



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 01:59 PM EDT

PDB ID : 3G6O  
Title : Crystal structure of P. aeruginosa bacteriophytochrome PaBphP photosensory core domain mutant Q188L  
Authors : Yang, X.; Kuk, J.; Moffat, K.  
Deposited on : 2009-02-07  
Resolution : 2.85 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

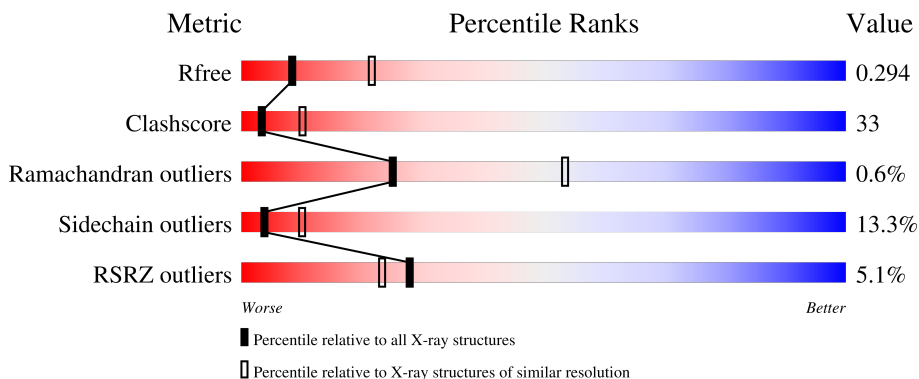
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	505	
1	B	505	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7512 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	3666	2313	653	680	20	0	6	0
1	B	457	3672	2316	654	682	20	0	7	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	GLN	engineered mutation	UNP Q9HWR3
A	498	LEU	-	expression tag	UNP Q9HWR3
A	499	GLU	-	expression tag	UNP Q9HWR3
A	500	HIS	-	expression tag	UNP Q9HWR3
A	501	HIS	-	expression tag	UNP Q9HWR3
A	502	HIS	-	expression tag	UNP Q9HWR3
A	503	HIS	-	expression tag	UNP Q9HWR3
A	504	HIS	-	expression tag	UNP Q9HWR3
A	505	HIS	-	expression tag	UNP Q9HWR3
B	188	LEU	GLN	engineered mutation	UNP Q9HWR3
B	498	LEU	-	expression tag	UNP Q9HWR3
B	499	GLU	-	expression tag	UNP Q9HWR3
B	500	HIS	-	expression tag	UNP Q9HWR3
B	501	HIS	-	expression tag	UNP Q9HWR3
B	502	HIS	-	expression tag	UNP Q9HWR3
B	503	HIS	-	expression tag	UNP Q9HWR3
B	504	HIS	-	expression tag	UNP Q9HWR3
B	505	HIS	-	expression tag	UNP Q9HWR3

