



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:49 am BST

PDB ID : 1WAF  
Title : DNA POLYMERASE FROM BACTERIOPHAGE RB69  
Authors : Wang, J.; Satter, A.K.M.A.; Wang, C.C.; Karam, J.D.; Konigsberg, W.H.;  
Steitz, T.A.  
Deposited on : 1997-04-13  
Resolution : 3.20 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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

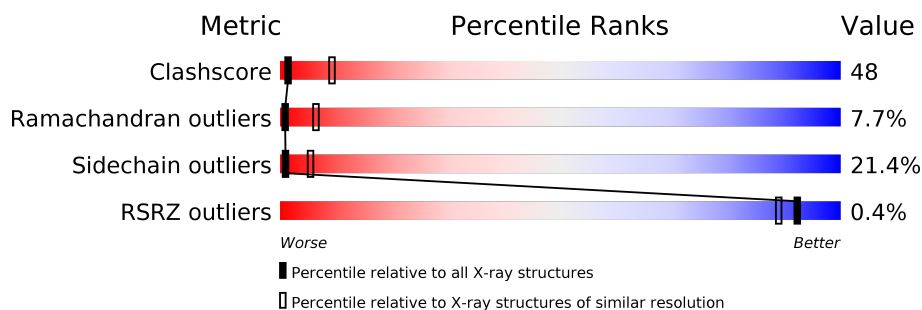
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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.

Mol	Chain	Length	Quality of chain
1	A	903	<div> <div></div> <div> <div></div> <div>29%</div> <div>51%</div> <div>17%</div> <div></div> </div> </div>
1	B	903	<div> <div></div> <div> <div></div> <div>30%</div> <div>52%</div> <div>16%</div> <div></div> </div> </div>

## 2 Entry composition [i](#)

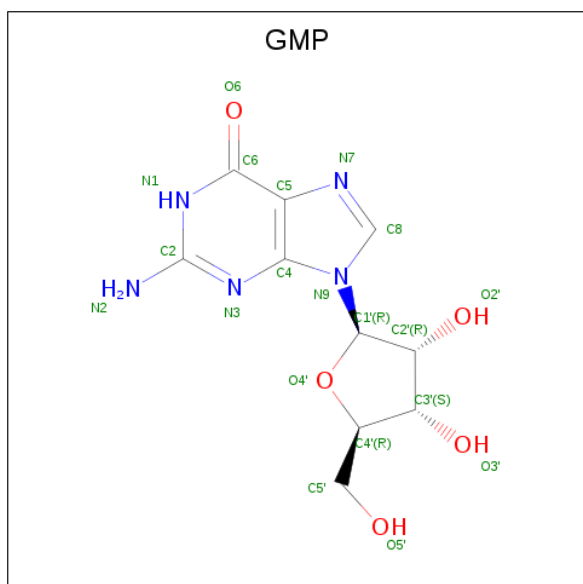
There are 2 unique types of molecules in this entry. The entry contains 14800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7380	4739	1226	1382	33			
1	B	903	Total	C	N	O	S	0	0	0
			7380	4739	1226	1382	33			

- Molecule 2 is GUANOSINE (three-letter code: GMP) (formula:  $C_{10}H_{13}N_5O_5$ ).

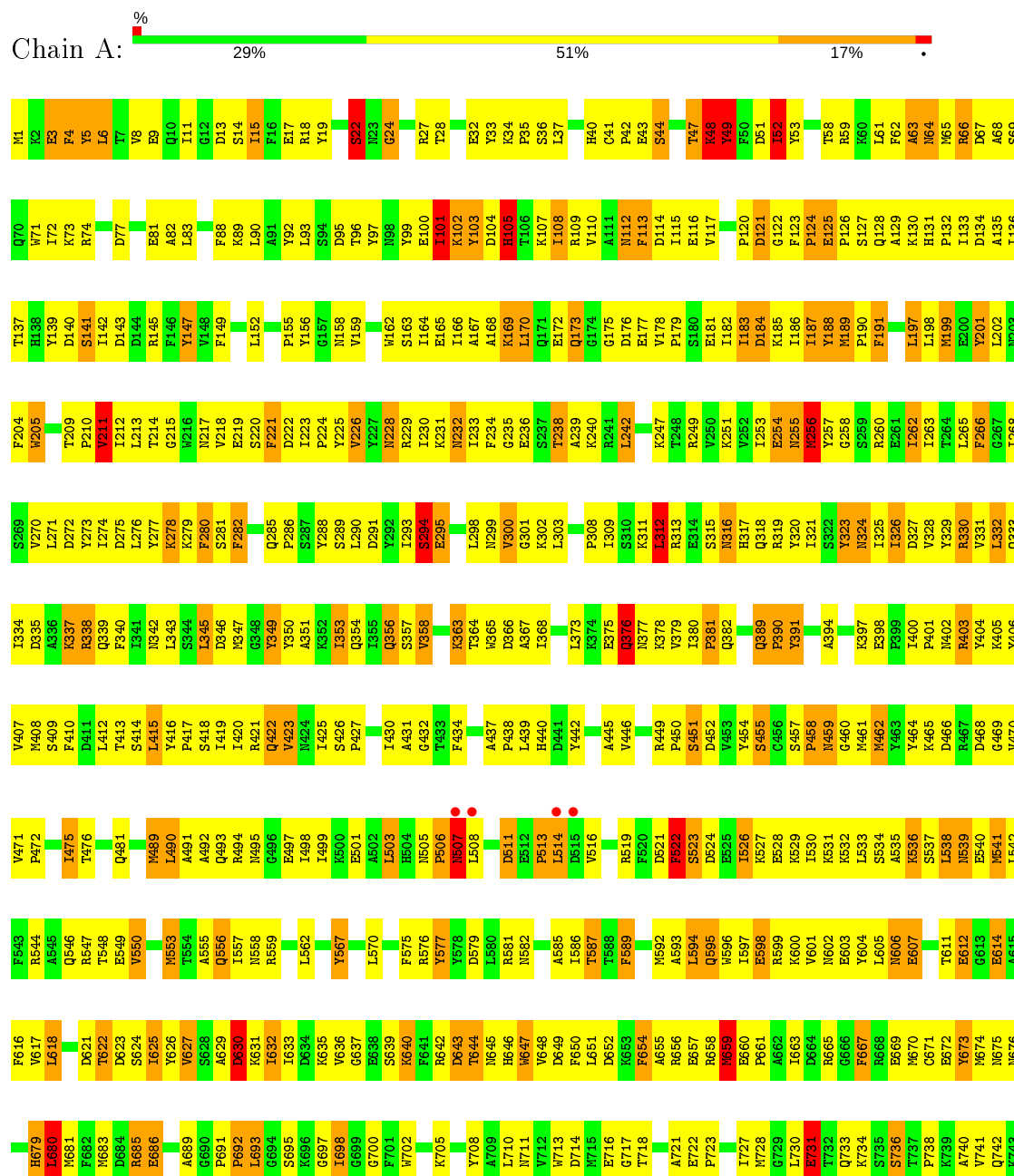


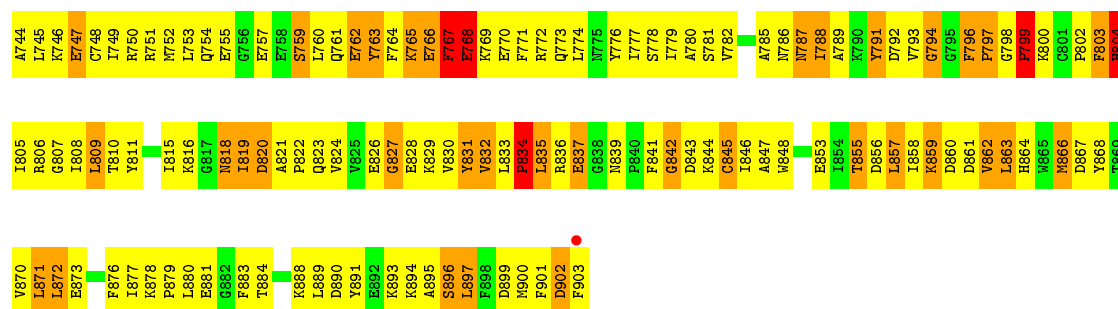
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	10	5	5		
2	B	1	Total	C	N	O	0	0
			20	10	5	5		

### 3 Residue-property plots

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

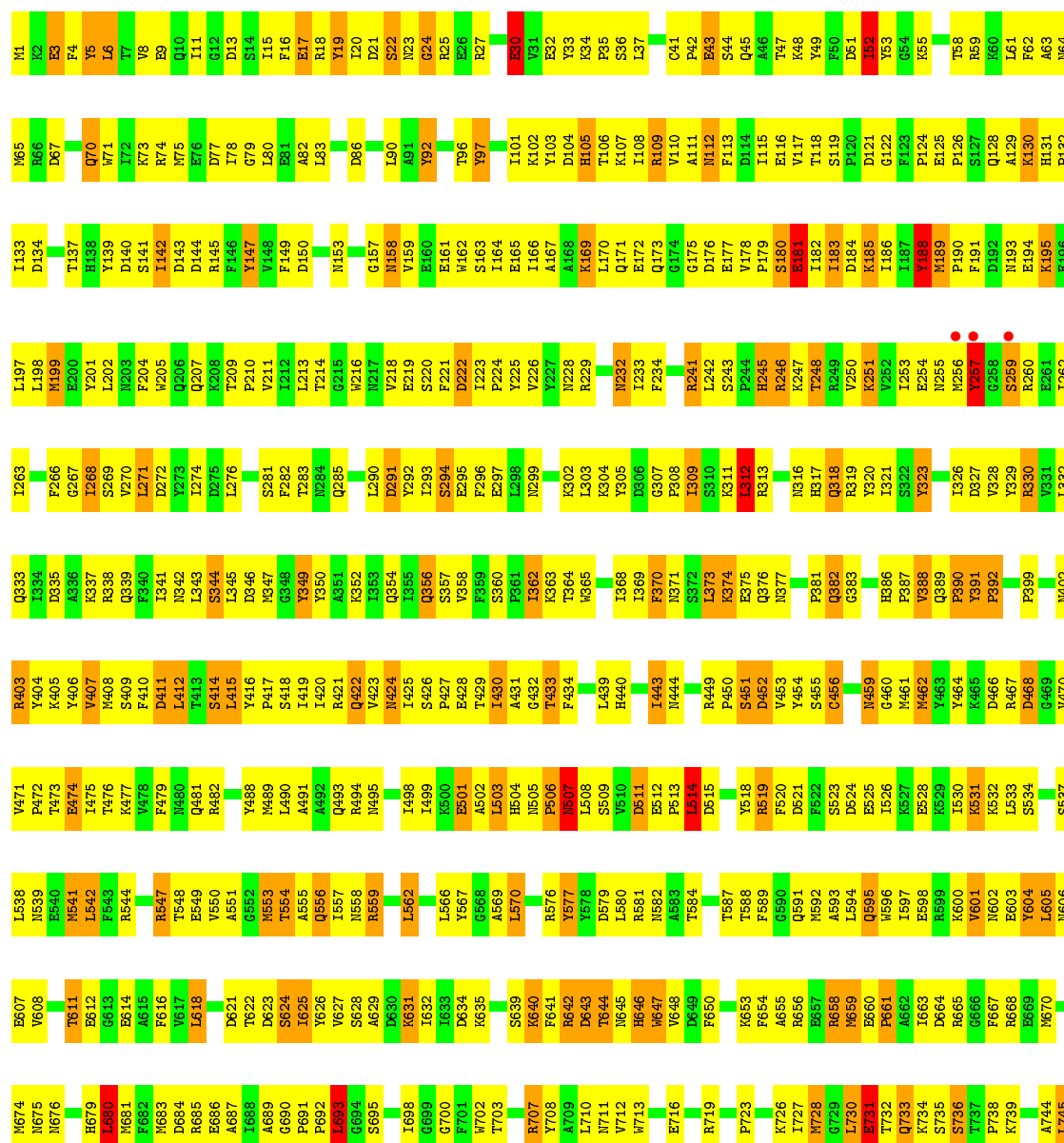
#### • Molecule 1: DNA POLYMERASE

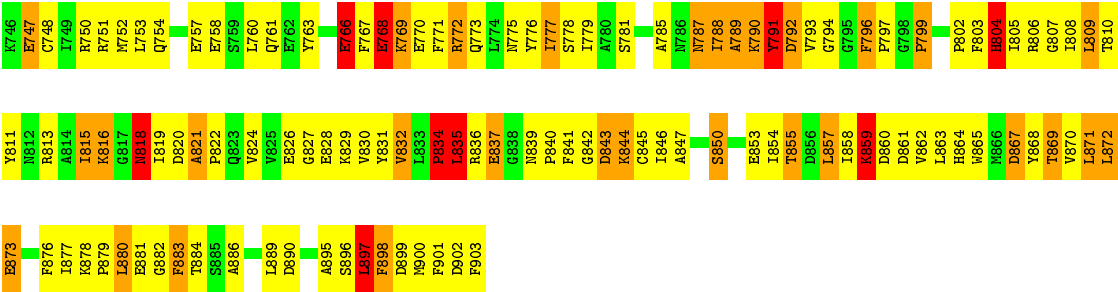




## • Molecule 1: DNA POLYMERASE

Chain B: 30% 52% 16%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.32Å 196.86Å 118.31Å 90.00° 92.57° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 29.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 82.3 (29.88-3.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.84 (at 3.18Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.198 , 0.274 0.221 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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](#)

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

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	0.90	2/7561 (0.0%)	1.01	24/10217 (0.2%)
1	B	0.88	1/7561 (0.0%)	0.99	13/10217 (0.1%)
All	All	0.89	3/15122 (0.0%)	1.00	37/20434 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	6
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	759	SER	CB-OG	-6.99	1.33	1.42
1	A	294	SER	CB-OG	-5.47	1.35	1.42
1	B	826	GLU	CG-CD	5.10	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	MET	N-CA-C	7.68	131.73	111.00
1	A	48	LYS	N-CA-C	-7.58	90.54	111.00
1	A	767	PHE	N-CA-C	-7.07	91.92	111.00
1	A	490	LEU	CA-CB-CG	-6.80	99.66	115.30
1	A	258	GLY	N-CA-C	-6.71	96.32	113.10
1	B	768	GLU	N-CA-C	-6.49	93.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	GLY	N-CA-C	6.31	128.87	113.10
1	B	745	LEU	CA-CB-CG	-6.28	100.87	115.30
1	A	24	GLY	N-CA-C	6.27	128.78	113.10
1	B	680	LEU	N-CA-C	6.26	127.90	111.00
1	A	831	TYR	N-CA-C	6.21	127.76	111.00
1	B	788	ILE	N-CA-C	-6.19	94.29	111.00
1	A	794	GLY	N-CA-C	-5.99	98.12	113.10
1	A	101	ILE	N-CA-C	5.97	127.12	111.00
1	B	30	GLU	N-CA-C	-5.89	95.11	111.00
1	A	680	LEU	N-CA-C	5.86	126.82	111.00
1	A	768	GLU	N-CA-C	-5.85	95.21	111.00
1	A	276	LEU	CA-CB-CG	5.83	128.70	115.30
1	B	490	LEU	CA-CB-CG	-5.73	102.12	115.30
1	A	221	PHE	N-CA-C	5.70	126.39	111.00
1	A	522	PHE	N-CA-C	5.62	126.17	111.00
1	A	785	ALA	N-CA-C	-5.57	95.97	111.00
1	B	570	LEU	CA-CB-CG	-5.49	102.68	115.30
1	B	625	ILE	CB-CA-C	-5.31	100.98	111.60
1	A	755	GLU	N-CA-C	5.23	125.13	111.00
1	B	407	VAL	CB-CA-C	-5.22	101.47	111.40
1	A	507	ASN	N-CA-C	5.22	125.10	111.00
1	A	679	HIS	N-CA-C	5.22	125.09	111.00
1	B	533	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	842	GLY	N-CA-C	-5.15	100.24	113.10
1	A	3	GLU	N-CA-C	5.12	124.83	111.00
1	B	3	GLU	N-CA-C	5.11	124.79	111.00
1	A	842	GLY	N-CA-C	-5.10	100.35	113.10
1	A	612	GLU	N-CA-C	5.07	124.69	111.00
1	A	211	VAL	N-CA-C	-5.04	97.40	111.00
1	B	514	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	835	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	TYR	Sidechain
1	A	349	TYR	Sidechain
1	A	350	TYR	Sidechain
1	A	567	TYR	Sidechain
1	B	188	TYR	Sidechain
1	B	323	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	349	TYR	Sidechain
1	B	350	TYR	Sidechain
1	B	464	TYR	Sidechain
1	B	577	TYR	Sidechain

## 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	7380	0	7265	722	0
1	B	7380	0	7265	674	0
2	A	20	0	13	2	0
2	B	20	0	13	2	0
All	All	14800	0	14556	1396	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 48.

