



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2021 – 12:26 PM EDT

PDB ID : 7JR5  
Title : Real Time Reaction Intermediates in Stigmatella Bacteriophytochrome P2  
Authors : Schmidt, M.  
Deposited on : 2020-08-11  
Resolution : 2.40 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 : 2.23.2  
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) : 2.23.2

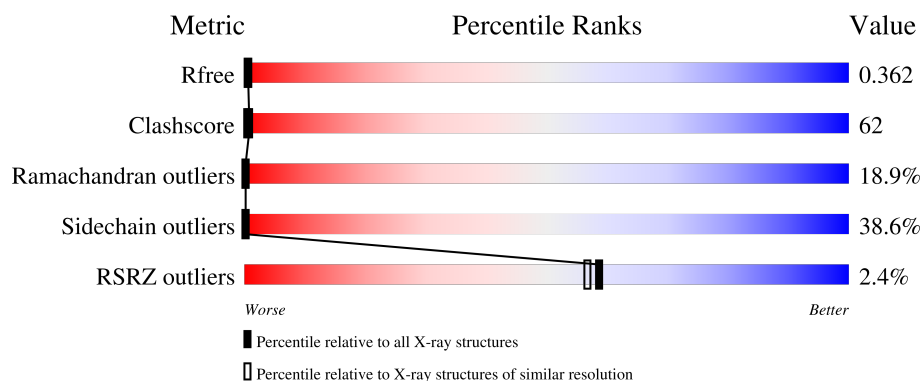
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

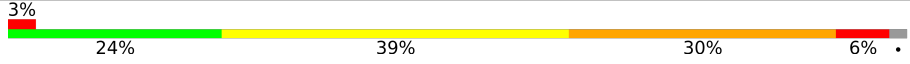
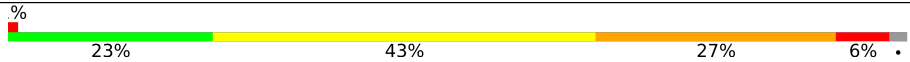
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	490	 3% 24% 39% 30% 6% .
1	B	490	 % 23% 43% 27% 6% .

## 2 Entry composition [i](#)

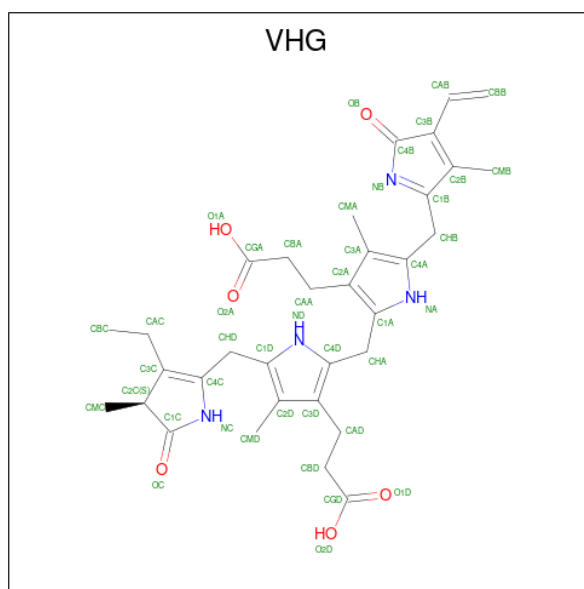
There are 4 unique types of molecules in this entry. The entry contains 7640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Photoreceptor-histidine kinase BphP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	3	0
			3686	2336	670	669	11			
1	B	482	Total	C	N	O	S	0	2	0
			3677	2330	668	668	11			

- Molecule 2 is 3-[2-[[5-[(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-2-yl)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1 {H}-pyrrol-2-yl)methyl]-5-[[3 {S}-4-ethyl-3-methyl-2-oxidanylidene-1,3-dihydropyrrol-5-yl)methyl]-4-methyl-1 {H}-pyrrol-3-yl]propanoic acid (three-letter code: VHG) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			86	66	8	12		
2	B	1	Total	C	N	O	0	1
			86	66	8	12		

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			9	7	2		

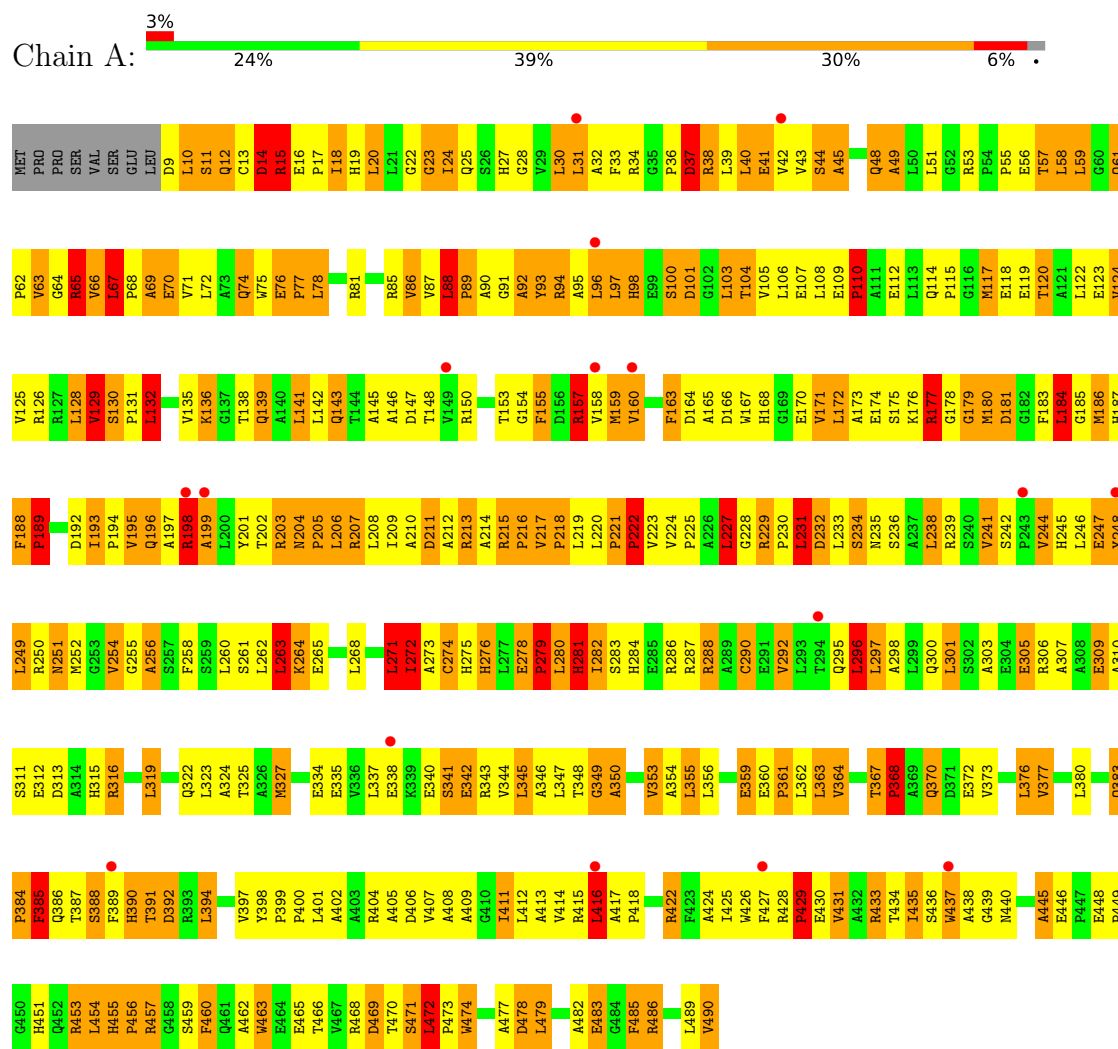
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	41	Total	O	0	0
			41	41		

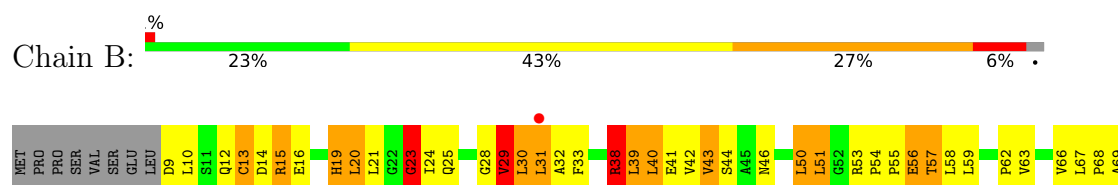
### 3 Residue-property plots

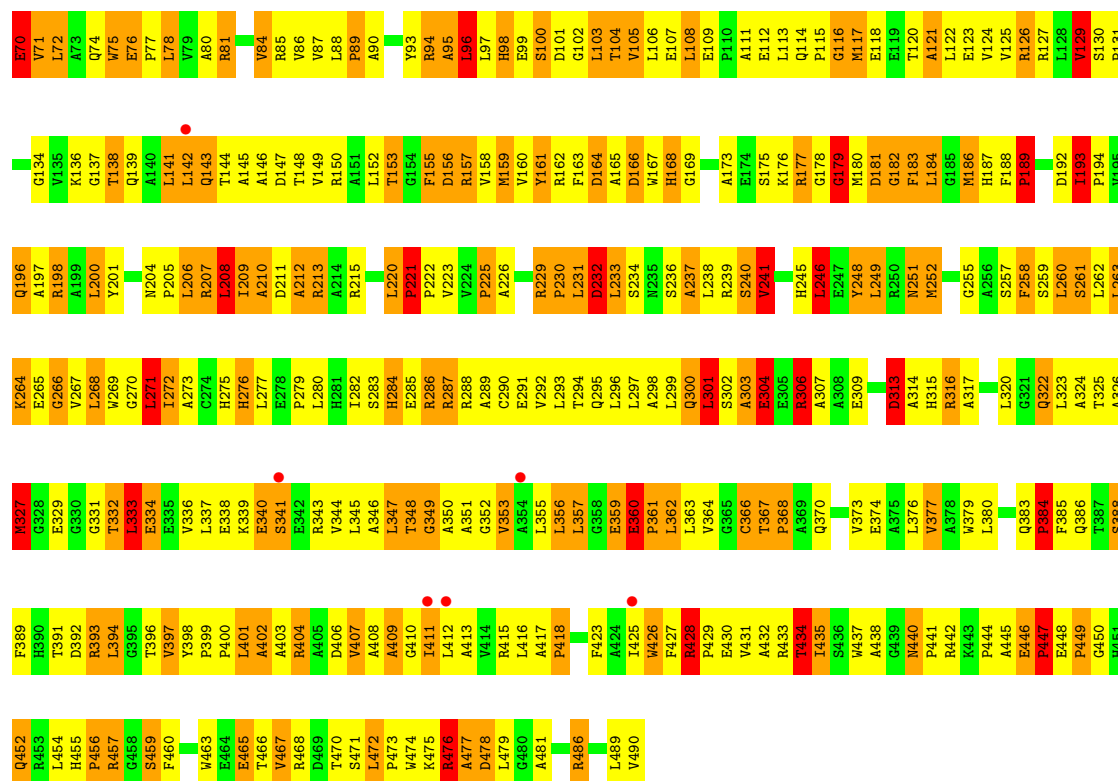
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.69Å 83.40Å 86.87Å 90.00° 107.63° 90.00°	Depositor
Resolution (Å)	19.97 – 2.40 19.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	85.2 (19.97-2.40) 73.7 (19.97-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.313 , 0.341 0.316 , 0.362	Depositor DCC
$R_{free}$ test set	2664 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	7640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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

### 5.1 Standard geometry

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

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	0.87	2/3772 (0.1%)	1.18	13/5145 (0.3%)
1	B	0.77	2/3759 (0.1%)	1.10	9/5127 (0.2%)
All	All	0.82	4/7531 (0.1%)	1.14	22/10272 (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	3	16
1	B	0	17
All	All	3	33

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13[A]	CYS	CB-SG	-17.98	1.51	1.82
1	A	13[B]	CYS	CB-SG	-17.98	1.51	1.82
1	B	13[A]	CYS	CB-SG	-6.06	1.72	1.82
1	B	13[B]	CYS	CB-SG	-6.06	1.72	1.82

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	PRO	N-CA-CB	-9.10	92.38	103.30
1	B	447	PRO	N-CA-CB	-7.89	93.83	103.30
1	A	189	PRO	N-CA-C	7.65	131.98	112.10
1	A	222	PRO	N-CA-CB	-7.18	94.68	103.30
1	B	181	ASP	CB-CA-C	6.16	122.72	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	CYS	CB-CA-C	6.12	122.64	110.40
1	B	189	PRO	N-CA-C	6.08	127.92	112.10
1	A	157	ARG	CG-CD-NE	6.07	124.56	111.80
1	B	189	PRO	N-CA-CB	-6.03	95.96	102.60
1	A	279	PRO	N-CA-CB	-5.73	96.30	102.60
1	B	384	PRO	N-CA-CB	-5.70	96.34	102.60
1	A	221	PRO	N-CA-CB	-5.62	96.42	102.60
1	B	428	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	177	ARG	CG-CD-NE	5.55	123.45	111.80
1	B	99	GLU	CB-CA-C	5.52	121.44	110.40
1	B	38	ARG	CB-CA-C	5.49	121.38	110.40
1	A	279	PRO	N-CA-C	5.46	126.29	112.10
1	A	429	PRO	N-CA-C	5.31	125.90	112.10
1	A	15	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	428	ARG	CG-CD-NE	5.11	122.52	111.80
1	A	222	PRO	N-CA-C	5.05	125.23	112.10
1	A	370	GLN	CB-CA-C	-5.02	100.35	110.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	106	LEU	CA
1	A	290	CYS	CA
1	A	296	LEU	CA

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	THR	Peptide
1	A	14	ASP	Peptide
1	A	15	ARG	Peptide
1	A	17	PRO	Peptide
1	A	186	MET	Peptide
1	A	198	ARG	Peptide
1	A	211	ASP	Peptide
1	A	231	LEU	Peptide
1	A	316	ARG	Peptide
1	A	325	THR	Peptide
1	A	37	ASP	Peptide
1	A	384	PRO	Peptide
1	A	416	LEU	Peptide
1	A	424	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	44	SER	Peptide
1	A	65	ARG	Peptide
1	B	111	ALA	Peptide
1	B	179	GLY	Peptide
1	B	208	LEU	Peptide
1	B	210	ALA	Peptide
1	B	221	PRO	Mainchain,Peptide
1	B	23	GLY	Peptide
1	B	232	ASP	Peptide
1	B	271	LEU	Peptide
1	B	289	ALA	Peptide
1	B	304	GLU	Peptide
1	B	313	ASP	Peptide
1	B	341	SER	Peptide
1	B	388	SER	Peptide
1	B	39	LEU	Peptide
1	B	426	TRP	Peptide
1	B	434	THR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3686	0	3721	453	0
1	B	3677	0	3709	469	0
2	A	86	0	0	13	0
2	B	86	0	0	21	0
3	B	9	0	7	0	0
4	A	55	0	0	22	0
4	B	41	0	0	15	1
All	All	7640	0	7437	927	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 62.