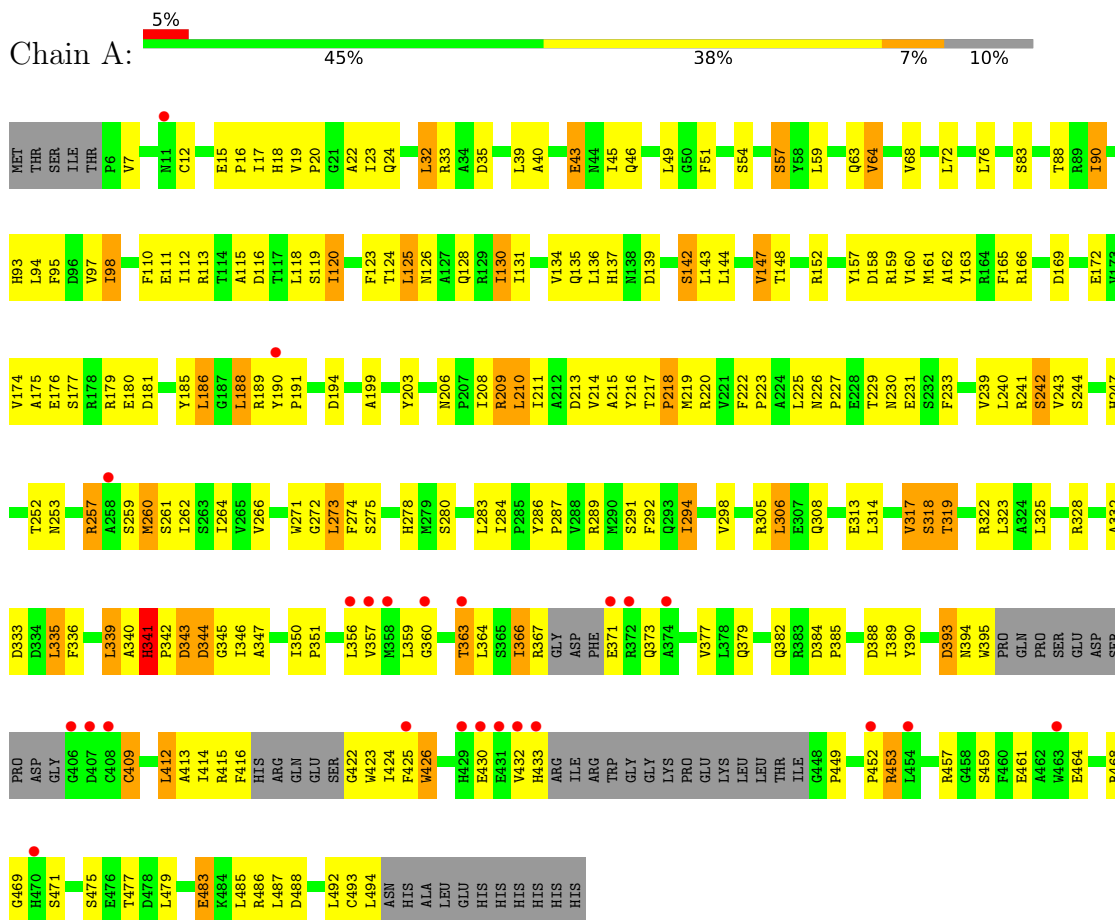
- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C<sub>33</sub>H<sub>34</sub>N<sub>4</sub>O<sub>6</sub>).



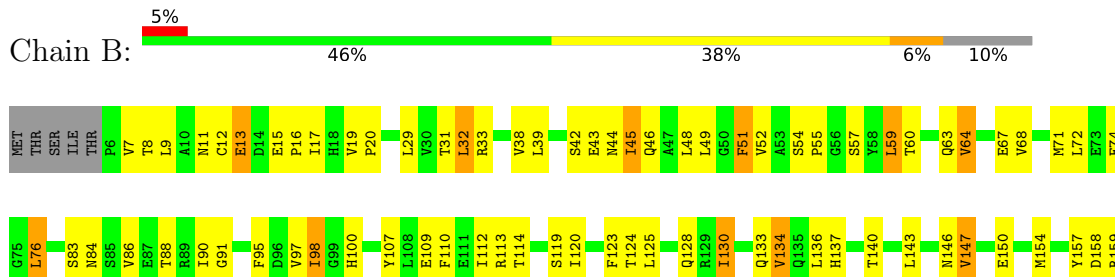
### 3 Residue-property plots [i](#)

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: Bacteriophytochrome



- Molecule 1: Bacteriophytochrome



V160	Y237	R321	GLN	H470
M161	S238	R322	PRO	S471
A162	V239	L323	SER	W474
Y163	L240	A324	GLU	E483
R164	R241	SER	ASP	K484
E172	S242	R328	PRO	L486
V173	Y243	A329	ASP	L486
V174	S244	R330	GLY	L487
A175	N253	F336	G406	L488
E176	R257	L339	C409	L489
S177	A258	A340	G410	D488
R178	S259	H341	W411	M490
R179	M260	P342	L412	E491
E180	S261	D343	A413	L492
D181	I262	G344	I414	C493
L182	S263	D345	R415	L494
Y185	L264	I346	F416	ASN
L186	V265	G354	HIS	HIS
G187	V266	A355	ALA	LEU
L188	W271	L356	GLN	GLU
R189	G272	V357	GLU	HIS
Y190	L273	M358	SER	HIS
D194	F274	L359	G422	HIS
Q198	S275	G360	W423	HIS
R201	C276	G361	I424	HIS
L202	H277	R362	F425	HIS
Y203	H278	T363	W426	
N206	P281	L364	E430	
P207	I284	S365	E431	
I208	P285	I366	W432	
R209	Y286	R367	H433	
L210	P287	GLY	ARG	
I211	V288	ASP	ILE	
A212	R289	PHE	ARG	
D213	M290	E371	TRP	
V214	S291	R372	GLY	
A215	F292	Q373	GLY	
Y216	Q293	N376	LYS	
T217	I294	V377	PRO	
P218	F295	L378	GLU	
M219	S296	Q379	LYS	
R220	Q297	R380	LEU	
V221	V298	L381	LEU	
N226	I302	R382	THR	
T229	R305	E386	ILE	
N230	L306	R387	G448	
E231	E313	D388	P449	
S232	V317	I389	L454	
F233	S318	Y390	T455	
D234	T319	D393	W463	
S236	E320	N394	V466	
		W395	W467	
		PRO	R468	
			C469	