All (1396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ILE:CG2	1:B:260:ARG:HB2	1.63	1.26
1:B:246:ARG:HG2	1:B:246:ARG:HH11	1.06	1.13
1:B:253:ILE:HG22	1:B:260:ARG:HB2	1.20	1.12
1:B:253:ILE:HG12	1:B:254:GLU:H	1.18	1.09
1:A:796:PHE:HB3	1:A:797:PRO:HD2	1.33	1.08
1:B:246:ARG:HH11	1:B:246:ARG:CG	1.71	1.04
1:B:489:MET:SD	1:B:553:MET:HB2	1.97	1.03
1:B:34:LYS:HD2	1:B:63:ALA:HA	1.44	0.99
1:B:149:PHE:HB3	1:B:197:LEU:HD11	1.42	0.98
1:B:223:ILE:HB	1:B:224:PRO:HD3	1.45	0.97
1:A:857:LEU:HD23	1:A:857:LEU:H	1.27	0.97
1:B:514:LEU:HD21	1:B:530:ILE:HD11	1.47	0.96
1:A:162:TRP:HB3	1:A:188:TYR:HE2	1.29	0.93
1:B:41:CYS:HB2	1:B:45:GLN:HG3	1.48	0.93
1:A:103:TYR:HE2	1:A:346:ASP:HA	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:GLN:H	1:B:356:GLN:HE21	1.14	0.92
1:B:171:GLN:HG2	1:B:177:GLU:HG3	1.51	0.92
1:A:605:LEU:HB3	1:A:616:PHE:CE2	2.06	0.91
1:A:508:LEU:HD22	1:A:532:LYS:HA	1.54	0.90
1:A:164:ILE:HD12	1:A:164:ILE:H	1.37	0.89
1:B:246:ARG:HG2	1:B:246:ARG:NH1	1.87	0.88
1:B:644:THR:HB	1:B:692:PRO:O	1.73	0.88
1:A:642:ARG:O	1:A:643:ASP:HB2	1.74	0.87
1:A:832:VAL:H	1:A:847:ALA:HA	1.39	0.87
1:A:303:LEU:HD23	1:A:323:TYR:HB2	1.56	0.87
1:A:661:PRO:O	1:A:665:ARG:HG3	1.74	0.87
1:B:164:ILE:HD12	1:B:164:ILE:H	1.39	0.87
1:B:253:ILE:HG22	1:B:260:ARG:CB	2.04	0.87
1:A:27:ARG:HG3	1:A:28:THR:H	1.39	0.86
1:A:752:MET:HG2	1:A:760:LEU:HD12	1.57	0.86
1:B:272:ASP:OD1	1:B:274:ILE:HG22	1.76	0.85
1:B:182:ILE:HA	1:B:185:LYS:HG3	1.55	0.85
1:A:788:ILE:HB	1:A:791:TYR:HD2	1.40	0.85
1:A:52:ILE:HD13	1:A:52:ILE:H	1.39	0.84
1:B:11:ILE:HD13	1:B:247:LYS:HG3	1.59	0.84
1:B:330:ARG:HA	1:B:333:GLN:NE2	1.91	0.84
1:A:162:TRP:HB3	1:A:188:TYR:CE2	2.12	0.84
1:B:547:ARG:NH1	1:B:547:ARG:HB3	1.93	0.84
1:B:855:THR:HB	1:B:857:LEU:CD2	2.08	0.83
1:B:356:GLN:N	1:B:356:GLN:HE21	1.76	0.83
1:A:163:SER:HB3	1:A:166:ILE:HD12	1.61	0.83
1:A:640:LYS:N	1:A:640:LYS:HD3	1.92	0.83
1:B:854:ILE:HG22	1:B:859:LYS:HB2	1.61	0.82
1:B:256:MET:SD	1:B:788:ILE:HG12	2.20	0.82
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.61	0.82
1:A:656:ARG:HH11	1:A:656:ARG:HB3	1.44	0.82
1:A:356:GLN:NE2	1:A:356:GLN:H	1.78	0.82
1:B:167:ALA:HA	1:B:176:ASP:HB2	1.62	0.81
1:B:291:ASP:HB3	1:B:302:LYS:HB2	1.61	0.81
1:B:253:ILE:HG21	1:B:260:ARG:HB2	1.58	0.81
1:A:713:TRP:CH2	1:A:723:PRO:HG3	2.15	0.81
1:A:356:GLN:HE21	1:A:356:GLN:H	1.26	0.81
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.63	0.81
1:A:117:VAL:HG13	1:A:132:PRO:O	1.81	0.80
1:B:303:LEU:HD23	1:B:323:TYR:HA	1.63	0.80
1:B:482:ARG:HG3	1:B:556:GLN:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD11	1:A:363:LYS:HE3	1.63	0.80
1:A:576:ARG:HD2	1:A:577:TYR:CE1	2.17	0.80
1:A:577:TYR:H	1:A:577:TYR:HD1	1.30	0.80
1:B:233:ILE:HG13	1:B:234:PHE:HD1	1.48	0.79
1:A:605:LEU:HB3	1:A:616:PHE:CD2	2.17	0.79
1:B:253:ILE:HG12	1:B:254:GLU:N	1.96	0.79
1:B:642:ARG:O	1:B:643:ASP:HB3	1.80	0.79
1:A:593:ALA:HA	1:A:670:MET:HE3	1.63	0.79
1:B:149:PHE:HB3	1:B:197:LEU:CD1	2.12	0.79
1:B:233:ILE:HG13	1:B:234:PHE:CD1	2.17	0.79
1:B:880:LEU:HA	1:B:883:PHE:CE2	2.17	0.79
1:B:356:GLN:H	1:B:356:GLN:NE2	1.80	0.79
1:A:101:ILE:HG21	1:A:349:TYR:HB3	1.65	0.78
1:B:581:ARG:HH11	1:B:581:ARG:HG3	1.48	0.78
1:A:339:GLN:NE2	1:A:342:ASN:HB2	1.98	0.78
1:B:219:GLU:HA	1:B:223:ILE:HD12	1.64	0.78
1:B:434:PHE:CZ	1:B:460:GLY:HA2	2.18	0.78
1:B:195:LYS:H	1:B:195:LYS:HD2	1.48	0.78
1:A:320:TYR:HD1	1:A:321:ILE:HD12	1.49	0.78
1:B:3:GLU:HB3	1:B:21:ASP:HA	1.63	0.78
1:A:233:ILE:HG13	1:A:234:PHE:HD1	1.49	0.77
1:A:421:ARG:HD2	1:A:475:ILE:HG22	1.66	0.77
1:B:112:ASN:HD22	1:B:113:PHE:N	1.82	0.77
1:A:763:TYR:O	1:A:766:GLU:HB2	1.85	0.77
1:B:4:PHE:HA	1:B:97:TYR:HE2	1.47	0.77
1:A:421:ARG:HD2	1:A:475:ILE:CG2	2.14	0.77
1:B:253:ILE:CG1	1:B:254:GLU:H	1.95	0.77
1:B:481:GLN:HE21	1:B:559:ARG:NH1	1.83	0.77
1:B:414:SER:O	1:B:417:PRO:HD2	1.85	0.77
1:A:830:VAL:HG12	1:A:831:TYR:H	1.48	0.76
1:B:593:ALA:HA	1:B:670:MET:HE1	1.67	0.76
1:A:214:THR:HG22	1:A:215:GLY:H	1.48	0.76
1:A:9:GLU:HG2	1:A:266:PHE:HD1	1.48	0.76
1:B:295:GLU:O	1:B:299:ASN:HA	1.86	0.76
1:B:511:ASP:HB2	1:B:534:SER:OG	1.86	0.76
1:A:763:TYR:HD1	1:A:763:TYR:O	1.67	0.76
1:B:748:CYS:O	1:B:752:MET:HG3	1.86	0.76
1:B:832:VAL:HG22	1:B:847:ALA:HB2	1.67	0.76
1:A:818:ASN:HA	1:A:822:PRO:HG3	1.68	0.76
1:B:423:VAL:HB	1:B:425:ILE:HG13	1.67	0.76
1:B:645:ASN:HD21	1:B:719:ARG:HH11	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLN:O	1:A:550:VAL:HG23	1.86	0.75
1:A:788:ILE:HB	1:A:791:TYR:CD2	2.21	0.75
1:A:163:SER:OG	1:A:165:GLU:HG2	1.86	0.74
1:A:647:TRP:O	1:A:650:PHE:HB3	1.87	0.74
1:A:899:ASP:C	1:A:900:MET:SD	2.65	0.74
1:B:250:VAL:HG12	1:B:251:LYS:H	1.53	0.74
1:B:880:LEU:HA	1:B:883:PHE:CD2	2.22	0.74
1:B:661:PRO:O	1:B:665:ARG:HG3	1.87	0.74
1:A:315:SER:O	1:A:316:ASN:HB2	1.87	0.74
1:A:577:TYR:N	1:A:577:TYR:CD1	2.54	0.74
1:B:404:TYR:CZ	1:B:618:LEU:HD21	2.22	0.74
1:A:291:ASP:HB3	1:A:302:LYS:HB2	1.68	0.74
1:B:647:TRP:O	1:B:650:PHE:HB3	1.88	0.73
1:B:832:VAL:HA	1:B:846:ILE:O	1.87	0.73
1:A:188:TYR:HD1	1:A:189:MET:N	1.87	0.73
1:A:131:HIS:HB3	1:A:132:PRO:HD2	1.69	0.73
1:B:806:ARG:HH21	1:B:843:ASP:HA	1.53	0.73
1:A:748:CYS:O	1:A:752:MET:HG3	1.89	0.73
1:A:214:THR:HG22	1:A:215:GLY:N	2.03	0.73
1:A:356:GLN:N	1:A:356:GLN:HE21	1.87	0.73
1:B:514:LEU:HD21	1:B:530:ILE:CD1	2.19	0.73
1:A:247:LYS:O	1:A:266:PHE:HB2	1.88	0.72
1:A:159:VAL:HG21	1:A:317:HIS:CD2	2.24	0.72
1:A:523:SER:HB3	1:A:526:ILE:HG12	1.72	0.72
1:B:18:ARG:NH2	1:B:211:VAL:HA	2.04	0.72
1:A:796:PHE:HB3	1:A:797:PRO:CD	2.16	0.72
1:A:123:PHE:CE2	1:A:828:GLU:HB3	2.24	0.72
1:B:147:TYR:N	1:B:147:TYR:HD1	1.88	0.72
1:B:281:SER:O	1:B:282:PHE:HB2	1.90	0.72
1:B:504:HIS:O	1:B:506:PRO:HD3	1.90	0.71
1:B:514:LEU:HD12	1:B:541:MET:SD	2.29	0.71
1:A:740:ALA:HB2	1:A:778:SER:HB2	1.72	0.71
1:B:831:TYR:CE2	1:B:850:SER:HA	2.25	0.71
1:A:834:PRO:HB3	1:A:867:ASP:HB3	1.71	0.71
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.72	0.71
1:B:606:ASN:HB2	1:B:611:THR:O	1.89	0.71
1:B:855:THR:HB	1:B:857:LEU:HD21	1.71	0.71
1:A:773:GLN:HA	1:B:78:ILE:HD11	1.73	0.71
1:A:233:ILE:HG13	1:A:234:PHE:CD1	2.26	0.71
1:A:680:LEU:HD23	1:A:680:LEU:H	1.55	0.71
1:B:246:ARG:CG	1:B:246:ARG:NH1	2.41	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLN:HE21	1:B:339:GLN:HA	1.56	0.71
1:B:834:PRO:O	1:B:835:LEU:HD23	1.91	0.71
1:A:291:ASP:CB	1:A:302:LYS:HB2	2.21	0.70
1:B:169:LYS:HB2	1:B:175:GLY:HA3	1.71	0.70
1:A:897:LEU:H	1:A:897:LEU:HD12	1.55	0.70
1:B:526:ILE:O	1:B:530:ILE:HG12	1.90	0.70
1:B:544:ARG:O	1:B:548:THR:HG23	1.90	0.70
1:A:873:GLU:HA	1:A:877:ILE:HD12	1.73	0.70
1:A:280:PHE:N	1:A:280:PHE:CD1	2.58	0.70
1:B:222:ASP:O	1:B:226:VAL:HG23	1.92	0.70
1:A:547:ARG:HA	1:A:550:VAL:HG23	1.74	0.69
1:A:643:ASP:HB3	1:A:646:HIS:H	1.57	0.69
1:A:47:THR:HB	1:A:48:LYS:O	1.92	0.69
1:A:806:ARG:O	1:A:810:THR:HG22	1.92	0.69
1:A:173:GLN:H	1:A:173:GLN:HE21	1.37	0.69
1:A:162:TRP:HE3	1:A:188:TYR:CD2	2.09	0.69
1:B:213:LEU:HB2	1:B:268:ILE:HD11	1.75	0.69
1:A:414:SER:HB2	1:A:417:PRO:HG3	1.73	0.69
1:B:188:TYR:HE1	1:B:190:PRO:HB3	1.58	0.69
1:B:707:ARG:HB2	1:B:707:ARG:HH11	1.58	0.69
1:B:4:PHE:HA	1:B:97:TYR:CE2	2.27	0.69
1:A:878:LYS:O	1:A:881:GLU:HB3	1.91	0.69
1:B:788:ILE:HG22	1:B:791:TYR:CD2	2.27	0.69
1:A:162:TRP:CE3	1:A:188:TYR:CD2	2.81	0.69
1:A:727:ILE:HG22	1:A:733:GLN:HE22	1.58	0.69
1:B:597:ILE:HB	1:B:667:PHE:CE1	2.28	0.69
1:A:232:ASN:N	1:A:232:ASN:HD22	1.91	0.69
1:A:593:ALA:HA	1:A:670:MET:CE	2.23	0.69
1:B:223:ILE:HB	1:B:224:PRO:CD	2.20	0.69
1:B:449:ARG:NH1	1:B:451:SER:O	2.25	0.68
1:A:145:ARG:HH21	1:A:185:LYS:HD2	1.57	0.68
1:A:381:PRO:HD2	1:A:576:ARG:HD3	1.75	0.68
1:A:167:ALA:HA	1:A:176:ASP:HB2	1.75	0.68
1:A:644:THR:HB	1:A:692:PRO:O	1.93	0.68
1:A:728:MET:HA	1:A:728:MET:HE2	1.76	0.68
1:B:303:LEU:HD23	1:B:323:TYR:CA	2.23	0.68
1:B:767:PHE:HA	1:B:770:GLU:HG2	1.76	0.68
1:B:873:GLU:HA	1:B:877:ILE:HD13	1.75	0.68
1:A:776:TYR:O	1:A:779:ILE:HG12	1.92	0.68
1:A:821:ALA:N	1:A:822:PRO:HD2	2.09	0.68
1:B:877:ILE:HD12	1:B:877:ILE:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TYR:CD1	1:B:147:TYR:N	2.58	0.68
1:B:53:TYR:HE1	1:B:428:GLU:HA	1.59	0.68
1:B:538:LEU:O	1:B:539:ASN:HB2	1.91	0.68
1:A:109:ARG:HA	1:A:142:ILE:HG12	1.76	0.68
1:A:162:TRP:CE3	1:A:188:TYR:HD2	2.12	0.68
1:A:403:ARG:HH11	1:A:888:LYS:HB2	1.58	0.68
1:B:460:GLY:O	1:B:461:MET:HG2	1.94	0.68
1:B:750:ARG:HG2	1:B:754:GLN:OE1	1.94	0.68
1:B:897:LEU:H	1:B:897:LEU:HD12	1.59	0.68
1:B:162:TRP:HB3	1:B:188:TYR:HE2	1.60	0.67
1:A:105:HIS:HA	1:A:108:ILE:HG13	1.76	0.67
1:A:120:PRO:HD3	1:A:156:TYR:HE2	1.59	0.67
1:A:163:SER:HG	1:A:165:GLU:HG2	1.57	0.67
1:A:270:VAL:O	1:A:271:LEU:HD23	1.94	0.67
1:B:389:GLN:NE2	1:B:390:PRO:HD2	2.09	0.67
1:A:163:SER:OG	1:A:166:ILE:HG13	1.94	0.67
1:B:481:GLN:HE21	1:B:559:ARG:HH11	1.41	0.67
1:B:97:TYR:HB3	1:B:101:ILE:HD11	1.77	0.67
1:B:52:ILE:H	1:B:52:ILE:HD13	1.59	0.67
1:A:353:ILE:HG12	1:A:354:GLN:N	2.07	0.67
1:A:655:ALA:HA	1:A:659:MET:HB2	1.75	0.67
1:B:632:ILE:O	1:B:635:LYS:HB3	1.95	0.67
1:A:280:PHE:N	1:A:280:PHE:HD1	1.90	0.67
1:A:830:VAL:HG12	1:A:831:TYR:N	2.09	0.67
1:A:330:ARG:HA	1:A:333:GLN:HE21	1.59	0.66
1:B:162:TRP:CE3	1:B:188:TYR:CD2	2.84	0.66
1:B:869:THR:O	1:B:873:GLU:HG3	1.96	0.66
1:A:514:LEU:HB2	1:A:541:MET:HE1	1.76	0.66
1:A:804:HIS:N	1:A:804:HIS:ND1	2.40	0.66
1:B:747:GLU:HG3	1:B:763:TYR:CE2	2.30	0.66
1:A:82:ALA:O	1:A:382:GLN:HB3	1.95	0.66
1:B:449:ARG:HH12	1:B:452:ASP:HA	1.60	0.66
1:A:52:ILE:CD1	1:A:52:ILE:H	2.07	0.66
1:A:691:PRO:HB3	1:A:697:GLY:O	1.96	0.66
1:A:741:VAL:O	1:A:744:ALA:HB3	1.96	0.66
1:B:499:ILE:HG21	1:B:542:LEU:HB2	1.78	0.66
1:B:191:PHE:CD1	1:B:197:LEU:HD13	2.31	0.66
1:A:833:LEU:O	1:A:845:CYS:HA	1.96	0.65
1:A:727:ILE:HG22	1:A:733:GLN:NE2	2.09	0.65
1:A:321:ILE:O	1:A:325:ILE:HD12	1.97	0.65
1:A:730:LEU:O	1:A:731:GLU:HG2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:TYR:CE2	1:B:618:LEU:HD21	2.30	0.65
1:B:421:ARG:NH2	1:B:476:THR:HG23	2.12	0.65
1:A:120:PRO:HD3	1:A:156:TYR:CE2	2.32	0.65
1:A:581:ARG:HH11	1:A:581:ARG:HG3	1.61	0.65
1:A:303:LEU:HD23	1:A:323:TYR:CB	2.27	0.65
1:B:391:TYR:HB2	1:B:392:PRO:HD2	1.78	0.65
1:B:757:GLU:O	1:B:761:GLN:HG3	1.96	0.65
1:B:809:LEU:O	1:B:813:ARG:HG3	1.95	0.65
1:A:489:MET:CE	1:A:490:LEU:HG	2.27	0.65
1:B:6:LEU:HB2	1:B:18:ARG:O	1.97	0.65
1:A:188:TYR:C	1:A:189:MET:HG3	2.18	0.64
1:A:513:PRO:HG3	1:A:537:SER:O	1.98	0.64
1:A:640:LYS:HD3	1:A:640:LYS:H	1.62	0.64
1:A:416:TYR:N	1:A:417:PRO:HD2	2.10	0.64
1:A:577:TYR:N	1:A:577:TYR:HD1	1.92	0.64
1:B:163:SER:OG	1:B:166:ILE:HG13	1.96	0.64
1:A:454:TYR:HD2	1:A:462:MET:HG2	1.62	0.64
1:A:738:PRO:O	1:A:742:GLN:HG3	1.97	0.64
1:A:765:LYS:O	1:A:768:GLU:HB3	1.97	0.64
1:B:205:TRP:HZ3	1:B:242:LEU:O	1.79	0.64
1:A:152:LEU:HD11	1:A:190:PRO:HB2	1.78	0.64
1:B:647:TRP:HZ3	1:B:693:LEU:HB2	1.60	0.64
1:B:83:LEU:N	1:B:83:LEU:HD12	2.13	0.64
1:A:702:TRP:CE3	1:A:708:TYR:HB3	2.32	0.64
1:A:74:ARG:O	1:A:77:ASP:HB2	1.97	0.64
1:A:544:ARG:O	1:A:548:THR:HG23	1.96	0.64
1:B:402:ASN:CG	1:B:403:ARG:H	2.01	0.64
1:A:128:GLN:OE1	1:A:128:GLN:N	2.31	0.64
1:A:19:TYR:CD1	1:A:19:TYR:N	2.66	0.64
1:B:475:ILE:HD11	1:B:566:LEU:HD23	1.78	0.64
1:B:593:ALA:HA	1:B:670:MET:CE	2.28	0.64
1:A:170:LEU:HB2	1:A:173:GLN:NE2	2.13	0.63
1:A:103:TYR:CE2	1:A:346:ASP:HA	2.23	0.63
1:A:679:HIS:O	1:A:681:MET:N	2.28	0.63
1:B:163:SER:HG	1:B:165:GLU:HG2	1.63	0.63
1:B:193:ASN:HD22	1:B:195:LYS:HD3	1.62	0.63
1:A:647:TRP:HZ3	1:A:693:LEU:HB2	1.63	0.63
1:B:647:TRP:HH2	1:B:691:PRO:O	1.80	0.63
1:B:75:MET:HG3	1:B:82:ALA:HB2	1.80	0.63
1:B:867:ASP:HB3	1:B:870:VAL:HB	1.79	0.63
1:A:133:ILE:HD12	1:A:198:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LEU:O	1:A:618:LEU:HD22	1.98	0.63
1:A:643:ASP:HB3	1:A:646:HIS:HB2	1.80	0.63
1:A:313:ARG:HG2	1:A:313:ARG:HH11	1.64	0.63
1:A:835:LEU:HD12	1:A:845:CYS:H	1.64	0.63
1:B:707:ARG:NH1	1:B:707:ARG:HB2	2.13	0.63
1:A:820:ASP:C	1:A:822:PRO:HD2	2.19	0.63
1:B:511:ASP:HB3	1:B:537:SER:OG	1.98	0.63
1:A:857:LEU:CD2	1:A:857:LEU:H	2.06	0.63
1:B:228:ASN:O	1:B:232:ASN:HB2	1.98	0.63
1:A:832:VAL:HA	1:A:846:ILE:O	1.99	0.63
1:B:897:LEU:HD12	1:B:897:LEU:N	2.14	0.63
1:B:374:LYS:HA	2:B:999:GMP:N2	2.13	0.62
1:B:663:ILE:HG22	1:B:664:ASP:N	2.14	0.62
1:A:135:ALA:O	1:A:136:ILE:HG13	1.99	0.62
1:A:317:HIS:O	1:A:321:ILE:HD13	1.99	0.62
1:B:164:ILE:H	1:B:164:ILE:CD1	2.10	0.62
1:B:303:LEU:HD22	1:B:326:ILE:HG13	1.79	0.62
1:B:42:PRO:O	1:B:45:GLN:HG2	1.98	0.62
1:B:772:ARG:HA	1:B:868:TYR:CE2	2.34	0.62
1:A:112:ASN:HD22	1:A:113:PHE:N	1.97	0.62
1:A:35:PRO:HG2	1:A:62:PHE:HB2	1.79	0.62
1:A:857:LEU:HD23	1:A:857:LEU:N	2.07	0.62
1:B:117:VAL:HG22	1:B:133:ILE:HA	1.80	0.62
1:B:680:LEU:HD23	1:B:680:LEU:H	1.65	0.62
1:B:180:SER:O	1:B:183:ILE:HG12	1.98	0.62
1:A:728:MET:HA	1:A:728:MET:CE	2.30	0.62
1:A:625:ILE:HD11	1:A:683:MET:SD	2.40	0.62
1:B:547:ARG:HH11	1:B:547:ARG:HB3	1.60	0.62
1:B:541:MET:HE2	1:B:541:MET:HA	1.81	0.62
1:A:186:ILE:HG22	1:A:187:ILE:N	2.15	0.62
1:A:9:GLU:HG2	1:A:266:PHE:CD1	2.33	0.61
1:B:125:GLU:HB3	1:B:128:GLN:OE1	2.00	0.61
1:B:139:TYR:CZ	1:B:141:SER:HA	2.34	0.61
1:B:653:LYS:HA	1:B:656:ARG:NH1	2.15	0.61
1:A:279:LYS:HB2	1:A:280:PHE:CD1	2.35	0.61
1:B:835:LEU:HD12	1:B:839:ASN:CG	2.20	0.61
1:A:178:VAL:HG12	1:A:183:ILE:HD11	1.81	0.61
1:B:140:ASP:OD1	1:B:142:ILE:HB	2.00	0.61
1:A:172:GLU:CD	1:A:172:GLU:H	2.02	0.61
1:B:584:THR:O	1:B:588:THR:HG23	2.00	0.61
1:B:426:SER:HB3	1:B:429:THR:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:ILE:HG22	1:A:847:ALA:N	2.16	0.61
1:A:37:LEU:CD1	1:A:72:ILE:HD11	2.31	0.61
1:B:434:PHE:CE2	1:B:460:GLY:HA2	2.35	0.61
1:B:645:ASN:HD21	1:B:719:ARG:NH1	1.97	0.61
1:A:834:PRO:CB	1:A:867:ASP:HB3	2.30	0.60
1:B:116:GLU:HB3	1:B:320:TYR:OH	2.01	0.60
1:B:303:LEU:HD11	1:B:319:ARG:HE	1.65	0.60
1:B:52:ILE:N	1:B:52:ILE:HD13	2.16	0.60
1:B:653:LYS:HD2	1:B:656:ARG:NH1	2.16	0.60
1:A:855:THR:CG2	1:A:857:LEU:HD21	2.31	0.60
1:A:27:ARG:HG3	1:A:28:THR:N	2.15	0.60
1:A:803:PHE:O	1:A:806:ARG:HB3	2.00	0.60
1:B:20:ILE:HG23	1:B:24:GLY:HA2	1.83	0.60
1:B:730:LEU:O	1:B:731:GLU:HG2	2.01	0.60
1:A:164:ILE:H	1:A:164:ILE:CD1	2.09	0.60
1:A:205:TRP:CH2	1:A:210:PRO:HD2	2.37	0.60
1:A:771:PHE:HA	1:A:774:LEU:HD12	1.83	0.60
1:B:247:LYS:O	1:B:266:PHE:HB2	2.01	0.60
1:B:647:TRP:CZ3	1:B:693:LEU:HB2	2.37	0.60
1:A:231:LYS:O	1:A:235:GLY:N	2.34	0.60
1:A:576:ARG:HD2	1:A:577:TYR:HE1	1.64	0.60
1:A:859:LYS:O	1:A:863:LEU:HD12	2.01	0.60
1:B:110:VAL:HG12	1:B:111:ALA:N	2.16	0.60
1:B:806:ARG:NH2	1:B:843:ASP:HA	2.15	0.60
1:A:173:GLN:N	1:A:173:GLN:NE2	2.49	0.60
1:A:265:LEU:HB3	1:A:268:ILE:HD11	1.82	0.60
1:A:281:SER:O	1:A:282:PHE:HB2	2.01	0.60
1:A:656:ARG:HB3	1:A:656:ARG:NH1	2.15	0.60
1:B:406:TYR:HE1	1:B:647:TRP:CZ2	2.19	0.60
1:B:518:TYR:CE2	1:B:544:ARG:HB3	2.36	0.60
1:A:406:TYR:CB	1:A:629:ALA:HB3	2.32	0.60
1:A:823:GLN:HG2	1:A:824:VAL:N	2.16	0.60
1:B:621:ASP:O	1:B:623:ASP:N	2.35	0.60
1:A:173:GLN:N	1:A:173:GLN:HE21	2.00	0.60
1:B:647:TRP:CH2	1:B:691:PRO:O	2.55	0.60
1:A:657:GLU:O	1:A:661:PRO:HG2	2.01	0.60
1:A:410:PHE:O	1:A:624:SER:HA	2.02	0.59
1:B:159:VAL:HG21	1:B:317:HIS:CD2	2.37	0.59
1:A:366:ASP:OD1	1:A:576:ARG:NH1	2.35	0.59
1:B:362:ILE:HG22	1:B:363:LYS:N	2.17	0.59
1:B:449:ARG:NH1	1:B:452:ASP:HA	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ARG:O	1:B:646:HIS:HB2	2.02	0.59
1:B:685:ARG:HG2	1:B:686:GLU:H	1.68	0.59
1:A:538:LEU:O	1:A:540:GLU:N	2.35	0.59
1:B:318:GLN:OE1	1:B:318:GLN:HA	2.01	0.59
1:A:529:LYS:O	1:A:533:LEU:HD13	2.02	0.59
1:A:597:ILE:O	1:A:601:VAL:HG23	2.02	0.59
1:A:605:LEU:HD13	1:A:616:PHE:HD2	1.68	0.59
1:A:776:TYR:CE1	1:A:777:ILE:HG13	2.37	0.59
1:A:823:GLN:HG2	1:A:824:VAL:H	1.66	0.59
1:A:4:PHE:HA	1:A:97:TYR:CE2	2.38	0.59
1:B:103:TYR:OH	1:B:346:ASP:HB2	2.03	0.59
1:A:303:LEU:HD11	1:A:319:ARG:HE	1.68	0.59
1:A:126:PRO:O	1:A:228:ASN:ND2	2.36	0.59
1:A:389:GLN:HA	1:A:389:GLN:HE21	1.68	0.59
1:A:597:ILE:HD13	1:A:667:PHE:CE1	2.38	0.59
1:A:832:VAL:H	1:A:847:ALA:CA	2.14	0.59
1:A:835:LEU:H	1:A:867:ASP:H	1.51	0.59
1:B:455:SER:OG	1:B:676:ASN:HA	2.02	0.59
1:B:402:ASN:HA	1:B:886:ALA:O	2.03	0.59
1:B:270:VAL:C	1:B:271:LEU:HD23	2.23	0.59
1:B:443:ILE:HG22	1:B:592:MET:HG3	1.85	0.59
1:B:679:HIS:O	1:B:681:MET:N	2.34	0.59
1:A:253:ILE:HG22	1:A:254:GLU:N	2.17	0.59
1:B:105:HIS:C	1:B:107:LYS:H	2.06	0.59
1:B:245:HIS:CE1	1:B:267:GLY:HA3	2.37	0.59
1:B:268:ILE:HD12	1:B:268:ILE:C	2.23	0.59
1:A:295:GLU:O	1:A:299:ASN:N	2.35	0.58
1:A:873:GLU:HA	1:A:877:ILE:CD1	2.33	0.58
1:B:347:MET:HE1	1:B:358:VAL:HG13	1.84	0.58
1:B:685:ARG:HG2	1:B:686:GLU:N	2.17	0.58
1:B:846:ILE:HG22	1:B:847:ALA:H	1.68	0.58
1:A:145:ARG:HB2	1:A:147:TYR:CE1	2.38	0.58
1:A:415:LEU:HD22	1:A:623:ASP:HB3	1.86	0.58
1:B:481:GLN:NE2	1:B:559:ARG:NH1	2.51	0.58
1:B:647:TRP:CD1	1:B:648:VAL:N	2.71	0.58
1:B:645:ASN:ND2	1:B:719:ARG:HH11	1.99	0.58
1:A:802:PRO:HB2	1:A:804:HIS:ND1	2.18	0.58
1:A:842:GLY:O	1:A:843:ASP:HB2	2.03	0.58
1:A:407:VAL:HG12	1:A:408:MET:N	2.19	0.58
1:A:13:ASP:OD1	1:A:66:ARG:HB3	2.04	0.58
1:A:454:TYR:CD2	1:A:462:MET:HG2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:SER:HA	1:A:782:VAL:O	2.02	0.58
1:A:126:PRO:HG3	1:A:221:PHE:CD1	2.38	0.58
1:A:763:TYR:C	1:A:763:TYR:HD1	2.07	0.58
1:B:169:LYS:HB2	1:B:175:GLY:CA	2.33	0.58
1:B:78:ILE:HG22	1:B:79:GLY:N	2.17	0.58
1:B:830:VAL:HG12	1:B:831:TYR:N	2.19	0.58
1:A:116:GLU:HG3	1:A:324:ASN:ND2	2.18	0.58
1:A:427:PRO:O	1:A:430:ILE:HG22	2.03	0.58
1:B:74:ARG:O	1:B:77:ASP:HB2	2.03	0.58
1:B:52:ILE:CD1	1:B:52:ILE:H	2.17	0.58
1:B:579:ASP:HB3	1:B:582:ASN:ND2	2.19	0.58
1:A:679:HIS:O	1:A:679:HIS:CG	2.57	0.57
1:A:767:PHE:HA	1:A:770:GLU:HG2	1.85	0.57
1:B:494:ARG:O	1:B:498:ILE:HD13	2.04	0.57
1:A:649:ASP:O	1:A:652:ASP:HB3	2.04	0.57
1:A:772:ARG:HH11	1:A:772:ARG:HG3	1.67	0.57
1:A:83:LEU:HD12	1:A:83:LEU:N	2.19	0.57
1:B:406:TYR:HB3	1:B:629:ALA:HB3	1.86	0.57
1:A:291:ASP:HB3	1:A:302:LYS:HD2	1.85	0.57
1:A:320:TYR:HD1	1:A:321:ILE:CD1	2.14	0.57
1:A:830:VAL:HG12	1:A:847:ALA:HB1	1.85	0.57
1:A:380:ILE:HG12	2:A:999:GMP:O6	2.04	0.57
1:B:104:ASP:CG	1:B:107:LYS:HD2	2.24	0.57
1:B:455:SER:O	1:B:462:MET:HA	2.05	0.57
1:B:830:VAL:CG1	1:B:831:TYR:N	2.66	0.57
1:A:163:SER:H	1:A:318:GLN:HE22	1.53	0.57
1:A:523:SER:HB3	1:A:526:ILE:CG1	2.35	0.57
1:A:493:GLN:HB2	1:A:549:GLU:HG3	1.87	0.57
1:A:492:ALA:HA	1:A:495:ASN:HB2	1.86	0.57
1:A:406:TYR:HB2	1:A:629:ALA:HB3	1.86	0.57
1:A:90:LEU:HD11	1:A:363:LYS:CE	2.33	0.57
1:B:431:ALA:HB1	1:B:454:TYR:CE2	2.39	0.57
1:A:353:ILE:HD11	1:A:357:SER:HB2	1.86	0.57
1:A:589:PHE:O	1:A:592:MET:HB3	2.05	0.57
1:A:839:ASN:OD1	1:A:841:PHE:HB2	2.04	0.57
1:A:604:TYR:O	1:A:607:GLU:HB3	2.05	0.57
1:B:188:TYR:CD1	1:B:190:PRO:HD3	2.40	0.57
1:B:425:ILE:HG22	1:B:425:ILE:O	2.04	0.57
1:B:92:TYR:C	1:B:92:TYR:CD1	2.78	0.57
1:A:335:ASP:O	1:A:339:GLN:N	2.37	0.57
1:A:595:GLN:HA	1:A:598:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LEU:O	1:A:654:PHE:HB3	2.05	0.57
1:A:685:ARG:NH2	1:A:716:GLU:H	2.02	0.57
1:A:432:GLY:HA3	1:A:462:MET:HE2	1.87	0.57
1:A:52:ILE:HD11	1:A:381:PRO:HG3	1.85	0.57
1:B:602:ASN:OD1	1:B:616:PHE:HB2	2.05	0.57
1:B:752:MET:HG2	1:B:760:LEU:HD12	1.86	0.57
1:B:807:GLY:O	1:B:810:THR:HG22	2.05	0.57
1:A:121:ASP:HB2	1:A:826:GLU:OE1	2.05	0.56
1:A:403:ARG:HH22	1:A:889:LEU:HD21	1.69	0.56
1:A:605:LEU:HB3	1:A:616:PHE:HE2	1.65	0.56
1:A:752:MET:CG	1:A:760:LEU:HD12	2.32	0.56
1:A:101:ILE:HG22	1:A:102:LYS:N	2.20	0.56
1:A:844:LYS:O	1:A:845:CYS:HB3	2.03	0.56
1:A:469:GLY:O	1:A:472:PRO:HG2	2.06	0.56
1:B:305:TYR:OH	1:B:309:ILE:HB	2.05	0.56
1:B:432:GLY:O	1:B:433:THR:HB	2.06	0.56
1:A:4:PHE:HA	1:A:97:TYR:HE2	1.71	0.56
1:B:702:TRP:CZ3	1:B:708:TYR:CD2	2.93	0.56
1:B:772:ARG:HA	1:B:868:TYR:HE2	1.69	0.56
1:A:894:LYS:HA	1:A:894:LYS:HE2	1.86	0.56
1:B:51:ASP:C	1:B:53:TYR:H	2.08	0.56
1:B:711:ASN:HB2	1:B:753:LEU:HB3	1.87	0.56
1:A:129:ALA:HB1	1:A:225:TYR:CE1	2.41	0.56
1:A:308:PRO:HD2	1:A:311:LYS:CG	2.36	0.56
1:A:303:LEU:HD23	1:A:323:TYR:CA	2.35	0.56
1:A:654:PHE:HD1	1:A:654:PHE:C	2.09	0.56
1:A:654:PHE:CD1	1:A:654:PHE:C	2.77	0.56
1:B:101:ILE:HG21	1:B:349:TYR:HD1	1.69	0.56
1:A:414:SER:HB2	1:A:417:PRO:CG	2.34	0.56
1:A:763:TYR:C	1:A:763:TYR:CD1	2.79	0.56
1:B:347:MET:CE	1:B:358:VAL:HG13	2.36	0.56
1:A:291:ASP:HB3	1:A:302:LYS:CB	2.36	0.56
1:A:767:PHE:C	1:A:767:PHE:CD1	2.79	0.56
1:B:205:TRP:CZ3	1:B:242:LEU:O	2.58	0.56
1:A:228:ASN:O	1:A:232:ASN:ND2	2.39	0.56
1:A:506:PRO:HG3	1:A:535:ALA:HB2	1.88	0.56
1:B:162:TRP:CE3	1:B:188:TYR:HD2	2.23	0.56
