:A:423:PHE:HB2	1:A:458:PHE:CD2	2.38	0.57
1:A:325:ARG:HG2	1:A:326:ASP:N	2.19	0.57
1:C:67:LEU:O	1:C:71:ASP:HB2	2.04	0.57
1:C:315:ILE:HG12	1:C:344:THR:HB	1.86	0.57
1:A:388:VAL:HG12	1:A:390:GLY:H	1.68	0.57
1:B:107:ASN:HB3	1:B:296:VAL:HG11	1.86	0.57
2:F:308:LEU:HD21	2:F:344:TYR:CE2	2.39	0.57
2:D:315:TYR:CD1	2:D:329:VAL:HG11	2.40	0.57
1:C:512:TRP:HE1	1:C:529:LYS:HB3	1.70	0.56
2:D:35:TRP:HD1	2:D:36:ASP:H	1.53	0.56
1:A:342:ILE:HD12	1:A:372:VAL:HG12	1.87	0.56
2:E:43:PHE:HE1	2:E:120:PHE:CD2	2.23	0.56
1:C:379:ILE:HD11	2:D:243:PRO:HG2	1.88	0.56
1:A:50:GLY:HA2	1:A:449:LYS:HB3	1.88	0.56
2:D:117:ILE:HD12	2:D:366:LYS:HE3	1.88	0.56
1:B:61:MET:O	1:B:126:SER:OG	2.22	0.56
1:A:188:ASP:HB3	1:A:191:TRP:O	2.05	0.56
1:A:360:LEU:HB3	1:A:405:LYS:HB2	1.87	0.56
1:C:411:ARG:O	1:C:438:GLY:HA2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:HA	1:A:405:LYS:HE2	1.88	0.56
1:C:543:ASP:OD1	1:C:543:ASP:N	2.37	0.56
1:C:133:SER:HB2	1:C:153:ARG:HD3	1.87	0.56
1:C:188:ASP:OD1	1:C:189:LYS:N	2.37	0.56
2:E:115:ILE:HG22	2:E:122:GLU:HA	1.88	0.56
1:A:235:ARG:HG2	1:A:281:ASP:HB2	1.88	0.55
1:A:549:ASP:OD1	1:A:549:ASP:N	2.37	0.55
1:A:562:PRO:HA	1:A:580:GLN:HE21	1.71	0.55
1:A:360:LEU:HD22	1:A:405:LYS:HG3	1.88	0.55
1:B:322:ASP:HB3	1:B:324:LYS:HE3	1.87	0.55
2:D:253:ARG:HB3	2:D:263:LYS:HB2	1.88	0.55
1:C:571:SER:HB2	2:D:333:ILE:HG23	1.88	0.55
1:B:362:THR:OG1	1:B:403:SER:OG	2.12	0.55
2:E:285:LEU:HD23	2:E:295:MET:O	2.06	0.55
2:F:283:ASP:OD1	2:F:283:ASP:N	2.37	0.55
1:B:63:GLU:HG3	1:B:635:THR:HG21	1.89	0.55
2:D:333:ILE:HD12	2:D:339:GLY:HA2	1.88	0.55
2:E:283:ASP:N	2:E:283:ASP:OD1	2.39	0.55
2:F:285:LEU:HD23	2:F:295:MET:O	2.06	0.55
1:C:212:ASP:OD1	2:D:87:LYS:HD3	2.06	0.55
1:A:571:SER:HB2	2:E:333:ILE:HG23	1.88	0.55
2:D:43:PHE:HE1	2:D:120:PHE:HD2	1.55	0.55
1:C:65:ILE:HG12	1:C:169:VAL:HG21	1.88	0.55
2:D:172:MET:HG2	2:D:177:GLY:HA2	1.89	0.55
2:F:41:GLU:OE1	2:F:82:ARG:NE	2.39	0.55
2:F:232:TRP:HA	2:F:252:TYR:O	2.06	0.55
1:C:509:ILE:HB	1:C:531:VAL:HG22	1.89	0.54
1:C:358:LYS:HE2	1:C:408:PRO:HA	1.87	0.54
2:F:41:GLU:N	2:F:82:ARG:O	2.39	0.54
1:C:260:LEU:HD12	1:C:297:LEU:HD12	1.88	0.54
1:C:413:ALA:HB3	1:C:437:ASP:OD1	2.07	0.54
1:B:243:HIS:CE1	1:B:265:ILE:HD11	2.42	0.54
1:A:543:ASP:OD1	1:A:543:ASP:N	2.39	0.54
1:B:549:ASP:OD1	1:B:549:ASP:N	2.40	0.54
1:C:216:ASN:HB2	1:C:218:TYR:CE1	2.43	0.54
1:C:211:ARG:HG2	2:D:37:TYR:CD2	2.43	0.54
1:B:325:ARG:HG2	1:B:326:ASP:N	2.23	0.54
2:D:43:PHE:HE1	2:D:120:PHE:CD2	2.26	0.54
1:C:467:LEU:HD21	2:D:241:GLY:O	2.08	0.54
1:B:419:ARG:HB2	1:B:431:ILE:HG23	1.90	0.54
1:A:87:ALA:HB1	1:A:269:ARG:NE	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:THR:HG21	1:B:149:GLY:HA3	1.90	0.53
2:D:330:ALA:HB1	2:D:360:PRO:HG2	1.90	0.53
1:C:445:ASN:OD1	1:C:489:SER:N	2.42	0.53
1:C:105:THR:HA	1:C:109:MET:O	2.08	0.53
2:E:43:PHE:HE1	2:E:120:PHE:HD2	1.56	0.53
1:A:608:TYR:HA	1:A:629:TYR:O	2.09	0.53
1:C:477:GLU:HG2	1:C:512:TRP:HA	1.90	0.53
1:A:322:ASP:HB3	1:A:324:LYS:HE3	1.91	0.53
1:C:117:GLY:N	1:C:460:THR:HG21	2.24	0.53
1:C:262:ALA:HB1	1:C:293:PHE:CE2	2.42	0.53
1:C:531:VAL:HG11	1:C:581:LEU:HD11	1.89	0.53
1:A:125:PRO:HG2	1:A:128:PHE:HB2	1.91	0.53
1:B:146:GLY:HA2	1:B:456:TYR:O	2.09	0.53
1:B:255:GLY:O	1:B:301:ARG:HA	2.09	0.53
1:B:360:LEU:HB3	1:B:405:LYS:HB2	1.91	0.53
2:E:274:SER:OG	2:E:288:ILE:HG12	2.09	0.53
1:A:576:SER:O	1:A:576:SER:OG	2.24	0.53
1:B:644:TRP:O	1:B:682:PRO:HA	2.08	0.53
1:A:235:ARG:NH1	1:A:277:ASP:O	2.39	0.52
1:A:265:ILE:HG22	1:A:292:THR:H	1.74	0.52
1:A:45:PRO:HB2	1:A:407:ARG:HH12	1.75	0.52
1:A:188:ASP:OD1	1:A:189:LYS:N	2.41	0.52
1:C:576:SER:OG	1:C:576:SER:O	2.26	0.52