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.79Å 109.79Å 189.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.47 – 2.85 42.47 – 2.62	Depositor EDS
% Data completeness (in resolution range)	82.8 (42.47-2.85) 67.1 (42.47-2.62)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.229 , 0.298 0.223 , 0.294	Depositor DCC
$R_{free}$ test set	1331 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.5	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/3746	0.58	0/5083
1	B	0.31	0/3752	0.56	0/5091
All	All	0.32	0/7498	0.57	0/10174

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	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	LEU	Peptide
1	A	341	HIS	Peptide
1	A	90	ILE	Peptide

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

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3666	0	3592	240	0
1	B	3672	0	3596	233	0
2	A	86	0	62	18	0
2	B	86	0	62	31	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
All	All	7512	0	7312	486	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 33.

All (486) 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:209[A]:ARG:HH11	1:A:209[A]:ARG:HG2	1.21	1.04
2:A:900[A]:BLA:HMC1	2:A:900[A]:BLA:HBC1	1.38	1.01
1:A:194:ASP:HB3	2:A:900[A]:BLA:HHB	1.45	0.97
1:A:33:ARG:HB3	1:A:39:LEU:HD11	1.48	0.95
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.34	0.93
2:B:900[A]:BLA:HMC1	2:B:900[A]:BLA:HBC1	1.51	0.91
1:A:294:ILE:HD11	1:B:294:ILE:HD11	1.51	0.89
1:B:468:ARG:HE	1:B:468:ARG:HA	1.37	0.89
1:B:488:ASP:O	1:B:491:GLU:HB3	1.72	0.89
2:B:900[B]:BLA:HBC1	2:B:900[B]:BLA:HMC1	1.53	0.88
1:B:468:ARG:HA	1:B:468:ARG:NE	1.88	0.88
1:A:203[B]:TYR:OH	2:A:900[B]:BLA:HHA	1.75	0.87
1:B:394:ASN:HB3	1:B:469:GLY:O	1.75	0.87
1:A:188:LEU:HD13	1:A:190[B]:TYR:OH	1.74	0.86
1:A:363:THR:HG21	1:A:371:GLU:HB2	1.54	0.86
1:B:157:TYR:HE1	1:B:284:ILE:HD11	1.41	0.85
1:B:20:PRO:HD2	1:B:235:LEU:HD12	1.58	0.85
1:A:203[B]:TYR:CZ	2:A:900[B]:BLA:HAA1	2.11	0.85
1:A:229:THR:HG23	1:A:231:GLU:H	1.42	0.84
1:B:202:LEU:HB3	1:B:209[B]:ARG:HH22	1.42	0.84
1:B:157:TYR:CE1	1:B:284:ILE:HD11	2.14	0.83
2:A:900[A]:BLA:CMA	2:A:900[A]:BLA:HMB3	2.09	0.83
1:A:203[B]:TYR:OH	2:A:900[B]:BLA:HAA1	1.79	0.82
1:B:210:LEU:HD12	1:B:289:ARG:HD3	1.59	0.82
1:B:203[B]:TYR:OH	2:B:900[B]:BLA:HAA1	1.79	0.82
1:A:51:PHE:HB3	1:A:63:GLN:HG2	1.60	0.81