1:B:309:ILE:O	1:B:309:ILE:HD13	2.06	0.56
1:B:329:TYR:O	1:B:332:LEU:HB2	2.06	0.56
1:B:604:TYR:CD1	1:B:605:LEU:HD23	2.40	0.56
1:B:419:ILE:HD13	1:B:589:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:TYR:HD1	1:A:391:TYR:H	1.54	0.55
1:B:423:VAL:O	1:B:424:ASN:HB3	2.06	0.55
1:B:163:SER:OG	1:B:165:GLU:HG2	2.07	0.55
1:B:19:TYR:N	1:B:19:TYR:CD1	2.73	0.55
1:B:553:MET:HG3	1:B:554:THR:N	2.21	0.55
1:B:455:SER:HA	1:B:675:ASN:O	2.06	0.55
1:A:465:LYS:HD3	1:A:675:ASN:O	2.06	0.55
1:B:471:VAL:HB	1:B:472:PRO:CD	2.36	0.55
1:A:51:ASP:HB2	1:A:52:ILE:HD13	1.88	0.55
1:B:201:TYR:O	1:B:204:PHE:HB3	2.07	0.55
1:B:857:LEU:N	1:B:857:LEU:HD23	2.21	0.55
1:A:173:GLN:H	1:A:173:GLN:NE2	2.04	0.55
1:A:214:THR:CG2	1:A:215:GLY:H	2.18	0.55
1:A:33:TYR:HD2	1:A:65:MET:HE1	1.71	0.55
1:A:409:SER:HA	1:A:625:ILE:O	2.06	0.55
1:A:647:TRP:CD1	1:A:648:VAL:N	2.75	0.55
1:A:750:ARG:HG2	1:A:754:GLN:OE1	2.06	0.55
1:A:416:TYR:O	1:A:419:ILE:HB	2.07	0.55
1:A:498:ILE:HG22	1:A:499:ILE:HG13	1.87	0.55
1:A:147:TYR:CD2	1:A:204:PHE:HE1	2.24	0.55
1:A:883:PHE:CD1	1:A:883:PHE:N	2.70	0.55
1:B:339:GLN:HA	1:B:339:GLN:NE2	2.21	0.55
1:B:41:CYS:CB	1:B:45:GLN:HG3	2.31	0.55
1:A:254:GLU:O	1:A:255:ASN:HB2	2.06	0.55
1:A:893:LYS:HG2	1:A:894:LYS:N	2.22	0.55
1:B:370:PHE:CD1	1:B:370:PHE:C	2.78	0.55
1:B:443:ILE:HG22	1:B:592:MET:CG	2.37	0.55
1:A:272:ASP:CG	1:A:274:ILE:HG22	2.28	0.55
1:B:181:GLU:CD	1:B:181:GLU:H	2.10	0.55
1:B:193:ASN:ND2	1:B:195:LYS:HD3	2.21	0.55
1:B:423:VAL:HB	1:B:425:ILE:CG1	2.36	0.55
1:B:479:PHE:CD1	1:B:479:PHE:C	2.80	0.55
1:A:205:TRP:CZ3	1:A:209:THR:HG23	2.42	0.54
1:A:808:ILE:O	1:A:811:TYR:HB3	2.07	0.54
1:A:403:ARG:NH1	1:A:888:LYS:HB2	2.22	0.54
1:B:195:LYS:O	1:B:199:MET:HB2	2.07	0.54
1:B:689:ALA:HB1	1:B:711:ASN:O	2.07	0.54
1:A:291:ASP:HB3	1:A:302:LYS:CD	2.37	0.54
1:A:547:ARG:HA	1:A:550:VAL:CG2	2.37	0.54
1:A:836:ARG:NH1	1:A:864:HIS:O	2.40	0.54
1:B:117:VAL:HG13	1:B:132:PRO:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:O	1:B:175:GLY:HA2	2.07	0.54
1:B:321:ILE:N	1:B:321:ILE:HD12	2.23	0.54
1:B:369:ILE:HG21	1:B:577:TYR:CZ	2.42	0.54
1:A:379:VAL:HG12	1:A:380:ILE:O	2.07	0.54
1:A:425:ILE:O	1:A:472:PRO:HD3	2.07	0.54
1:A:597:ILE:HB	1:A:667:PHE:CE1	2.43	0.54
1:B:604:TYR:C	1:B:604:TYR:CD1	2.81	0.54
1:A:147:TYR:CD1	1:A:147:TYR:N	2.73	0.54
1:A:166:ILE:O	1:A:175:GLY:HA2	2.07	0.54
1:A:235:GLY:O	1:A:238:THR:HG23	2.08	0.54
1:A:489:MET:HE2	1:A:490:LEU:HG	1.88	0.54
1:A:514:LEU:CD1	1:A:533:LEU:HD21	2.38	0.54
1:A:598:GLU:HG3	1:A:599:ARG:N	2.21	0.54
1:A:669:GLU:O	1:A:672:GLU:HB3	2.08	0.54
1:A:796:PHE:HD1	1:A:796:PHE:N	2.05	0.54
1:A:117:VAL:HG22	1:A:133:ILE:HA	1.89	0.54
1:A:855:THR:HB	1:A:857:LEU:HD21	1.90	0.54
1:B:271:LEU:N	1:B:271:LEU:HD23	2.23	0.54
1:A:576:ARG:HB3	1:A:577:TYR:CD1	2.43	0.54
1:A:643:ASP:O	1:A:646:HIS:HB3	2.07	0.54
1:A:72:ILE:HD12	1:A:72:ILE:H	1.73	0.54
1:B:456:CYS:HB3	1:B:462:MET:N	2.23	0.54
1:B:834:PRO:O	1:B:845:CYS:HA	2.07	0.54
1:A:40:HIS:HE1	1:A:81:GLU:OE1	1.91	0.54
1:B:830:VAL:CG1	1:B:847:ALA:HB1	2.38	0.54
1:B:421:ARG:CZ	1:B:476:THR:HG23	2.36	0.54
1:B:547:ARG:CZ	1:B:547:ARG:HB3	2.38	0.54
1:B:702:TRP:N	1:B:702:TRP:CD1	2.75	0.54
1:B:766:GLU:O	1:B:769:LYS:HB3	2.07	0.54
1:B:810:THR:HB	1:B:843:ASP:OD2	2.08	0.54
1:A:475:ILE:HG22	1:A:476:THR:N	2.23	0.54
1:A:837:GLU:HB2	1:A:844:LYS:HE2	1.90	0.54
1:B:689:ALA:HB3	1:B:710:LEU:HD22	1.89	0.54
1:A:162:TRP:HE3	1:A:188:TYR:CE2	2.26	0.54
1:A:353:ILE:HD11	1:A:357:SER:O	2.08	0.54
1:A:870:VAL:HG12	1:A:871:LEU:N	2.23	0.54
1:B:282:PHE:O	1:B:283:THR:HG23	2.07	0.54
1:B:459:ASN:HD21	1:B:461:MET:CG	2.21	0.54
1:B:728:MET:HA	1:B:728:MET:CE	2.33	0.54
1:B:149:PHE:CD1	1:B:149:PHE:N	2.75	0.53
1:B:248:THR:HA	1:B:266:PHE:HD1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASP:OD2	1:A:107:LYS:N	2.42	0.53
1:A:145:ARG:HH21	1:A:185:LYS:CD	2.21	0.53
1:A:214:THR:CG2	1:A:215:GLY:N	2.71	0.53
1:B:53:TYR:CE1	1:B:428:GLU:CB	2.91	0.53
1:B:751:ARG:NH1	1:B:763:TYR:HB2	2.23	0.53
1:A:101:ILE:CG2	1:A:102:LYS:N	2.72	0.53
1:A:320:TYR:CD1	1:A:321:ILE:HD12	2.37	0.53
1:B:658:ARG:C	1:B:661:PRO:HD2	2.29	0.53
1:A:152:LEU:O	1:A:158:ASN:HA	2.09	0.53
1:B:808:ILE:O	1:B:811:TYR:HB3	2.07	0.53
1:A:116:GLU:CG	1:A:324:ASN:ND2	2.71	0.53
1:A:810:THR:HG21	1:A:845:CYS:O	2.07	0.53
1:A:899:ASP:HB2	1:A:900:MET:SD	2.49	0.53
1:A:434:PHE:CE2	1:A:460:GLY:HA2	2.44	0.53
1:A:602:ASN:OD1	1:A:617:VAL:HG23	2.07	0.53
1:B:245:HIS:HE1	1:B:267:GLY:HA3	1.74	0.53
1:B:653:LYS:HD2	1:B:656:ARG:HH11	1.73	0.53
1:A:285:GLN:HG3	1:A:286:PRO:HD2	1.91	0.53
1:A:594:LEU:O	1:A:597:ILE:HG22	2.08	0.53
1:A:62:PHE:HD2	1:A:67:ASP:HB3	1.73	0.53
1:A:767:PHE:HD1	1:A:767:PHE:C	2.12	0.53
1:A:788:ILE:O	1:A:791:TYR:CD2	2.62	0.53
1:B:253:ILE:CG2	1:B:260:ARG:CB	2.59	0.53
1:B:802:PRO:HD2	1:B:805:ILE:HB	1.90	0.53
1:B:167:ALA:HB1	1:B:178:VAL:HG21	1.91	0.53
1:B:499:ILE:HD11	1:B:541:MET:HB3	1.90	0.53
1:B:555:ALA:O	1:B:558:ASN:HB3	2.08	0.53
1:B:803:PHE:CZ	1:B:845:CYS:HB3	2.44	0.53
1:A:270:VAL:C	1:A:271:LEU:HD23	2.29	0.53
1:A:471:VAL:HB	1:A:472:PRO:CD	2.38	0.53
1:A:494:ARG:HA	1:A:497:GLU:HG2	1.91	0.53
1:A:165:GLU:O	1:A:168:ALA:HB3	2.08	0.53
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.23	0.53
1:B:321:ILE:CD1	1:B:321:ILE:N	2.72	0.53
1:B:329:TYR:CD2	1:B:333:GLN:NE2	2.77	0.53
1:B:752:MET:CG	1:B:760:LEU:HD12	2.39	0.53
1:B:899:ASP:C	1:B:901:PHE:H	2.12	0.53
1:A:288:TYR:HA	1:A:293:ILE:CD1	2.39	0.52
1:A:796:PHE:CD1	1:A:796:PHE:N	2.75	0.52
1:A:821:ALA:N	1:A:822:PRO:CD	2.71	0.52
1:A:123:PHE:CZ	1:A:828:GLU:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASP:OD2	1:B:185:LYS:HE3	2.09	0.52
1:B:33:TYR:O	1:B:35:PRO:HD3	2.09	0.52
1:B:423:VAL:O	1:B:424:ASN:CB	2.57	0.52
1:A:167:ALA:HA	1:A:176:ASP:CB	2.39	0.52
1:A:636:VAL:O	1:A:636:VAL:HG12	2.09	0.52
1:A:792:ASP:O	1:A:794:GLY:N	2.43	0.52
1:B:129:ALA:O	1:B:229:ARG:HD3	2.10	0.52
1:B:581:ARG:NH1	1:B:581:ARG:HG3	2.17	0.52
1:A:33:TYR:CD2	1:A:65:MET:HE1	2.44	0.52
1:B:495:ASN:OD1	1:B:521:ASP:HA	2.09	0.52
1:B:4:PHE:O	1:B:19:TYR:HB2	2.09	0.52
1:B:867:ASP:O	1:B:871:LEU:HB2	2.09	0.52
1:A:219:GLU:HA	1:A:223:ILE:HD12	1.90	0.52
1:A:511:ASP:HB2	1:A:537:SER:HB3	1.92	0.52
1:A:647:TRP:HH2	1:A:691:PRO:O	1.93	0.52
1:A:818:ASN:CA	1:A:822:PRO:HG3	2.37	0.52
1:B:164:ILE:HD12	1:B:164:ILE:N	2.17	0.52
1:B:776:TYR:CE2	1:B:777:ILE:HG12	2.44	0.52
1:A:434:PHE:CZ	1:A:460:GLY:HA2	2.44	0.52
1:B:101:ILE:HG21	1:B:349:TYR:CD1	2.44	0.52
1:B:626:TYR:CD1	1:B:626:TYR:N	2.77	0.52
1:A:506:PRO:HG2	1:A:507:ASN:H	1.74	0.52
1:B:549:GLU:O	1:B:553:MET:HB3	2.09	0.52
1:B:744:ALA:CB	1:B:767:PHE:CE2	2.93	0.52
1:B:489:MET:SD	1:B:553:MET:CB	2.87	0.52
1:A:308:PRO:HD2	1:A:311:LYS:HB2	1.91	0.52
1:A:419:ILE:O	1:A:423:VAL:HG23	2.10	0.52
1:A:489:MET:HG3	1:A:553:MET:HB3	1.91	0.52
1:A:62:PHE:O	1:A:64:ASN:N	2.42	0.52
1:A:858:ILE:HG13	1:A:859:LYS:N	2.25	0.52
1:B:167:ALA:HA	1:B:176:ASP:CB	2.37	0.52
1:A:421:ARG:HD2	1:A:475:ILE:HG21	1.89	0.52
1:A:647:TRP:CZ3	1:A:693:LEU:HB2	2.44	0.51
1:B:186:ILE:HD12	1:B:186:ILE:N	2.26	0.51
1:B:16:PHE:HE1	1:B:30:GLU:HG3	1.76	0.51
1:A:169:LYS:HB2	1:A:175:GLY:CA	2.39	0.51
1:A:781:SER:O	1:A:831:TYR:O	2.28	0.51
1:B:504:HIS:C	1:B:506:PRO:HD3	2.30	0.51
1:B:788:ILE:HG22	1:B:791:TYR:CG	2.45	0.51
1:A:155:PRO:HG2	1:A:156:TYR:CD1	2.45	0.51
1:A:280:PHE:CD2	1:A:343:LEU:HD13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ILE:HD13	1:A:667:PHE:CD1	2.46	0.51
1:B:23:ASN:O	1:B:25:ARG:N	2.43	0.51
1:B:103:TYR:CE1	1:B:346:ASP:HA	2.46	0.51
1:B:4:PHE:CE2	1:B:103:TYR:HA	2.46	0.51
1:A:127:SER:HB2	1:A:128:GLN:OE1	2.10	0.51
1:A:167:ALA:HA	1:A:176:ASP:OD2	2.09	0.51
1:A:186:ILE:CG2	1:A:187:ILE:N	2.73	0.51
1:A:822:PRO:O	1:A:822:PRO:HG2	2.09	0.51
1:B:188:TYR:CE1	1:B:190:PRO:HD3	2.45	0.51
1:B:205:TRP:CZ3	1:B:209:THR:HG23	2.45	0.51
1:B:663:ILE:HD13	1:B:683:MET:HE3	1.93	0.51
1:B:70:GLN:HA	1:B:70:GLN:OE1	2.09	0.51
1:A:232:ASN:H	1:A:232:ASN:HD22	1.59	0.51
1:B:108:ILE:O	1:B:110:VAL:N	2.44	0.51
1:B:6:LEU:HD12	1:B:211:VAL:HG11	1.91	0.51
1:B:53:TYR:CE1	1:B:428:GLU:HB2	2.46	0.51
1:B:541:MET:CE	1:B:541:MET:HA	2.39	0.51
1:A:274:ILE:HG23	1:A:275:ASP:H	1.75	0.51
1:A:321:ILE:CD1	1:A:321:ILE:N	2.73	0.51
1:A:356:GLN:C	1:A:358:VAL:H	2.12	0.51
1:A:413:THR:O	1:A:415:LEU:N	2.42	0.51
1:A:656:ARG:NH1	1:A:656:ARG:CB	2.74	0.51
1:A:818:ASN:O	1:A:822:PRO:HG3	2.11	0.51
1:A:811:TYR:HB2	1:A:846:ILE:HG23	1.91	0.51
1:B:788:ILE:O	1:B:790:LYS:HG3	2.11	0.51
1:A:274:ILE:HG23	1:A:275:ASP:N	2.26	0.51
1:A:338:ARG:HG3	1:A:340:PHE:CE1	2.45	0.51
1:A:52:ILE:N	1:A:52:ILE:HD13	2.18	0.51
1:A:582:ASN:O	1:A:585:ALA:HB3	2.11	0.51
1:A:5:TYR:HA	1:A:19:TYR:HB3	1.92	0.51
1:A:273:TYR:OH	1:A:335:ASP:HA	2.11	0.51
1:A:899:ASP:O	1:A:900:MET:SD	2.68	0.51
1:B:83:LEU:HD12	1:B:83:LEU:H	1.75	0.51
1:B:858:ILE:HG13	1:B:859:LYS:N	2.26	0.51
1:A:680:LEU:HD23	1:A:680:LEU:N	2.22	0.51
1:B:246:ARG:N	1:B:246:ARG:CD	2.74	0.51
1:B:711:ASN:OD1	1:B:723:PRO:HB2	2.11	0.51
1:A:437:ALA:O	1:A:442:TYR:HE2	1.94	0.51
1:A:642:ARG:O	1:A:643:ASP:CB	2.53	0.51
1:A:68:ALA:O	1:A:71:TRP:HB3	2.11	0.51
1:A:763:TYR:O	1:A:763:TYR:CD1	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:ILE:CD1	1:B:541:MET:HB3	2.41	0.51
1:B:71:TRP:CZ3	1:B:82:ALA:HB1	2.46	0.51
1:A:125:GLU:CB	1:A:128:GLN:HE22	2.24	0.50
1:B:139:TYR:CE1	1:B:144:ASP:HA	2.46	0.50
1:B:188:TYR:HE1	1:B:190:PRO:CB	2.22	0.50
1:B:327:ASP:O	1:B:328:VAL:C	2.49	0.50
1:B:606:ASN:O	1:B:611:THR:N	2.42	0.50
1:A:191:PHE:CD1	1:A:197:LEU:HD22	2.47	0.50
1:A:191:PHE:CD1	1:A:191:PHE:N	2.78	0.50
1:A:332:LEU:HD23	1:A:332:LEU:H	1.75	0.50
1:A:491:ALA:O	1:A:495:ASN:N	2.43	0.50
1:A:625:ILE:C	1:A:626:TYR:CD1	2.84	0.50
1:A:744:ALA:HB2	1:A:767:PHE:HE2	1.74	0.50
1:B:439:LEU:O	1:B:440:HIS:C	2.49	0.50
1:B:499:ILE:HD13	1:B:542:LEU:N	2.27	0.50
1:B:8:VAL:HG12	1:B:17:GLU:HB2	1.93	0.50
1:A:110:VAL:HG22	1:A:212:ILE:HB	1.94	0.50
1:A:321:ILE:HD12	1:A:321:ILE:N	2.25	0.50
1:A:412:LEU:HD13	1:A:683:MET:HB2	1.93	0.50
1:A:776:TYR:CD1	1:A:777:ILE:N	2.80	0.50
1:B:218:VAL:O	1:B:223:ILE:HG13	2.11	0.50
1:B:255:ASN:HB3	1:B:257:TYR:CE2	2.46	0.50
1:A:184:ASP:OD1	1:A:184:ASP:N	2.45	0.50
1:A:205:TRP:CZ2	1:A:210:PRO:HD2	2.46	0.50
1:A:744:ALA:CB	1:A:767:PHE:CE2	2.94	0.50
1:A:744:ALA:CB	1:A:767:PHE:HE2	2.25	0.50
1:B:128:GLN:OE1	1:B:128:GLN:N	2.45	0.50
1:B:311:LYS:NZ	1:B:821:ALA:HA	2.26	0.50
1:A:626:TYR:N	1:A:626:TYR:CD1	2.79	0.50
1:B:241:ARG:HD3	1:B:246:ARG:NH1	2.26	0.50
1:B:604:TYR:HD1	1:B:605:LEU:HD23	1.76	0.50
1:A:222:ASP:O	1:A:226:VAL:HG23	2.11	0.50
1:A:787:ASN:C	1:A:789:ALA:H	2.14	0.50
1:A:863:LEU:HA	1:A:866:MET:HB2	1.93	0.50
1:B:188:TYR:HD1	1:B:189:MET:N	2.10	0.50
1:B:345:LEU:O	1:B:349:TYR:HD2	1.95	0.50
1:B:733:GLN:O	1:B:734:LYS:C	2.47	0.50
1:B:188:TYR:CD1	1:B:189:MET:N	2.80	0.50
1:B:250:VAL:HG12	1:B:251:LYS:N	2.25	0.50
1:B:605:LEU:O	1:B:607:GLU:N	2.45	0.50
1:B:1:MET:O	1:B:22:SER:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ILE:HG22	1:B:260:ARG:O	2.11	0.50
1:B:459:ASN:HD21	1:B:461:MET:HG3	1.76	0.50
1:A:229:ARG:O	1:A:232:ASN:HB2	2.11	0.49
1:A:324:ASN:O	1:A:327:ASP:HB2	2.12	0.49
1:A:744:ALA:HB2	1:A:767:PHE:CE2	2.47	0.49
1:B:119:SER:HB2	1:B:131:HIS:ND1	2.27	0.49
1:B:165:GLU:CD	1:B:165:GLU:H	2.15	0.49
1:B:312:LEU:O	1:B:312:LEU:HD13	2.12	0.49
1:B:600:LYS:O	1:B:603:GLU:HB3	2.12	0.49
1:B:763:TYR:C	1:B:763:TYR:CD1	2.84	0.49
1:A:169:LYS:HB3	1:A:173:GLN:HB2	1.94	0.49
1:A:255:ASN:C	1:A:257:TYR:H	2.14	0.49
1:B:139:TYR:HE1	1:B:144:ASP:HA	1.76	0.49
1:B:343:LEU:O	1:B:345:LEU:N	2.44	0.49
1:B:391:TYR:CD1	1:B:391:TYR:N	2.80	0.49
1:A:647:TRP:CD1	1:A:647:TRP:C	2.85	0.49
1:A:201:TYR:O	1:A:204:PHE:HB3	2.13	0.49
1:A:536:LYS:C	1:A:536:LYS:HD3	2.33	0.49
1:B:456:CYS:HB3	1:B:462:MET:HA	1.95	0.49
1:B:854:ILE:CG2	1:B:859:LYS:HB2	2.37	0.49
1:A:815:ILE:CG2	1:A:815:ILE:O	2.60	0.49
1:B:431:ALA:HB3	1:B:462:MET:O	2.12	0.49
1:B:507:ASN:O	1:B:508:LEU:HD12	2.12	0.49
1:B:625:ILE:C	1:B:626:TYR:CD1	2.86	0.49
1:A:328:VAL:O	1:A:332:LEU:HD23	2.12	0.49
1:B:53:TYR:CD1	1:B:428:GLU:HB2	2.47	0.49
1:B:689:ALA:CB	1:B:710:LEU:HD22	2.42	0.49
1:A:116:GLU:CG	1:A:324:ASN:HD21	2.26	0.49
1:A:262:ILE:O	1:A:262:ILE:HG13	2.13	0.49
1:A:41:CYS:HB2	1:A:42:PRO:HD2	1.94	0.49
1:A:380:ILE:HD12	1:A:576:ARG:CZ	2.42	0.49
1:B:162:TRP:HB3	1:B:188:TYR:CE2	2.44	0.49
1:B:431:ALA:HB1	1:B:454:TYR:CD2	2.47	0.49
1:B:857:LEU:H	1:B:857:LEU:CD2	2.26	0.49
1:A:658:ARG:HH11	1:A:658:ARG:HG3	1.78	0.49
1:B:162:TRP:CE3	1:B:188:TYR:CE2	3.01	0.49
1:B:303:LEU:CD2	1:B:326:ILE:HG13	2.42	0.49
1:B:41:CYS:HB3	1:B:58:THR:HG23	1.94	0.49
1:B:45:GLN:OE1	1:B:45:GLN:HA	2.12	0.49
1:A:6:LEU:HB2	1:A:18:ARG:O	2.13	0.49
1:A:451:SER:OG	1:A:454:TYR:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:O	1:A:93:LEU:HG	2.13	0.49
1:B:456:CYS:HB3	1:B:462:MET:CA	2.42	0.49
1:B:481:GLN:NE2	1:B:559:ARG:HH11	2.08	0.49
1:B:410:PHE:O	1:B:624:SER:HA	2.13	0.49
1:B:654:PHE:CD1	1:B:654:PHE:C	2.86	0.49
1:B:820:ASP:C	1:B:822:PRO:HD2	2.34	0.49
1:A:169:LYS:HB2	1:A:175:GLY:HA3	1.94	0.49
1:A:364:THR:HG22	1:A:368:ILE:HD11	1.94	0.49
1:A:430:ILE:HG23	1:A:430:ILE:O	2.12	0.49
1:A:459:ASN:H	1:A:459:ASN:HD22	1.61	0.49
1:B:428:GLU:OE2	1:B:470:VAL:HG23	2.12	0.49
1:B:791:TYR:CD1	1:B:791:TYR:C	2.86	0.49
1:B:837:GLU:HA	1:B:837:GLU:OE1	2.12	0.48
1:A:167:ALA:CA	1:A:176:ASP:HB2	2.42	0.48
1:A:455:SER:HA	1:A:675:ASN:O	2.13	0.48
1:A:614:GLU:HG3	1:A:616:PHE:HE1	1.78	0.48
1:B:61:LEU:HD13	1:B:62:PHE:N	2.28	0.48
1:A:556:GLN:OE1	1:A:557:ILE:HD13	2.12	0.48
1:A:844:LYS:O	1:A:845:CYS:CB	2.62	0.48
1:B:188:TYR:CE1	1:B:190:PRO:HB3	2.43	0.48
1:B:381:PRO:HD2	1:B:576:ARG:HD3	1.94	0.48
1:B:433:THR:HG23	1:B:434:PHE:N	2.27	0.48
1:B:474:GLU:O	1:B:477:LYS:HB3	2.13	0.48
1:B:744:ALA:O	1:B:747:GLU:HB2	2.13	0.48
1:B:884:THR:HB	1:B:889:LEU:O	2.14	0.48
1:A:291:ASP:HA	1:A:294:SER:OG	2.13	0.48
1:A:421:ARG:HB2	1:A:680:LEU:CD1	2.43	0.48
1:A:643:ASP:HB3	1:A:646:HIS:N	2.26	0.48
1:A:832:VAL:N	1:A:847:ALA:HA	2.19	0.48
1:A:897:LEU:N	1:A:897:LEU:HD12	2.27	0.48
1:A:8:VAL:HG11	1:A:93:LEU:HD21	1.95	0.48
1:A:104:ASP:O	1:A:105:HIS:CD2	2.66	0.48
1:A:339:GLN:HE22	1:A:342:ASN:HB2	1.77	0.48
1:A:592:MET:HG2	1:A:670:MET:HE1	1.94	0.48
1:A:68:ALA:O	1:A:72:ILE:HD12	2.14	0.48
1:A:835:LEU:CD1	1:A:845:CYS:H	2.26	0.48
1:B:857:LEU:CD2	1:B:857:LEU:N	2.76	0.48
1:A:255:ASN:OD1	1:A:256:MET:N	2.44	0.48
1:A:514:LEU:HD13	1:A:533:LEU:HD21	1.94	0.48
1:A:654:PHE:HD1	1:A:654:PHE:O	1.97	0.48
1:B:112:ASN:ND2	1:B:113:PHE:N	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:ASN:O	1:B:790:LYS:HG2	2.14	0.48
1:A:113:PHE:HE1	1:A:218:VAL:HG23	1.78	0.48
1:A:408:MET:O	1:A:627:VAL:HG23	2.14	0.48
1:A:655:ALA:HA	1:A:659:MET:CB	2.43	0.48
1:A:818:ASN:O	1:A:819:ILE:HB	2.12	0.48
1:A:866:MET:HE3	1:A:871:LEU:HD12	1.96	0.48
1:B:170:LEU:HB3	1:B:172:GLU:OE1	2.14	0.48
1:B:577:TYR:CD1	1:B:577:TYR:N	2.81	0.48
1:A:104:ASP:CG	1:A:107:LYS:HD2	2.34	0.48
1:B:18:ARG:NH2	1:B:210:PRO:O	2.46	0.48
1:B:221:PHE:CD2	1:B:222:ASP:N	2.82	0.48
1:B:834:PRO:O	1:B:835:LEU:HB2	2.14	0.48
1:B:843:ASP:O	1:B:844:LYS:HE3	2.14	0.48
1:A:291:ASP:HB2	1:A:302:LYS:HB2	1.94	0.48
1:B:873:GLU:HA	1:B:877:ILE:CD1	2.41	0.48
1:A:254:GLU:O	1:A:255:ASN:CB	2.62	0.48
1:A:323:TYR:O	1:A:324:ASN:C	2.52	0.48
1:A:9:GLU:CG	1:A:266:PHE:CD1	2.97	0.48
1:B:364:THR:O	1:B:368:ILE:HG12	2.13	0.48
1:B:402:ASN:CG	1:B:403:ARG:N	2.66	0.48
1:A:211:VAL:HG12	1:A:212:ILE:HG13	1.96	0.47
1:A:347:MET:CE	1:A:358:VAL:HG22	2.43	0.47
1:B:880:LEU:HD23	1:B:883:PHE:CE2	2.49	0.47
1:A:872:LEU:HD23	1:A:876:PHE:HB3	1.94	0.47
1:B:343:LEU:C	1:B:343:LEU:HD23	2.35	0.47
1:B:365:TRP:O	1:B:368:ILE:HB	2.13	0.47
1:B:712:VAL:CG1	1:B:713:TRP:N	2.77	0.47
1:B:831:TYR:O	1:B:832:VAL:HB	2.14	0.47
1:B:859:LYS:HG2	1:B:863:LEU:HD11	1.96	0.47
1:A:449:ARG:NH1	1:A:452:ASP:HA	2.29	0.47
1:A:883:PHE:HD1	1:A:883:PHE:N	2.11	0.47
1:B:305:TYR:HE1	1:B:307:GLY:O	1.97	0.47
1:B:727:ILE:HG21	1:B:732:THR:OG1	2.15	0.47
1:B:832:VAL:HG22	1:B:847:ALA:CB	2.41	0.47
1:A:103:TYR:C	1:A:103:TYR:CD1	2.88	0.47
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.14	0.47
1:A:524:ASP:HA	1:A:527:LYS:HB2	1.96	0.47
1:A:644:THR:HG23	1:A:645:ASN:H	1.80	0.47
1:A:796:PHE:CB	1:A:797:PRO:HD2	2.22	0.47
1:A:806:ARG:HG2	1:A:806:ARG:NH1	2.29	0.47
1:A:873:GLU:HA	1:A:877:ILE:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:HB1	1:B:229:ARG:HB2	1.96	0.47
1:B:370:PHE:CD1	1:B:371:ASN:N	2.82	0.47
1:B:530:ILE:C	1:B:532:LYS:N	2.68	0.47
1:B:562:LEU:HA	1:B:562:LEU:HD12	1.56	0.47
1:A:188:TYR:CD1	1:A:189:MET:N	2.75	0.47
1:A:674:MET:HB2	1:A:676:ASN:ND2	2.30	0.47
1:A:831:TYR:CD2	1:A:848:TRP:CE2	3.03	0.47
1:B:166:ILE:HA	1:B:169:LYS:HG2	1.97	0.47
1:B:612:GLU:HA	1:B:612:GLU:OE1	2.15	0.47
1:A:18:ARG:NH2	1:A:210:PRO:O	2.47	0.47
1:A:692:PRO:O	1:A:693:LEU:CB	2.62	0.47
1:A:806:ARG:HH11	1:A:806:ARG:HG2	1.79	0.47
1:A:830:VAL:CG1	1:A:831:TYR:H	2.23	0.47
1:A:99:TYR:HD2	1:A:100:GLU:O	1.97	0.47
1:B:263:ILE:HD12	1:B:263:ILE:N	2.29	0.47
1:B:405:LYS:O	1:B:690:GLY:HA2	2.15	0.47
1:B:416:TYR:O	1:B:420:ILE:HG13	2.13	0.47
1:B:468:ASP:HB3	1:B:473:THR:CG2	2.44	0.47
1:B:872:LEU:HD22	1:B:877:ILE:CD1	2.45	0.47
1:A:331:VAL:O	1:A:334:ILE:N	2.48	0.47
1:A:37:LEU:HD22	1:A:83:LEU:O	2.15	0.47
1:B:213:LEU:HA	1:B:213:LEU:HD12	1.72	0.47
1:A:156:TYR:HD1	1:A:156:TYR:N	2.12	0.47
1:A:275:ASP:O	1:A:279:LYS:HG2	2.15	0.47
1:A:288:TYR:HA	1:A:293:ILE:HD11	1.95	0.47
1:B:551:ALA:O	1:B:554:THR:HG22	2.14	0.47
1:A:300:VAL:HG23	1:A:301:GLY:N	2.30	0.47
1:A:389:GLN:NE2	1:A:390:PRO:HD2	2.30	0.47
1:A:503:LEU:HA	1:A:506:PRO:HB3	1.97	0.47
1:A:570:LEU:HD23	1:A:575:PHE:CD2	2.50	0.47
1:A:644:THR:HG23	1:A:645:ASN:N	2.30	0.47
1:B:616:PHE:HE1	1:B:631:LYS:HB2	1.80	0.47
1:A:101:ILE:HG22	1:A:102:LYS:H	1.78	0.47
1:A:103:TYR:HE2	1:A:346:ASP:CA	2.18	0.47
1:A:211:VAL:HG12	1:A:212:ILE:CG1	2.45	0.47
1:A:420:ILE:HD12	1:A:420:ILE:N	2.30	0.47
1:A:570:LEU:HD23	1:A:570:LEU:HA	1.56	0.47
1:B:338:ARG:HA	1:B:338:ARG:HD2	1.57	0.47
1:B:415:LEU:HA	1:B:415:LEU:HD12	1.61	0.47
1:B:392:PRO:HG2	1:B:587:THR:HG23	1.95	0.47
1:B:589:PHE:C	1:B:589:PHE:CD1	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:ALA:HB1	1:B:767:PHE:CE2	2.49	0.47
1:A:113:PHE:HE1	1:A:218:VAL:CG2	2.27	0.47
1:A:115:ILE:HD12	1:A:116:GLU:N	2.29	0.47
1:A:188:TYR:HE1	1:A:190:PRO:HB3	1.80	0.47
1:A:335:ASP:O	1:A:339:GLN:HA	2.15	0.47
1:A:897:LEU:H	1:A:897:LEU:CD1	2.24	0.47
1:B:182:ILE:O	1:B:186:ILE:CD1	2.62	0.47
1:B:386:HIS:HB3	1:B:387:PRO:HD2	1.96	0.47
1:B:412:LEU:HA	1:B:412:LEU:HD13	1.76	0.47
1:B:427:PRO:O	1:B:430:ILE:HG22	2.14	0.47
1:B:775:ASN:O	1:B:778:SER:OG	2.31	0.47
1:B:804:HIS:HB2	1:B:805:ILE:H	1.55	0.47
1:B:821:ALA:N	1:B:822:PRO:HD2	2.30	0.47
1:A:162:TRP:CE3	1:A:188:TYR:CE2	3.02	0.46
1:A:522:PHE:O	1:A:523:SER:CB	2.63	0.46
1:A:89:LYS:HB2	1:A:89:LYS:NZ	2.30	0.46
1:A:702:TRP:CZ3	1:A:708:TYR:CD2	3.03	0.46
1:B:112:ASN:HA	1:B:214:THR:HG22	1.96	0.46
1:B:188:TYR:O	1:B:189:MET:HG3	2.15	0.46
1:B:195:LYS:CD	1:B:195:LYS:H	2.23	0.46
1:B:268:ILE:HD12	1:B:269:SER:N	2.30	0.46
1:A:337:LYS:HG3	1:A:338:ARG:N	2.30	0.46
1:A:339:GLN:HE21	1:A:339:GLN:CA	2.27	0.46
1:A:491:ALA:HA	1:A:494:ARG:NH2	2.29	0.46
1:A:495:ASN:OD1	1:A:521:ASP:HA	2.15	0.46
1:A:663:ILE:H	1:A:663:ILE:HD12	1.80	0.46
1:B:216:TRP:C	1:B:218:VAL:N	2.69	0.46
1:A:155:PRO:HG2	1:A:156:TYR:HD1	1.80	0.46
1:A:15:ILE:HG21	1:A:92:TYR:CE2	2.51	0.46
1:A:426:SER:HB2	1:A:472:PRO:HD2	1.98	0.46
1:B:118:THR:HB	1:B:134:ASP:OD2	2.15	0.46
1:B:896:SER:O	1:B:898:PHE:N	2.49	0.46
1:A:156:TYR:CD1	1:A:156:TYR:N	2.83	0.46
1:A:236:GLU:O	1:A:239:ALA:N	2.48	0.46
1:A:234:PHE:HB3	1:A:238:THR:HG21	1.98	0.46
1:A:692:PRO:O	1:A:693:LEU:HB3	2.15	0.46
1:A:878:LYS:HB3	1:A:879:PRO:CD	2.46	0.46
1:B:472:PRO:O	1:B:473:THR:C	2.54	0.46
1:B:653:LYS:HA	1:B:653:LYS:HD2	1.62	0.46
1:B:4:PHE:CA	1:B:97:TYR:HE2	2.25	0.46
1:A:178:VAL:HG12	1:A:183:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:THR:HG21	1:A:891:TYR:HD2	1.80	0.46
1:B:23:ASN:ND2	1:B:25:ARG:HD2	2.31	0.46
1:B:365:TRP:HA	1:B:368:ILE:HG13	1.97	0.46
1:B:596:TRP:CB	1:B:670:MET:HE1	2.45	0.46
1:B:640:LYS:O	1:B:640:LYS:HG3	2.16	0.46
1:B:183:ILE:HA	1:B:186:ILE:HD13	1.97	0.46
1:B:129:ALA:HA	1:B:225:TYR:CZ	2.51	0.46
1:B:604:TYR:HD1	1:B:605:LEU:N	2.13	0.46
1:A:303:LEU:HB3	1:A:323:TYR:HD1	1.80	0.46
1:A:49:TYR:HA	1:A:377:ASN:O	2.16	0.46
1:A:408:MET:HE2	1:A:685:ARG:HG3	1.97	0.46
1:A:691:PRO:HA	1:A:692:PRO:HD3	1.73	0.46