1:B:517:PRO:HG3	1:B:523:PHE:CZ	2.45	0.52
1:B:528:LEU:HD12	1:B:529:LYS:HG3	1.92	0.52
1:B:559:SER:OG	1:B:588:SER:OG	2.18	0.52
2:F:237:GLY:HA2	2:F:247:GLU:HG2	1.90	0.52
1:A:276:THR:OG1	2:E:61:SER:OG	2.24	0.52
1:B:576:SER:OG	1:B:576:SER:O	2.26	0.52
2:F:274:SER:OG	2:F:288:ILE:HG12	2.09	0.52
1:C:219:ASP:HB3	1:C:225:ILE:CD1	2.29	0.52
1:C:452:ILE:HG12	1:C:482:TYR:HB2	1.92	0.52
1:A:271:LEU:HB3	1:A:286:ASN:HB3	1.92	0.52
1:B:202:SER:HB3	1:B:239:TYR:CE2	2.45	0.52
2:D:115:ILE:HG22	2:D:122:GLU:HA	1.92	0.52
1:C:117:GLY:H	1:C:460:THR:HG21	1.74	0.52
1:A:81:VAL:HG22	1:A:92:VAL:HG12	1.90	0.52
2:F:340:ILE:HD12	2:F:355:TYR:CE1	2.45	0.52
1:C:407:ARG:HB2	1:C:413:ALA:HB2	1.92	0.52
1:A:406:TRP:CZ2	1:A:408:PRO:HG3	2.45	0.52
2:E:91:VAL:HB	2:E:107:ASN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:H	1:B:67:LEU:HD12	1.76	0.52
1:C:375:ALA:HA	1:C:390:GLY:HA3	1.91	0.51
1:C:591:VAL:HG12	1:C:606:TRP:CE3	2.45	0.51
1:A:169:VAL:HG22	1:A:181:PHE:HD2	1.74	0.51
1:A:358:LYS:O	1:A:406:TRP:HD1	1.93	0.51
1:C:429:PRO:HB2	1:C:454:ARG:HH21	1.75	0.51
1:B:75:PHE:HA	1:B:590:THR:HG21	1.91	0.51
2:E:107:ASN:OD1	2:E:131:SER:OG	2.24	0.51
2:F:199:ARG:NH1	2:F:213:GLU:OE1	2.44	0.51
2:F:271:ASP:HB3	2:F:289:ASN:OD1	2.10	0.51
1:C:358:LYS:O	1:C:406:TRP:HD1	1.94	0.51
1:C:580:GLN:NE2	1:C:584:VAL:O	2.44	0.51
1:B:313:GLY:N	1:B:346:TYR:HB3	2.23	0.51
1:B:392:ASP:N	1:B:392:ASP:OD1	2.43	0.51
1:A:357:GLU:HG3	1:A:358:LYS:N	2.26	0.51
1:B:114:PRO:HG3	1:B:370:HIS:ND1	2.25	0.51
2:D:152:ARG:HA	2:D:167:ILE:O	2.11	0.51
2:D:254:ILE:HG12	2:D:261:VAL:HG22	1.91	0.51
2:E:45:VAL:HG22	2:E:46:SER:H	1.76	0.51
1:C:446:ILE:HA	1:C:487:SER:O	2.10	0.51
1:B:358:LYS:O	1:B:406:TRP:HD1	1.93	0.51
1:B:571:SER:HB2	2:F:333:ILE:HG23	1.93	0.51
2:D:308:LEU:HD21	2:D:344:TYR:CE2	2.45	0.51
2:F:333:ILE:HG21	2:F:337:GLN:HE21	1.75	0.51
1:C:666:SER:CB	2:D:61:SER:HB2	2.40	0.51
1:B:50:GLY:HA2	1:B:449:LYS:HB3	1.93	0.51
1:B:357:GLU:HG3	1:B:358:LYS:N	2.26	0.51
1:B:529:LYS:HE2	1:B:565:ASN:HD21	1.76	0.51
2:E:156:ILE:HG22	2:E:163:ILE:HA	1.93	0.51
1:A:214:LYS:HE3	1:A:229:TYR:CZ	2.46	0.51
1:A:429:PRO:HG2	1:A:456:TYR:CZ	2.46	0.51
2:D:45:VAL:HG22	2:D:46:SER:H	1.76	0.51
1:A:413:ALA:HB3	1:A:437:ASP:OD1	2.11	0.50
1:A:539:ASN:HB3	1:A:557:THR:HG22	1.92	0.50
1:B:403:SER:HB3	1:B:417:VAL:HG12	1.93	0.50
2:D:340:ILE:HD12	2:D:355:TYR:CE1	2.46	0.50
1:A:125:PRO:HD3	1:A:243:HIS:CE1	2.46	0.50
2:F:234:ILE:HD11	2:F:267:PHE:HE2	1.76	0.50
1:A:75:PHE:HA	1:A:590:THR:HG21	1.92	0.50
1:B:401:SER:HB3	1:B:419:ARG:HG2	1.93	0.50
1:C:541:HIS:HB3	1:C:555:ASN:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:SER:HB3	1:A:239:TYR:CE2	2.46	0.50
2:D:222:SER:HB3	2:D:275:GLU:HB2	1.93	0.50
1:C:357:GLU:HG3	1:C:358:LYS:N	2.26	0.50
1:B:211:ARG:HD2	2:F:35:TRP:CE3	2.47	0.50
2:F:45:VAL:HG22	2:F:46:SER:H	1.77	0.50
1:C:138:THR:O	1:C:141:VAL:HG12	2.12	0.50
1:C:214:LYS:HE3	1:C:229:TYR:CZ	2.47	0.50
1:C:357:GLU:HG3	1:C:358:LYS:H	1.77	0.50
1:B:649:LEU:HD12	1:B:678:ILE:HG12	1.93	0.50
2:E:292:ILE:HD13	2:E:308:LEU:HD22	1.94	0.50
1:B:67:LEU:O	1:B:71:ASP:HB2	2.12	0.49
1:A:212:ASP:OD1	2:E:87:LYS:HD3	2.11	0.49
1:A:255:GLY:HA3	1:A:302:VAL:O	2.11	0.49
2:D:331:ASP:OD1	2:D:340:ILE:HG22	2.11	0.49
1:C:430:VAL:O	1:C:432:PRO:HD3	2.13	0.49
1:C:446:ILE:HD11	1:C:486:LEU:HD23	1.94	0.49
2:E:286:TYR:HB3	2:E:318:LEU:HD21	1.94	0.49
1:C:87:ALA:HB1	1:C:269:ARG:NE	2.27	0.49
1:C:405:LYS:HD3	1:C:415:SER:CB	2.41	0.49
1:A:405:LYS:HD3	1:A:415:SER:HB2	1.93	0.49
1:C:624:GLY:HA2	1:C:665:LEU:HD11	1.94	0.49
1:B:591:VAL:HG12	1:B:606:TRP:CE3	2.47	0.49
1:A:591:VAL:HG12	1:A:606:TRP:CE3	2.47	0.49