All (927) 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:A:345:LEU:HD12	1:A:345:LEU:O	1.33	1.29
1:A:10:LEU:N	1:A:14:ASP:OD1	1.68	1.26
1:B:97:LEU:HD13	1:B:105:VAL:O	1.43	1.17
1:B:182:GLY:O	1:B:183:PHE:CD2	1.98	1.16
1:A:345:LEU:O	1:A:345:LEU:CD1	1.96	1.14
1:A:128:LEU:O	1:A:128:LEU:HD22	1.50	1.11
1:B:97:LEU:HD13	1:B:105:VAL:C	1.69	1.10
1:B:402:ALA:O	1:B:404:ARG:N	1.88	1.07
1:B:385:PHE:O	1:B:415:ARG:NH1	1.89	1.05
1:B:192:ASP:O	1:B:194:PRO:HD3	1.56	1.05
1:A:232:ASP:OD1	1:A:234:SER:OG	1.72	1.04
1:A:468:ARG:NH1	4:A:602:HOH:O	1.86	1.04
1:A:198:ARG:HG3	1:A:268:LEU:HD22	1.37	1.01
1:A:411:ILE:HA	1:A:426:TRP:O	1.60	1.00
1:A:96:LEU:HD23	1:A:284:HIS:ND1	1.78	0.99
1:A:109:GLU:HG2	1:A:110:PRO:CD	1.93	0.97
1:B:394:LEU:CD1	1:B:408:ALA:HB1	1.94	0.96
1:A:93:TYR:HB3	1:A:109:GLU:C	1.86	0.96
1:A:346:ALA:CA	1:A:350:ALA:HB2	1.95	0.95
1:B:345:LEU:HD11	1:B:352:GLY:CA	1.97	0.95
1:A:188:PHE:N	1:A:437:TRP:HZ3	1.65	0.94
1:A:64:GLY:HA3	1:A:72:LEU:HD21	1.45	0.94
2:B:602[A]:VHG:CMA	2:B:602[A]:VHG:C2B	2.46	0.94
1:A:306:ARG:O	4:A:601:HOH:O	1.85	0.93
1:A:88:LEU:HB2	1:A:89:PRO:CD	1.98	0.93
1:B:29:VAL:HG21	1:B:108:LEU:HG	1.51	0.92
1:B:141:LEU:HD21	1:B:300:GLN:NE2	1.85	0.92
1:A:109:GLU:HG2	1:A:110:PRO:HD2	1.51	0.91
2:B:602[A]:VHG:CMA	2:B:602[A]:VHG:CMB	2.48	0.91
1:B:23:GLY:O	1:B:240:SER:OG	1.89	0.91
1:B:258:PHE:HE2	1:B:290:CYS:HG	0.93	0.90
1:B:248[B]:TYR:HB2	1:B:456:PRO:HB3	1.51	0.90
1:A:346:ALA:N	1:A:350:ALA:HB2	1.87	0.89
1:B:187:HIS:O	1:B:437:TRP:HA	1.73	0.89
1:A:315[B]:HIS:O	1:A:315[B]:HIS:CD2	2.27	0.88
1:B:25:GLN:HE21	1:B:238:LEU:HB3	1.39	0.87
1:B:25:GLN:NE2	1:B:238:LEU:HB3	1.90	0.87
1:A:356:LEU:HD22	1:A:377:VAL:HG21	1.57	0.87
1:A:335:GLU:O	1:A:338:GLU:HG3	1.75	0.85
1:A:346:ALA:HA	1:A:350:ALA:HB2	1.59	0.84
1:B:192:ASP:O	1:B:194:PRO:CD	2.25	0.84
1:A:229:ARG:HH12	1:A:232:ASP:HB2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PHE:N	1:A:437:TRP:CZ3	2.45	0.83
2:B:602[B]:VHG:CBC	2:B:602[B]:VHG:CMC	2.56	0.83
1:A:334:GLU:OE1	1:A:334:GLU:N	2.12	0.83
1:B:12:GLN:HA	1:B:15:ARG:HB2	1.59	0.83
1:B:366:CYS:O	1:B:366:CYS:SG	2.37	0.83
1:A:188:PHE:HA	1:A:437:TRP:CZ3	2.13	0.83
1:A:38:ARG:HD3	1:A:75:TRP:CH2	2.14	0.83
1:A:53:ARG:NH2	4:A:604:HOH:O	1.99	0.83
1:A:100:SER:OG	1:A:100:SER:O	1.91	0.82
1:B:304:GLU:OE2	4:B:701:HOH:O	1.97	0.81
1:A:346:ALA:HA	1:A:350:ALA:CB	2.10	0.81
1:A:109:GLU:OE1	4:A:603:HOH:O	1.98	0.81
1:A:112:GLU:HG3	1:A:117:MET:HG2	1.62	0.81
1:A:353:VAL:HG11	1:A:364:VAL:HG22	1.61	0.81
1:B:97:LEU:CD1	1:B:105:VAL:O	2.28	0.80
1:A:131:PRO:HD3	1:B:295:GLN:HE21	1.44	0.80
1:A:142:LEU:HD13	1:A:301:LEU:HD21	1.65	0.78
1:B:344:VAL:HA	1:B:347:LEU:HG	1.64	0.78
2:B:602[A]:VHG:CBC	2:B:602[A]:VHG:CMC	2.61	0.78
1:B:260:LEU:HD11	1:B:290:CYS:HB3	1.65	0.78
1:B:102:GLY:O	1:B:103:LEU:HD23	1.83	0.78
1:B:42:VAL:HA	1:B:220:LEU:O	1.84	0.78
1:A:112:GLU:OE1	1:A:283:SER:HB3	1.84	0.77
1:A:282:ILE:HB	1:A:286:ARG:HD2	1.66	0.77
1:A:32:ALA:HB2	1:A:105:VAL:HG12	1.64	0.77
1:A:188:PHE:CA	1:A:437:TRP:CZ3	2.68	0.77
1:B:96:LEU:HD13	1:B:96:LEU:N	1.99	0.77
2:A:500[B]:VHG:C4A	2:A:500[B]:VHG:CMB	2.63	0.77
2:A:500[B]:VHG:CMB	2:A:500[B]:VHG:C3A	2.63	0.77
1:A:448:GLU:OE1	1:A:453:ARG:HG3	1.85	0.77
1:A:100:SER:O	1:A:101:ASP:HB2	1.83	0.77
1:A:210:ALA:HA	1:A:256:ALA:HB1	1.67	0.77
1:B:229:ARG:H	1:B:229:ARG:HD3	1.49	0.77
1:B:345:LEU:HD11	1:B:352:GLY:N	2.00	0.76
1:B:198:ARG:HA	1:B:201:TYR:CD2	2.20	0.76
1:B:211:ASP:OD1	1:B:279:PRO:HG3	1.85	0.76
1:B:411:ILE:HB	1:B:425:ILE:HG23	1.65	0.76
1:A:363:LEU:HD13	1:A:363:LEU:C	2.06	0.76
1:B:78:LEU:C	1:B:78:LEU:HD12	2.05	0.76
1:A:11:SER:O	1:A:14:ASP:N	2.15	0.76
2:B:602[A]:VHG:CMB	2:B:602[A]:VHG:C3A	2.63	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASN:HD21	1:A:456:PRO:HG2	1.51	0.76
1:B:352:GLY:O	1:B:426:TRP:HB2	1.86	0.76
1:A:30:LEU:O	1:A:44:SER:HB3	1.87	0.75
1:A:353:VAL:HG11	1:A:364:VAL:CG2	2.16	0.75
1:A:88:LEU:CB	1:A:89:PRO:HD3	2.17	0.75
1:B:258:PHE:CD1	1:B:258:PHE:C	2.60	0.75
1:B:94:ARG:HG3	1:B:96:LEU:HD11	1.67	0.75
1:B:315:HIS:CG	1:B:315:HIS:O	2.38	0.74
1:A:128:LEU:O	1:A:128:LEU:CD2	2.31	0.74
1:A:10:LEU:CA	1:A:14:ASP:OD1	2.35	0.74
1:A:416:LEU:HG	1:A:489:LEU:HD22	1.70	0.74
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.68	0.74
1:A:177:ARG:HG3	1:A:177:ARG:HH11	1.52	0.74
1:A:457:ARG:HG3	1:A:457:ARG:HH11	1.52	0.74
1:B:437:TRP:CD2	1:B:441:PRO:HB3	2.23	0.74
1:A:88:LEU:N	1:A:88:LEU:HD13	2.02	0.74
1:B:78:LEU:HD21	1:B:97:LEU:HD23	1.70	0.73
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.51	0.73
1:A:216:PRO:O	1:A:217:VAL:HG13	1.88	0.73
1:A:316:ARG:NH1	1:A:477:ALA:O	2.19	0.73
1:A:391:THR:HA	4:A:632:HOH:O	1.88	0.73
1:B:184:LEU:C	1:B:184:LEU:HD12	2.08	0.73
1:B:139:GLN:N	4:B:704:HOH:O	2.22	0.73
1:B:209:ILE:HG12	1:B:241:VAL:HG11	1.71	0.72
1:A:248[A]:TYR:O	1:A:248[A]:TYR:CD2	2.42	0.72
1:B:25:GLN:OE1	1:B:239:ARG:O	2.07	0.72
1:B:94:ARG:N	1:B:109:GLU:O	2.22	0.72
1:A:187:HIS:C	1:A:437:TRP:HZ3	1.92	0.72
1:B:50:LEU:O	1:B:51:LEU:HB2	1.90	0.72
1:B:97:LEU:HD12	1:B:98:HIS:H	1.55	0.72
2:A:500[A]:VHG:CBC	2:A:500[A]:VHG:CMC	2.68	0.71
1:B:394:LEU:HD13	1:B:408:ALA:HB1	1.71	0.71
1:A:10:LEU:C	1:A:14:ASP:OD1	2.28	0.71
1:B:149:VAL:O	1:B:153:THR:HG23	1.90	0.71
1:B:265:GLU:N	4:B:702:HOH:O	2.18	0.71
4:A:605:HOH:O	1:B:324:ALA:CB	2.39	0.71
1:A:248[B]:TYR:CG	1:A:248[B]:TYR:O	2.43	0.71
1:A:215:ARG:O	1:A:216:PRO:O	2.08	0.71
1:A:122:LEU:O	1:A:125:VAL:HB	1.91	0.70
1:A:187:HIS:C	1:A:437:TRP:CZ3	2.65	0.70
1:B:208:LEU:HD12	1:B:210:ALA:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HD11	1:B:290:CYS:CB	2.21	0.70
1:A:203:ARG:NE	4:A:607:HOH:O	2.25	0.70
1:B:356:LEU:CD2	1:B:377:VAL:HG11	2.21	0.70
1:B:161:TYR:CE2	1:B:193:ILE:HD11	2.27	0.70
1:B:345:LEU:HD11	1:B:352:GLY:C	2.11	0.70
1:A:431:VAL:HG12	1:A:431:VAL:O	1.92	0.69
1:B:265:GLU:O	4:B:702:HOH:O	2.10	0.69
1:B:264:LYS:HG2	4:B:702:HOH:O	1.93	0.69
1:B:260:LEU:HD13	1:B:294:THR:HG23	1.73	0.69
1:B:25:GLN:HE22	1:B:239:ARG:N	1.90	0.69
1:B:248[B]:TYR:HB3	1:B:456:PRO:HG3	1.73	0.69
1:B:435:ILE:HD11	1:B:465:GLU:OE1	1.93	0.69
1:B:206:LEU:HD21	1:B:291:GLU:HB2	1.76	0.68
1:B:182:GLY:O	1:B:183:PHE:CG	2.46	0.68
1:A:58:LEU:HD22	1:A:58:LEU:H	1.57	0.68
1:A:248[A]:TYR:O	1:A:248[A]:TYR:CG	2.47	0.68
1:A:457:ARG:HG3	1:A:457:ARG:NH1	2.07	0.68
1:A:483:GLU:OE1	4:A:605:HOH:O	2.12	0.68
1:A:204:ASN:O	1:A:205:PRO:O	2.12	0.68
1:A:319:LEU:HD12	1:A:347:LEU:HD21	1.75	0.68
1:A:437:TRP:HA	1:A:437:TRP:CE3	2.27	0.68
1:B:356:LEU:HD23	1:B:377:VAL:HG11	1.75	0.68
1:A:388:SER:HA	1:A:413:ALA:HB3	1.76	0.68
1:A:174:GLU:OE2	1:A:174:GLU:HA	1.95	0.67
1:B:317:ALA:O	1:B:320:LEU:N	2.26	0.67
1:B:248[B]:TYR:CB	1:B:456:PRO:HB3	2.25	0.67
1:A:349:GLY:HA3	1:A:428:ARG:HH22	1.59	0.67
1:B:161:TYR:HE2	1:B:193:ILE:HD11	1.56	0.67
1:A:238:LEU:O	1:A:238:LEU:HD23	1.94	0.67
1:B:14:ASP:HA	1:B:196:GLN:HE21	1.60	0.67
1:B:100:SER:O	4:B:703:HOH:O	2.11	0.67
1:B:117:MET:SD	1:B:286:ARG:HB2	2.33	0.67
1:A:155:PHE:HA	1:A:276:HIS:CD2	2.31	0.67
1:A:184:LEU:HD23	4:A:637:HOH:O	1.92	0.66
1:A:394:LEU:CD1	1:A:411:ILE:HD13	2.25	0.66
1:B:138:THR:N	4:B:704:HOH:O	2.28	0.66
1:A:455:HIS:N	1:A:455:HIS:CD2	2.63	0.66
1:A:428:ARG:HD2	1:A:474:TRP:CZ3	2.31	0.66
1:A:38:ARG:HD3	1:A:75:TRP:HH2	1.58	0.66
1:A:223:VAL:HB	1:A:228:GLY:O	1.96	0.66
2:A:500[A]:VHG:CBA	2:A:500[A]:VHG:CMA	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ALA:O	1:B:124:VAL:HB	1.94	0.66
1:A:28:GLY:HA3	1:A:238:LEU:HG	1.78	0.66
1:A:48:GLN:HG2	1:A:49:ALA:H	1.61	0.66
1:A:154:GLY:O	1:A:155:PHE:O	2.14	0.66
1:A:354:ALA:CB	1:A:425:ILE:HG23	2.26	0.66
1:B:14:ASP:HA	1:B:196:GLN:NE2	2.11	0.65
1:B:54:PRO:HB2	1:B:57:THR:OG1	1.96	0.65
1:B:337:LEU:O	1:B:341:SER:HB2	1.96	0.65
1:B:31:LEU:HD23	1:B:40:LEU:HD11	1.77	0.65
1:B:97:LEU:HD12	1:B:98:HIS:N	2.12	0.65
1:A:319:LEU:HD12	1:A:347:LEU:CD2	2.27	0.65
1:A:364:VAL:HG23	1:A:364:VAL:O	1.97	0.65
1:B:30:LEU:O	1:B:31:LEU:C	2.35	0.65
1:B:176:LYS:HE3	1:B:180:MET:HB2	1.79	0.65
1:B:472:LEU:HB3	1:B:473:PRO:HD2	1.79	0.65
1:A:100:SER:CB	4:A:606:HOH:O	2.44	0.65
1:A:123:GLU:HA	1:A:126:ARG:HG2	1.79	0.65
1:B:29:VAL:CG2	1:B:108:LEU:HG	2.25	0.65
1:A:143:GLN:OE1	1:A:147:ASP:OD2	2.15	0.65
1:B:141:LEU:HD11	1:B:300:GLN:HE21	1.61	0.64
1:B:182:GLY:O	1:B:183:PHE:HD2	1.72	0.64
1:A:490:VAL:HG23	1:B:327:MET:HG2	1.79	0.64
1:A:171:VAL:HG11	1:A:183:PHE:HB2	1.79	0.64
2:A:500[B]:VHG:CBC	2:A:500[B]:VHG:CMC	2.74	0.64
1:B:259:SER:HA	1:B:272:ILE:O	1.96	0.64
1:B:316:ARG:HG3	1:B:316:ARG:HH11	1.63	0.64
1:B:402:ALA:C	1:B:404:ARG:H	2.00	0.64
1:B:156:ASP:N	1:B:156:ASP:OD1	2.31	0.64
1:A:65:ARG:O	1:A:66:VAL:HG13	1.97	0.64
1:A:345:LEU:C	1:A:350:ALA:CB	2.66	0.64
1:B:98:HIS:N	1:B:98:HIS:ND1	2.46	0.64
1:A:217:VAL:O	1:A:218:PRO:O	2.16	0.64
1:A:344:VAL:HA	1:A:347:LEU:HD12	1.79	0.64
1:A:437:TRP:HA	1:A:437:TRP:HE3	1.62	0.64
1:A:448:GLU:CD	1:A:455:HIS:CE1	2.71	0.64
1:B:204:ASN:ND2	1:B:234:SER:O	2.30	0.64
1:A:187:HIS:ND1	1:A:437:TRP:CZ3	2.62	0.63
1:B:168:HIS:CD2	1:B:437:TRP:CH2	2.86	0.63
1:A:354:ALA:O	1:A:355:LEU:HB2	1.97	0.63
1:A:433:ARG:HH11	1:A:433:ARG:CG	2.11	0.63
1:A:473:PRO:HA	4:A:621:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:HH21	1:B:207:ARG:HB2	1.62	0.63
1:B:77:PRO:HA	1:B:80:ALA:HB3	1.79	0.63
1:B:258:PHE:HE2	1:B:290:CYS:SG	2.11	0.63
1:A:86:VAL:HG13	1:A:94:ARG:HA	1.78	0.63
1:A:126:ARG:NE	1:B:292:VAL:HG21	2.13	0.63
1:A:131:PRO:HD3	1:B:295:GLN:NE2	2.13	0.63
1:B:141:LEU:HD21	1:B:300:GLN:HE21	1.61	0.63
1:A:124:VAL:HG12	1:A:148:THR:HB	1.81	0.63
1:A:445:ALA:HB1	1:A:456:PRO:HA	1.80	0.63
1:A:349:GLY:HA3	1:A:428:ARG:NH2	2.14	0.63
1:B:245:HIS:O	1:B:246:LEU:HB2	1.98	0.63
1:A:193:ILE:HG23	4:A:644:HOH:O	1.98	0.62
1:A:398:TYR:O	1:A:398:TYR:CD2	2.52	0.62
1:B:293:LEU:N	1:B:293:LEU:HD23	2.13	0.62
1:B:263:LEU:N	4:B:707:HOH:O	2.31	0.62
1:B:33:PHE:HA	1:B:39:LEU:O	1.98	0.62
1:B:265:GLU:O	1:B:267:VAL:N	2.31	0.62
1:B:376:LEU:HD12	1:B:376:LEU:O	1.98	0.62
1:A:394:LEU:HD13	1:A:411:ILE:HD13	1.81	0.62
1:B:164:ASP:O	1:B:166:ASP:N	2.31	0.62
1:B:209:ILE:HD12	1:B:212:ALA:CB	2.29	0.62
1:A:345:LEU:O	1:A:345:LEU:HD13	1.94	0.62
1:B:194:PRO:HD2	1:B:197:ALA:HB3	1.81	0.62
1:A:11:SER:N	1:A:14:ASP:OD2	2.32	0.62
1:A:188:PHE:HB2	1:A:189:PRO:HD2	1.81	0.62
1:A:209:ILE:O	1:A:256:ALA:HB1	1.99	0.62
1:A:247:GLU:OE2	1:A:455:HIS:HA	2.00	0.62
1:A:12:GLN:HB3	1:A:454:LEU:HD11	1.82	0.62
1:B:115:PRO:O	1:B:116:GLY:C	2.38	0.62
1:B:275:HIS:CE1	2:B:602[B]:VHG:CBB	2.82	0.62
1:A:128:LEU:HD23	1:A:145:ALA:HB2	1.82	0.61
1:B:74:GLN:HA	1:B:77:PRO:HD2	1.83	0.61
1:B:283:SER:O	1:B:284:HIS:C	2.37	0.61
1:B:343:ARG:O	1:B:347:LEU:HD23	2.00	0.61
1:A:204:ASN:O	1:A:204:ASN:ND2	2.33	0.61
1:B:391:THR:O	1:B:410:GLY:HA2	2.01	0.61
1:A:88:LEU:CB	1:A:89:PRO:CD	2.71	0.61
1:B:212:ALA:O	1:B:246:LEU:HD21	2.01	0.61
1:A:130:SER:HA	1:B:295:GLN:NE2	2.14	0.61
1:A:238:LEU:O	1:A:238:LEU:CD2	2.49	0.61
1:A:387:THR:HG21	1:A:486:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:HIS:HB3	1:B:234:SER:OG	2.00	0.61
1:B:122:LEU:O	1:B:123:GLU:C	2.36	0.61
1:B:438:ALA:HB1	1:B:460:PHE:HA	1.81	0.61
1:A:109:GLU:O	1:A:110:PRO:O	2.18	0.61
1:B:75:TRP:CD1	1:B:75:TRP:C	2.73	0.61
1:A:139:GLN:O	1:A:143:GLN:HB2	2.01	0.61
1:B:184:LEU:HD12	1:B:184:LEU:O	1.99	0.61
1:A:25:GLN:HG2	1:A:27:HIS:CE1	2.36	0.60
1:A:192:ASP:O	1:A:194:PRO:HD3	2.01	0.60
1:A:97:LEU:CD1	1:A:97:LEU:C	2.70	0.60
1:B:260:LEU:CD1	1:B:290:CYS:HB3	2.31	0.60
1:A:109:GLU:HG2	1:A:110:PRO:HD3	1.81	0.60
1:A:297:LEU:HA	1:A:300:GLN:HB2	1.83	0.60
1:A:344:VAL:O	1:A:347:LEU:HB2	2.02	0.60
1:A:412:LEU:O	1:A:425:ILE:HA	2.01	0.60
1:B:150:ARG:HD3	1:B:175:SER:OG	2.02	0.60
1:B:160:VAL:HG23	1:B:173:ALA:HB3	1.84	0.60
1:A:284:HIS:CD2	1:A:288:ARG:HD2	2.37	0.60
1:B:23:GLY:C	1:B:240:SER:HG	1.97	0.60
1:A:126:ARG:HE	1:B:292:VAL:HG21	1.67	0.60
1:A:239:ARG:NH2	2:A:500[B]:VHG:O2D	2.34	0.60
1:A:301:LEU:O	1:A:305:GLU:HG2	2.02	0.60
1:A:363:LEU:HB2	1:A:367:THR:HG21	1.84	0.60
1:B:428:ARG:NH1	1:B:474:TRP:CH2	2.70	0.60
1:B:29:VAL:CG2	1:B:108:LEU:O	2.49	0.59
1:B:428:ARG:NH1	1:B:474:TRP:CZ3	2.70	0.59
1:A:469:ASP:HB3	4:A:639:HOH:O	2.02	0.59
1:B:394:LEU:HD12	1:B:409:ALA:N	2.17	0.59
1:A:251:ASN:N	1:A:251:ASN:OD1	2.31	0.59
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.66	0.59
1:B:176:LYS:NZ	1:B:181:ASP:O	2.22	0.59
1:B:447:PRO:HB3	1:B:454:LEU:CB	2.32	0.59
1:B:489:LEU:O	1:B:490:VAL:O	2.20	0.59
1:B:196:GLN:OE1	1:B:197:ALA:HB2	2.02	0.59
1:B:373:VAL:O	1:B:376:LEU:HB3	2.03	0.59
1:B:380:LEU:HD23	1:B:425:ILE:HD11	1.83	0.59
1:B:437:TRP:CE3	1:B:441:PRO:HB3	2.37	0.59
1:B:448:GLU:O	1:B:450:GLY:O	2.20	0.59
1:A:146:ALA:HB2	1:A:160:VAL:HG21	1.85	0.59
1:B:341:SER:HA	1:B:344:VAL:H	1.68	0.59
1:A:45:ALA:HB2	1:A:218:PRO:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:C	1:A:172:LEU:HD12	2.23	0.59
1:A:457:ARG:O	1:A:457:ARG:HG2	2.01	0.59
1:B:303:ALA:O	1:B:306:ARG:HB2	2.03	0.59
1:A:128:LEU:HD21	1:A:296:LEU:HD22	1.84	0.59
1:A:394:LEU:O	1:A:394:LEU:HG	2.03	0.59
1:A:233:LEU:O	1:A:239:ARG:HD3	2.03	0.59
1:A:440:ASN:ND2	1:A:463:TRP:CE2	2.71	0.59
1:A:319:LEU:O	1:A:322:GLN:HB2	2.03	0.58
1:A:25:GLN:HB3	1:A:238:LEU:HB2	1.84	0.58
1:A:30:LEU:HD13	1:A:30:LEU:C	2.24	0.58
1:A:88:LEU:HD13	1:A:88:LEU:H	1.67	0.58
1:A:119:GLU:HA	1:B:118:GLU:OE2	2.02	0.58
1:B:260:LEU:HD13	1:B:294:THR:CG2	2.32	0.58
1:B:209:ILE:HD12	1:B:212:ALA:HB2	1.85	0.58
1:B:313:ASP:OD1	1:B:313:ASP:O	2.21	0.58
1:A:392:ASP:OD1	1:A:392:ASP:C	2.41	0.58
1:A:439:GLY:C	1:A:440:ASN:HD22	2.06	0.58
1:A:337:LEU:O	1:A:341:SER:N	2.36	0.58