1:A:799:PRO:O	1:A:800:LYS:HB3	2.16	0.46
1:A:818:ASN:O	1:A:822:PRO:CD	2.64	0.46
1:A:835:LEU:HG	1:A:845:CYS:HA	1.98	0.46
1:A:856:ASP:HA	1:A:859:LYS:CB	2.46	0.46
1:B:115:ILE:C	1:B:115:ILE:HD12	2.36	0.46
1:B:35:PRO:HG2	1:B:62:PHE:HB2	1.96	0.46
1:B:71:TRP:HZ3	1:B:82:ALA:HB1	1.81	0.46
1:A:169:LYS:HA	1:A:169:LYS:NZ	2.30	0.46
1:A:240:LYS:O	1:A:242:LEU:N	2.49	0.46
1:A:182:ILE:O	1:A:185:LYS:HB2	2.16	0.46
1:A:606:ASN:C	1:A:606:ASN:HD22	2.20	0.46
1:A:659:MET:HB3	1:A:660:GLU:H	1.55	0.46
1:A:757:GLU:O	1:A:761:GLN:HG3	2.15	0.46
1:B:726:LYS:HA	1:B:726:LYS:HD2	1.76	0.46
1:B:794:GLY:C	1:B:796:PHE:H	2.19	0.46
1:A:365:TRP:CE3	1:A:368:ILE:HD12	2.52	0.45
1:A:579:ASP:O	1:A:582:ASN:HB2	2.16	0.45
1:A:663:ILE:HG12	1:A:683:MET:CE	2.46	0.45
1:A:863:LEU:HD12	1:A:863:LEU:H	1.81	0.45
1:A:772:ARG:HA	1:A:868:TYR:CE2	2.51	0.45
1:A:214:THR:HG21	1:A:273:TYR:HD1	1.82	0.45
1:A:394:ALA:CB	1:A:622:THR:HG23	2.45	0.45
1:B:566:LEU:O	1:B:569:ALA:N	2.49	0.45
1:B:605:LEU:O	1:B:608:VAL:HG12	2.16	0.45
1:B:776:TYR:CD2	1:B:777:ILE:HG12	2.52	0.45
1:A:211:VAL:HG12	1:A:212:ILE:N	2.31	0.45
1:B:502:ALA:HB1	1:B:531:LYS:HA	1.98	0.45
1:B:788:ILE:O	1:B:791:TYR:HB3	2.16	0.45
1:B:880:LEU:HA	1:B:883:PHE:HE2	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:HB3	1:A:128:GLN:NE2	2.32	0.45
1:A:409:SER:OG	1:A:686:GLU:HG3	2.16	0.45
1:A:491:ALA:O	1:A:495:ASN:HB2	2.16	0.45
1:A:499:ILE:CG2	1:A:542:LEU:HB2	2.46	0.45
1:B:304:LYS:O	1:B:319:ARG:HD3	2.17	0.45
1:B:382:GLN:HG3	1:B:383:GLY:N	2.31	0.45
1:B:828:GLU:CG	1:B:829:LYS:H	2.28	0.45
1:B:828:GLU:HA	1:B:828:GLU:OE1	2.15	0.45
1:B:897:LEU:CD1	1:B:897:LEU:N	2.80	0.45
1:A:178:VAL:CG1	1:A:183:ILE:HD11	2.45	0.45
1:A:325:ILE:O	1:A:326:ILE:C	2.54	0.45
1:A:397:LYS:HG2	1:A:398:GLU:O	2.17	0.45
1:A:540:GLU:HG3	1:A:544:ARG:CZ	2.45	0.45
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.81	0.45
1:A:347:MET:HA	1:A:558:ASN:HD21	1.81	0.45
1:A:576:ARG:CD	1:A:577:TYR:CE1	2.96	0.45
1:A:855:THR:CB	1:A:857:LEU:HD21	2.46	0.45
1:B:145:ARG:HB2	1:B:147:TYR:HE1	1.82	0.45
1:B:416:TYR:HD2	1:B:567:TYR:CG	2.35	0.45
1:B:489:MET:SD	1:B:553:MET:CE	3.05	0.45
1:B:48:LYS:O	1:B:49:TYR:HB2	2.17	0.45
1:A:115:ILE:C	1:A:115:ILE:HD12	2.37	0.45
1:A:218:VAL:HG22	1:A:223:ILE:HD11	1.99	0.45
1:A:329:TYR:O	1:A:332:LEU:HB2	2.17	0.45
1:A:391:TYR:N	1:A:391:TYR:CD1	2.85	0.45
1:A:8:VAL:O	1:A:8:VAL:HG23	2.17	0.45
1:B:112:ASN:HA	1:B:214:THR:CG2	2.47	0.45
1:B:137:THR:HB	1:B:328:VAL:HG21	1.99	0.45
1:B:409:SER:HB3	1:B:626:TYR:CD2	2.52	0.45
1:B:5:TYR:H	1:B:5:TYR:HD1	1.64	0.45
1:A:131:HIS:CD2	1:A:131:HIS:N	2.84	0.45
1:A:274:ILE:O	1:A:277:TYR:HB3	2.16	0.45
1:A:342:ASN:O	1:A:345:LEU:HB2	2.16	0.45
1:A:51:ASP:OD1	1:A:53:TYR:HB2	2.17	0.45
1:B:19:TYR:HD1	1:B:19:TYR:N	2.15	0.45
1:B:431:ALA:CB	1:B:454:TYR:CD2	2.99	0.45
1:B:597:ILE:HD12	1:B:597:ILE:HA	1.91	0.45
1:B:877:ILE:HD12	1:B:877:ILE:N	2.30	0.45
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.88	0.45
1:A:298:LEU:HB2	1:A:300:VAL:HG22	1.98	0.45
1:A:439:LEU:O	1:A:442:TYR:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:ASP:HA	1:A:859:LYS:HB2	1.98	0.45
1:B:162:TRP:HE3	1:B:188:TYR:CD2	2.34	0.45
1:B:167:ALA:HB1	1:B:178:VAL:CG2	2.46	0.45
1:B:700:GLY:HA3	1:B:710:LEU:HD23	1.99	0.45
1:B:731:GLU:HB3	1:B:734:LYS:HD2	1.98	0.45
1:B:733:GLN:CD	1:B:733:GLN:H	2.19	0.45
1:A:291:ASP:HB3	1:A:302:LYS:CG	2.46	0.45
1:A:698:ILE:HD11	1:A:752:MET:HB3	1.99	0.45
1:B:389:GLN:HA	1:B:389:GLN:HE21	1.82	0.45
1:B:686:GLU:HG3	1:B:687:ALA:N	2.32	0.45
1:B:811:TYR:O	1:B:815:ILE:HB	2.17	0.45
2:B:999:GMP:O5'	2:B:999:GMP:H2'	2.16	0.45
1:A:334:ILE:O	1:A:335:ASP:C	2.53	0.44
1:A:507:ASN:N	1:A:534:SER:HA	2.32	0.44
1:A:596:TRP:CZ3	1:A:599:ARG:NH2	2.85	0.44
1:A:689:ALA:HB1	1:A:711:ASN:O	2.17	0.44
1:A:700:GLY:N	1:A:753:LEU:HD22	2.32	0.44
1:B:204:PHE:O	1:B:207:GLN:HB3	2.17	0.44
1:A:105:HIS:C	1:A:107:LYS:N	2.70	0.44
1:A:489:MET:HG2	1:A:489:MET:O	2.16	0.44
1:A:689:ALA:HB1	1:A:711:ASN:C	2.37	0.44
1:A:800:LYS:HG2	1:A:800:LYS:O	2.17	0.44
1:A:902:ASP:N	1:A:902:ASP:OD1	2.51	0.44
1:A:18:ARG:HA	1:A:27:ARG:O	2.17	0.44
1:A:137:THR:HG21	1:A:325:ILE:HA	1.99	0.44
1:A:92:TYR:CD1	1:A:92:TYR:C	2.90	0.44
1:B:820:ASP:O	1:B:822:PRO:N	2.49	0.44
1:B:834:PRO:O	1:B:835:LEU:CB	2.65	0.44
1:A:103:TYR:O	1:A:103:TYR:CD1	2.71	0.44
1:A:116:GLU:HG2	1:A:324:ASN:HD21	1.82	0.44
1:B:15:ILE:HA	1:B:15:ILE:HD13	1.69	0.44
1:B:170:LEU:C	1:B:172:GLU:H	2.21	0.44
1:A:832:VAL:O	1:A:833:LEU:HG	2.17	0.44
1:B:218:VAL:HG22	1:B:223:ILE:HG13	1.98	0.44
1:B:126:PRO:HG3	1:B:221:PHE:CD1	2.52	0.44
1:B:605:LEU:HB3	1:B:616:PHE:CE2	2.53	0.44
1:B:698:ILE:HD12	1:B:753:LEU:HD23	2.00	0.44
1:A:17:GLU:O	1:A:28:THR:HA	2.17	0.44
1:A:1:MET:HB3	1:A:22:SER:O	2.18	0.44
1:A:280:PHE:HD2	1:A:343:LEU:HD13	1.81	0.44
1:A:65:MET:HE1	1:A:88:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:TYR:N	1:A:97:TYR:CD1	2.85	0.44
1:B:216:TRP:C	1:B:218:VAL:H	2.21	0.44
1:B:343:LEU:C	1:B:345:LEU:N	2.71	0.44
1:B:834:PRO:HG2	1:B:871:LEU:HB2	1.99	0.44
1:A:139:TYR:CE2	1:A:141:SER:HA	2.52	0.44
1:A:145:ARG:HB2	1:A:147:TYR:HE1	1.81	0.44
1:A:126:PRO:HG3	1:A:221:PHE:CE1	2.52	0.44
1:A:713:TRP:CZ2	1:A:723:PRO:HG3	2.53	0.44
1:A:72:ILE:O	1:A:73:LYS:C	2.55	0.44
1:A:888:LYS:O	1:A:889:LEU:HD23	2.17	0.44
1:B:528:GLU:C	1:B:530:ILE:H	2.21	0.44
1:B:550:VAL:O	1:B:553:MET:HG3	2.18	0.44
1:B:605:LEU:C	1:B:607:GLU:N	2.71	0.44
1:B:606:ASN:HB2	1:B:611:THR:C	2.37	0.44
1:B:412:LEU:HD22	1:B:683:MET:HB2	1.99	0.44
1:A:1:MET:O	1:A:22:SER:HA	2.18	0.44
1:A:253:ILE:CG2	1:A:254:GLU:N	2.81	0.44
1:A:402:ASN:HB3	1:A:404:TYR:CZ	2.53	0.44
1:B:194:GLU:O	1:B:197:LEU:HB3	2.18	0.44
1:B:233:ILE:HG13	1:B:234:PHE:CE1	2.50	0.44
1:B:292:TYR:C	1:B:292:TYR:CD1	2.91	0.44
1:B:785:ALA:C	1:B:787:ASN:N	2.69	0.44
1:B:97:TYR:CD1	1:B:97:TYR:N	2.86	0.44
1:A:112:ASN:C	1:A:112:ASN:HD22	2.18	0.44
1:A:187:ILE:O	1:A:187:ILE:HG22	2.17	0.44
1:A:265:LEU:CB	1:A:268:ILE:HD11	2.47	0.44
1:A:339:GLN:NE2	1:A:339:GLN:CA	2.81	0.44
1:A:33:TYR:CD2	1:A:65:MET:CE	3.01	0.44
1:A:832:VAL:H	1:A:847:ALA:CB	2.31	0.44
1:B:110:VAL:HG12	1:B:111:ALA:H	1.83	0.44
1:B:332:LEU:HD13	1:B:332:LEU:HA	1.73	0.44
1:B:503:LEU:HD11	1:B:539:ASN:ND2	2.33	0.44
1:B:389:GLN:HB3	1:B:580:LEU:HD22	2.00	0.44
1:B:454:TYR:O	1:B:675:ASN:HB3	2.18	0.44
1:B:693:LEU:C	1:B:695:SER:H	2.21	0.44
1:B:880:LEU:HA	1:B:883:PHE:HD2	1.80	0.44
1:A:401:PRO:O	1:A:402:ASN:HB2	2.17	0.43
1:A:407:VAL:HA	1:A:627:VAL:O	2.17	0.43
1:A:62:PHE:CE2	1:A:68:ALA:HA	2.53	0.43
1:A:751:ARG:CZ	1:A:763:TYR:HB2	2.47	0.43
1:B:846:ILE:HG22	1:B:847:ALA:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:PRO:O	1:B:882:GLY:N	2.51	0.43
1:A:555:ALA:HA	1:A:558:ASN:HB2	1.99	0.43
1:A:772:ARG:HA	1:A:868:TYR:HE2	1.83	0.43
1:B:124:PRO:O	1:B:126:PRO:HD3	2.17	0.43
1:B:601:VAL:O	1:B:604:TYR:HB3	2.17	0.43
1:B:806:ARG:NH1	1:B:806:ARG:HG2	2.33	0.43
1:A:855:THR:HG22	1:A:857:LEU:CD2	2.49	0.43
1:B:404:TYR:CG	1:B:618:LEU:HD11	2.53	0.43
1:B:450:PRO:O	1:B:451:SER:O	2.35	0.43
1:B:49:TYR:HA	1:B:377:ASN:O	2.18	0.43
1:B:752:MET:HG2	1:B:760:LEU:CD1	2.48	0.43
1:A:115:ILE:CD1	1:A:117:VAL:HG23	2.49	0.43
1:A:188:TYR:CE1	1:A:190:PRO:HD3	2.53	0.43
1:A:744:ALA:O	1:A:747:GLU:N	2.51	0.43
1:A:767:PHE:O	1:A:768:GLU:CB	2.65	0.43
1:A:772:ARG:HH11	1:A:772:ARG:CG	2.29	0.43
1:B:194:GLU:O	1:B:197:LEU:N	2.52	0.43
1:B:859:LYS:O	1:B:862:VAL:HB	2.18	0.43
1:A:189:MET:O	1:A:191:PHE:HE1	2.01	0.43
1:A:526:ILE:O	1:A:530:ILE:HG12	2.19	0.43
1:A:503:LEU:HD21	1:A:539:ASN:ND2	2.33	0.43
1:A:576:ARG:HB3	1:A:577:TYR:CE1	2.54	0.43
1:A:656:ARG:HG2	1:A:656:ARG:O	2.18	0.43
1:A:831:TYR:HD2	1:A:848:TRP:CE2	2.37	0.43
1:B:139:TYR:HE1	1:B:144:ASP:CA	2.31	0.43
1:B:243:SER:HB3	1:B:247:LYS:N	2.34	0.43
1:B:253:ILE:HG22	1:B:260:ARG:CA	2.46	0.43
1:B:806:ARG:HH11	1:B:806:ARG:HG2	1.83	0.43
1:A:223:ILE:HB	1:A:224:PRO:CD	2.41	0.43
1:A:289:SER:O	1:A:290:LEU:C	2.57	0.43
1:A:331:VAL:HG12	1:A:332:LEU:N	2.34	0.43
1:A:632:ILE:O	1:A:635:LYS:HB3	2.17	0.43
1:A:745:LEU:O	1:A:746:LYS:C	2.57	0.43
1:A:830:VAL:HG13	1:A:848:TRP:C	2.39	0.43
1:A:899:ASP:C	1:A:901:PHE:H	2.22	0.43
1:B:105:HIS:C	1:B:107:LYS:N	2.71	0.43
1:B:199:MET:O	1:B:202:LEU:HB3	2.17	0.43
1:B:243:SER:HB3	1:B:247:LYS:H	1.83	0.43
1:B:243:SER:O	1:B:246:ARG:HD2	2.18	0.43
1:B:494:ARG:O	1:B:498:ILE:CD1	2.66	0.43
1:B:411:ASP:HA	1:B:623:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:LYS:C	1:B:792:ASP:H	2.22	0.43
1:B:9:GLU:HG2	1:B:266:PHE:CD2	2.53	0.43
1:A:163:SER:HB3	1:A:166:ILE:CD1	2.42	0.43
1:A:804:HIS:HB2	1:A:805:ILE:H	1.68	0.43
1:B:835:LEU:HD12	1:B:839:ASN:ND2	2.33	0.43
1:A:215:GLY:HA3	1:A:218:VAL:HB	2.00	0.43
1:A:330:ARG:HA	1:A:333:GLN:NE2	2.32	0.43
1:A:797:PRO:HB2	1:A:798:GLY:H	1.65	0.43
1:A:894:LYS:O	1:A:896:SER:N	2.51	0.43
1:B:170:LEU:C	1:B:172:GLU:N	2.72	0.43
1:B:373:LEU:O	1:B:374:LYS:C	2.57	0.43
1:B:601:VAL:HG12	1:B:602:ASN:N	2.34	0.43
1:B:680:LEU:N	1:B:680:LEU:HD23	2.27	0.43
1:B:731:GLU:HA	1:B:734:LYS:HG3	2.00	0.43
1:B:831:TYR:O	1:B:832:VAL:CB	2.67	0.43
1:B:861:ASP:O	1:B:864:HIS:HB3	2.19	0.43
1:A:407:VAL:CG1	1:A:408:MET:N	2.82	0.43
1:A:762:GLU:HG3	1:A:763:TYR:N	2.34	0.43
1:B:109:ARG:HB3	1:B:211:VAL:HG23	2.01	0.43
1:B:606:ASN:HB3	1:B:614:GLU:HB2	2.01	0.43
1:B:790:LYS:O	1:B:792:ASP:N	2.52	0.43
1:B:828:GLU:HG3	1:B:829:LYS:H	1.83	0.43
1:A:300:VAL:HG23	1:A:301:GLY:H	1.83	0.43
1:A:740:ALA:HB2	1:A:778:SER:CB	2.47	0.43
1:B:130:LYS:H	1:B:130:LYS:HG3	1.45	0.43
1:B:511:ASP:HB2	1:B:534:SER:CB	2.48	0.43
1:B:51:ASP:O	1:B:53:TYR:N	2.52	0.43
1:A:191:PHE:CD2	1:A:197:LEU:HA	2.54	0.42
1:A:901:PHE:N	1:A:901:PHE:CD1	2.84	0.42
1:B:143:ASP:C	1:B:145:ARG:N	2.71	0.42
1:B:253:ILE:CG1	1:B:254:GLU:N	2.63	0.42
1:B:262:ILE:O	1:B:262:ILE:HD12	2.19	0.42
1:B:343:LEU:O	1:B:346:ASP:N	2.52	0.42
1:B:408:MET:HE1	1:B:655:ALA:HB2	2.00	0.42
1:B:601:VAL:O	1:B:602:ASN:C	2.57	0.42
1:B:645:ASN:OD1	1:B:645:ASN:C	2.57	0.42
1:B:653:LYS:HA	1:B:656:ARG:HH12	1.84	0.42
1:A:308:PRO:HD2	1:A:311:LYS:CB	2.48	0.42
1:A:508:LEU:HD13	1:A:531:LYS:O	2.19	0.42
1:A:663:ILE:HG21	1:A:683:MET:HE2	2.01	0.42
1:B:293:ILE:HG22	1:B:294:SER:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:PRO:HD2	1:B:311:LYS:HG3	2.02	0.42
1:B:656:ARG:HH11	1:B:656:ARG:HB3	1.83	0.42
1:B:456:CYS:O	1:B:674:MET:HB3	2.18	0.42
1:B:745:LEU:HA	1:B:745:LEU:HD23	1.61	0.42
1:A:176:ASP:O	1:A:177:GLU:HB2	2.19	0.42
1:A:406:TYR:HB3	1:A:629:ALA:HB3	2.01	0.42
1:A:647:TRP:O	1:A:650:PHE:N	2.52	0.42
1:A:714:ASP:OD1	1:A:717:GLY:N	2.52	0.42
1:A:763:TYR:HE1	1:A:767:PHE:CB	2.31	0.42
1:B:112:ASN:O	1:B:113:PHE:HB3	2.19	0.42
1:B:189:MET:O	1:B:191:PHE:CE1	2.71	0.42
1:B:341:ILE:O	1:B:345:LEU:CD2	2.67	0.42
1:B:352:LYS:N	1:B:352:LYS:HD3	2.34	0.42
1:B:604:TYR:O	1:B:607:GLU:HB3	2.19	0.42
1:B:643:ASP:O	1:B:646:HIS:CB	2.68	0.42
1:B:690:GLY:O	1:B:713:TRP:NE1	2.52	0.42
1:A:15:ILE:HD13	1:A:15:ILE:HA	1.75	0.42
1:A:190:PRO:C	1:A:191:PHE:CD1	2.92	0.42
1:A:232:ASN:ND2	1:A:232:ASN:N	2.60	0.42
1:A:446:VAL:O	1:A:446:VAL:HG12	2.19	0.42
1:B:256:MET:O	1:B:257:TYR:CD1	2.73	0.42
1:B:664:ASP:O	1:B:668:ARG:HG3	2.20	0.42
1:B:713:TRP:CZ3	1:B:723:PRO:HD3	2.54	0.42
1:B:840:PRO:HD2	1:B:865:TRP:CD1	2.55	0.42
1:A:680:LEU:CD2	1:A:680:LEU:H	2.24	0.42
1:B:246:ARG:HD2	1:B:246:ARG:N	2.33	0.42
1:B:305:TYR:CE1	1:B:307:GLY:O	2.73	0.42
1:B:52:ILE:CD1	1:B:52:ILE:N	2.80	0.42
1:B:596:TRP:CE2	1:B:670:MET:HB2	2.54	0.42
1:B:710:LEU:HD23	1:B:710:LEU:HA	1.84	0.42
1:B:730:LEU:O	1:B:732:THR:N	2.52	0.42
1:A:36:SER:HB2	2:A:999:GMP:O4'	2.20	0.42
1:A:791:TYR:CD1	1:A:791:TYR:C	2.92	0.42
1:B:290:LEU:O	1:B:290:LEU:HD12	2.19	0.42
1:B:591:GLN:O	1:B:595:GLN:HG2	2.19	0.42
1:B:660:GLU:N	1:B:661:PRO:CD	2.83	0.42
1:A:420:ILE:CD1	1:A:420:ILE:H	2.33	0.42
1:A:422:GLN:HE21	1:A:422:GLN:HB2	1.55	0.42
1:A:767:PHE:HD1	1:A:768:GLU:N	2.18	0.42
1:B:13:ASP:O	1:B:32:GLU:HA	2.20	0.42
1:B:162:TRP:HE3	1:B:188:TYR:CE2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLN:HA	1:B:390:PRO:HD3	1.83	0.42
1:B:391:TYR:HD1	1:B:391:TYR:N	2.17	0.42
1:B:426:SER:OG	1:B:427:PRO:HD2	2.20	0.42
1:B:789:ALA:HA	1:B:805:ILE:HG21	2.01	0.42
1:B:96:THR:C	1:B:97:TYR:CD1	2.93	0.42
1:A:188:TYR:CD1	1:A:190:PRO:HD3	2.55	0.42
1:A:255:ASN:HB3	1:A:257:TYR:CE2	2.55	0.42
1:A:600:LYS:HD3	1:A:600:LYS:HA	1.82	0.42
1:A:605:LEU:C	1:A:607:GLU:H	2.23	0.42
1:A:786:ASN:O	1:A:788:ILE:N	2.53	0.42
1:B:18:ARG:HH22	1:B:211:VAL:HA	1.83	0.42
1:B:330:ARG:HD2	1:B:333:GLN:HE22	1.85	0.42
1:B:859:LYS:HD2	1:B:860:ASP:OD1	2.19	0.42
1:A:226:VAL:O	1:A:230:ILE:HG13	2.20	0.42
1:A:373:LEU:HG	1:A:378:LYS:HB2	2.01	0.42
1:A:605:LEU:C	1:A:607:GLU:N	2.73	0.42
1:B:246:ARG:HD2	1:B:246:ARG:H	1.85	0.42
1:B:37:LEU:HA	1:B:37:LEU:HD23	1.83	0.42
1:B:414:SER:HB2	1:B:417:PRO:HG2	2.01	0.42
1:B:872:LEU:HD22	1:B:877:ILE:HD11	2.02	0.42
1:B:92:TYR:C	1:B:92:TYR:HD1	2.22	0.42
1:A:420:ILE:HD12	1:A:420:ILE:H	1.84	0.42
1:A:655:ALA:O	1:A:659:MET:HB3	2.20	0.42
1:A:695:SER:HB2	1:A:754:GLN:O	2.20	0.42
1:B:153:ASN:HA	1:B:158:ASN:ND2	2.35	0.42
1:B:404:TYR:CD1	1:B:618:LEU:HD11	2.55	0.42
1:B:454:TYR:N	1:B:454:TYR:CD1	2.88	0.42
1:B:488:TYR:CD2	1:B:519:ARG:HG2	2.55	0.42
1:B:51:ASP:C	1:B:53:TYR:N	2.72	0.42
1:B:625:ILE:CD1	1:B:683:MET:SD	3.08	0.42
1:A:113:PHE:CD1	1:A:113:PHE:C	2.92	0.41
1:A:409:SER:C	1:A:410:PHE:CD1	2.93	0.41
1:A:450:PRO:O	1:A:451:SER:O	2.37	0.41
1:A:489:MET:SD	1:A:553:MET:HB2	2.60	0.41
1:A:567:TYR:CD1	1:A:567:TYR:O	2.73	0.41
1:A:64:ASN:OD1	1:A:66:ARG:N	2.53	0.41
1:A:807:GLY:HA2	1:A:845:CYS:O	2.20	0.41
1:B:680:LEU:H	1:B:680:LEU:CD2	2.27	0.41
1:A:312:LEU:HA	1:A:312:LEU:HD23	1.83	0.41
1:A:353:ILE:CG1	1:A:357:SER:HB2	2.50	0.41
1:B:198:LEU:CD1	1:B:233:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:HB3	1:B:67:ASP:OD2	2.20	0.41
1:B:738:PRO:HG3	1:B:781:SER:HA	2.01	0.41
1:B:776:TYR:O	1:B:779:ILE:CG1	2.68	0.41
1:A:763:TYR:O	1:A:764:PHE:C	2.58	0.41
1:B:1:MET:HB3	1:B:22:SER:HA	2.02	0.41
1:B:345:LEU:HA	1:B:345:LEU:HD13	1.83	0.41
1:B:347:MET:HE2	1:B:358:VAL:HG22	2.02	0.41
1:B:389:GLN:CD	1:B:390:PRO:HD2	2.41	0.41
1:B:531:LYS:H	1:B:531:LYS:HG3	1.53	0.41
1:B:728:MET:HA	1:B:728:MET:HE1	2.01	0.41
1:A:147:TYR:CD2	1:A:204:PHE:CE1	3.07	0.41
1:A:274:ILE:CG1	1:A:278:LYS:HE3	2.51	0.41
1:A:330:ARG:O	1:A:334:ILE:HG13	2.21	0.41
1:A:431:ALA:HB2	1:A:464:TYR:CE1	2.55	0.41
1:A:489:MET:HE3	1:A:490:LEU:HG	2.02	0.41
1:A:547:ARG:O	1:A:550:VAL:HB	2.20	0.41
1:A:570:LEU:HD23	1:A:575:PHE:HD2	1.85	0.41
1:A:604:TYR:CD1	1:A:604:TYR:C	2.93	0.41
1:B:169:LYS:HB3	1:B:169:LYS:HE3	1.93	0.41
1:B:109:ARG:HD2	1:B:210:PRO:HA	2.03	0.41
1:B:402:ASN:ND2	1:B:403:ARG:H	2.18	0.41
1:B:422:GLN:HE21	1:B:422:GLN:HB2	1.48	0.41
1:B:5:TYR:HA	1:B:19:TYR:HB3	2.02	0.41
1:B:776:TYR:O	1:B:779:ILE:HG12	2.19	0.41
1:B:858:ILE:HG13	1:B:859:LYS:H	1.84	0.41
1:A:663:ILE:HG12	1:A:683:MET:HE1	2.01	0.41
1:B:178:VAL:HA	1:B:179:PRO:HD3	1.87	0.41
1:B:150:ASP:HB3	1:B:190:PRO:HA	2.03	0.41
1:B:330:ARG:HA	1:B:333:GLN:HE21	1.80	0.41
1:B:335:ASP:O	1:B:339:GLN:HA	2.20	0.41
1:A:125:GLU:HB3	1:A:128:GLN:HE22	1.83	0.41
1:A:113:PHE:CE1	1:A:218:VAL:HG23	2.55	0.41
1:A:400:ILE:HA	1:A:401:PRO:HD3	1.86	0.41
1:A:621:ASP:O	1:A:623:ASP:N	2.50	0.41
1:A:663:ILE:N	1:A:663:ILE:HD12	2.35	0.41
1:A:745:LEU:O	1:A:748:CYS:N	2.54	0.41
1:B:243:SER:CB	1:B:247:LYS:H	2.33	0.41
1:B:373:LEU:O	1:B:376:GLN:HB2	2.20	0.41
1:B:760:LEU:O	1:B:761:GLN:C	2.59	0.41
1:B:807:GLY:O	1:B:810:THR:CG2	2.67	0.41
1:A:253:ILE:HG22	1:A:254:GLU:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.41
1:A:343:LEU:O	1:A:346:ASP:HB3	2.20	0.41
1:A:373:LEU:O	1:A:376:GLN:HB3	2.20	0.41
1:B:139:TYR:CD1	1:B:140:ASP:N	2.89	0.41
1:B:157:GLY:O	1:B:313:ARG:NH2	2.46	0.41
1:B:182:ILE:O	1:B:186:ILE:HD13	2.20	0.41
1:B:41:CYS:SG	1:B:45:GLN:HB2	2.61	0.41
1:B:462:MET:HE2	1:B:462:MET:HB2	1.84	0.41
1:B:512:GLU:OE1	1:B:513:PRO:HD2	2.21	0.41
1:B:792:ASP:O	1:B:794:GLY:N	2.53	0.41
1:B:51:ASP:HB3	1:B:83:LEU:CD2	2.51	0.41
1:A:189:MET:O	1:A:191:PHE:CE1	2.73	0.41
1:A:9:GLU:HG3	1:A:266:PHE:CE1	2.56	0.41
1:A:364:THR:O	1:A:367:ALA:HB3	2.19	0.41
1:A:364:THR:O	1:A:368:ILE:HG13	2.20	0.41
1:A:629:ALA:O	1:A:630:ASP:C	2.58	0.41
1:A:633:ILE:HD13	1:A:633:ILE:HA	1.88	0.41
1:A:866:MET:HE2	1:A:868:TYR:CD1	2.56	0.41
1:B:293:ILE:HG23	1:B:297:GLU:HG3	2.03	0.41
1:B:345:LEU:O	1:B:349:TYR:HB2	2.21	0.41
1:B:456:CYS:HB3	1:B:462:MET:H	1.85	0.41
1:B:475:ILE:HD11	1:B:566:LEU:CD2	2.46	0.41
1:B:570:LEU:HA	1:B:570:LEU:HD23	1.44	0.41
1:B:597:ILE:HB	1:B:667:PHE:HE1	1.82	0.41
1:B:767:PHE:O	1:B:768:GLU:HB3	2.20	0.41
1:A:109:ARG:HH12	1:A:142:ILE:HG21	1.86	0.41
1:A:108:ILE:HG22	1:A:211:VAL:HG11	2.03	0.41
1:A:363:LYS:HD3	1:A:363:LYS:HA	1.77	0.41
1:A:434:PHE:HD1	1:A:462:MET:SD	2.43	0.41
1:A:457:SER:HA	1:A:458:PRO:HD3	1.69	0.41
1:A:656:ARG:HA	1:A:660:GLU:HG3	2.02	0.41
1:A:757:GLU:HG2	1:A:761:GLN:HG3	2.03	0.41
1:A:796:PHE:C	1:A:809:LEU:HD13	2.41	0.41
1:A:867:ASP:O	1:A:871:LEU:HB2	2.21	0.41
1:B:354:GLN:O	1:B:357:SER:HB2	2.21	0.41
1:B:78:ILE:HG22	1:B:80:LEU:N	2.36	0.41
1:B:816:LYS:HE2	1:B:816:LYS:HB3	1.86	0.41
1:B:877:ILE:O	1:B:878:LYS:C	2.59	0.41
1:A:347:MET:HE2	1:A:358:VAL:HG22	2.03	0.41
1:A:64:ASN:OD1	1:A:64:ASN:C	2.58	0.41
1:A:650:PHE:C	1:A:650:PHE:CD1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:LYS:CA	1:A:749:ILE:HD12	2.51	0.41
1:B:373:LEU:HA	1:B:373:LEU:HD12	1.80	0.41
1:B:592:MET:SD	1:B:670:MET:HE2	2.61	0.41
1:B:606:ASN:N	1:B:616:PHE:HE2	2.19	0.41
1:B:625:ILE:HD11	1:B:683:MET:SD	2.61	0.41
1:B:641:PHE:HE2	1:B:647:TRP:HA	1.86	0.41
1:B:770:GLU:O	1:B:771:PHE:C	2.58	0.41
1:B:815:ILE:HA	1:B:815:ILE:HD12	1.82	0.41
1:A:198:LEU:CD1	1:A:233:ILE:HD11	2.51	0.41
1:A:439:LEU:O	1:A:440:HIS:C	2.59	0.41
1:A:51:ASP:C	1:A:53:TYR:H	2.24	0.41
1:A:611:THR:O	1:A:612:GLU:OE2	2.39	0.41
1:A:751:ARG:NH1	1:A:759:SER:O	2.54	0.41
1:B:150:ASP:O	1:B:191:PHE:N	2.54	0.41
1:B:186:ILE:CD1	1:B:186:ILE:N	2.83	0.41
1:B:205:TRP:C	1:B:207:GLN:N	2.73	0.41
1:B:248:THR:HA	1:B:266:PHE:CD1	2.55	0.41
1:B:501:GLU:C	1:B:503:LEU:H	2.24	0.41
1:B:747:GLU:O	1:B:750:ARG:N	2.54	0.41
1:A:445:ALA:HA	1:A:673:TYR:CE2	2.55	0.40
1:A:391:TYR:CD2	1:A:587:THR:HG21	2.55	0.40
1:B:362:ILE:O	1:B:363:LYS:C	2.59	0.40
1:B:491:ALA:O	1:B:493:GLN:N	2.53	0.40
1:B:787:ASN:O	1:B:790:LYS:CG	2.70	0.40
1:B:791:TYR:CG	1:B:791:TYR:O	2.74	0.40
1:A:815:ILE:O	1:A:815:ILE:HG22	2.21	0.40
1:B:53:TYR:CE1	1:B:428:GLU:HA	2.48	0.40
1:B:61:LEU:HD13	1:B:61:LEU:C	2.40	0.40
1:B:876:PHE:O	1:B:879:PRO:HG2	2.20	0.40
1:A:128:GLN:O	1:A:129:ALA:HB3	2.20	0.40
1:A:228:ASN:O	1:A:229:ARG:C	2.60	0.40
1:A:365:TRP:O	1:A:366:ASP:C	2.58	0.40
1:A:419:ILE:O	1:A:420:ILE:C	2.60	0.40
1:A:858:ILE:O	1:A:859:LYS:C	2.59	0.40
1:A:861:ASP:O	1:A:862:VAL:C	2.59	0.40
1:B:205:TRP:O	1:B:209:THR:N	2.53	0.40
1:B:419:ILE:HG22	1:B:420:ILE:N	2.34	0.40
1:B:49:TYR:OH	1:B:59:ARG:HD2	2.20	0.40
1:B:645:ASN:O	1:B:646:HIS:C	2.59	0.40
1:B:64:ASN:OD1	1:B:65:MET:N	2.55	0.40
1:A:140:ASP:HB3	1:A:143:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:HD1	1:A:147:TYR:N	2.17	0.40
1:A:263:ILE:HD12	1:A:263:ILE:N	2.36	0.40
1:A:14:SER:HA	1:A:32:GLU:HA	2.03	0.40
1:A:34:LYS:HB3	1:A:34:LYS:HE3	1.77	0.40
1:A:647:TRP:O	1:A:650:PHE:CB	2.64	0.40
1:A:667:PHE:HA	1:A:667:PHE:HD1	1.73	0.40
1:A:685:ARG:HG2	1:A:686:GLU:N	2.37	0.40
1:A:738:PRO:HG3	1:A:780:ALA:O	2.21	0.40
1:B:109:ARG:HA	1:B:142:ILE:HG12	2.03	0.40
1:B:145:ARG:HE	1:B:185:LYS:HA	1.87	0.40
1:B:327:ASP:O	1:B:330:ARG:N	2.54	0.40
1:B:343:LEU:C	1:B:343:LEU:CD2	2.89	0.40
1:B:511:ASP:CB	1:B:537:SER:OG	2.67	0.40
1:B:6:LEU:CD1	1:B:211:VAL:HG11	2.51	0.40
1:B:713:TRP:CH2	1:B:723:PRO:HB3	2.57	0.40
1:B:818:ASN:HD22	1:B:819:ILE:H	1.70	0.40
1:A:198:LEU:O	1:A:199:MET:C	2.59	0.40
1:A:218:VAL:HG22	1:A:223:ILE:CD1	2.52	0.40
1:A:249:ARG:HG2	1:A:251:LYS:HE3	2.03	0.40
1:A:274:ILE:HG12	1:A:278:LYS:HE3	2.03	0.40
1:A:351:ALA:HB3	1:A:353:ILE:CG2	2.52	0.40
1:A:34:LYS:CE	1:A:63:ALA:HA	2.51	0.40
1:A:746:LYS:HA	1:A:749:ILE:HD12	2.03	0.40
1:B:209:THR:HA	1:B:210:PRO:HD3	1.82	0.40
1:B:430:ILE:O	1:B:430:ILE:HG23	2.22	0.40
1:B:482:ARG:HB2	1:B:559:ARG:HB2	2.03	0.40
1:B:727:ILE:HG23	1:B:728:MET:N	2.37	0.40
1:B:767:PHE:O	1:B:768:GLU:CB	2.70	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	901/903 (100%)	657 (73%)	170 (19%)	74 (8%)	1	5
1	B	901/903 (100%)	659 (73%)	177 (20%)	65 (7%)	1	7
All	All	1802/1806 (100%)	1316 (73%)	347 (19%)	139 (8%)	1	6