1:C:114:PRO:HG3	1:C:370:HIS:ND1	2.28	0.49
1:C:392:ASP:OD1	1:C:392:ASP:N	2.45	0.49
1:C:546:LEU:H	1:C:546:LEU:HD23	1.77	0.49
1:A:452:ILE:HG12	1:A:482:TYR:HB2	1.94	0.49
1:C:83:ASN:OD1	1:C:88:THR:HG21	2.13	0.49
1:C:219:ASP:OD2	1:B:190:HIS:NE2	2.44	0.49
1:C:360:LEU:HD22	1:C:405:LYS:HG3	1.94	0.49
1:C:528:LEU:HD12	1:C:529:LYS:HG3	1.93	0.49
1:B:446:ILE:HA	1:B:487:SER:O	2.12	0.49
1:C:47:LYS:O	1:C:47:LYS:NZ	2.34	0.49
1:C:633:ASN:HB2	1:C:653:ILE:O	2.13	0.49
1:A:243:HIS:CG	1:A:265:ILE:HD11	2.48	0.49
1:A:475:LYS:NZ	1:A:511:ASP:OD2	2.42	0.49
2:D:285:LEU:HD23	2:D:295:MET:O	2.12	0.49
2:E:35:TRP:HD1	2:E:36:ASP:H	1.61	0.49
1:A:97:THR:HG22	1:A:98:SER:O	2.12	0.49
1:A:204:ASN:O	1:A:234:ASN:HB3	2.13	0.49
1:B:247:GLU:HB3	1:B:261:ASN:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:TRP:HE3	1:B:523:PHE:HB3	1.76	0.49
1:C:96:GLY:N	1:C:561:THR:OG1	2.46	0.48
1:C:302:VAL:HG12	1:C:307:LYS:HB3	1.95	0.48
1:C:276:THR:HB	2:D:89:GLY:HA2	1.95	0.48
1:C:512:TRP:HD1	1:C:529:LYS:O	1.95	0.48
1:B:97:THR:HG22	1:B:98:SER:O	2.13	0.48
2:F:151:TYR:HB2	2:F:172:MET:HB3	1.94	0.48
2:F:219:GLN:HB2	2:F:236:ASP:OD1	2.12	0.48
1:C:549:ASP:N	1:C:549:ASP:OD1	2.46	0.48
1:A:474:LEU:HD11	1:A:525:PRO:HB2	1.95	0.48
1:B:216:ASN:HB3	1:B:224:ILE:HG13	1.94	0.48
1:C:534:TYR:HE1	1:C:562:PRO:HG2	1.78	0.48
1:C:313:GLY:H	1:C:346:TYR:HB3	1.77	0.48
1:C:540:ALA:O	1:C:555:ASN:HA	2.12	0.48
1:A:513:ILE:HG22	1:A:527:ASN:ND2	2.28	0.48
1:A:166:LEU:HA	1:A:183:ARG:O	2.13	0.48
1:A:248:ILE:HG12	1:A:260:LEU:HD22	1.95	0.48
1:A:560:TRP:NE1	1:A:562:PRO:HG3	2.28	0.48
1:B:141:VAL:HG11	1:B:433:ALA:CB	2.43	0.48
1:B:243:HIS:CD2	1:B:265:ILE:HD11	2.49	0.48
1:B:615:MET:HE1	1:B:621:THR:HG21	1.96	0.48
2:F:105:VAL:CG1	2:F:132:PRO:HB2	2.44	0.48
1:A:441:SER:OG	1:A:443:LYS:HB3	2.14	0.48
2:D:90:ASP:HB3	2:D:108:ASN:HB3	1.94	0.48
1:A:306:TRP:CD1	1:A:308:VAL:HG13	2.49	0.48
1:A:442:LYS:HD2	1:A:442:LYS:N	2.18	0.48
1:A:467:LEU:HD21	2:E:241:GLY:O	2.14	0.48
1:B:292:THR:HB	1:B:317:THR:HA	1.94	0.48
1:B:337:ARG:CZ	1:B:339:ARG:HD2	2.43	0.48
1:B:543:ASP:N	1:B:543:ASP:OD1	2.45	0.48
1:A:315:ILE:HG12	1:A:344:THR:HB	1.95	0.48
1:A:392:ASP:OD1	1:A:392:ASP:N	2.47	0.48
1:B:181:PHE:HB2	1:B:198:VAL:HG22	1.95	0.48
2:F:234:ILE:HG13	2:F:250:SER:O	2.14	0.48
1:A:75:PHE:HB3	1:A:605:LYS:HD2	1.95	0.47
1:A:520:LYS:HD2	2:E:236:ASP:HB2	1.95	0.47
1:B:82:LYS:O	1:B:90:SER:HA	2.14	0.47
1:B:258:PHE:CE2	1:B:299:TRP:HD1	2.32	0.47
1:C:81:VAL:HA	1:C:91:THR:O	2.14	0.47
1:C:97:THR:HG21	1:C:149:GLY:HA3	1.96	0.47
1:A:411:ARG:O	1:A:438:GLY:HA2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:VAL:HG12	1:A:606:TRP:HE3	1.78	0.47
1:B:59:ILE:HG21	1:B:594:ARG:CZ	2.45	0.47
2:F:254:ILE:HG12	2:F:261:VAL:HG22	1.97	0.47
1:C:604:TYR:CD2	1:C:634:VAL:HB	2.50	0.47
1:B:106:TRP:HB3	1:B:111:ILE:HD11	1.97	0.47
1:B:164:PHE:HE1	1:B:184:LEU:HB3	1.79	0.47
1:B:211:ARG:HB3	2:F:37:TYR:HB3	1.96	0.47
1:C:109:MET:HG2	1:C:346:TYR:CD2	2.49	0.47
1:C:360:LEU:HB3	1:C:405:LYS:HB2	1.95	0.47
1:A:306:TRP:HD1	1:A:308:VAL:HG13	1.79	0.47
1:A:530:LYS:H	1:A:567:SER:HB3	1.80	0.47
1:B:171:GLY:HA3	1:B:677:PHE:CD1	2.47	0.47
1:B:405:LYS:HD3	1:B:415:SER:CB	2.43	0.47
2:E:232:TRP:HA	2:E:252:TYR:O	2.13	0.47
1:C:59:ILE:HG21	1:C:594:ARG:NH1	2.29	0.47
1:C:367:VAL:HG22	1:C:398:PHE:HB2	1.96	0.47
1:C:431:ILE:HG13	1:C:455:ASN:HA	1.95	0.47
1:A:105:THR:HA	1:A:109:MET:O	2.15	0.47
1:B:105:THR:HA	1:B:109:MET:O	2.15	0.47
1:B:512:TRP:HE1	1:B:529:LYS:HB2	1.80	0.47
1:B:372:VAL:CG2	1:B:393:LYS:H	2.27	0.47
1:B:411:ARG:O	1:B:438:GLY:HA2	2.15	0.47
1:B:413:ALA:HB3	1:B:437:ASP:OD1	2.15	0.47
2:F:281:THR:OG1	2:F:283:ASP:OD1	2.30	0.47