2:B:602[A]:VHG:CMB	2:B:602[A]:VHG:C4A	2.81	0.58
1:A:315[B]:HIS:O	1:A:315[B]:HIS:CG	2.56	0.58
1:A:448:GLU:HG2	1:A:455:HIS:CE1	2.38	0.58
1:A:123:GLU:OE1	1:B:288:ARG:NH2	2.27	0.58
1:B:43:VAL:CG2	1:B:59:LEU:HG	2.33	0.58
1:B:28:GLY:C	1:B:29:VAL:HG22	2.23	0.58
1:B:54:PRO:HB2	1:B:57:THR:HG1	1.69	0.58
1:B:95:ALA:O	1:B:107:GLU:O	2.20	0.58
1:B:40:LEU:HD12	1:B:43:VAL:HG13	1.86	0.58
1:B:388:SER:HA	1:B:413:ALA:HB3	1.85	0.58
2:A:500[A]:VHG:ND	2:A:500[A]:VHG:NC	2.52	0.58
1:B:258:PHE:C	1:B:258:PHE:HD1	2.04	0.57
1:A:229:ARG:NH1	1:A:232:ASP:HB2	2.17	0.57
1:A:416:LEU:HG	1:A:489:LEU:CD2	2.34	0.57
2:B:602[A]:VHG:CMA	2:B:602[A]:VHG:CBA	2.82	0.57
1:A:390:HIS:HB2	1:A:474:TRP:NE1	2.19	0.57
1:B:88:LEU:HB2	1:B:89:PRO:HD2	1.85	0.57
1:B:251:ASN:O	1:B:251:ASN:ND2	2.27	0.57
1:A:22:GLY:HA3	4:A:641:HOH:O	2.02	0.57
1:B:129:VAL:HG12	1:B:129:VAL:O	2.04	0.57
1:A:188:PHE:CB	1:A:189:PRO:HD2	2.34	0.57
1:A:363:LEU:HD22	1:A:363:LEU:O	2.04	0.57
1:A:345:LEU:C	1:A:350:ALA:HB1	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:TYR:HE1	1:B:169:GLY:C	2.08	0.57
1:B:398:TYR:C	1:B:400:PRO:HD2	2.25	0.57
1:B:345:LEU:HD21	1:B:351:ALA:C	2.25	0.57
1:B:401:LEU:HD22	1:B:404:ARG:HG3	1.87	0.57
1:A:345:LEU:C	1:A:350:ALA:HB2	2.25	0.57
1:B:239:ARG:HH22	2:B:602[A]:VHG:CGD	2.17	0.57
1:A:411:ILE:HB	1:A:425:ILE:HG13	1.87	0.56
1:B:70:GLU:HB2	1:B:86:VAL:HG23	1.87	0.56
1:B:143:GLN:O	1:B:146:ALA:HB3	2.05	0.56
1:B:232:ASP:OD1	1:B:232:ASP:O	2.24	0.56
1:A:255:GLY:O	1:A:256:ALA:HB2	2.06	0.56
1:B:351:ALA:O	1:B:366:CYS:HB3	2.05	0.56
1:B:472:LEU:HB3	1:B:473:PRO:CD	2.35	0.56
1:B:486:ARG:HH11	1:B:486:ARG:HB3	1.71	0.56
1:B:122:LEU:HB3	1:B:126:ARG:HH22	1.71	0.56
1:B:252:MET:CE	1:B:275:HIS:HE1	2.18	0.56
1:A:97:LEU:HB2	1:A:105:VAL:O	2.05	0.56
1:A:198:ARG:HA	1:A:201:TYR:HB2	1.88	0.56
1:B:139:GLN:HB2	4:B:704:HOH:O	2.03	0.56
1:A:390:HIS:HB2	1:A:474:TRP:CD1	2.41	0.56
1:B:13[A]:CYS:HA	2:B:602[A]:VHG:CAC	2.34	0.56
1:A:448:GLU:CG	1:A:455:HIS:CE1	2.88	0.56
1:B:248[B]:TYR:HB3	1:B:456:PRO:CG	2.36	0.56
1:B:316:ARG:HH11	1:B:316:ARG:CG	2.19	0.56
1:A:38:ARG:HB3	1:A:63:VAL:CG2	2.35	0.56
1:B:117:MET:CE	1:B:286:ARG:CB	2.84	0.56
1:B:284:HIS:O	1:B:287:ARG:HD3	2.06	0.56
2:B:602[A]:VHG:CMA	2:B:602[A]:VHG:C1B	2.83	0.56
1:A:473:PRO:CA	4:A:621:HOH:O	2.53	0.56
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.19	0.56
1:B:455:HIS:HB3	1:B:456:PRO:CD	2.36	0.56
1:B:30:LEU:CD1	1:B:105:VAL:HG23	2.36	0.56
1:B:38:ARG:CB	1:B:63:VAL:HG13	2.36	0.56
1:A:33:PHE:HD1	1:A:40:LEU:HG	1.71	0.55
1:A:78:LEU:CD1	1:A:97:LEU:HG	2.36	0.55
1:A:93:TYR:HB3	1:A:109:GLU:O	2.05	0.55
1:A:131:PRO:CD	1:B:295:GLN:HE21	2.16	0.55
1:B:97:LEU:HD11	1:B:104:THR:C	2.26	0.55
1:B:283:SER:HG	1:B:285:GLU:CD	2.10	0.55
1:A:12:GLN:HE22	1:A:15:ARG:HE	1.54	0.55
1:A:25:GLN:CG	1:A:27:HIS:CE1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG12	2:A:500[B]:VHG:O2D	2.06	0.55
1:B:260:LEU:HD21	1:B:290:CYS:HB3	1.89	0.55
1:B:265:GLU:C	4:B:702:HOH:O	2.45	0.55
1:B:393:ARG:HB2	1:B:396:THR:HB	1.88	0.55
1:A:96:LEU:HD23	1:A:284:HIS:CG	2.42	0.55
1:B:117:MET:HE2	1:B:286:ARG:HB3	1.87	0.55
1:A:354:ALA:HB3	1:A:425:ILE:HG23	1.87	0.55
1:A:38:ARG:HG2	1:A:63:VAL:HG22	1.89	0.55
1:A:479:LEU:C	1:A:479:LEU:HD23	2.27	0.55
1:B:29:VAL:HG23	1:B:108:LEU:O	2.06	0.55
1:B:209:ILE:HG23	1:B:212:ALA:HB2	1.88	0.55
1:B:388:SER:CB	1:B:413:ALA:O	2.55	0.55
1:B:40:LEU:HB3	1:B:59:LEU:HA	1.88	0.55
1:B:97:LEU:HD21	1:B:104:THR:HG22	1.89	0.55
1:A:367:THR:HG23	1:A:368:PRO:O	2.07	0.55
1:B:124:VAL:HA	1:B:127:ARG:HD3	1.88	0.55
1:A:88:LEU:HB2	1:A:89:PRO:HD2	1.86	0.55
1:A:416:LEU:HD11	1:A:489:LEU:HB2	1.89	0.55
1:A:394:LEU:HD13	1:A:411:ILE:HG23	1.89	0.54
1:B:313:ASP:HA	1:B:316:ARG:HB2	1.88	0.54
2:B:602[B]:VHG:O2D	2:B:602[B]:VHG:CMD	2.55	0.54
1:B:30:LEU:O	1:B:31:LEU:O	2.24	0.54
1:A:30:LEU:O	1:A:44:SER:CB	2.55	0.54
1:A:171:VAL:HG23	1:A:188:PHE:CZ	2.42	0.54
1:B:260:LEU:CG	1:B:290:CYS:HB3	2.37	0.54
1:B:455:HIS:CB	1:B:456:PRO:CD	2.86	0.54
1:A:44:SER:O	1:A:44:SER:OG	2.15	0.54
2:A:500[A]:VHG:CMA	2:A:500[A]:VHG:NB	2.70	0.54
1:A:199:ALA:O	1:A:203:ARG:NH1	2.41	0.54
1:A:448:GLU:CD	1:A:455:HIS:NE2	2.61	0.54
1:B:32:ALA:HB1	1:B:103:LEU:HD13	1.90	0.54
1:B:252:MET:HE1	2:B:602[A]:VHG:NB	2.23	0.54
1:B:309:GLU:HG2	1:B:475:LYS:CE	2.38	0.54
1:A:399:PRO:N	1:A:400:PRO:HD2	2.23	0.54
1:A:31:LEU:HD13	1:A:31:LEU:O	2.08	0.54
1:B:86:VAL:HG13	1:B:86:VAL:O	2.08	0.54
1:B:96:LEU:N	1:B:96:LEU:CD1	2.69	0.54
1:A:61:GLN:OE1	1:A:65:ARG:NH1	2.40	0.54
1:A:159:MET:O	1:A:173:ALA:HB3	2.06	0.54
1:A:433:ARG:HH11	1:A:433:ARG:HB3	1.73	0.54
1:A:383:GLN:HG2	1:A:384:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:O	1:A:207:ARG:NE	2.42	0.53
1:A:398:TYR:CZ	1:A:400:PRO:HG2	2.44	0.53
1:A:471:SER:O	1:A:472:LEU:C	2.46	0.53
1:B:184:LEU:C	1:B:184:LEU:CD1	2.76	0.53
1:B:260:LEU:HB3	1:B:294:THR:HG21	1.91	0.53
1:A:406:ASP:OD2	1:A:407:VAL:HG12	2.07	0.53
1:B:366:CYS:HG	1:B:407:VAL:HG11	1.73	0.53
1:B:78:LEU:C	1:B:78:LEU:CD1	2.76	0.53
1:B:189:PRO:HD3	1:B:437:TRP:HE3	1.73	0.53
1:B:206:LEU:C	1:B:207:ARG:HD3	2.28	0.53
1:B:162:ARG:HA	1:B:270:GLY:HA3	1.89	0.53
1:A:356:LEU:HG	1:A:361:PRO:HG3	1.91	0.53
1:B:391:THR:HG21	1:B:397:VAL:HG21	1.91	0.53
1:B:394:LEU:HD11	1:B:408:ALA:HB1	1.85	0.53
1:A:399:PRO:CA	1:A:402:ALA:HB2	2.39	0.53
1:B:360:GLU:CB	1:B:361:PRO:CD	2.87	0.53
1:A:56:GLU:O	1:A:59:LEU:HD23	2.08	0.53
1:A:124:VAL:CG1	1:A:148:THR:HB	2.38	0.53
1:A:126:ARG:HE	1:B:292:VAL:CG2	2.22	0.53
1:B:168:HIS:HE1	1:B:187:HIS:ND1	2.06	0.53
1:B:211:ASP:HA	1:B:279:PRO:HB3	1.90	0.53
1:B:258:PHE:HD1	1:B:258:PHE:O	1.92	0.53
1:A:204:ASN:O	1:A:204:ASN:CG	2.48	0.53
1:B:74:GLN:HB3	1:B:84:VAL:HG11	1.91	0.53
1:B:95:ALA:O	1:B:107:GLU:C	2.47	0.53
1:B:112:GLU:O	1:B:113:LEU:HB2	2.09	0.53
1:B:147:ASP:O	1:B:150:ARG:HG2	2.09	0.53
1:B:155:PHE:CE1	1:B:276:HIS:HB2	2.44	0.53
1:B:355:LEU:HB3	1:B:357:LEU:HD21	1.91	0.53
1:A:210:ALA:CA	1:A:256:ALA:HB1	2.39	0.52
1:B:282:ILE:HG22	1:B:286:ARG:HG2	1.91	0.52
1:A:66:VAL:O	1:A:67:LEU:O	2.26	0.52
1:A:431:VAL:O	1:A:431:VAL:CG1	2.57	0.52
1:B:124:VAL:HG13	1:B:148:THR:HB	1.90	0.52
1:B:194:PRO:O	1:B:198:ARG:HG2	2.09	0.52
1:B:265:GLU:OE2	1:B:306:ARG:NH2	2.42	0.52
1:B:30:LEU:HD13	1:B:105:VAL:HG23	1.91	0.52
1:A:112:GLU:CG	1:A:117:MET:HG2	2.37	0.52
1:B:112:GLU:HG2	1:B:117:MET:HG3	1.91	0.52
1:A:459:SER:C	1:A:460:PHE:CD1	2.83	0.52
1:B:24:ILE:CA	1:B:240:SER:OG	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HD22	1:B:294:THR:HG21	1.92	0.52
1:A:177:ARG:HH11	1:A:177:ARG:CG	2.22	0.52
1:A:248[A]:TYR:OH	2:A:500[A]:VHG:CMB	2.58	0.52
1:A:296:LEU:O	1:A:297:LEU:C	2.47	0.52
1:B:150:ARG:HD3	1:B:175:SER:CB	2.40	0.52
1:A:31:LEU:HD12	1:A:31:LEU:N	2.25	0.52
1:B:122:LEU:O	1:B:125:VAL:N	2.43	0.52
1:B:141:LEU:HD21	1:B:300:GLN:HB3	1.92	0.52
1:B:334:GLU:N	1:B:334:GLU:OE1	2.43	0.52
1:B:385:PHE:CD1	1:B:389:PHE:HB2	2.44	0.52
1:B:209:ILE:HG23	1:B:212:ALA:CB	2.40	0.52
1:A:399:PRO:HA	1:A:402:ALA:HB2	1.92	0.52
1:B:296:LEU:HD12	1:B:296:LEU:O	2.09	0.52
1:B:356:LEU:CD1	1:B:361:PRO:HB3	2.40	0.52
1:A:45:ALA:CB	1:A:218:PRO:O	2.58	0.51
1:A:309:GLU:O	1:A:312:GLU:N	2.42	0.51
1:A:16:GLU:OE2	1:A:242:SER:HB2	2.10	0.51
1:A:322:GLN:HE21	1:A:343:ARG:CZ	2.24	0.51
1:B:12:GLN:NE2	1:B:452:GLN:O	2.43	0.51
1:B:212:ALA:N	1:B:255:GLY:O	2.43	0.51
1:A:70:GLU:OE2	1:A:88:LEU:HA	2.09	0.51
1:A:188:PHE:HB3	1:A:438:ALA:HB3	1.92	0.51
1:A:242:SER:C	1:A:244:VAL:H	2.14	0.51
1:A:292:VAL:HA	1:A:295:GLN:NE2	2.25	0.51
1:A:435:ILE:HG22	1:A:465:GLU:HB3	1.92	0.51
1:A:160:VAL:HA	1:A:272:ILE:HB	1.92	0.51
1:A:211:ASP:OD1	1:A:279:PRO:HG3	2.09	0.51
1:B:107:GLU:O	1:B:108:LEU:CB	2.58	0.51
1:B:431:VAL:O	1:B:431:VAL:HG23	2.10	0.51
1:B:13[B]:CYS:HA	2:B:602[B]:VHG:CAC	2.39	0.51
1:B:59:LEU:HD11	1:B:220:LEU:HB3	1.93	0.51
1:B:157:ARG:HG2	1:B:275:HIS:HB2	1.93	0.51
1:B:332:THR:O	1:B:336:VAL:HG22	2.11	0.51
1:A:135:VAL:HG12	1:A:135:VAL:O	2.10	0.51
1:B:324:ALA:O	1:B:327:MET:HB2	2.11	0.51
1:B:391:THR:O	1:B:410:GLY:CA	2.59	0.51
1:B:470:THR:HG22	1:B:471:SER:H	1.74	0.51
1:A:97:LEU:C	1:A:97:LEU:HD13	2.31	0.51
1:A:433:ARG:HB3	1:A:433:ARG:NH1	2.26	0.51
1:A:448:GLU:CD	1:A:455:HIS:HE2	2.14	0.51
1:B:348:THR:O	1:B:349:GLY:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HA	1:B:66:VAL:HB	1.91	0.51
1:B:97:LEU:HB2	1:B:106:LEU:HA	1.93	0.51
1:A:261:SER:HB3	1:A:263:LEU:HG	1.93	0.51
1:B:345:LEU:CD1	1:B:352:GLY:O	2.58	0.51
1:A:276:HIS:HB3	1:A:278:GLU:H	1.75	0.50
1:B:67:LEU:HB2	1:B:72:LEU:HG	1.93	0.50
1:B:189:PRO:HD3	1:B:437:TRP:CE3	2.46	0.50
1:B:323:LEU:HD12	1:B:323:LEU:C	2.31	0.50
1:B:345:LEU:HG	1:B:350:ALA:O	2.10	0.50
1:B:394:LEU:HD13	1:B:408:ALA:CB	2.40	0.50
1:A:157:ARG:HH11	1:A:157:ARG:CG	2.23	0.50
1:A:307:ALA:O	1:A:310:ALA:N	2.44	0.50
1:B:252:MET:CE	1:B:275:HIS:CE1	2.94	0.50
1:B:367:THR:OG1	1:B:368:PRO:N	2.43	0.50
1:B:434:THR:O	1:B:435:ILE:C	2.49	0.50
1:A:248[A]:TYR:HE1	1:A:460:PHE:HE2	1.59	0.50
1:B:211:ASP:C	1:B:213:ARG:H	2.15	0.50
1:A:377:VAL:HA	1:A:380:LEU:HB2	1.94	0.50
1:B:248[B]:TYR:HA	1:B:251:ASN:ND2	2.25	0.50
1:B:380:LEU:CD2	1:B:425:ILE:HD11	2.41	0.50
1:A:48:GLN:CG	1:A:53:ARG:O	2.59	0.50
1:A:141:LEU:HD13	1:A:141:LEU:C	2.32	0.50
1:A:262:LEU:O	1:A:263:LEU:C	2.49	0.50
1:A:297:LEU:N	1:A:297:LEU:HD22	2.26	0.50
1:A:76:GLU:HB3	1:A:77:PRO:CD	2.41	0.50
1:A:222:PRO:C	4:A:617:HOH:O	2.50	0.50
1:B:341:SER:OG	1:B:344:VAL:CG2	2.60	0.50
1:B:38:ARG:O	1:B:39:LEU:HB2	2.11	0.50
1:B:87:VAL:HG22	1:B:87:VAL:O	2.12	0.50
1:A:157:ARG:O	1:A:274:CYS:HA	2.11	0.50
1:A:211:ASP:O	1:A:214:ALA:N	2.42	0.50
1:B:209:ILE:HG22	1:B:209:ILE:O	2.11	0.50
1:A:280:LEU:O	1:A:281:HIS:HB2	2.12	0.50
1:B:78:LEU:HD11	1:B:97:LEU:HB3	1.93	0.50
1:A:128:LEU:HD21	1:A:296:LEU:CD2	2.41	0.49
1:A:474:TRP:HA	1:A:478:ASP:OD2	2.11	0.49
1:B:163:PHE:HA	1:B:168:HIS:O	2.12	0.49
1:A:58:LEU:HD22	1:A:58:LEU:N	2.27	0.49
1:A:183:PHE:O	1:A:185:GLY:N	2.45	0.49
1:A:288:ARG:NH2	1:B:123:GLU:OE2	2.44	0.49
1:B:313:ASP:OD1	1:B:313:ASP:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:HB3	1:A:437:TRP:CE3	2.47	0.49
1:B:303:ALA:O	1:B:306:ARG:CB	2.61	0.49
1:B:345:LEU:CD1	1:B:352:GLY:C	2.80	0.49
1:B:351:ALA:O	1:B:366:CYS:N	2.45	0.49
1:A:224:VAL:O	1:A:225:PRO:C	2.50	0.49
1:B:455:HIS:HB3	1:B:456:PRO:HD2	1.94	0.49
1:A:96:LEU:O	1:A:107:GLU:HB2	2.12	0.49
1:A:181:ASP:OD1	1:A:181:ASP:N	2.44	0.49
1:A:319:LEU:CD1	1:A:347:LEU:HD21	2.40	0.49
1:B:388:SER:HB2	1:B:413:ALA:O	2.12	0.49
1:A:178:GLY:O	1:A:179:GLY:C	2.51	0.49
1:B:21:LEU:N	1:B:21:LEU:HD12	2.28	0.49
1:A:48:GLN:HG3	1:A:53:ARG:O	2.13	0.49
1:A:399:PRO:HB3	1:A:402:ALA:HB2	1.94	0.49
1:B:122:LEU:O	1:B:124:VAL:N	2.46	0.49
1:B:248[A]:TYR:CD1	1:B:248[A]:TYR:C	2.85	0.49
1:B:25:GLN:NE2	1:B:238:LEU:CB	2.69	0.49
1:B:430:GLU:HA	1:B:470:THR:O	2.11	0.49
1:A:69:ALA:O	1:A:72:LEU:HB2	2.12	0.49
1:B:168:HIS:NE2	1:B:437:TRP:CZ2	2.80	0.49
1:B:78:LEU:HD21	1:B:97:LEU:HB3	1.95	0.49
1:B:302:SER:O	1:B:306:ARG:HB2	2.13	0.49
1:B:348:THR:HG23	1:B:478:ASP:CG	2.33	0.49
1:A:28:GLY:HA3	1:A:238:LEU:CD1	2.43	0.48
1:A:117:MET:SD	1:A:117:MET:C	2.91	0.48
1:A:324:ALA:HB3	1:B:486:ARG:HH12	1.78	0.48
1:B:93:TYR:HB2	1:B:108:LEU:HD11	1.94	0.48
1:B:155:PHE:HE1	1:B:276:HIS:HB2	1.77	0.48
1:B:476:ARG:O	1:B:477:ALA:CB	2.61	0.48
1:B:96:LEU:HD13	1:B:96:LEU:H	1.75	0.48
1:A:275:HIS:CE1	2:A:500[B]:VHG:CBB	2.95	0.48
1:B:260:LEU:HD22	1:B:294:THR:CG2	2.43	0.48
1:A:101:ASP:OD2	1:A:227:LEU:HD21	2.14	0.48
1:B:229:ARG:O	1:B:230:PRO:O	2.31	0.48
1:B:394:LEU:HB2	1:B:409:ALA:HA	1.94	0.48
1:B:50:LEU:CD1	1:B:88:LEU:HD11	2.44	0.48
1:B:101:ASP:N	1:B:101:ASP:OD1	2.46	0.48
1:B:206:LEU:HD13	1:B:287:ARG:O	2.13	0.48
1:B:399:PRO:N	1:B:400:PRO:CD	2.77	0.48
1:B:447:PRO:HB3	1:B:454:LEU:HB2	1.96	0.48
1:A:346:ALA:HA	1:A:350:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:HB3	1:B:63:VAL:HG13	1.96	0.48
1:B:124:VAL:O	1:B:127:ARG:HB2	2.13	0.48
1:B:129:VAL:O	1:B:129:VAL:CG1	2.61	0.48
1:A:18:ILE:O	1:A:18:ILE:HG12	2.13	0.48
1:A:448:GLU:O	1:A:449:PRO:C	2.52	0.48
1:A:471:SER:O	1:A:471:SER:OG	2.25	0.48
1:B:149:VAL:O	1:B:153:THR:CG2	2.60	0.48
1:B:345:LEU:HD11	1:B:352:GLY:O	2.13	0.48
1:B:379:TRP:CE2	1:B:383:GLN:OE1	2.67	0.48
1:A:349:GLY:CA	1:A:428:ARG:NH2	2.77	0.48
1:B:229:ARG:C	1:B:230:PRO:O	2.52	0.48
1:B:315:HIS:O	1:B:315:HIS:CD2	2.66	0.48
1:A:33:PHE:O	1:A:38:ARG:CZ	2.61	0.47
1:A:88:LEU:N	1:A:88:LEU:CD1	2.72	0.47
1:A:201:TYR:CE2	1:A:207:ARG:NH2	2.82	0.47
1:A:356:LEU:HD11	1:A:373:VAL:HG12	1.96	0.47
1:A:398:TYR:CE2	1:A:400:PRO:HG2	2.49	0.47
1:B:159:MET:HE1	2:B:602[B]:VHG:CBB	2.44	0.47
1:B:187:HIS:NE2	1:B:435:ILE:HG22	2.29	0.47
1:B:428:ARG:HG3	1:B:428:ARG:HH11	1.79	0.47
1:B:46:ASN:OD1	1:B:46:ASN:O	2.32	0.47
1:B:141:LEU:CD2	1:B:300:GLN:NE2	2.69	0.47
1:B:207:ARG:HH21	1:B:207:ARG:CB	2.27	0.47
1:A:95:ALA:HB1	1:A:107:GLU:H	1.79	0.47
1:A:183:PHE:O	1:A:186:MET:N	2.43	0.47
1:B:389:PHE:N	1:B:413:ALA:HB3	2.29	0.47
1:B:417:ALA:HB1	1:B:418:PRO:CD	2.45	0.47
1:A:251:ASN:HD21	1:A:456:PRO:CG	2.23	0.47
1:A:96:LEU:O	1:A:96:LEU:HD12	2.14	0.47
1:A:264:LYS:NZ	1:A:305:GLU:OE2	2.36	0.47
1:A:387:THR:O	1:A:388:SER:O	2.32	0.47
1:A:437:TRP:O	1:A:463:TRP:N	2.48	0.47
1:B:76:GLU:HB3	1:B:77:PRO:HD3	1.96	0.47
1:B:163:PHE:N	1:B:163:PHE:CD1	2.83	0.47
1:B:189:PRO:HG2	1:B:457:ARG:NH1	2.29	0.47
1:B:292:VAL:C	1:B:293:LEU:HD23	2.35	0.47
1:B:346:ALA:HB2	4:B:724:HOH:O	2.14	0.47
1:A:10:LEU:C	1:A:14:ASP:CG	2.73	0.47
1:A:24:ILE:HD13	1:A:24:ILE:H	1.79	0.47
1:A:93:TYR:N	1:A:93:TYR:CD1	2.83	0.47