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	255	ASN
1	A	312	LEU
1	A	316	ASN
1	A	405	LYS
1	A	451	SER
1	A	462	MET
1	A	523	SER
1	A	539	ASN
1	A	643	ASP
1	A	680	LEU
1	A	692	PRO
1	A	766	GLU
1	A	768	GLU
1	A	787	ASN
1	A	797	PRO
1	A	799	PRO
1	A	819	ILE
1	A	827	GLY
1	A	829	LYS
1	A	845	CYS
1	A	895	ALA
1	B	24	GLY
1	B	161	GLU
1	B	259	SER
1	B	388	VAL
1	B	451	SER
1	B	507	ASN
1	B	622	THR
1	B	680	LEU
1	B	731	GLU
1	B	766	GLU
1	B	768	GLU
1	B	787	ASN
1	B	791	TYR

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Mol	Chain	Res	Type
1	B	793	VAL
1	B	799	PRO
1	B	804	HIS
1	B	818	ASN
1	B	834	PRO
1	B	835	LEU
1	B	897	LEU
1	A	24	GLY
1	A	49	TYR
1	A	101	ILE
1	A	122	GLY
1	A	376	GLN
1	A	458	PRO
1	A	507	ASN
1	A	550	VAL
1	A	637	GLY
1	A	659	MET
1	A	721	ALA
1	A	804	HIS
1	A	859	LYS
1	A	862	VAL
1	A	866	MET
1	B	43	GLU
1	B	102	LYS
1	B	109	ARG
1	B	122	GLY
1	B	181	GLU
1	B	312	LEU
1	B	344	SER
1	B	415	LEU
1	B	433	THR
1	B	509	SER
1	B	646	HIS
1	B	736	SER
1	B	789	ALA
1	B	797	PRO
1	B	832	VAL
1	B	836	ARG
1	B	895	ALA
1	A	44	SER
1	A	105	HIS
1	A	181	GLU