1:C:305:LYS:NZ	1:C:355:PRO:HA	2.29	0.47
1:B:423:PHE:HB2	1:B:458:PHE:CD2	2.50	0.47
1:A:447:VAL:HG13	1:A:487:SER:HB3	1.97	0.47
1:C:612:ARG:HE	1:C:626:LEU:HD13	1.81	0.46
1:B:417:VAL:HG22	1:B:433:ALA:HB3	1.96	0.46
1:B:452:ILE:HG23	1:B:482:TYR:HB3	1.97	0.46
1:B:530:LYS:H	1:B:567:SER:HB3	1.80	0.46
1:A:255:GLY:O	1:A:301:ARG:HA	2.15	0.46
1:B:667:ARG:HD3	1:B:667:ARG:HA	1.77	0.46
2:F:202:LYS:HB3	2:F:212:ASP:HB3	1.97	0.46
1:C:403:SER:HB3	1:C:417:VAL:HG12	1.97	0.46
1:C:572:PRO:HD2	2:D:313:THR:HG22	1.97	0.46
1:A:292:THR:OG1	1:A:317:THR:HG22	2.15	0.46
1:A:531:VAL:HG11	1:A:581:LEU:HD11	1.97	0.46
2:D:50:LEU:HD13	2:D:365:TRP:CE2	2.51	0.46
2:D:78:GLU:O	2:D:82:ARG:HG3	2.16	0.46
2:F:152:ARG:HA	2:F:167:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:HB3	1:A:224:ILE:HG13	1.97	0.46
1:B:65:ILE:HG12	1:B:169:VAL:CG2	2.45	0.46
1:B:214:LYS:HE3	1:B:229:TYR:CZ	2.51	0.46
2:D:335:TYR:HB3	2:D:359:ILE:HD11	1.98	0.46
2:F:237:GLY:HA3	2:F:247:GLU:O	2.16	0.46
1:A:93:ALA:HB1	1:A:97:THR:O	2.15	0.46
1:B:54:THR:HB	1:B:134:LEU:HB3	1.97	0.46
1:C:65:ILE:HG12	1:C:169:VAL:CG2	2.46	0.46
1:C:446:ILE:HD12	1:C:487:SER:O	2.15	0.46
1:A:452:ILE:HG23	1:A:482:TYR:HB3	1.97	0.46
1:B:148:LEU:HD13	1:B:457:ARG:HB2	1.97	0.46
1:B:262:ALA:HB1	1:B:293:PHE:HE2	1.80	0.46
1:B:615:MET:HE2	2:F:358:ILE:HD11	1.97	0.46
2:F:331:ASP:OD1	2:F:331:ASP:O	2.34	0.46
1:A:142:ASN:HB3	1:A:417:VAL:HG11	1.97	0.46
1:B:459:PRO:HG2	1:B:464:LEU:HD11	1.97	0.46
2:F:333:ILE:HD12	2:F:339:GLY:HA2	1.97	0.46
1:A:546:LEU:H	1:A:546:LEU:HD23	1.81	0.46
1:B:393:LYS:HG3	1:B:465:TYR:CG	2.51	0.46
1:B:614:THR:OG1	1:B:624:GLY:O	2.24	0.46
2:D:251:LEU:HD21	2:D:285:LEU:HD11	1.97	0.46
2:D:274:SER:OG	2:D:288:ILE:HG12	2.15	0.46
1:C:417:VAL:HG22	1:C:433:ALA:HB3	1.97	0.46
1:C:549:ASP:OD2	1:C:598:ARG:NH1	2.49	0.46
1:A:258:PHE:CE2	1:A:299:TRP:HD1	2.34	0.46
2:E:203:ILE:HG12	2:E:210:VAL:HG22	1.97	0.46
2:F:41:GLU:O	2:F:83:ALA:HA	2.16	0.46
2:D:308:LEU:HD21	2:D:344:TYR:CD2	2.51	0.45
2:E:117:ILE:HD12	2:E:366:LYS:HE3	1.98	0.45
1:A:213:LYS:HG3	1:A:278:TYR:CZ	2.51	0.45
2:D:64:THR:HG21	2:D:78:GLU:HG2	1.97	0.45
1:A:633:ASN:HB2	1:A:653:ILE:O	2.17	0.45
1:C:108:GLY:O	1:C:346:TYR:OH	2.27	0.45
1:A:125:PRO:HD3	1:A:243:HIS:ND1	2.32	0.45
2:F:43:PHE:CE1	2:F:120:PHE:CD2	3.03	0.45
1:C:615:MET:HE3	1:C:621:THR:HG21	1.98	0.45
1:B:204:ASN:O	1:B:234:ASN:HB3	2.17	0.45
1:C:75:PHE:HA	1:C:590:THR:HG21	1.98	0.45
1:C:379:ILE:CD1	2:D:244:TYR:HB2	2.47	0.45
1:A:515:TRP:CZ3	1:A:525:PRO:HD3	2.52	0.45
1:B:114:PRO:HG3	1:B:370:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:THR:HA	1:B:419:ARG:CZ	2.47	0.45
1:B:188:ASP:OD1	1:B:189:LYS:N	2.50	0.45
2:D:84:ASN:HB3	2:D:86:PHE:CE1	2.52	0.45
2:F:310:PHE:CZ	2:F:312:ASP:HA	2.51	0.45
1:A:65:ILE:HG12	1:A:169:VAL:HG21	1.99	0.45
1:A:541:HIS:HB3	1:A:555:ASN:HB3	1.98	0.45
1:A:633:ASN:HB3	1:A:654:ASN:HA	1.99	0.45
1:B:422:MET:HB2	1:B:427:TRP:CE3	2.52	0.45
1:C:144:THR:HA	1:C:419:ARG:CZ	2.47	0.44
1:C:467:LEU:HB3	1:C:468:PRO:HD3	1.98	0.44
1:B:360:LEU:HD22	1:B:405:LYS:HG3	1.98	0.44
1:B:389:VAL:O	1:B:467:LEU:HB3	2.18	0.44
1:B:534:TYR:CE1	1:B:562:PRO:HG2	2.51	0.44
1:B:572:PRO:HD2	2:F:313:THR:HG22	1.99	0.44
2:D:105:VAL:CG1	2:D:132:PRO:HB2	2.45	0.44
1:C:325:ARG:NH2	2:D:128:GLY:O	2.50	0.44
1:C:615:MET:HE2	2:D:358:ILE:HD11	1.98	0.44
2:D:330:ALA:HB2	2:D:363:PHE:HZ	1.81	0.44
2:E:152:ARG:HA	2:E:167:ILE:O	2.16	0.44
2:E:167:ILE:HD13	2:E:208:ASP:O	2.17	0.44
2:F:307:PHE:CE2	2:F:308:LEU:HD13	2.51	0.44
1:C:338:SER:HB2	1:C:376:ASP:HA	1.98	0.44
1:A:243:HIS:ND1	1:A:265:ILE:HD11	2.31	0.44
1:B:292:THR:OG1	1:B:317:THR:HG22	2.18	0.44