1:A:404:ARG:C	1:A:406:ASP:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLY:C	4:B:704:HOH:O	2.52	0.47
1:A:281:HIS:HD1	1:A:282:ILE:H	1.62	0.47
1:A:433:ARG:HH11	1:A:433:ARG:CB	2.27	0.47
1:B:122:LEU:HB3	1:B:126:ARG:NH2	2.30	0.47
1:A:356:LEU:HD11	1:A:373:VAL:CG1	2.45	0.47
1:B:117:MET:CE	1:B:286:ARG:HB3	2.45	0.47
1:A:97:LEU:HD13	1:A:98:HIS:N	2.30	0.46
1:A:209:ILE:HD12	1:A:209:ILE:H	1.80	0.46
1:A:210:ALA:HA	1:A:256:ALA:CB	2.41	0.46
1:A:353:VAL:HG12	4:A:613:HOH:O	2.16	0.46
1:B:160:VAL:HG12	1:B:160:VAL:O	2.15	0.46
1:B:237:ALA:HB1	1:B:287:ARG:HH21	1.78	0.46
1:B:401:LEU:HD13	1:B:404:ARG:HG3	1.97	0.46
1:A:211:ASP:O	1:A:213:ARG:N	2.48	0.46
1:A:385:PHE:HD1	1:A:385:PHE:O	1.98	0.46
1:B:476:ARG:O	1:B:477:ALA:HB2	2.15	0.46
1:B:33:PHE:CZ	1:B:63:VAL:HG11	2.50	0.46
1:B:168:HIS:NE2	1:B:437:TRP:CH2	2.84	0.46
1:B:168:HIS:CE1	1:B:187:HIS:HB3	2.51	0.46
1:B:353:VAL:HG23	1:B:426:TRP:HB3	1.97	0.46
1:B:441:PRO:HD3	1:B:463:TRP:CE3	2.50	0.46
1:A:416:LEU:HD13	1:A:416:LEU:HA	1.69	0.46
1:A:37:ASP:O	1:A:37:ASP:CG	2.54	0.46
1:A:61:GLN:HA	1:A:62:PRO:HD2	1.80	0.46
1:A:31:LEU:O	1:A:31:LEU:CD1	2.63	0.46
1:A:468:ARG:O	1:A:469:ASP:CG	2.53	0.46
1:B:24:ILE:HA	1:B:240:SER:OG	2.15	0.46
1:B:95:ALA:HA	1:B:108:LEU:HB2	1.98	0.46
1:A:76:GLU:HB3	1:A:77:PRO:HD3	1.97	0.46
1:A:125:VAL:O	1:A:129:VAL:HB	2.15	0.46
1:A:128:LEU:O	1:A:128:LEU:CG	2.63	0.46
1:B:291:GLU:O	1:B:295:GLN:HB2	2.16	0.46
1:A:278:GLU:CB	1:A:279:PRO:HD2	2.45	0.46
1:A:388:SER:OG	1:A:413:ALA:O	2.25	0.46
1:B:66:VAL:HG12	1:B:67:LEU:HD23	1.98	0.46
1:B:84:VAL:O	1:B:94:ARG:NH1	2.44	0.46
1:A:163:PHE:CD1	1:A:163:PHE:N	2.83	0.46
1:A:272:ILE:O	1:A:272:ILE:HD13	2.15	0.46
1:A:354:ALA:HB3	1:A:425:ILE:H	1.81	0.46
1:B:275:HIS:NE2	2:B:602[B]:VHG:CBB	2.79	0.46
1:B:301:LEU:O	1:B:302:SER:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:THR:OG1	1:B:426:TRP:HZ2	1.99	0.46
1:A:117:MET:HG3	1:A:118:GLU:HG3	1.98	0.45
1:A:233:LEU:CD1	1:A:236:SER:HB3	2.46	0.45
1:A:260:LEU:HB2	1:A:272:ILE:HG23	1.98	0.45
1:A:385:PHE:CD2	1:A:389:PHE:HB2	2.52	0.45
1:A:440:ASN:ND2	1:A:440:ASN:N	2.65	0.45
1:B:144:THR:O	1:B:145:ALA:C	2.54	0.45
1:B:148:THR:O	1:B:152:LEU:N	2.49	0.45
1:B:220:LEU:HA	1:B:221:PRO:HA	1.76	0.45
1:B:261:SER:HA	1:B:271:LEU:HD13	1.98	0.45
1:B:340:GLU:OE1	1:B:343:ARG:NH1	2.49	0.45
1:B:345:LEU:HD11	1:B:352:GLY:HA2	1.93	0.45
1:B:399:PRO:N	1:B:400:PRO:HD2	2.31	0.45
1:A:34:ARG:CB	1:A:103:LEU:HB3	2.46	0.45
1:A:39:LEU:HD12	1:A:62:PRO:N	2.31	0.45
1:A:48:GLN:HG3	1:A:53:ARG:N	2.30	0.45
1:A:252:MET:O	1:A:254:VAL:HG12	2.17	0.45
1:A:380:LEU:HD22	1:A:385:PHE:CZ	2.51	0.45
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.78	0.45
1:A:439:GLY:C	1:A:440:ASN:ND2	2.69	0.45
1:B:332:THR:O	1:B:333:LEU:C	2.54	0.45
1:B:408:ALA:HB2	1:B:427:PHE:HD1	1.81	0.45
1:A:33:PHE:HA	1:A:40:LEU:HA	1.97	0.45
1:A:109:GLU:HG3	1:A:238:LEU:HD12	1.97	0.45
1:A:363:LEU:C	1:A:363:LEU:CD1	2.78	0.45
1:A:401:LEU:HD22	1:A:404:ARG:CG	2.47	0.45
1:A:408:ALA:HB2	1:A:427:PHE:HB3	1.98	0.45
1:A:460:PHE:CD1	1:A:460:PHE:N	2.84	0.45
1:B:117:MET:O	1:B:121:ALA:CB	2.64	0.45
1:B:117:MET:O	1:B:121:ALA:N	2.48	0.45
1:B:204:ASN:O	1:B:205:PRO:C	2.55	0.45
1:A:11:SER:N	1:A:14:ASP:CG	2.69	0.45
1:A:120:THR:O	1:A:124:VAL:HG22	2.17	0.45
1:A:128:LEU:O	1:A:128:LEU:HD13	2.17	0.45
1:A:248[A]:TYR:CE1	1:A:460:PHE:HE2	2.35	0.45
1:A:387:THR:HA	1:A:415:ARG:HG2	1.98	0.45
1:B:156:ASP:OD1	1:B:276:HIS:ND1	2.50	0.45
1:A:172:LEU:C	1:A:172:LEU:CD1	2.85	0.45
1:B:28:GLY:O	1:B:29:VAL:HG13	2.16	0.45
1:B:302:SER:O	1:B:303:ALA:C	2.55	0.45
1:B:362:LEU:O	1:B:362:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLN:HA	1:B:386:GLN:NE2	2.31	0.45
1:A:141:LEU:HD21	1:A:300:GLN:OE1	2.16	0.45
1:A:193:ILE:CG1	1:A:193:ILE:O	2.63	0.45
1:A:251:ASN:ND2	1:A:456:PRO:HG2	2.28	0.45
1:B:209:ILE:HD12	1:B:212:ALA:HB1	1.97	0.45
1:B:322:GLN:HG2	1:B:343:ARG:CZ	2.46	0.45
1:A:367:THR:O	1:A:407:VAL:HG21	2.17	0.45
1:A:473:PRO:HB3	4:A:621:HOH:O	2.15	0.45
1:B:68:PRO:HD2	1:B:71:VAL:HG12	1.99	0.45
1:B:489:LEU:O	1:B:490:VAL:C	2.55	0.45
1:A:394:LEU:HB3	1:A:409:ALA:O	2.17	0.45
1:B:71:VAL:HG23	1:B:86:VAL:HB	1.98	0.45
1:B:125:VAL:HG12	1:B:293:LEU:HD21	1.99	0.45
1:B:248[A]:TYR:HD1	1:B:249:LEU:HD23	1.82	0.45
1:B:374:GLU:OE2	1:B:374:GLU:HA	2.15	0.45
1:B:412:LEU:HG	1:B:474:TRP:CZ3	2.51	0.45
1:A:33:PHE:CD1	1:A:40:LEU:HG	2.50	0.45
1:A:64:GLY:HA2	1:A:66:VAL:O	2.17	0.45
1:A:367:THR:C	1:A:407:VAL:HG21	2.38	0.45
1:B:248[B]:TYR:CD1	1:B:248[B]:TYR:C	2.90	0.45
1:B:287:ARG:HA	1:B:290:CYS:HB2	1.99	0.45
1:A:205:PRO:HB2	1:A:206:LEU:HD12	1.99	0.45
1:A:244:VAL:O	1:A:247:GLU:HB3	2.17	0.45
1:A:346:ALA:N	1:A:350:ALA:CB	2.68	0.45
2:A:500[B]:VHG:CBA	2:A:500[B]:VHG:CMA	2.95	0.45
1:B:177:ARG:O	1:B:179:GLY:N	2.50	0.45
1:A:78:LEU:HD11	1:A:97:LEU:HG	1.98	0.44
1:A:163:PHE:CE2	1:A:268:LEU:HD23	2.51	0.44
1:B:477:ALA:O	1:B:481:ALA:HB2	2.17	0.44
1:A:376:LEU:HD22	1:A:398:TYR:CZ	2.53	0.44
1:A:312:GLU:HB3	1:A:477:ALA:CB	2.48	0.44
1:B:264:LYS:HB3	1:B:298:ALA:O	2.17	0.44
1:B:446:GLU:HA	1:B:447:PRO:HD3	1.83	0.44
1:A:345:LEU:O	1:A:350:ALA:HB1	2.17	0.44
1:A:348:THR:HG21	1:A:426:TRP:CD2	2.52	0.44
1:B:157:ARG:HA	1:B:175:SER:O	2.18	0.44
1:B:393:ARG:CB	1:B:396:THR:HB	2.47	0.44
1:A:22:GLY:O	1:A:23:GLY:O	2.36	0.44
1:A:159:MET:O	1:A:160:VAL:HB	2.18	0.44
1:A:292:VAL:HA	1:A:295:GLN:HE21	1.81	0.44
1:A:297:LEU:HD22	1:A:297:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:HIS:CD2	1:A:455:HIS:H	2.31	0.44
1:B:25:GLN:HE22	1:B:238:LEU:C	2.21	0.44
1:A:28:GLY:HA3	1:A:238:LEU:CG	2.44	0.44
1:B:97:LEU:HD12	1:B:98:HIS:O	2.17	0.44
1:B:459:SER:OG	1:B:460:PHE:N	2.49	0.44
1:A:170:GLU:HB2	1:A:187:HIS:HA	1.98	0.44
1:B:43:VAL:HG21	1:B:59:LEU:HG	1.99	0.44
1:B:248[B]:TYR:CB	1:B:456:PRO:CG	2.96	0.44
1:B:252:MET:HE2	1:B:275:HIS:HE1	1.81	0.44
1:B:393:ARG:HH11	1:B:393:ARG:HG2	1.83	0.44
1:A:249:LEU:O	1:A:252:MET:N	2.51	0.44
1:B:19:HIS:CB	1:B:234:SER:OG	2.65	0.44
1:B:130:SER:HB2	1:B:131:PRO:HD2	2.00	0.44
1:B:448:GLU:CD	1:B:455:HIS:NE2	2.71	0.44
1:B:468:ARG:HA	4:B:714:HOH:O	2.16	0.44
2:B:602[B]:VHG:CBA	2:B:602[B]:VHG:CMA	2.96	0.44
1:A:178:GLY:O	1:A:180:MET:N	2.50	0.43
1:A:203:ARG:CD	4:A:607:HOH:O	2.64	0.43
1:B:75:TRP:O	1:B:75:TRP:CG	2.71	0.43
1:B:130:SER:CB	1:B:131:PRO:CD	2.96	0.43
1:B:239:ARG:HH22	2:B:602[B]:VHG:CGD	2.31	0.43
1:A:171:VAL:CG2	1:A:188:PHE:CZ	3.01	0.43
1:A:428:ARG:O	1:A:429:PRO:O	2.36	0.43
1:B:100:SER:HB3	1:B:103:LEU:HB2	2.00	0.43
1:B:159:MET:CE	2:B:602[B]:VHG:CBB	2.96	0.43
1:B:181:ASP:HB3	4:B:728:HOH:O	2.18	0.43
1:B:388:SER:HA	1:B:413:ALA:O	2.18	0.43
1:A:94:ARG:HG2	1:A:94:ARG:HH21	1.83	0.43
1:B:233:LEU:HD23	1:B:236:SER:OG	2.19	0.43
1:B:248[B]:TYR:CD1	1:B:248[B]:TYR:O	2.71	0.43
1:A:58:LEU:HG	1:A:66:VAL:HG12	2.00	0.43
1:B:389:PHE:H	1:B:413:ALA:HB3	1.82	0.43
1:A:66:VAL:C	1:A:67:LEU:HG	2.39	0.43
1:A:69:ALA:O	1:A:72:LEU:N	2.51	0.43
1:A:177:ARG:HG3	1:A:177:ARG:NH1	2.24	0.43
1:A:344:VAL:C	1:A:346:ALA:H	2.22	0.43
1:A:479:LEU:C	1:A:479:LEU:CD2	2.87	0.43
1:B:38:ARG:HB2	1:B:63:VAL:HG13	2.00	0.43
1:B:211:ASP:OD1	1:B:279:PRO:CG	2.63	0.43
1:B:260:LEU:O	1:B:261:SER:O	2.36	0.43
1:B:299:LEU:O	1:B:302:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:HD11	1:B:347:LEU:CD1	2.49	0.43
1:A:20:LEU:HD12	1:A:20:LEU:O	2.18	0.43
1:A:39:LEU:HD12	1:A:62:PRO:HA	2.01	0.43
1:A:207:ARG:HH21	1:A:207:ARG:CG	2.32	0.43
1:B:33:PHE:HB3	1:B:38:ARG:HA	2.00	0.43
1:B:260:LEU:HD11	1:B:290:CYS:CA	2.49	0.43
1:A:58:LEU:HG	1:A:66:VAL:CG1	2.49	0.43
1:B:194:PRO:HG2	1:B:196:GLN:HE22	1.82	0.43
1:B:200:LEU:O	1:B:200:LEU:HD13	2.19	0.43
1:B:379:TRP:O	1:B:379:TRP:CG	2.71	0.43
1:A:131:PRO:O	1:A:132:LEU:HB2	2.19	0.43
1:A:157:ARG:CD	1:A:275:HIS:CE1	3.02	0.43
1:A:258:PHE:O	1:A:273:ALA:HA	2.19	0.43
1:A:354:ALA:O	1:A:355:LEU:CB	2.67	0.43
1:B:70:GLU:HG3	1:B:88:LEU:HB3	2.01	0.43
1:B:267:VAL:HG12	4:B:702:HOH:O	2.19	0.43
1:B:273:ALA:CB	2:B:602[A]:VHG:CAB	2.97	0.43
1:B:320:LEU:CD1	1:B:347:LEU:CD1	2.97	0.43
1:B:344:VAL:O	1:B:345:LEU:C	2.57	0.43
1:B:437:TRP:HB2	1:B:441:PRO:HG3	2.01	0.43
1:A:48:GLN:NE2	1:A:53:ARG:O	2.50	0.42
1:A:287:ARG:NH2	4:A:603:HOH:O	2.50	0.42
1:A:359:GLU:OE1	1:A:360:GLU:O	2.37	0.42
1:A:368:PRO:HB2	1:A:372:GLU:OE2	2.19	0.42
1:B:167:TRP:HB3	1:B:198:ARG:NH1	2.34	0.42
1:B:248[A]:TYR:O	1:B:251:ASN:ND2	2.52	0.42
1:A:93:TYR:HD2	1:A:110:PRO:N	2.17	0.42
1:B:33:PHE:CD1	1:B:38:ARG:HB3	2.54	0.42
1:B:130:SER:HB2	1:B:131:PRO:CD	2.50	0.42
1:B:408:ALA:HB2	1:B:427:PHE:CD1	2.53	0.42
1:A:129:VAL:O	1:A:130:SER:C	2.57	0.42
1:A:398:TYR:C	1:A:400:PRO:HD2	2.39	0.42
1:A:404:ARG:HD3	1:A:404:ARG:HA	1.89	0.42
1:B:260:LEU:O	1:B:260:LEU:CD2	2.68	0.42
1:B:428:ARG:HH11	1:B:428:ARG:CG	2.33	0.42
1:A:230:PRO:O	1:A:231:LEU:C	2.58	0.42
1:A:250:ARG:HA	1:A:254:VAL:HG11	2.00	0.42
1:A:324:ALA:HA	1:A:327:MET:HB2	2.02	0.42
1:B:78:LEU:HD21	1:B:97:LEU:CD2	2.42	0.42
1:B:265:GLU:O	1:B:266:GLY:C	2.57	0.42
1:B:283:SER:O	1:B:286:ARG:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:HG3	1:B:343:ARG:HD2	2.01	0.42
1:B:355:LEU:N	1:B:355:LEU:HD12	2.34	0.42
1:B:393:ARG:CG	1:B:393:ARG:NH1	2.82	0.42
1:A:264:LYS:HD2	1:A:298:ALA:O	2.19	0.42
1:A:292:VAL:O	1:A:295:GLN:HB2	2.19	0.42
1:A:383:GLN:HG2	1:A:384:PRO:CD	2.48	0.42
1:B:20:LEU:N	1:B:20:LEU:HD13	2.34	0.42
1:B:59:LEU:O	1:B:59:LEU:HD23	2.20	0.42
1:B:95:ALA:O	1:B:96:LEU:O	2.37	0.42
1:B:322:GLN:C	1:B:324:ALA:H	2.23	0.42
1:A:41:GLU:HG3	4:A:629:HOH:O	2.19	0.42
1:A:143:GLN:OE1	1:A:143:GLN:C	2.58	0.42
1:A:479:LEU:HD23	1:A:479:LEU:O	2.19	0.42
1:B:90:ALA:HB3	1:B:93:TYR:HE2	1.84	0.42
1:A:88:LEU:H	1:A:92:ALA:HB1	1.85	0.42
1:B:94:ARG:HA	1:B:94:ARG:HD3	1.64	0.42
1:B:314:ALA:O	1:B:317:ALA:N	2.53	0.42
1:A:399:PRO:CB	1:A:402:ALA:HB2	2.50	0.42
1:A:45:ALA:O	1:A:55:PRO:CG	2.67	0.42
1:A:86:VAL:CG2	1:A:88:LEU:HD11	2.50	0.42
1:A:322:GLN:HE21	1:A:343:ARG:NH2	2.17	0.42
1:A:353:VAL:HG11	1:A:364:VAL:HG23	1.96	0.42
1:A:197:ALA:O	1:A:198:ARG:CB	2.68	0.42
1:A:198:ARG:HA	1:A:201:TYR:H	1.84	0.42
1:A:245:HIS:ND1	2:A:500[A]:VHG:CHA	2.83	0.42
1:B:142:LEU:HG	1:B:160:VAL:HG11	2.02	0.42
1:B:182:GLY:C	1:B:183:PHE:CG	2.93	0.42
1:B:263:LEU:O	1:B:298:ALA:CB	2.67	0.42
1:B:320:LEU:CD1	1:B:347:LEU:HD13	2.50	0.42
1:A:90:ALA:O	1:A:92:ALA:N	2.53	0.41
1:A:202:THR:HA	1:A:263:LEU:CD2	2.49	0.41
1:B:466:THR:O	1:B:467:VAL:C	2.57	0.41
1:A:281:HIS:HD1	1:A:282:ILE:N	2.17	0.41
1:A:307:ALA:HB2	1:B:306:ARG:HH11	1.85	0.41
1:A:416:LEU:O	1:A:422:ARG:HB2	2.20	0.41
1:B:205:PRO:HB2	1:B:206:LEU:HD23	2.02	0.41
1:B:435:ILE:O	1:B:435:ILE:HD12	2.21	0.41
1:A:184:LEU:C	1:A:184:LEU:CD2	2.89	0.41
1:B:78:LEU:HD12	1:B:78:LEU:O	2.19	0.41
1:B:248[B]:TYR:CB	1:B:456:PRO:CB	2.95	0.41
1:B:260:LEU:CD2	1:B:290:CYS:HB3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ALA:HA	1:B:349:GLY:HA2	2.01	0.41
1:B:440:ASN:HA	1:B:441:PRO:HD3	1.89	0.41
1:B:157:ARG:CG	1:B:275:HIS:HB2	2.50	0.41
1:B:341:SER:OG	1:B:344:VAL:HG21	2.20	0.41
1:B:401:LEU:HD13	1:B:404:ARG:HB2	2.02	0.41
1:B:412:LEU:HD12	1:B:426:TRP:CZ2	2.54	0.41
1:B:486:ARG:HB3	1:B:486:ARG:NH1	2.34	0.41
1:A:48:GLN:CB	1:A:53:ARG:O	2.68	0.41
1:A:124:VAL:HG12	1:A:148:THR:CB	2.49	0.41
1:A:388:SER:HA	1:A:413:ALA:CB	2.46	0.41
1:A:86:VAL:CG2	1:A:88:LEU:CD1	2.98	0.41
1:A:225:PRO:HG3	4:A:629:HOH:O	2.19	0.41
1:B:81:ARG:NH1	1:B:81:ARG:HB3	2.35	0.41
1:B:117:MET:SD	1:B:286:ARG:CB	3.07	0.41
1:A:38:ARG:HB3	1:A:63:VAL:HG22	2.02	0.41
1:A:94:ARG:HH21	1:A:94:ARG:CG	2.34	0.41
1:A:260:LEU:O	1:A:271:LEU:CB	2.68	0.41
1:B:97:LEU:CD1	1:B:98:HIS:O	2.68	0.41
1:B:207:ARG:HD3	1:B:207:ARG:N	2.35	0.41
1:B:236:SER:C	1:B:238:LEU:H	2.24	0.41
1:A:74:GLN:O	1:A:75:TRP:C	2.59	0.41
1:A:155:PHE:CE2	1:A:258:PHE:HB2	2.56	0.41
1:A:28:GLY:CA	1:A:238:LEU:HG	2.47	0.41
1:A:183:PHE:O	1:A:184:LEU:C	2.60	0.41
1:A:183:PHE:CD1	1:A:183:PHE:N	2.86	0.41
1:A:348:THR:HG21	1:A:426:TRP:CE3	2.56	0.41
1:B:156:ASP:HB2	1:B:157:ARG:H	1.76	0.41
1:B:161:TYR:CE1	1:B:169:GLY:C	2.92	0.41
1:B:205:PRO:HB2	1:B:206:LEU:CD2	2.50	0.41
1:B:345:LEU:HD12	1:B:345:LEU:HA	1.89	0.41
1:B:360:GLU:HB3	1:B:361:PRO:HD3	2.02	0.41
2:B:602[B]:VHG:CAA	2:B:602[B]:VHG:CAD	2.99	0.41
1:A:38:ARG:NH1	1:A:104:THR:OG1	2.54	0.41
1:B:168:HIS:NE2	1:B:187:HIS:HB3	2.36	0.41
1:B:223:VAL:O	1:B:223:VAL:CG2	2.68	0.41
1:A:34:ARG:HB3	1:A:103:LEU:HB3	2.04	0.40
1:A:56:GLU:O	1:A:57:THR:C	2.59	0.40
1:A:25:GLN:HG3	1:A:27:HIS:CE1	2.56	0.40
1:A:303:ALA:HA	1:A:306:ARG:HG2	2.02	0.40
1:A:485:PHE:O	1:A:486:ARG:C	2.59	0.40
1:B:75:TRP:CD1	1:B:75:TRP:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ALA:O	1:B:147:ASP:C	2.59	0.40
1:A:16:GLU:OE2	1:A:242:SER:CB	2.69	0.40
1:A:188:PHE:HB2	1:A:189:PRO:CD	2.49	0.40
1:A:385:PHE:HD2	1:A:389:PHE:HB2	1.86	0.40
1:A:388:SER:HA	1:A:413:ALA:C	2.42	0.40
1:A:93:TYR:HD2	1:A:110:PRO:CD	2.33	0.40
1:A:241:VAL:O	1:A:242:SER:C	2.59	0.40
1:A:248[A]:TYR:HE1	1:A:460:PHE:CE2	2.38	0.40
1:A:306:ARG:HD3	1:B:307:ALA:HB2	2.02	0.40
1:B:142:LEU:O	1:B:145:ALA:HB3	2.21	0.40
1:B:379:TRP:NE1	1:B:383:GLN:OE1	2.55	0.40
1:A:19:HIS:NE2	1:A:20:LEU:HD23	2.36	0.40
1:A:107:GLU:OE2	1:A:238:LEU:HD22	2.21	0.40
1:A:209:ILE:HD12	1:A:209:ILE:N	2.37	0.40
1:A:312:GLU:HB3	1:A:477:ALA:HB1	2.04	0.40
1:B:76:GLU:CB	1:B:77:PRO:HD3	2.52	0.40
1:B:168:HIS:CG	1:B:169:GLY:N	2.90	0.40
1:B:193:ILE:HD12	1:B:271:LEU:HD23	2.03	0.40
1:B:211:ASP:HA	1:B:279:PRO:CB	2.51	0.40
1:B:288:ARG:O	1:B:291:GLU:HB3	2.22	0.40
1:B:309:GLU:O	1:B:313:ASP:N	2.54	0.40
1:B:401:LEU:HD22	1:B:401:LEU:HA	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:735:HOH:O	4:B:736:HOH:O[2_444]	1.87	0.33