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Mol	Chain	Res	Type
1	A	226	VAL
1	A	256	MET
1	A	381	PRO
1	A	415	LEU
1	A	506	PRO
1	A	522	PHE
1	A	630	ASP
1	A	731	GLU
1	A	734	LYS
1	A	832	VAL
1	A	834	PRO
1	B	241	ARG
1	B	390	PRO
1	B	523	SER
1	B	605	LEU
1	B	693	LEU
1	B	821	ALA
1	B	843	ASP
1	B	873	GLU
1	A	22	SER
1	A	63	ALA
1	A	183	ILE
1	A	228	ASN
1	A	278	LYS
1	A	519	ARG
1	A	538	LEU
1	A	586	ILE
1	B	52	ILE
1	B	257	TYR
1	B	414	SER
1	B	424	ASN
1	B	506	PRO
1	B	661	PRO
1	B	827	GLY
1	A	102	LYS
1	A	124	PRO
1	A	295	GLU
1	A	603	GLU
1	A	793	VAL
1	A	796	PHE
1	B	222	ASP
1	B	316	ASN

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Mol	Chain	Res	Type
1	B	318	GLN
1	B	362	ILE
1	B	462	MET
1	B	601	VAL
1	B	643	ASP
1	B	730	LEU
1	B	758	GLU
1	B	859	LYS
1	A	3	GLU
1	A	187	ILE
1	A	622	THR
1	A	718	THR
1	B	374	LYS
1	B	659	MET
1	A	300	VAL
1	B	392	PRO
1	A	470	VAL
1	A	52	ILE
1	A	326	ILE
1	A	390	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	802/802 (100%)	634 (79%)	168 (21%)	1	6
1	B	802/802 (100%)	627 (78%)	175 (22%)	1	5
All	All	1604/1604 (100%)	1261 (79%)	343 (21%)	1	5