2:E:105:VAL:CG1	2:E:132:PRO:HB2	2.45	0.44
1:C:51:VAL:HG13	1:C:139:SER:HB2	2.00	0.44
1:A:95:ARG:HE	1:A:537:GLU:HB3	1.82	0.44
1:A:136:HIS:O	1:A:139:SER:OG	2.33	0.44
1:A:405:LYS:HD3	1:A:415:SER:CB	2.48	0.44
1:B:375:ALA:HA	1:B:390:GLY:HA3	1.98	0.44
2:F:227:LYS:HB2	2:F:282:ARG:HB2	1.99	0.44
1:C:358:LYS:HZ3	1:C:406:TRP:HE1	1.65	0.44
1:C:434:PHE:O	1:C:451:SER:HA	2.17	0.44
1:A:61:MET:HG2	1:A:72:VAL:HG11	1.99	0.44
1:B:605:LYS:HB2	1:B:633:ASN:OD1	2.18	0.44
2:E:326:GLU:HG2	2:E:345:SER:HA	1.99	0.44
2:F:90:ASP:HB3	2:F:108:ASN:HB3	1.99	0.44
1:A:216:ASN:HB2	1:A:218:TYR:CE1	2.52	0.44
1:B:546:LEU:HD23	1:B:546:LEU:H	1.83	0.44
2:F:117:ILE:HD12	2:F:366:LYS:HE3	1.99	0.44
1:A:403:SER:HB3	1:A:417:VAL:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:ASP:OD1	2:D:331:ASP:O	2.34	0.44
2:D:340:ILE:HG13	2:D:354:PHE:O	2.17	0.44
2:F:307:PHE:CD2	2:F:308:LEU:HD13	2.52	0.44
1:A:87:ALA:HB1	1:A:269:ARG:HE	1.82	0.44
1:A:365:VAL:HG23	1:A:398:PHE:HE1	1.82	0.44
1:B:188:ASP:HB3	1:B:191:TRP:O	2.18	0.44
1:B:618:ASN:N	1:B:618:ASN:HD22	2.15	0.44
1:C:46:MET:C	1:C:48:ASP:H	2.21	0.44
2:F:358:ILE:HG22	2:F:359:ILE:HG13	1.99	0.44
1:B:75:PHE:HB3	1:B:605:LYS:HD2	2.00	0.43
1:B:167:GLN:HG3	1:B:681:THR:HG22	2.00	0.43
2:E:190:TYR:HA	2:E:201:LEU:O	2.18	0.43
1:C:61:MET:HG2	1:C:72:VAL:HG11	2.00	0.43
1:C:151:LEU:HG	1:C:152:VAL:N	2.33	0.43
1:B:59:ILE:HG21	1:B:594:ARG:NH1	2.32	0.43
1:B:125:PRO:HG2	1:B:128:PHE:HB2	2.00	0.43
1:B:611:GLN:HG3	1:B:626:LEU:O	2.18	0.43
1:C:591:VAL:HG12	1:C:606:TRP:HE3	1.81	0.43
1:A:434:PHE:O	1:A:451:SER:HA	2.18	0.43
1:B:53:ARG:HB3	1:B:135:LEU:HD23	1.99	0.43
1:B:212:ASP:OD1	2:F:87:LYS:HD3	2.18	0.43
2:E:151:TYR:HB2	2:E:172:MET:HB3	1.99	0.43
2:E:199:ARG:NH1	2:E:213:GLU:OE1	2.51	0.43
1:C:606:TRP:HD1	1:C:632:ASN:OD1	2.02	0.43
1:A:306:TRP:HB3	1:A:353:TYR:HD1	1.84	0.43
1:B:626:LEU:HD23	1:B:626:LEU:HA	1.76	0.43
1:C:602:LEU:HD12	1:C:636:LEU:HB3	1.99	0.43
1:A:46:MET:HG2	1:A:49:ILE:HD11	2.01	0.43
1:A:446:ILE:HA	1:A:487:SER:O	2.19	0.43
1:B:346:TYR:CZ	1:B:348:SER:HB2	2.54	0.43
2:F:344:TYR:CD1	2:F:350:LEU:HA	2.53	0.43
1:A:564:ILE:H	1:A:564:ILE:HG13	1.60	0.43
1:B:429:PRO:HG2	1:B:456:TYR:CZ	2.54	0.43
1:B:594:ARG:HB2	1:B:602:LEU:O	2.19	0.43
2:D:235:THR:O	2:D:249:PRO:HB2	2.19	0.43
1:C:65:ILE:HD12	1:C:65:ILE:H	1.83	0.43
1:C:372:VAL:CG2	1:C:393:LYS:H	2.31	0.43
1:A:94:PHE:HD2	1:A:149:GLY:C	2.22	0.43
1:A:211:ARG:HD2	2:E:35:TRP:CE3	2.53	0.43
2:D:251:LEU:HD13	2:D:276:VAL:HG11	2.01	0.43
1:C:217:ILE:O	1:C:225:ILE:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LYS:NZ	1:C:406:TRP:HE1	2.17	0.43
1:C:460:THR:N	1:C:463:ASP:HB2	2.34	0.43
1:B:643:ARG:O	1:B:644:TRP:C	2.57	0.43
1:C:292:THR:HB	1:C:317:THR:HA	2.00	0.43
1:C:395:ARG:HB2	1:C:424:GLY:HA2	1.99	0.43
1:C:496:TYR:HA	1:C:544:ILE:HA	2.00	0.43
1:C:643:ARG:HD3	1:C:643:ARG:HA	1.74	0.43
1:A:214:LYS:HB2	2:E:86:PHE:CD1	2.53	0.43
1:A:572:PRO:HD2	2:E:313:THR:HG22	2.01	0.43
1:B:122:SER:OG	1:B:269:ARG:NH2	2.51	0.43
2:E:42:ASP:N	2:E:42:ASP:OD1	2.52	0.43
2:F:220:PRO:HA	2:F:235:THR:HA	2.01	0.43
1:C:292:THR:OG1	1:C:317:THR:HG22	2.18	0.43
1:B:52:GLN:CD	1:B:503:ASN:HD21	2.21	0.43
1:B:175:PHE:CE2	1:B:206:TYR:HB3	2.54	0.43
2:F:50:LEU:HD13	2:F:365:TRP:CE2	2.54	0.43
1:A:64:ASN:H	1:A:67:LEU:HD12	1.84	0.42
2:D:167:ILE:HD13	2:D:208:ASP:O	2.18	0.42
2:F:150:ASP:HA	2:F:174:MET:SD	2.59	0.42
2:F:203:ILE:HG12	2:F:210:VAL:HG22	2.01	0.42
1:C:103:GLN:O	1:C:151:LEU:HA	2.19	0.42
1:B:46:MET:C	1:B:48:ASP:H	2.23	0.42
1:B:117:GLY:N	1:B:460:THR:HG21	2.34	0.42
1:B:543:ASP:HA	1:B:552:LEU:O	2.20	0.42
1:B:681:THR:N	1:B:682:PRO:HD3	2.34	0.42