## 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	483/490 (99%)	267 (55%)	123 (26%)	93 (19%)	0	0
1	B	482/490 (98%)	288 (60%)	106 (22%)	88 (18%)	0	0
All	All	965/980 (98%)	555 (58%)	229 (24%)	181 (19%)	0	0

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	GLY
1	A	36	PRO
1	A	37	ASP
1	A	57	THR
1	A	66	VAL
1	A	67	LEU
1	A	88	LEU
1	A	91	GLY
1	A	101	ASP
1	A	110	PRO
1	A	132	LEU
1	A	136	LYS
1	A	155	PHE
1	A	175	SER
1	A	184	LEU
1	A	189	PRO
1	A	195	VAL
1	A	198	ARG
1	A	199	ALA
1	A	205	PRO
1	A	206	LEU
1	A	212	ALA
1	A	216	PRO
1	A	218	PRO
1	A	222	PRO
1	A	231	LEU
1	A	232	ASP
1	A	254	VAL
1	A	279	PRO
1	A	281	HIS
1	A	350	ALA
1	A	355	LEU
1	A	362	LEU
1	A	364	VAL

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Mol	Chain	Res	Type
1	A	405	ALA
1	A	418	PRO
1	A	429	PRO
1	B	23	GLY
1	B	29	VAL
1	B	38	ARG
1	B	69	ALA
1	B	70	GLU
1	B	105	VAL
1	B	108	LEU
1	B	165	ALA
1	B	168	HIS
1	B	186	MET
1	B	189	PRO
1	B	193	ILE
1	B	222	PRO
1	B	225	PRO
1	B	226	ALA
1	B	231	LEU
1	B	232	ASP
1	B	241	VAL
1	B	246	LEU
1	B	252	MET
1	B	261	SER
1	B	284	HIS
1	B	333	LEU
1	B	349	GLY
1	B	359	GLU
1	B	366	CYS
1	B	402	ALA
1	B	403	ALA
1	B	432	ALA
1	B	447	PRO
1	B	449	PRO
1	A	14	ASP
1	A	41	GLU
1	A	49	ALA
1	A	63	VAL
1	A	70	GLU
1	A	166	ASP
1	A	179	GLY
1	A	213	ARG