All (343) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	5	TYR
1	A	6	LEU

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Mol	Chain	Res	Type
1	A	11	ILE
1	A	15	ILE
1	A	22	SER
1	A	44	SER
1	A	47	THR
1	A	48	LYS
1	A	49	TYR
1	A	52	ILE
1	A	58	THR
1	A	59	ARG
1	A	61	LEU
1	A	64	ASN
1	A	66	ARG
1	A	69	SER
1	A	95	ASP
1	A	96	THR
1	A	103	TYR
1	A	105	HIS
1	A	108	ILE
1	A	112	ASN
1	A	113	PHE
1	A	114	ASP
1	A	121	ASP
1	A	124	PRO
1	A	125	GLU
1	A	130	LYS
1	A	134	ASP
1	A	141	SER
1	A	147	TYR
1	A	149	PHE
1	A	169	LYS
1	A	170	LEU
1	A	173	GLN
1	A	184	ASP
1	A	188	TYR
1	A	189	MET
1	A	191	PHE
1	A	197	LEU
1	A	199	MET
1	A	201	TYR
1	A	202	LEU
1	A	205	TRP

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Mol	Chain	Res	Type
1	A	211	VAL
1	A	213	LEU
1	A	217	ASN
1	A	220	SER
1	A	232	ASN
1	A	238	THR
1	A	242	LEU
1	A	254	GLU
1	A	256	MET
1	A	260	ARG
1	A	262	ILE
1	A	266	PHE
1	A	280	PHE
1	A	282	PHE
1	A	294	SER
1	A	309	ILE
1	A	312	LEU
1	A	324	ASN
1	A	330	ARG
1	A	332	LEU
1	A	337	LYS
1	A	338	ARG
1	A	345	LEU
1	A	353	ILE
1	A	356	GLN
1	A	358	VAL
1	A	363	LYS
1	A	375	GLU
1	A	376	GLN
1	A	389	GLN
1	A	391	TYR
1	A	403	ARG
1	A	418	SER
1	A	422	GLN
1	A	423	VAL
1	A	438	PRO
1	A	455	SER
1	A	459	ASN
1	A	466	ASP
1	A	468	ASP
1	A	475	ILE
1	A	481	GLN

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Mol	Chain	Res	Type
1	A	489	MET
1	A	501	GLU
1	A	503	LEU
1	A	505	ASN
1	A	507	ASN
1	A	511	ASP
1	A	513	PRO
1	A	514	LEU
1	A	516	VAL
1	A	526	ILE
1	A	528	GLU
1	A	536	LYS
1	A	541	MET
1	A	553	MET
1	A	556	GLN
1	A	559	ARG
1	A	562	LEU
1	A	577	TYR
1	A	587	THR
1	A	589	PHE
1	A	594	LEU
1	A	595	GLN
1	A	598	GLU
1	A	606	ASN
1	A	607	GLU
1	A	614	GLU
1	A	618	LEU
1	A	625	ILE
1	A	627	VAL
1	A	630	ASP
1	A	631	LYS
1	A	632	ILE
1	A	639	SER
1	A	640	LYS
1	A	644	THR
1	A	647	TRP
1	A	654	PHE
1	A	659	MET
1	A	667	PHE
1	A	671	CYS
1	A	673	TYR
1	A	680	LEU

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Mol	Chain	Res	Type
1	A	685	ARG
1	A	686	GLU
1	A	693	LEU
1	A	698	ILE
1	A	705	LYS
1	A	710	LEU
1	A	722	GLU
1	A	731	GLU
1	A	736	SER
1	A	747	GLU
1	A	762	GLU
1	A	763	TYR
1	A	765	LYS
1	A	767	PHE
1	A	769	LYS
1	A	788	ILE
1	A	791	TYR
1	A	799	PRO
1	A	803	PHE
1	A	804	HIS
1	A	809	LEU
1	A	816	LYS
1	A	818	ASN
1	A	820	ASP
1	A	834	PRO
1	A	837	GLU
1	A	853	GLU
1	A	855	THR
1	A	857	LEU
1	A	860	ASP
1	A	863	LEU
1	A	871	LEU
1	A	872	LEU
1	A	880	LEU
1	A	890	ASP
1	A	896	SER
1	A	897	LEU
1	A	902	ASP
1	A	903	PHE
1	B	5	TYR
1	B	6	LEU
1	B	17	GLU

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Mol	Chain	Res	Type
1	B	19	TYR
1	B	22	SER
1	B	27	ARG
1	B	30	GLU
1	B	36	SER
1	B	43	GLU
1	B	44	SER
1	B	47	THR
1	B	52	ILE
1	B	55	LYS
1	B	70	GLN
1	B	73	LYS
1	B	86	ASP
1	B	90	LEU
1	B	92	TYR
1	B	97	TYR
1	B	105	HIS
1	B	106	THR
1	B	112	ASN
1	B	121	ASP
1	B	130	LYS
1	B	142	ILE
1	B	147	TYR
1	B	158	ASN
1	B	169	LYS
1	B	173	GLN
1	B	180	SER
1	B	181	GLU
1	B	183	ILE
1	B	184	ASP
1	B	185	LYS
1	B	188	TYR
1	B	189	MET
1	B	195	LYS
1	B	199	MET
1	B	220	SER
1	B	232	ASN
1	B	245	HIS
1	B	246	ARG
1	B	248	THR
1	B	251	LYS
1	B	257	TYR

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Mol	Chain	Res	Type
1	B	259	SER
1	B	268	ILE
1	B	271	LEU
1	B	276	LEU
1	B	285	GLN
1	B	291	ASP
1	B	294	SER
1	B	296	PHE
1	B	309	ILE
1	B	312	LEU
1	B	330	ARG
1	B	337	LYS
1	B	342	ASN
1	B	344	SER
1	B	356	GLN
1	B	360	SER
1	B	370	PHE
1	B	373	LEU
1	B	375	GLU
1	B	382	GLN
1	B	388	VAL
1	B	391	TYR
1	B	399	PRO
1	B	403	ARG
1	B	407	VAL
1	B	411	ASP
1	B	412	LEU
1	B	418	SER
1	B	422	GLN
1	B	430	ILE
1	B	443	ILE
1	B	444	ASN
1	B	452	ASP
1	B	453	VAL
1	B	456	CYS
1	B	459	ASN
1	B	466	ASP
1	B	467	ARG
1	B	468	ASP
1	B	474	GLU
1	B	501	GLU
1	B	503	LEU