1:C:211:ARG:HD2	2:D:35:TRP:CE3	2.54	0.42
1:C:515:TRP:HE3	1:C:523:PHE:HB3	1.85	0.42
1:A:365:VAL:HG23	1:A:398:PHE:CE1	2.54	0.42
1:B:138:THR:O	1:B:141:VAL:HG12	2.20	0.42
1:B:367:VAL:HG22	1:B:398:PHE:HB2	2.01	0.42
1:C:66:ALA:O	1:C:68:SER:N	2.52	0.42
1:B:512:TRP:HE1	1:B:529:LYS:CB	2.32	0.42
2:E:95:MET:HA	2:E:103:TRP:O	2.19	0.42
1:C:431:ILE:HD11	1:C:455:ASN:OD1	2.19	0.42
1:C:539:ASN:N	1:C:539:ASN:OD1	2.53	0.42
1:A:371:LEU:HD12	1:A:394:GLY:HA3	2.00	0.42
1:A:604:TYR:CD2	1:A:634:VAL:HB	2.54	0.42
1:C:616:SER:HB2	2:D:336:GLN:HB3	2.02	0.42
1:A:431:ILE:HG13	1:A:454:ARG:O	2.20	0.42
1:B:243:HIS:CG	1:B:265:ILE:HD11	2.55	0.42
1:B:284:PHE:CE1	1:B:325:ARG:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:267:PHE:HE1	2:F:302:VAL:HG21	1.85	0.42
2:F:340:ILE:HB	2:F:355:TYR:CD1	2.55	0.42
1:C:558:PHE:HD1	1:C:589:ALA:HB2	1.85	0.42
1:A:449:LYS:HE3	1:A:449:LYS:HB2	1.86	0.42
2:D:105:VAL:HA	2:D:112:ILE:HG12	2.02	0.42
2:F:178:SER:HB2	2:F:195:SER:HB3	2.01	0.42
1:C:162:GLU:HA	1:C:187:GLY:HA3	2.01	0.42
1:C:211:ARG:CG	2:D:37:TYR:HD2	2.32	0.42
1:A:163:GLY:O	1:A:186:TYR:HA	2.19	0.42
2:F:167:ILE:HD13	2:F:208:ASP:O	2.20	0.42
1:C:422:MET:HB2	1:C:427:TRP:CE3	2.55	0.42
1:A:511:ASP:HB3	1:A:527:ASN:O	2.20	0.42
1:B:125:PRO:HD3	1:B:243:HIS:HD2	1.77	0.42
1:B:591:VAL:HG12	1:B:606:TRP:HE3	1.85	0.42
1:B:606:TRP:HD1	1:B:632:ASN:OD1	2.02	0.42
1:A:141:VAL:HG11	1:A:433:ALA:CB	2.50	0.41
1:A:428:ALA:HB2	1:A:458:PHE:CE1	2.55	0.41
1:A:79:VAL:HG12	1:A:95:ARG:HH12	1.85	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.89	0.41
1:A:628:PRO:HB2	1:A:630:PHE:HE1	1.84	0.41
2:D:204:ASP:OD1	2:D:206:GLU:HB2	2.20	0.41
2:D:344:TYR:CD1	2:D:350:LEU:HA	2.55	0.41
2:F:107:ASN:OD1	2:F:131:SER:OG	2.31	0.41
1:C:75:PHE:CB	1:C:605:LYS:HD2	2.50	0.41
1:A:67:LEU:O	1:A:71:ASP:HB2	2.20	0.41
1:C:358:LYS:HE2	1:C:406:TRP:HE1	1.86	0.41
1:C:358:LYS:CE	1:C:406:TRP:HE1	2.33	0.41
1:A:65:ILE:HG12	1:A:169:VAL:CG2	2.50	0.41
1:B:615:MET:HG2	2:F:337:GLN:HA	2.01	0.41
2:E:235:THR:O	2:E:249:PRO:HB2	2.20	0.41
1:A:207:LYS:HD3	1:A:233:ARG:HG3	2.02	0.41
1:A:485:GLY:HA3	1:A:503:ASN:HA	2.02	0.41
1:B:211:ARG:HD2	2:F:35:TRP:CD2	2.55	0.41
1:B:403:SER:CB	1:B:417:VAL:HG12	2.50	0.41
2:E:295:MET:HG2	2:E:296:PRO:O	2.21	0.41
2:E:331:ASP:OD1	2:E:331:ASP:O	2.38	0.41
1:C:46:MET:HG2	1:C:49:ILE:HD11	2.02	0.41
1:C:169:VAL:CG2	1:C:181:PHE:HB3	2.51	0.41
1:A:444:GLY:O	1:A:489:SER:N	2.42	0.41
2:D:278:LEU:HD13	2:D:285:LEU:HA	2.01	0.41
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:HG23	1:A:102:THR:HG21	2.03	0.41
1:A:209:ARG:O	1:A:211:ARG:HG3	2.21	0.41
1:A:475:LYS:HB2	1:A:475:LYS:HE3	1.95	0.41
1:B:310:VAL:C	1:B:311:LYS:HG2	2.41	0.41
2:E:279:ASN:HB3	2:E:320:VAL:HG11	2.02	0.41
1:A:114:PRO:HG3	1:A:370:HIS:ND1	2.35	0.41
1:A:293:PHE:O	1:A:315:ILE:HA	2.20	0.41
1:B:467:LEU:HD21	2:F:241:GLY:O	2.21	0.41
1:B:560:TRP:NE1	1:B:562:PRO:HG3	2.35	0.41
1:C:169:VAL:HG22	1:C:181:PHE:HD2	1.86	0.41
1:C:216:ASN:HA	1:C:226:GLY:O	2.21	0.41
1:C:277:ASP:OD1	2:D:110:HIS:ND1	2.53	0.41
1:C:372:VAL:HG11	1:C:461:LEU:HD13	2.03	0.41
1:C:543:ASP:HA	1:C:552:LEU:O	2.21	0.41
1:A:71:ASP:HA	1:A:74:THR:HG22	2.02	0.41
1:A:125:PRO:HG2	1:A:128:PHE:CG	2.56	0.41
1:B:417:VAL:CG2	1:B:433:ALA:HB3	2.51	0.41
1:B:454:ARG:HE	1:B:456:TYR:HE1	1.69	0.41
1:B:564:ILE:H	1:B:564:ILE:HG13	1.64	0.41
2:D:326:GLU:OE1	2:D:343:ARG:NE	2.44	0.41
2:E:340:ILE:HB	2:E:355:TYR:CD1	2.56	0.41
1:A:101:HIS:HB3	1:A:148:LEU:HB2	2.03	0.41
1:A:335:MET:SD	2:E:130:THR:HG23	2.61	0.41
1:B:101:HIS:HE1	1:B:512:TRP:CE3	2.38	0.41
1:B:373:GLU:HA	1:B:392:ASP:HB3	2.03	0.41
2:D:91:VAL:HB	2:D:107:ASN:HB3	2.03	0.41