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Mol	Chain	Res	Type
1	A	256	ALA
1	A	361	PRO
1	A	469	ASP
1	A	479	LEU
1	B	31	LEU
1	B	41	GLU
1	B	43	VAL
1	B	51	LEU
1	B	56	GLU
1	B	62	PRO
1	B	95	ALA
1	B	96	LEU
1	B	116	GLY
1	B	129	VAL
1	B	178	GLY
1	B	230	PRO
1	B	266	GLY
1	B	268	LEU
1	B	269	TRP
1	B	326	ALA
1	B	327	MET
1	B	362	LEU
1	B	368	PRO
1	B	384	PRO
1	B	409	ALA
1	B	418	PRO
1	B	435	ILE
1	B	445	ALA
1	B	467	VAL
1	B	477	ALA
1	B	478	ASP
1	A	65	ARG
1	A	89	PRO
1	A	92	ALA
1	A	98	HIS
1	A	165	ALA
1	A	227	LEU
1	A	263	LEU
1	A	296	LEU
1	A	342	GLU
1	A	385	PHE
1	A	388	SER

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Mol	Chain	Res	Type
1	A	390	HIS
1	A	417	ALA
1	A	451	HIS
1	A	456	PRO
1	A	462	ALA
1	A	470	THR
1	A	478	ASP
1	A	482	ALA
1	B	55	PRO
1	B	117	MET
1	B	120	THR
1	B	212	ALA
1	B	301	LEU
1	B	303	ALA
1	B	306	ARG
1	B	332	THR
1	B	457	ARG
1	A	45	ALA
1	A	61	GLN
1	A	141	LEU
1	A	265	GLU
1	A	341	SER
1	A	414	VAL
1	A	472	LEU
1	B	161	TYR
1	B	221	PRO
1	B	360	GLU
1	B	361	PRO
1	B	429	PRO
1	B	433	ARG
1	B	459	SER
1	A	271	LEU
1	A	353	VAL
1	A	368	PRO
1	A	445	ALA
1	B	44	SER
1	B	179	GLY
1	B	237	ALA
1	B	353	VAL
1	B	479	LEU
1	A	11	SER
1	A	69	ALA

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Mol	Chain	Res	Type
1	A	160	VAL
1	A	272	ILE
1	A	280	LEU
1	A	349	GLY
1	B	89	PRO
1	B	121	ALA
1	B	134	GLY
1	B	182	GLY
1	B	331	GLY
1	B	476	ARG
1	A	129	VAL
1	A	171	VAL
1	B	444	PRO
1	A	77	PRO
1	A	115	PRO
1	A	68	PRO
1	A	87	VAL
1	B	76	GLU
1	B	456	PRO
1	A	221	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	378/383 (99%)	224 (59%)	154 (41%)	0	0
1	B	376/383 (98%)	239 (64%)	137 (36%)	0	0
All	All	754/766 (98%)	463 (61%)	291 (39%)	0	0

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	10	LEU
1	A	18	ILE

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Mol	Chain	Res	Type
1	A	20	LEU
1	A	24	ILE
1	A	30	LEU
1	A	31	LEU
1	A	37	ASP
1	A	38	ARG
1	A	40	LEU
1	A	42	VAL
1	A	43	VAL
1	A	48	GLN
1	A	51	LEU
1	A	58	LEU
1	A	59	LEU
1	A	67	LEU
1	A	71	VAL
1	A	74	GLN
1	A	76	GLU
1	A	78	LEU
1	A	81	ARG
1	A	85	ARG
1	A	86	VAL
1	A	88	LEU
1	A	93	TYR
1	A	94	ARG
1	A	96	LEU
1	A	97	LEU
1	A	100	SER
1	A	103	LEU
1	A	106	LEU
1	A	108	LEU
1	A	110	PRO
1	A	114	GLN
1	A	117	MET
1	A	120	THR
1	A	124	VAL
1	A	128	LEU
1	A	129	VAL
1	A	130	SER
1	A	132	LEU
1	A	136	LYS
1	A	138	THR
1	A	139	GLN

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Mol	Chain	Res	Type
1	A	143	GLN
1	A	150	ARG
1	A	153	THR
1	A	157	ARG
1	A	158	VAL
1	A	159	MET
1	A	163	PHE
1	A	164	ASP
1	A	167	TRP
1	A	168	HIS
1	A	172	LEU
1	A	176	LYS
1	A	177	ARG
1	A	180	MET
1	A	181	ASP
1	A	184	LEU
1	A	188	PHE
1	A	189	PRO
1	A	193	ILE
1	A	195	VAL
1	A	196	GLN
1	A	203	ARG
1	A	204	ASN
1	A	207	ARG
1	A	208	LEU
1	A	215	ARG
1	A	217	VAL
1	A	219	LEU
1	A	220	LEU
1	A	222	PRO
1	A	227	LEU
1	A	229	ARG
1	A	231	LEU
1	A	234	SER
1	A	235	ASN
1	A	238	LEU
1	A	241	VAL
1	A	244	VAL
1	A	246	LEU
1	A	247	GLU
1	A	248[A]	TYR
1	A	248[B]	TYR

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Mol	Chain	Res	Type
1	A	249	LEU
1	A	251	ASN
1	A	263	LEU
1	A	264	LYS
1	A	271	LEU
1	A	272	ILE
1	A	274	CYS
1	A	276	HIS
1	A	278	GLU
1	A	279	PRO
1	A	281	HIS
1	A	282	ILE
1	A	288	ARG
1	A	290	CYS
1	A	292	VAL
1	A	296	LEU
1	A	297	LEU
1	A	301	LEU
1	A	305	GLU
1	A	309	GLU
1	A	311	SER
1	A	313	ASP
1	A	319	LEU
1	A	323	LEU
1	A	327	MET
1	A	340	GLU
1	A	342	GLU
1	A	345	LEU
1	A	359	GLU
1	A	363	LEU
1	A	367	THR
1	A	368	PRO
1	A	370	GLN
1	A	376	LEU
1	A	377	VAL
1	A	383	GLN
1	A	385	PHE
1	A	386	GLN
1	A	391	THR
1	A	392	ASP
1	A	394	LEU
1	A	397	VAL

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Mol	Chain	Res	Type
1	A	411	ILE
1	A	416	LEU
1	A	422	ARG
1	A	430	GLU
1	A	431	VAL
1	A	433	ARG
1	A	434	THR
1	A	435	ILE
1	A	436	SER
1	A	437	TRP
1	A	446	GLU
1	A	453	ARG
1	A	454	LEU
1	A	455	HIS
1	A	457	ARG
1	A	460	PHE
1	A	463	TRP
1	A	466	THR
1	A	471	SER
1	A	472	LEU
1	A	474	TRP
1	A	483	GLU
1	A	485	PHE
1	A	486	ARG
1	A	490	VAL
1	B	9	ASP
1	B	10	LEU
1	B	15	ARG
1	B	16	GLU
1	B	19	HIS
1	B	20	LEU
1	B	29	VAL
1	B	30	LEU
1	B	40	LEU
1	B	50	LEU
1	B	53	ARG
1	B	56	GLU
1	B	57	THR
1	B	58	LEU
1	B	70	GLU
1	B	71	VAL
1	B	72	LEU

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Mol	Chain	Res	Type
1	B	75	TRP
1	B	78	LEU
1	B	81	ARG
1	B	84	VAL
1	B	85	ARG
1	B	94	ARG
1	B	96	LEU
1	B	98	HIS
1	B	100	SER
1	B	103	LEU
1	B	104	THR
1	B	114	GLN
1	B	126	ARG
1	B	129	VAL
1	B	136	LYS
1	B	138	THR
1	B	141	LEU
1	B	142	LEU
1	B	143	GLN
1	B	153	THR
1	B	155	PHE
1	B	156	ASP
1	B	157	ARG
1	B	158	VAL
1	B	159	MET
1	B	164	ASP
1	B	166	ASP
1	B	177	ARG
1	B	183	PHE
1	B	184	LEU
1	B	186	MET
1	B	188	PHE
1	B	189	PRO
1	B	193	ILE
1	B	196	GLN
1	B	198	ARG
1	B	200	LEU
1	B	206	LEU
1	B	207	ARG
1	B	208	LEU
1	B	209	ILE
1	B	213	ARG

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Mol	Chain	Res	Type
1	B	215	ARG
1	B	220	LEU
1	B	225	PRO
1	B	229	ARG
1	B	231	LEU
1	B	233	LEU
1	B	240	SER
1	B	241	VAL
1	B	246	LEU
1	B	248[A]	TYR
1	B	248[B]	TYR
1	B	249	LEU
1	B	251	ASN
1	B	257	SER
1	B	258	PHE
1	B	260	LEU
1	B	262	LEU
1	B	263	LEU
1	B	264	LYS
1	B	268	LEU
1	B	271	LEU
1	B	272	ILE
1	B	276	HIS
1	B	277	LEU
1	B	280	LEU
1	B	286	ARG
1	B	287	ARG
1	B	297	LEU
1	B	300	GLN
1	B	301	LEU
1	B	304	GLU
1	B	306	ARG
1	B	313	ASP
1	B	316	ARG
1	B	322	GLN
1	B	325	THR
1	B	327	MET
1	B	329	GLU
1	B	333	LEU
1	B	334	GLU
1	B	338	GLU
1	B	339	LYS

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Mol	Chain	Res	Type
1	B	340	GLU
1	B	347	LEU
1	B	348	THR
1	B	356	LEU
1	B	357	LEU
1	B	359	GLU
1	B	360	GLU
1	B	363	LEU
1	B	364	VAL
1	B	367	THR
1	B	370	GLN
1	B	377	VAL
1	B	384	PRO
1	B	392	ASP
1	B	393	ARG
1	B	394	LEU
1	B	397	VAL
1	B	401	LEU
1	B	404	ARG
1	B	406	ASP
1	B	407	VAL
1	B	411	ILE
1	B	416	LEU
1	B	423	PHE
1	B	428	ARG
1	B	434	THR
1	B	440	ASN
1	B	442	ARG
1	B	446	GLU
1	B	447	PRO
1	B	449	PRO
1	B	452	GLN
1	B	465	GLU
1	B	472	LEU
1	B	476	ARG
1	B	486	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	25	GLN

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Mol	Chain	Res	Type
1	A	74	GLN
1	A	204	ASN
1	A	235	ASN
1	A	275	HIS
1	A	276	HIS
1	A	295	GLN
1	A	322	GLN
1	A	440	ASN
1	B	25	GLN
1	B	168	HIS
1	B	275	HIS
1	B	284	HIS
1	B	295	GLN
1	B	300	GLN
1	B	370	GLN
1	B	386	GLN
1	B	452	GLN