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Mol	Chain	Res	Type
1	B	505	ASN
1	B	507	ASN
1	B	511	ASP
1	B	514	LEU
1	B	515	ASP
1	B	519	ARG
1	B	520	PHE
1	B	524	ASP
1	B	525	GLU
1	B	531	LYS
1	B	541	MET
1	B	542	LEU
1	B	547	ARG
1	B	553	MET
1	B	554	THR
1	B	556	GLN
1	B	559	ARG
1	B	562	LEU
1	B	594	LEU
1	B	595	GLN
1	B	598	GLU
1	B	604	TYR
1	B	611	THR
1	B	618	LEU
1	B	624	SER
1	B	627	VAL
1	B	628	SER
1	B	631	LYS
1	B	634	ASP
1	B	639	SER
1	B	640	LYS
1	B	642	ARG
1	B	644	THR
1	B	647	TRP
1	B	658	ARG
1	B	659	MET
1	B	684	ASP
1	B	693	LEU
1	B	703	THR
1	B	707	ARG
1	B	716	GLU
1	B	728	MET

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Mol	Chain	Res	Type
1	B	731	GLU
1	B	733	GLN
1	B	735	SER
1	B	736	SER
1	B	739	LYS
1	B	747	GLU
1	B	766	GLU
1	B	768	GLU
1	B	769	LYS
1	B	772	ARG
1	B	773	GLN
1	B	777	ILE
1	B	790	LYS
1	B	791	TYR
1	B	792	ASP
1	B	796	PHE
1	B	799	PRO
1	B	804	HIS
1	B	809	LEU
1	B	815	ILE
1	B	816	LYS
1	B	818	ASN
1	B	824	VAL
1	B	834	PRO
1	B	835	LEU
1	B	837	GLU
1	B	841	PHE
1	B	844	LYS
1	B	850	SER
1	B	853	GLU
1	B	855	THR
1	B	857	LEU
1	B	859	LYS
1	B	867	ASP
1	B	869	THR
1	B	871	LEU
1	B	872	LEU
1	B	880	LEU
1	B	881	GLU
1	B	883	PHE
1	B	890	ASP
1	B	897	LEU

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Mol	Chain	Res	Type
1	B	898	PHE
1	B	900	MET
1	B	902	ASP
1	B	903	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	112	ASN
1	A	131	HIS
1	A	173	GLN
1	A	232	ASN
1	A	318	GLN
1	A	324	ASN
1	A	333	GLN
1	A	339	GLN
1	A	356	GLN
1	A	389	GLN
1	A	422	GLN
1	A	480	ASN
1	A	481	GLN
1	A	558	ASN
1	A	606	ASN
1	A	818	ASN
1	B	112	ASN
1	B	158	ASN
1	B	173	GLN
1	B	193	ASN
1	B	232	ASN
1	B	245	HIS
1	B	333	GLN
1	B	339	GLN
1	B	356	GLN
1	B	389	GLN
1	B	402	ASN
1	B	422	GLN
1	B	444	ASN
1	B	459	ASN
1	B	481	GLN
1	B	493	GLN
1	B	539	ASN

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Mol	Chain	Res	Type
1	B	556	GLN
1	B	582	ASN
1	B	645	ASN
1	B	676	ASN
1	B	818	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GMP	B	999	-	18,22,22	2.61	6 (33%)	20,33,33	3.44	8 (40%)
2	GMP	A	999	-	18,22,22	2.62	6 (33%)	20,33,33	2.89	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GMP	B	999	-	-	0/2/22/22	0/3/3/3
2	GMP	A	999	-	-	0/2/22/22	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	GMP	C6-N1	7.57	1.46	1.33
2	B	999	GMP	C6-N1	6.60	1.44	1.33
2	B	999	GMP	O3'-C3'	4.54	1.53	1.43
2	B	999	GMP	C2-N1	4.29	1.43	1.35
2	A	999	GMP	C2'-C1'	3.73	1.59	1.53
2	A	999	GMP	C2-N1	3.61	1.41	1.35
2	B	999	GMP	C4-N3	3.36	1.40	1.35
2	B	999	GMP	O4'-C1'	3.20	1.45	1.41
2	A	999	GMP	C6-C5	2.94	1.46	1.41
2	B	999	GMP	C2-N2	2.47	1.38	1.33
2	A	999	GMP	O4'-C1'	2.29	1.44	1.41
2	A	999	GMP	C4-N3	2.17	1.39	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	GMP	C5-C6-N1	-8.87	111.30	123.43
2	A	999	GMP	C5-C6-N1	-8.41	111.93	123.43
2	B	999	GMP	C6-N1-C2	7.29	127.51	115.93
2	B	999	GMP	N3-C2-N1	-6.31	118.81	127.22
2	A	999	GMP	C6-N1-C2	5.77	125.10	115.93
2	A	999	GMP	N3-C2-N1	-4.85	120.75	127.22
2	B	999	GMP	C2'-C3'-C4'	-4.19	94.49	102.64
2	B	999	GMP	O4'-C1'-C2'	-3.49	101.82	106.93
2	A	999	GMP	C5'-C4'-C3'	-3.11	107.58	115.09
2	B	999	GMP	C4-C5-N7	3.03	112.56	109.40
2	B	999	GMP	C1'-N9-C4	3.01	131.94	126.64
2	B	999	GMP	N2-C2-N3	2.47	121.82	117.79
2	A	999	GMP	O4'-C4'-C5'	2.39	114.37	109.21
2	A	999	GMP	N2-C2-N3	2.08	121.17	117.79

There are no chirality outliers.

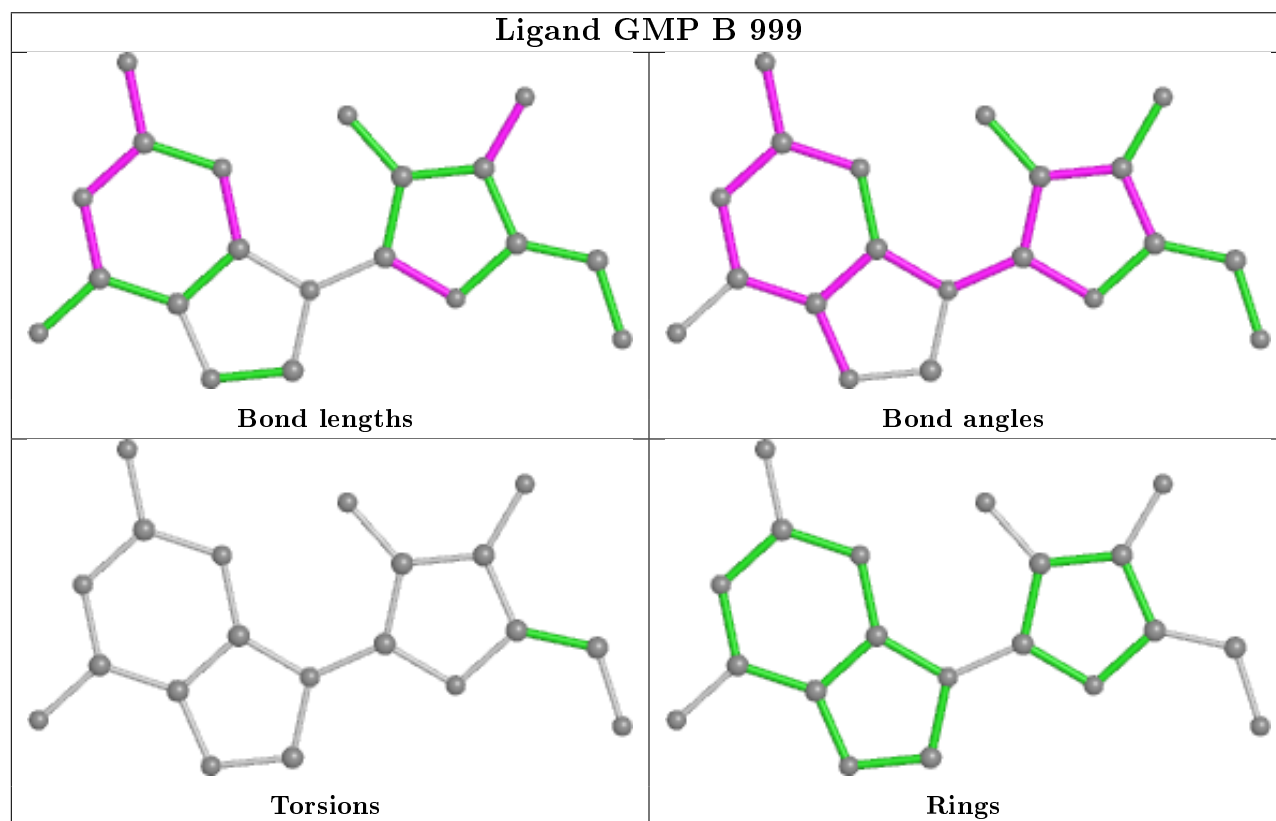
There are no torsion outliers.

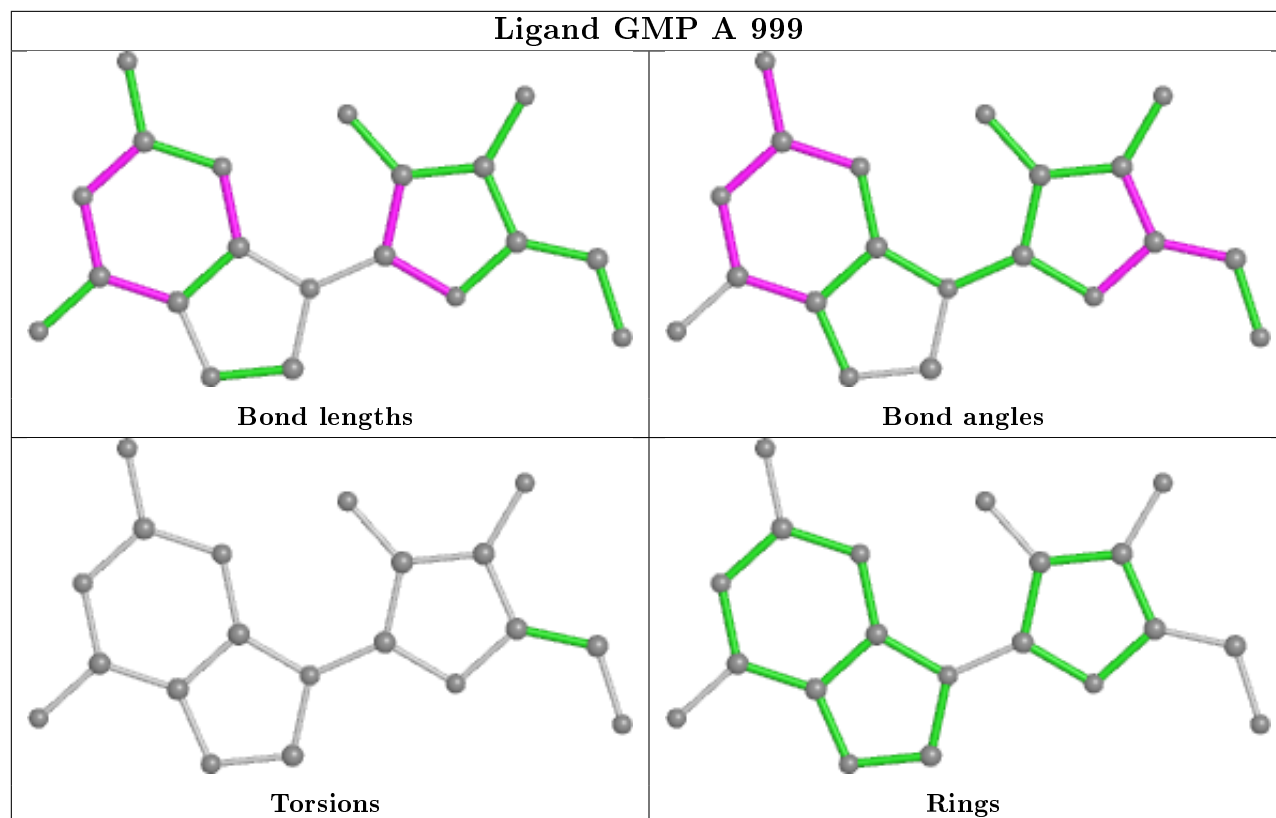
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	999	GMP	2	0
2	A	999	GMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	903/903 (100%)	-0.46	5 (0%) 89 83	40, 68, 100, 100	0
1	B	903/903 (100%)	-0.49	3 (0%) 94 92	39, 68, 100, 100	0
All	All	1806/1806 (100%)	-0.47	8 (0%) 92 89	39, 68, 100, 100	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	903	PHE	3.6
1	B	257	TYR	3.0
1	A	508	LEU	2.9
1	A	514	LEU	2.5
1	A	507	ASN	2.4
1	B	259	SER	2.4
1	A	515	ASP	2.3
1	B	256	MET	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.

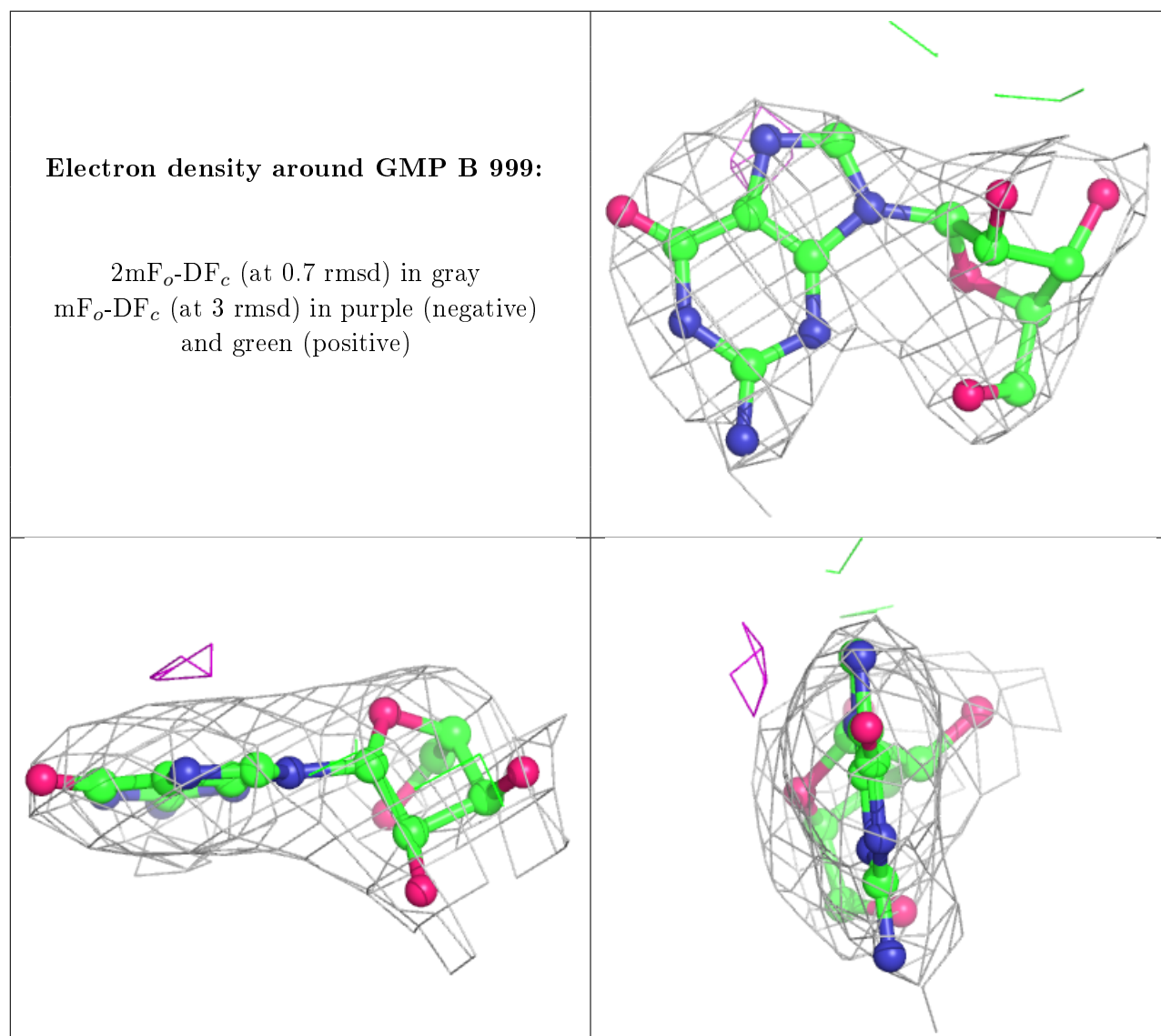
### 6.4 Ligands [i](#)

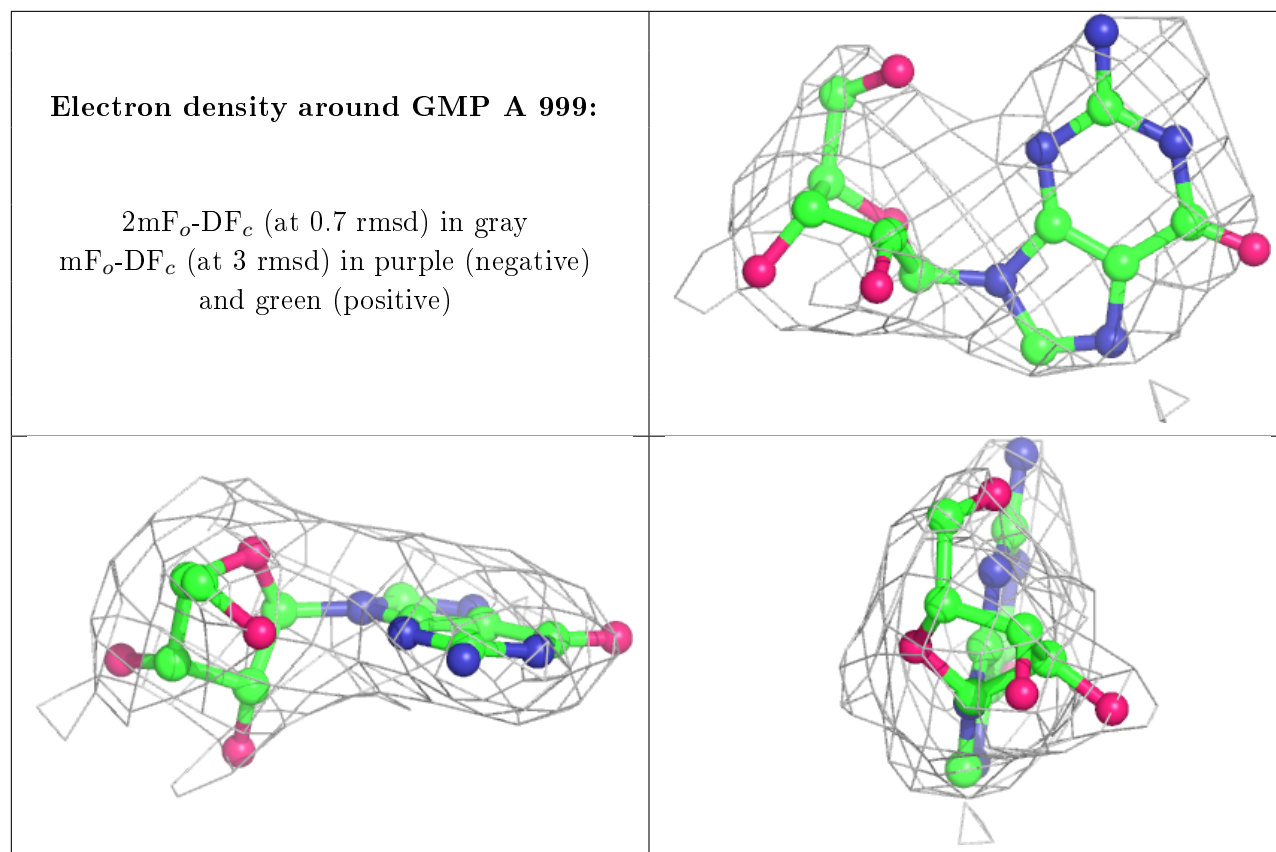
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GMP	B	999	20/20	0.96	0.20	82,82,84,84	0
2	GMP	A	999	20/20	0.96	0.18	81,82,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.