2:E:315:TYR:CD1	2:E:329:VAL:HG11	2.56	0.41
2:F:138:LEU:HD21	2:F:144:TYR:CD2	2.56	0.41
1:A:467:LEU:HB3	1:A:468:PRO:HD3	2.03	0.40
2:E:55:GLU:HG2	2:E:92:ALA:O	2.20	0.40
2:E:150:ASP:HA	2:E:174:MET:SD	2.61	0.40
2:E:307:PHE:CD2	2:E:308:LEU:HD13	2.56	0.40
2:E:340:ILE:HG13	2:E:354:PHE:O	2.21	0.40
1:C:97:THR:CG2	1:C:101:HIS:HB2	2.51	0.40
1:C:478:HIS:HB3	1:C:510:ASP:HB2	2.03	0.40
1:C:548:LYS:HA	1:C:548:LYS:HD2	1.89	0.40
1:A:210:ASN:OD1	1:A:213:LYS:HB3	2.22	0.40
1:B:581:LEU:HD23	1:B:581:LEU:HA	1.95	0.40
2:E:105:VAL:HA	2:E:112:ILE:HG12	2.02	0.40
1:C:170:GLN:OE1	1:C:180:GLU:HG3	2.22	0.40
1:C:580:GLN:HB3	1:C:618:ASN:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HB2	1:A:413:ALA:HB2	2.03	0.40
1:B:164:PHE:HZ	1:B:184:LEU:HD22	1.86	0.40
1:B:449:LYS:HE3	1:B:449:LYS:HB2	1.85	0.40
2:F:331:ASP:OD1	2:F:340:ILE:HG22	2.22	0.40
1:A:605:LYS:HB2	1:A:633:ASN:OD1	2.22	0.40
1:B:135:LEU:HD12	1:B:151:LEU:HD23	2.03	0.40
1:B:174:SER:OG	1:B:673:ASN:HB2	2.22	0.40
1:B:254:GLU:O	1:B:256:ASP:N	2.54	0.40
1:B:509:ILE:HG22	1:B:510:ASP:O	2.21	0.40
2:D:50:LEU:HD13	2:D:365:TRP:CD2	2.56	0.40
1:C:467:LEU:HD23	2:D:239:TYR:HE2	1.87	0.40
1:C:650:LYS:HG3	1:C:677:PHE:HB2	2.04	0.40
1:A:399:SER:HB2	1:A:419:ARG:HH21	1.86	0.40
1:B:650:LYS:HG3	1:B:677:PHE:HB2	2.04	0.40
2:D:57:ASN:O	2:D:60:TYR:HB2	2.22	0.40
2:F:98:ARG:HD3	2:F:137:PHE:CG	2.56	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	620/698 (89%)	575 (93%)	43 (7%)	2 (0%)	41 74
1	B	619/698 (89%)	575 (93%)	41 (7%)	3 (0%)	29 65
1	C	627/698 (90%)	584 (93%)	41 (6%)	2 (0%)	41 74
2	D	333/366 (91%)	313 (94%)	18 (5%)	2 (1%)	25 61
2	E	333/366 (91%)	314 (94%)	17 (5%)	2 (1%)	25 61
2	F	333/366 (91%)	314 (94%)	17 (5%)	2 (1%)	25 61
All	All	2865/3192 (90%)	2675 (93%)	177 (6%)	13 (0%)	29 65

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	68	SER
1	A	68	SER
1	A	306	TRP
1	B	68	SER
1	B	644	TRP
1	C	304	GLU
2	D	333	ILE
2	E	333	ILE
2	F	333	ILE
1	B	67	LEU
2	D	356	VAL
2	E	356	VAL
2	F	356	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	545/607 (90%)	532 (98%)	13 (2%)	49 <span style="background-color: #e0e0ff;">70</span>
1	B	543/607 (90%)	531 (98%)	12 (2%)	52 <span style="background-color: #e0e0ff;">72</span>
1	C	549/607 (90%)	534 (97%)	15 (3%)	44 <span style="background-color: #e0e0ff;">68</span>
2	D	297/327 (91%)	294 (99%)	3 (1%)	<span style="background-color: #e0e0ff;">76</span> <span style="background-color: #e0e0ff;">86</span>
2	E	297/327 (91%)	295 (99%)	2 (1%)	<span style="background-color: #e0e0ff;">84</span> <span style="background-color: #e0e0ff;">91</span>
2	F	297/327 (91%)	295 (99%)	2 (1%)	<span style="background-color: #e0e0ff;">84</span> <span style="background-color: #e0e0ff;">91</span>
All	All	2528/2802 (90%)	2481 (98%)	47 (2%)	<span style="background-color: #e0e0ff;">57</span> <span style="background-color: #e0e0ff;">76</span>

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	57	ASP
1	C	131	ASP
1	C	135	LEU
1	C	209	ARG

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Mol	Chain	Res	Type
1	C	212	ASP
1	C	223	ASN
1	C	283	ASP
1	C	323	TYR
1	C	376	ASP
1	C	422	MET
1	C	527	ASN
1	C	534	TYR
1	C	607	CYS
1	C	636	LEU
1	C	665	LEU
1	A	135	LEU
1	A	194	SER
1	A	207	LYS
1	A	209	ARG
1	A	212	ASP
1	A	283	ASP
1	A	323	TYR
1	A	441	SER
1	A	454	ARG
1	A	503	ASN
1	A	512	TRP
1	A	543	ASP
1	A	636	LEU
1	B	209	ARG
1	B	216	ASN
1	B	283	ASP
1	B	323	TYR
1	B	376	ASP
1	B	422	MET
1	B	505	PHE
1	B	512	TRP
1	B	546	LEU
1	B	618	ASN
1	B	636	LEU
1	B	665	LEU
2	D	33	MET
2	D	43	PHE
2	D	259	PHE
2	E	43	PHE
2	E	259	PHE
2	F	259	PHE