### 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](#)

5 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	VHG	A	500[A]	1	31,46,46	7.59	17 (54%)	28,67,67	1.73	9 (32%)
2	VHG	A	500[B]	1	31,46,46	7.54	15 (48%)	28,67,67	2.07	10 (35%)
2	VHG	B	602[A]	1	31,46,46	7.75	15 (48%)	28,67,67	3.02	15 (53%)
2	VHG	B	602[B]	1	31,46,46	7.87	15 (48%)	28,67,67	3.93	13 (46%)
3	BEN	B	601	-	9,9,9	0.40	0	7,11,11	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VHG	A	500[A]	1	-	11/18/58/58	0/4/4/4
2	VHG	A	500[B]	1	-	12/18/58/58	0/4/4/4
2	VHG	B	602[A]	1	-	11/18/58/58	0/4/4/4
2	VHG	B	602[B]	1	-	8/18/58/58	0/4/4/4
3	BEN	B	601	-	-	0/4/4/4	0/1/1/1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602[B]	VHG	CHA-C4D	-28.38	1.30	1.51
2	B	602[A]	VHG	CHA-C4D	-26.38	1.31	1.51
2	A	500[A]	VHG	CHA-C4D	-26.24	1.31	1.51
2	A	500[B]	VHG	CHA-C4D	-25.56	1.32	1.51
2	B	602[A]	VHG	CHB-C1B	-19.46	1.29	1.50
2	B	602[B]	VHG	CHB-C1B	-18.71	1.30	1.50
2	A	500[B]	VHG	CHB-C1B	-17.99	1.30	1.50
2	A	500[A]	VHG	CHB-C1B	-17.57	1.31	1.50
2	B	602[A]	VHG	C1C-NC	13.36	1.54	1.37
2	B	602[B]	VHG	C1C-NC	12.90	1.54	1.37
2	A	500[B]	VHG	C1C-NC	12.23	1.53	1.37
2	A	500[A]	VHG	C1C-NC	12.05	1.53	1.37
2	A	500[A]	VHG	C1B-NB	10.95	1.55	1.35
2	B	602[B]	VHG	C1B-NB	10.95	1.55	1.35
2	A	500[A]	VHG	CAC-C3C	-10.94	1.30	1.51
2	B	602[A]	VHG	CAC-C3C	-10.91	1.30	1.51
2	A	500[B]	VHG	CAC-C3C	-10.90	1.30	1.51
2	B	602[B]	VHG	CAC-C3C	-10.87	1.30	1.51
2	A	500[B]	VHG	C1B-NB	10.49	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500[A]	VHG	CHD-C4C	-10.19	1.32	1.50
2	A	500[B]	VHG	CHD-C4C	-10.06	1.32	1.50
2	B	602[A]	VHG	CHD-C4C	-10.05	1.32	1.50
2	A	500[B]	VHG	C4B-NB	9.53	1.54	1.37
2	B	602[A]	VHG	C1B-NB	9.50	1.52	1.35
2	B	602[A]	VHG	C4B-NB	9.42	1.54	1.37
2	B	602[B]	VHG	C4B-NB	9.25	1.54	1.37
2	A	500[A]	VHG	C3D-C4D	9.25	1.53	1.39
2	A	500[B]	VHG	C3D-C4D	9.20	1.53	1.39
2	B	602[B]	VHG	CHD-C4C	-8.96	1.34	1.50
2	A	500[A]	VHG	C4B-NB	8.96	1.53	1.37
2	B	602[A]	VHG	C3D-C4D	8.45	1.51	1.39
2	B	602[B]	VHG	C4C-NC	8.37	1.55	1.37
2	B	602[A]	VHG	C4C-NC	8.24	1.55	1.37
2	A	500[B]	VHG	C4C-NC	7.53	1.54	1.37
2	A	500[A]	VHG	C4C-NC	7.51	1.53	1.37
2	B	602[B]	VHG	C3D-C4D	6.67	1.49	1.39
2	B	602[B]	VHG	C2D-C1D	4.75	1.49	1.42
2	A	500[B]	VHG	C2D-C1D	3.91	1.48	1.42
2	A	500[A]	VHG	C2D-C1D	3.79	1.47	1.42
2	B	602[A]	VHG	OB-C4B	-3.64	1.17	1.23
2	B	602[A]	VHG	C2D-C1D	3.38	1.47	1.42
2	B	602[B]	VHG	C3D-C2D	3.32	1.47	1.37
2	B	602[A]	VHG	C3A-C4A	-3.17	1.37	1.42
2	B	602[B]	VHG	OB-C4B	-3.17	1.18	1.23
2	A	500[A]	VHG	OB-C4B	-3.13	1.18	1.23
2	A	500[B]	VHG	OB-C4B	-3.06	1.18	1.23
2	A	500[A]	VHG	C3D-C2D	3.04	1.46	1.37
2	A	500[A]	VHG	CHA-C1A	2.96	1.53	1.51
2	A	500[B]	VHG	CHA-C1A	2.94	1.53	1.51
2	B	602[A]	VHG	C3D-C2D	2.91	1.46	1.37
2	A	500[B]	VHG	C3D-C2D	2.87	1.46	1.37
2	B	602[B]	VHG	C2C-C1C	-2.81	1.48	1.51
2	A	500[A]	VHG	C2C-C1C	-2.80	1.48	1.51
2	B	602[A]	VHG	C2C-C1C	-2.75	1.48	1.51
2	A	500[B]	VHG	C2C-C1C	-2.73	1.48	1.51
2	B	602[B]	VHG	OC-C1C	-2.73	1.18	1.23
2	B	602[B]	VHG	C3A-C4A	-2.69	1.37	1.42
2	A	500[A]	VHG	C3B-C2B	2.59	1.42	1.37
2	B	602[A]	VHG	OC-C1C	-2.58	1.18	1.23
2	A	500[B]	VHG	C3A-C4A	-2.27	1.38	1.42
2	A	500[A]	VHG	C3A-C4A	-2.13	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500[A]	VHG	OC-C1C	-2.01	1.19	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602[B]	VHG	CAD-C3D-C4D	-17.02	115.34	127.30
2	B	602[A]	VHG	CAA-CBA-CGA	-6.33	102.06	112.67
2	B	602[A]	VHG	CAA-C2A-C1A	-6.32	122.86	127.30
2	B	602[B]	VHG	CAD-CBD-CGD	-5.91	102.76	112.67
2	B	602[A]	VHG	CAD-C3D-C4D	-5.72	123.28	127.30
2	A	500[B]	VHG	CHB-C1B-C2B	-4.90	120.36	129.53
2	B	602[A]	VHG	CHB-C1B-C2B	-4.67	120.80	129.53
2	B	602[A]	VHG	OC-C1C-NC	4.51	130.41	124.94
2	A	500[B]	VHG	CAA-CBA-CGA	-4.31	105.44	112.67
2	A	500[A]	VHG	CAD-C3D-C4D	-3.91	124.55	127.30
2	B	602[A]	VHG	CHD-C4C-NC	3.85	127.39	120.42
2	B	602[A]	VHG	OC-C1C-C2C	-3.83	122.58	126.28
2	A	500[B]	VHG	CAD-C3D-C4D	-3.56	124.80	127.30
2	B	602[B]	VHG	OC-C1C-NC	3.54	129.23	124.94
2	B	602[A]	VHG	CBD-CAD-C3D	-3.51	106.01	112.49
2	A	500[A]	VHG	CAA-C2A-C1A	-3.34	124.95	127.30
2	B	602[B]	VHG	CAA-C2A-C1A	-3.29	124.98	127.30
2	A	500[B]	VHG	CHD-C4C-NC	3.29	126.37	120.42
2	B	602[B]	VHG	CHD-C4C-NC	3.22	126.24	120.42
2	A	500[B]	VHG	CBA-CAA-C2A	-3.07	106.83	112.49
2	B	602[B]	VHG	CAD-C3D-C2D	3.05	136.00	127.25
2	B	602[A]	VHG	C3B-C4B-NB	-3.03	105.11	109.61
2	B	602[B]	VHG	CHB-C1B-C2B	-3.00	123.93	129.53
2	B	602[B]	VHG	CAA-CBA-CGA	-2.97	107.69	112.67
2	B	602[A]	VHG	CAD-CBD-CGD	-2.90	107.80	112.67
2	A	500[A]	VHG	C3B-C4B-NB	-2.89	105.32	109.61
2	B	602[B]	VHG	C3B-C4B-NB	-2.72	105.57	109.61
2	A	500[A]	VHG	CAA-CBA-CGA	-2.71	108.12	112.67
2	B	602[B]	VHG	OC-C1C-C2C	-2.70	123.67	126.28
2	A	500[B]	VHG	C3B-C4B-NB	-2.69	105.62	109.61
2	A	500[B]	VHG	CAB-C3B-C2B	-2.69	119.75	128.60
2	A	500[B]	VHG	CAD-CBD-CGD	-2.64	108.24	112.67
2	B	602[B]	VHG	CBB-CAB-C3B	-2.62	114.61	127.62
2	B	602[A]	VHG	CMC-C2C-C3C	-2.50	106.83	113.86
2	B	602[B]	VHG	OB-C4B-NB	2.44	129.31	124.36
2	B	602[A]	VHG	CBC-CAC-C3C	2.44	116.67	112.98
2	A	500[A]	VHG	CBA-CAA-C2A	-2.41	108.04	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602[B]	VHG	CBC-CAC-C3C	2.41	116.63	112.98
2	A	500[B]	VHG	CMC-C2C-C3C	-2.36	107.24	113.86
2	A	500[A]	VHG	CHD-C4C-NC	2.36	124.69	120.42
2	A	500[A]	VHG	CMC-C2C-C3C	-2.31	107.38	113.86
2	B	602[A]	VHG	CMB-C2B-C1B	-2.18	119.84	126.37
2	A	500[A]	VHG	CBB-CAB-C3B	-2.15	116.90	127.62
2	A	500[A]	VHG	CAD-CBD-CGD	-2.13	109.10	112.67
2	A	500[B]	VHG	CBB-CAB-C3B	-2.09	117.22	127.62
2	B	602[A]	VHG	CBB-CAB-C3B	-2.02	117.58	127.62
2	B	602[A]	VHG	CMD-C2D-C3D	2.00	128.72	124.94

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500[A]	VHG	C1A-C2A-CAA-CBA
2	A	500[A]	VHG	C3A-C2A-CAA-CBA
2	A	500[A]	VHG	C2D-C3D-CAD-CBD
2	A	500[A]	VHG	C4D-C3D-CAD-CBD
2	A	500[A]	VHG	C2A-CAA-CBA-CGA
2	A	500[B]	VHG	C2A-C1A-CHA-C4D
2	A	500[B]	VHG	NB-C1B-CHB-C4A
2	A	500[B]	VHG	C1A-C2A-CAA-CBA
2	A	500[B]	VHG	C3A-C2A-CAA-CBA
2	A	500[B]	VHG	C2B-C3B-CAB-CBB
2	A	500[B]	VHG	C4B-C3B-CAB-CBB
2	A	500[B]	VHG	C2C-C3C-CAC-CBC
2	A	500[B]	VHG	C3D-C4D-CHA-C1A
2	B	602[A]	VHG	NB-C1B-CHB-C4A
2	B	602[A]	VHG	C1A-C2A-CAA-CBA
2	B	602[A]	VHG	C3A-C2A-CAA-CBA
2	B	602[A]	VHG	C2C-C3C-CAC-CBC
2	B	602[A]	VHG	C4C-C3C-CAC-CBC
2	B	602[A]	VHG	C2D-C3D-CAD-CBD
2	B	602[A]	VHG	C4D-C3D-CAD-CBD
2	B	602[A]	VHG	C3A-C4A-CHB-C1B
2	B	602[A]	VHG	C3D-CAD-CBD-CGD
2	B	602[B]	VHG	C1A-C2A-CAA-CBA
2	B	602[B]	VHG	C3A-C2A-CAA-CBA
2	B	602[B]	VHG	C4C-C3C-CAC-CBC
2	B	602[B]	VHG	C2D-C3D-CAD-CBD
2	B	602[B]	VHG	C4D-C3D-CAD-CBD

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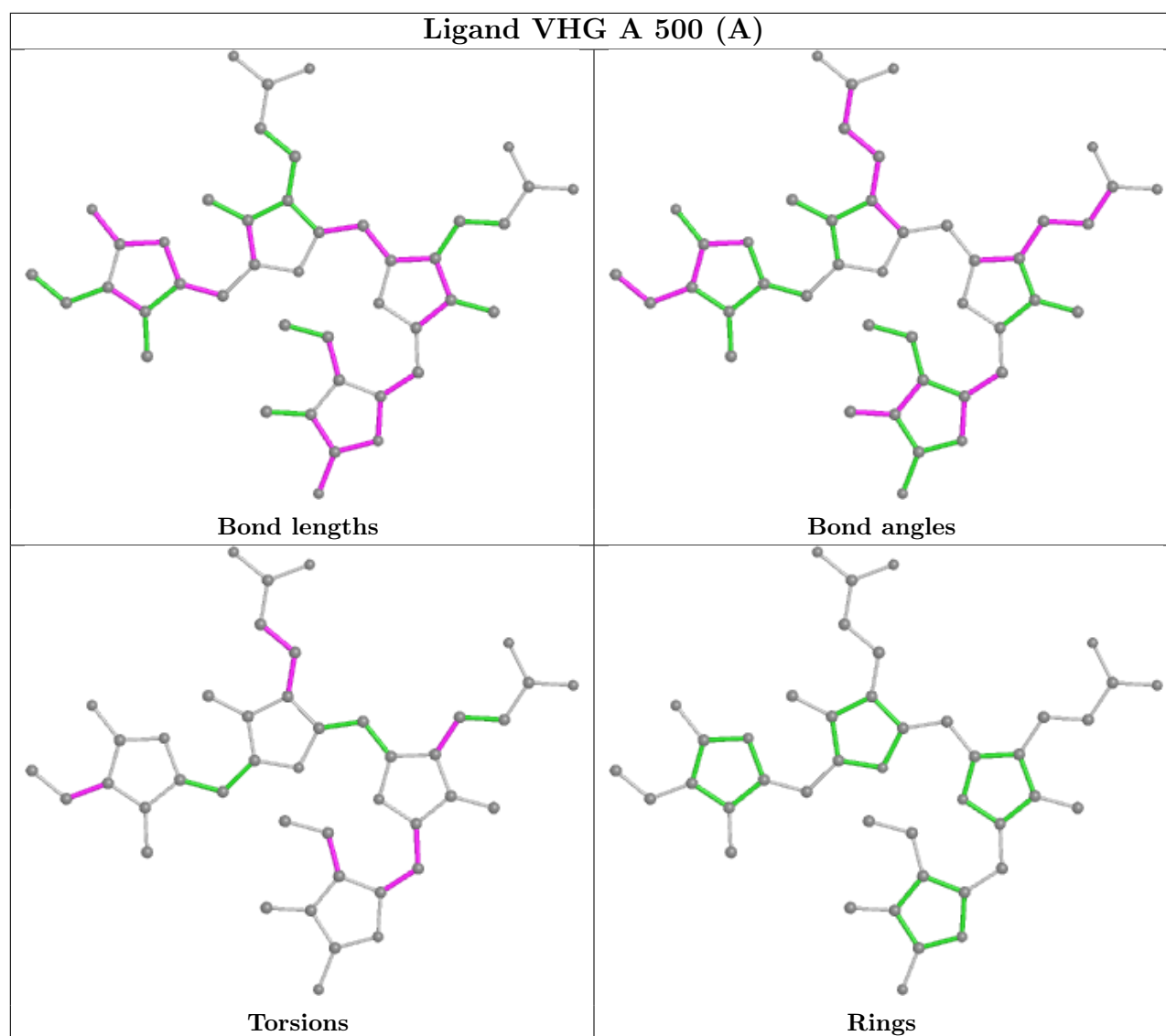
Mol	Chain	Res	Type	Atoms
2	B	602[B]	VHG	C3A-C4A-CHB-C1B
2	A	500[A]	VHG	C4B-C3B-CAB-CBB
2	A	500[A]	VHG	C2B-C3B-CAB-CBB
2	A	500[A]	VHG	C4C-C3C-CAC-CBC
2	A	500[A]	VHG	C2C-C3C-CAC-CBC
2	A	500[A]	VHG	NC-C4C-CHD-C1D
2	A	500[B]	VHG	NC-C4C-CHD-C1D
2	B	602[B]	VHG	C2C-C3C-CAC-CBC
2	B	602[B]	VHG	NC-C4C-CHD-C1D
2	A	500[B]	VHG	C2B-C1B-CHB-C4A
2	A	500[B]	VHG	C4C-C3C-CAC-CBC
2	A	500[A]	VHG	C2D-C1D-CHD-C4C
2	A	500[B]	VHG	C2D-C1D-CHD-C4C
2	B	602[A]	VHG	C2D-C1D-CHD-C4C
2	B	602[A]	VHG	C2B-C1B-CHB-C4A

There are no ring outliers.