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Mol	Chain	Res	Type
2	F	305	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	243	HIS
1	C	508	HIS
1	C	618	ASN
1	A	508	HIS
1	B	101	HIS
1	B	503	ASN
2	F	54	ASN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

### 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	628/698 (89%)	0.25	27 (4%) 35 29	77, 113, 166, 271	0
1	B	627/698 (89%)	0.31	37 (5%) 22 17	98, 141, 187, 248	0
1	C	633/698 (90%)	0.28	27 (4%) 35 29	72, 108, 158, 251	0
2	D	335/366 (91%)	0.38	14 (4%) 36 30	81, 109, 153, 214	0
2	E	335/366 (91%)	0.44	19 (5%) 23 19	88, 114, 153, 191	0
2	F	335/366 (91%)	0.56	33 (9%) 7 6	91, 135, 180, 260	0
All	All	2893/3192 (90%)	0.34	157 (5%) 25 22	72, 119, 173, 271	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	190	TYR	5.0
2	F	255	ASP	4.9
1	C	138	THR	4.9
2	F	278	LEU	4.8
1	B	131	ASP	4.7
1	C	95	ARG	4.6
1	B	52	GLN	4.5
1	B	95	ARG	4.3
1	C	150	GLY	4.3
1	C	352	ASP	4.2
1	C	133	SER	4.2
1	B	49	ILE	4.0
1	A	153	ARG	3.9
1	C	646	ASP	3.9
1	B	130	ASP	3.7
1	B	207	LYS	3.7
1	B	537	GLU	3.7
2	F	183	VAL	3.6
1	C	147	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	136	HIS	3.6
1	B	210	ASN	3.6
1	B	153	ARG	3.6
2	F	229	ASN	3.6
1	B	71	ASP	3.6
2	F	257	GLU	3.6
2	F	254	ILE	3.5
2	E	297	VAL	3.4
2	E	267	PHE	3.3
1	B	132	ALA	3.3
1	A	95	ARG	3.2
2	F	297	VAL	3.2
2	F	232	TRP	3.2
2	D	285	LEU	3.2
1	C	132	ALA	3.2
1	B	135	LEU	3.2
2	F	233	THR	3.1
2	D	297	VAL	3.1
1	C	455	ASN	3.1
1	B	50	GLY	3.1
1	C	52	GLN	3.1
2	F	223	LEU	3.1
2	D	183	VAL	3.1
1	B	133	SER	3.1
1	A	150	GLY	3.0
1	C	142	ASN	3.0
1	B	107	ASN	3.0
1	C	131	ASP	3.0
2	D	262	GLU	3.0
2	F	228	TYR	2.9
1	B	410	ASP	2.9
2	F	185	TYR	2.9
2	D	227	LYS	2.9
2	F	184	GLN	2.9
1	B	53	ARG	2.9
2	F	267	PHE	2.8
2	F	299	ALA	2.8
2	E	225	MET	2.8
2	E	233	THR	2.8
1	C	537	GLU	2.8
1	A	52	GLN	2.8
2	E	185	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	435	PHE	2.7
1	C	637	GLU	2.7
2	D	184	GLN	2.7
1	A	143	GLU	2.7
2	E	229	ASN	2.7
1	C	53	ARG	2.7
1	C	311	LYS	2.7
2	F	263	LYS	2.7
1	B	51	VAL	2.7
2	F	216	ILE	2.6
2	E	183	VAL	2.6
2	D	282	ARG	2.6
1	A	130	ASP	2.6
2	E	122	GLU	2.6
1	A	421	ASP	2.6
1	B	440	LEU	2.6
1	A	47	LYS	2.5
1	A	135	LEU	2.5
1	A	136	HIS	2.5
2	E	227	LYS	2.5
1	C	151	LEU	2.5
1	A	405	LYS	2.5
2	E	286	TYR	2.5
2	D	103	TRP	2.5
2	F	277	GLN	2.5
2	F	231	MET	2.5
1	A	449	LYS	2.5
1	B	483	ASP	2.5
1	B	151	LEU	2.5
2	F	210	VAL	2.5
1	A	660	GLU	2.5
1	A	675	GLU	2.4
1	A	414	ALA	2.4
1	C	601	SER	2.4
2	D	223	LEU	2.4
2	F	285	LEU	2.4
1	A	410	ASP	2.4
2	F	121	LYS	2.4
2	E	265	PHE	2.4
2	D	309	GLU	2.4
1	B	129	ILE	2.4
1	B	72	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	61	MET	2.4
2	D	283	ASP	2.4
2	F	194	TRP	2.4
1	C	47	LYS	2.3
1	C	313	GLY	2.3
2	D	265	PHE	2.3
2	E	228	TYR	2.3
1	A	152	VAL	2.3
2	F	230	LYS	2.3
1	C	483	ASP	2.3
2	F	251	LEU	2.3
2	F	188	TYR	2.3
1	B	536	ALA	2.3
1	A	477	GLU	2.3
2	F	226	ASP	2.3
1	A	594	ARG	2.2
1	B	143	GLU	2.2
1	A	420	GLU	2.2
1	A	142	ASN	2.2
1	A	102	THR	2.2
1	B	54	THR	2.2
2	F	282	ARG	2.2
2	D	252	TYR	2.2
2	E	285	LEU	2.2
1	A	455	ASN	2.2
1	C	647	LEU	2.2
2	E	223	LEU	2.2
1	A	133	SER	2.2
1	A	400	GLY	2.2
1	B	128	PHE	2.2
2	F	279	ASN	2.2
2	E	249	PRO	2.1
1	C	50	GLY	2.1
1	B	106	TRP	2.1
1	C	56	PHE	2.1
1	B	221	ASP	2.1
1	C	643	ARG	2.1
1	B	520	LYS	2.1
2	F	209	LYS	2.1
2	E	144	TYR	2.1
2	F	298	GLU	2.1
1	B	125	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	190	TYR	2.1
1	B	208	TYR	2.1
2	D	261	VAL	2.1
2	E	59	GLN	2.0
1	C	305	LYS	2.0
1	B	138	THR	2.0
2	E	300	ASP	2.0
1	B	229	TYR	2.0
1	B	305	LYS	2.0
1	A	214	LYS	2.0
2	F	182	MET	2.0
1	B	152	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.