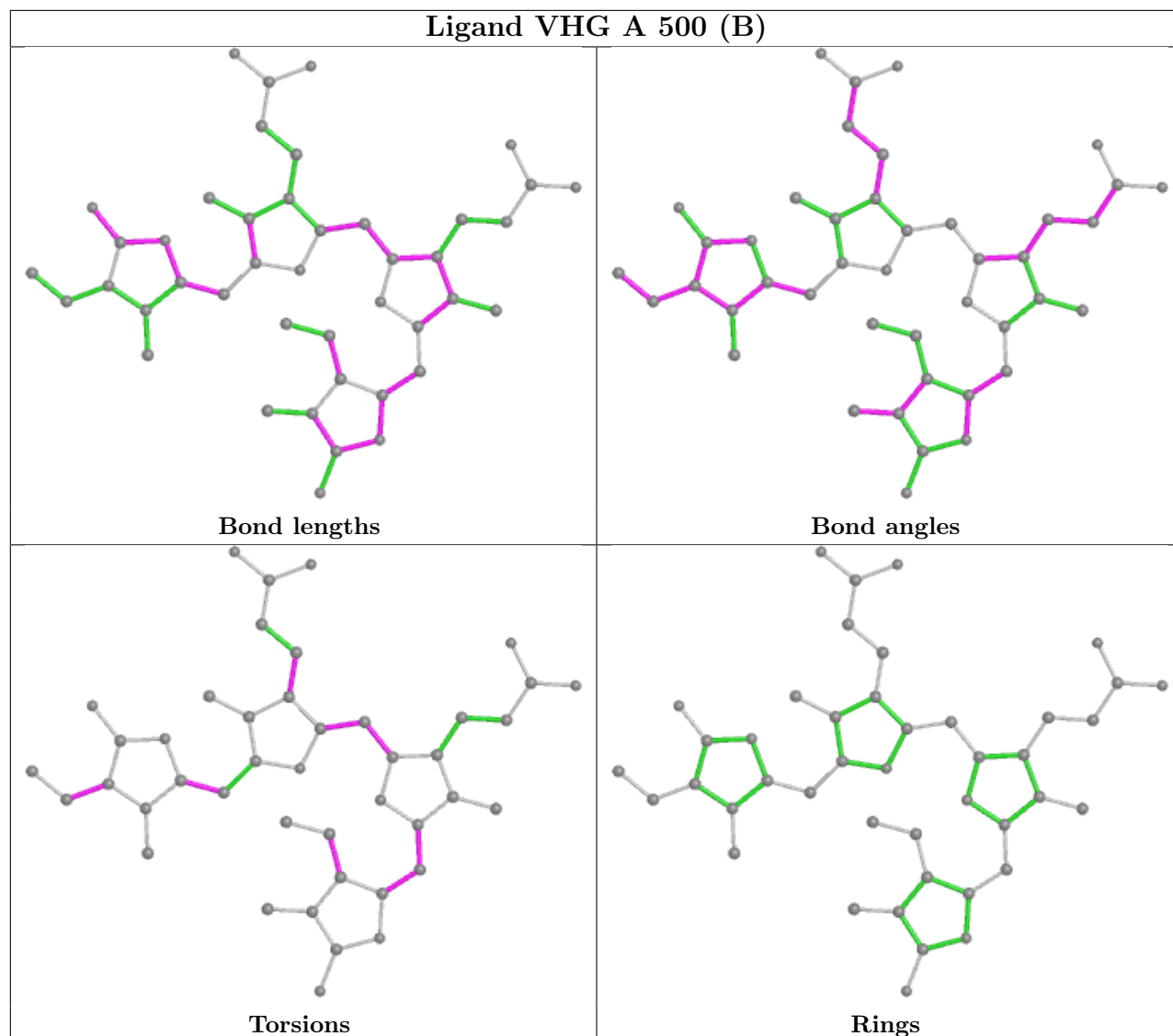
4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500[A]	VHG	6	0
2	A	500[B]	VHG	7	0
2	B	602[A]	VHG	11	0
2	B	602[B]	VHG	10	0

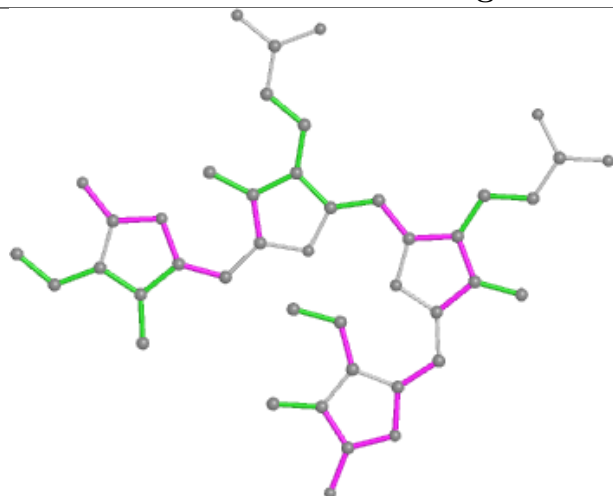
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



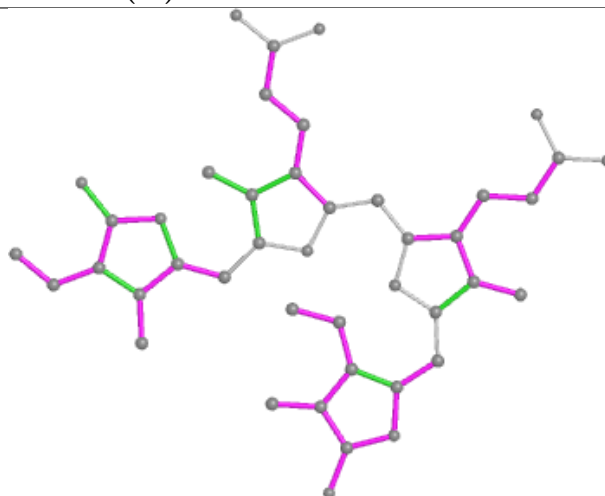
## Ligand VHG A 500 (B)



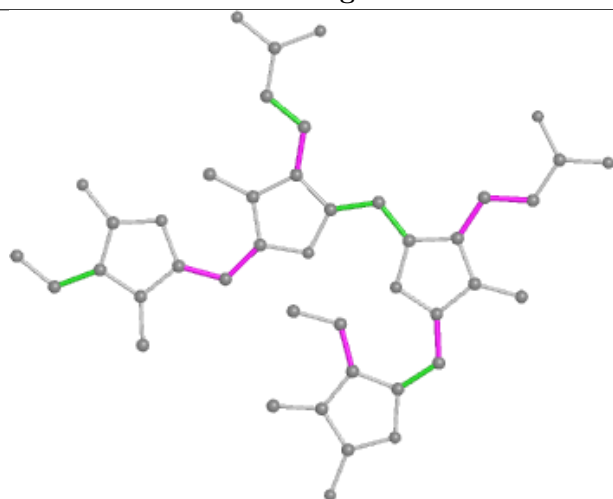
## Ligand VHG B 602 (A)



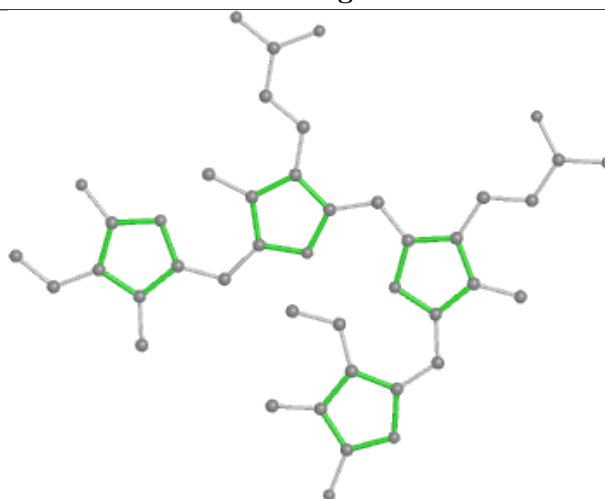
Bond lengths



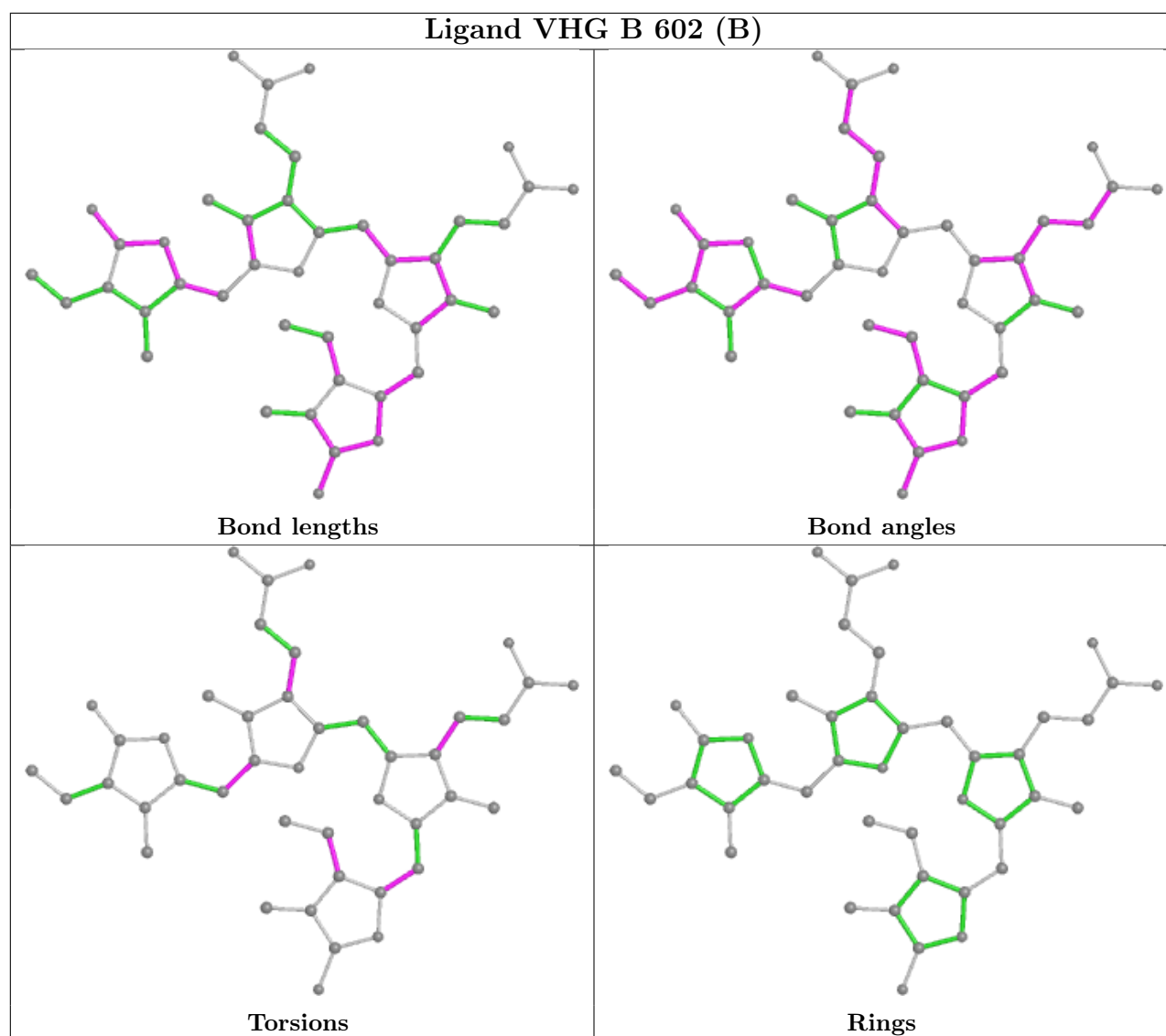
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	482/490 (98%)	0.01	16 (3%) 46 45	11, 26, 43, 62	0
1	B	482/490 (98%)	-0.10	7 (1%) 73 72	10, 23, 39, 61	0
All	All	964/980 (98%)	-0.05	23 (2%) 59 57	10, 24, 41, 62	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	ILE	4.8
1	B	425	ILE	4.2
1	B	341	SER	4.1
1	A	149	VAL	3.9
1	B	354	ALA	3.7
1	B	31	LEU	3.6
1	A	96	LEU	2.8
1	A	248[A]	TYR	2.7
1	A	160	VAL	2.5
1	A	427	PHE	2.5
1	A	42	VAL	2.4
1	A	437	TRP	2.4
1	A	416	LEU	2.3
1	A	199	ALA	2.3
1	A	31	LEU	2.3
1	B	412	LEU	2.3
1	A	389	PHE	2.3
1	A	198	ARG	2.2
1	A	338	GLU	2.2
1	A	158	VAL	2.1
1	A	294	THR	2.1
1	A	243	PRO	2.1
1	B	142	LEU	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

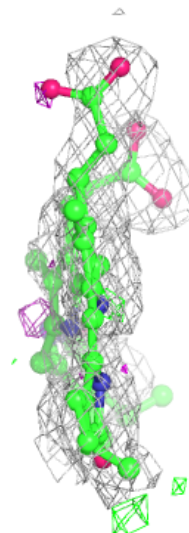
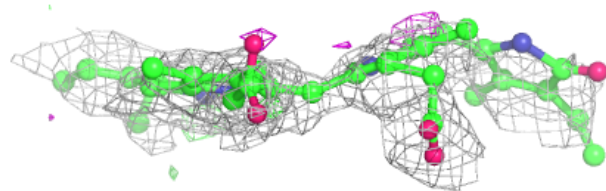
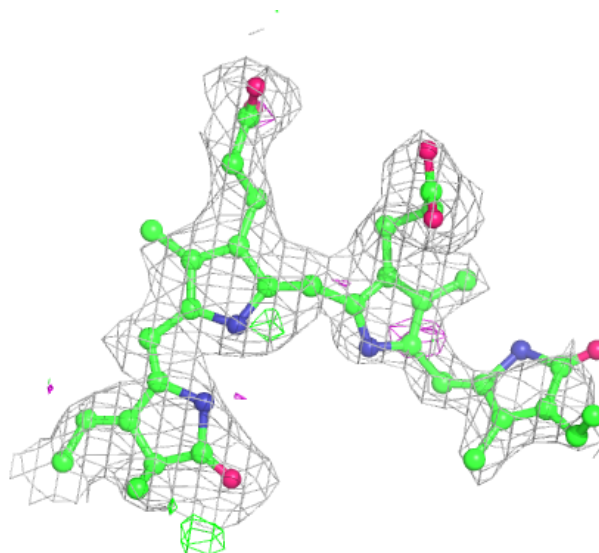
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	VHG	A	500[A]	43/43	0.80	0.29	22,24,33,34	43
2	VHG	A	500[B]	43/43	0.80	0.29	23,27,40,44	43
3	BEN	B	601	9/9	0.81	0.38	70,72,77,80	0
2	VHG	B	602[B]	43/43	0.82	0.26	14,19,21,22	43
2	VHG	B	602[A]	43/43	0.82	0.26	16,21,24,25	43

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.

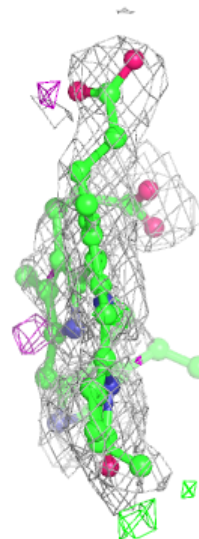
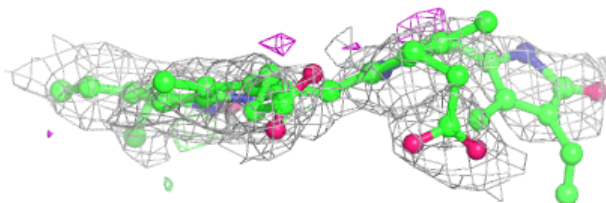
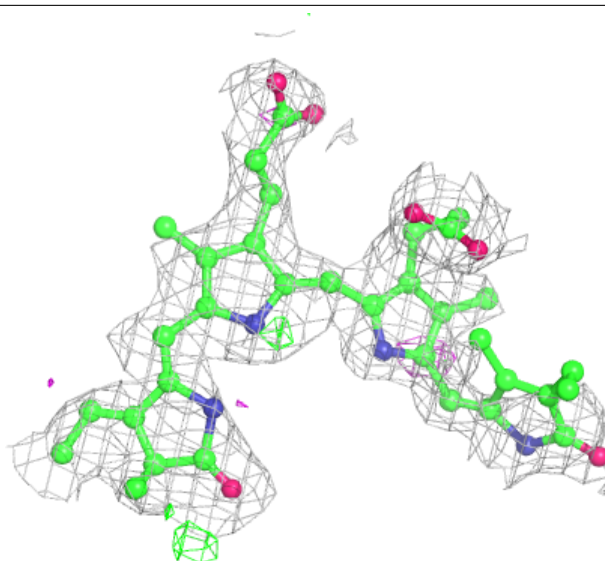
**Electron density around VHG A 500 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



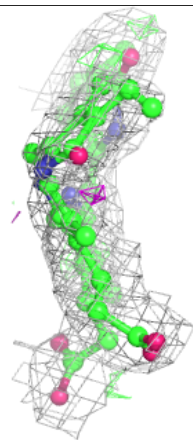
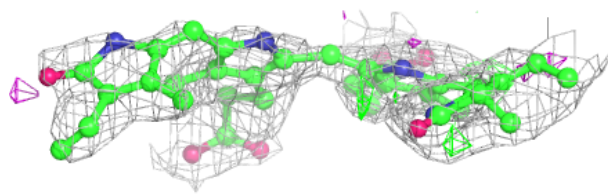
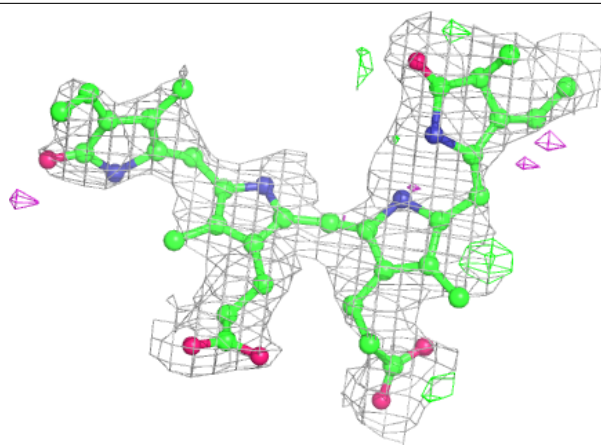
**Electron density around VHG A 500 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



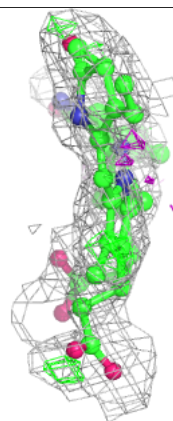
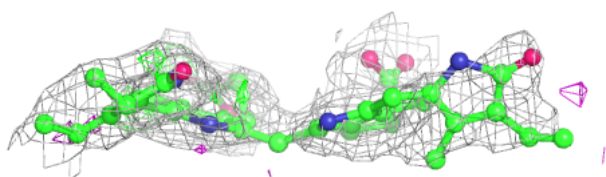
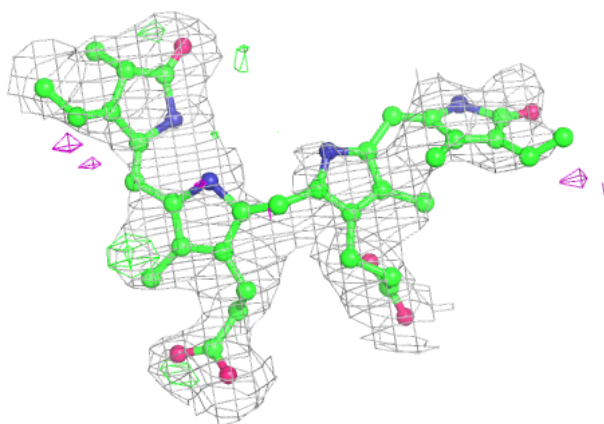
**Electron density around VHG B 602 (B):**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around VHG B 602 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.