1:A:123:PHE:HE2	1:B:123:PHE:HE2	1.27	0.81
1:B:188:LEU:HD22	1:B:190[B]:TYR:CE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:C	1:B:209[B]:ARG:HD3	2.00	0.80
1:B:229:THR:HG23	1:B:231:GLU:H	1.46	0.79
1:B:194:ASP:HB3	2:B:900[A]:BLA:HBB	1.65	0.79
1:A:209[B]:ARG:HG2	1:A:261:SER:HB2	1.66	0.78
1:A:45:ILE:HD12	1:A:46:GLN:H	1.49	0.77
1:B:51:PHE:HD2	1:B:52:VAL:H	1.33	0.77
1:A:379:GLN:HA	1:A:382:GLN:HG2	1.66	0.77
1:A:159:ARG:CZ	1:A:185:TYR:HE2	1.98	0.77
1:A:157:TYR:CE1	1:A:284:ILE:HD11	2.21	0.76
1:A:120:ILE:HD13	1:A:120:ILE:H	1.51	0.76
1:B:90:ILE:HG22	1:B:91:GLY:H	1.52	0.75
1:B:134:VAL:HA	1:B:143:LEU:HD21	1.67	0.75
1:A:123:PHE:HE2	1:B:123:PHE:CE2	2.04	0.75
1:B:163[B]:TYR:OH	1:B:190[B]:TYR:CD2	2.40	0.75
1:A:319:THR:HG22	1:A:322:ARG:NH2	2.02	0.74
1:B:185:TYR:HD1	1:B:188:LEU:HD12	1.51	0.74
1:A:287:PRO:HB3	1:B:120:ILE:HD13	1.70	0.74
1:B:33:ARG:HB3	1:B:39:LEU:HD11	1.70	0.74
1:B:190[B]:TYR:CZ	2:B:900[B]:BLA:HAB	2.24	0.73
1:A:257:ARG:HG2	1:A:257:ARG:NH1	1.98	0.73
1:B:416:PHE:HE1	1:B:424:ILE:HG13	1.53	0.72
1:B:190[B]:TYR:CE1	2:B:900[B]:BLA:HMB1	2.24	0.72
1:A:203[B]:TYR:HD1	1:A:209[B]:ARG:HD3	1.55	0.72
1:A:209[A]:ARG:HG2	1:A:209[A]:ARG:NH1	2.03	0.72
1:A:199:ALA:HB1	1:A:203[B]:TYR:CE2	2.25	0.72
1:A:335:LEU:HD11	1:A:492:LEU:HD23	1.72	0.72
1:A:209[A]:ARG:HH11	1:A:209[A]:ARG:CG	1.97	0.71
1:A:43:GLU:HG2	1:A:220:ARG:O	1.90	0.71
2:A:900[A]:BLA:HMB3	2:A:900[A]:BLA:HMA2	1.71	0.71
1:B:59:LEU:HD22	1:B:59:LEU:H	1.55	0.71
1:A:72:LEU:O	1:A:76:LEU:HD13	1.91	0.71
1:A:493:CYS:O	1:A:494:LEU:HB2	1.90	0.71
1:B:206:ASN:HB2	1:B:209[B]:ARG:CZ	2.21	0.71
1:A:319:THR:HG22	1:A:322:ARG:HH21	1.55	0.70
1:A:190[B]:TYR:CD1	2:A:900[B]:BLA:HMB1	2.26	0.70
1:A:64:VAL:HG13	1:A:68:VAL:HB	1.73	0.70
1:A:363:THR:HG21	1:A:371:GLU:CB	2.22	0.70
1:B:163[B]:TYR:OH	1:B:190[B]:TYR:HD2	1.74	0.70
1:A:123:PHE:CE2	1:B:123:PHE:CE2	2.80	0.69
1:A:157:TYR:HE1	1:A:284:ILE:HD11	1.55	0.69
1:B:257:ARG:HD2	1:B:281:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ARG:HB2	1:B:423:TRP:CH2	2.28	0.69
1:A:203[B]:TYR:CD1	1:A:209[B]:ARG:HD3	2.27	0.69
1:A:94:LEU:HD22	1:A:113:ARG:HD3	1.75	0.69
1:B:19:VAL:HG13	1:B:19:VAL:O	1.93	0.69
1:A:393:ASP:HA	1:A:409:CYS:O	1.94	0.68
1:B:203[B]:TYR:OH	2:B:900[B]:BLA:HHA	1.92	0.68
1:B:150:GLU:O	1:B:154:MET:HG3	1.92	0.68
1:A:341:HIS:O	1:A:343:ASP:N	2.26	0.68
1:A:286:TYR:HB3	1:A:287:PRO:HD3	1.76	0.68
1:B:235:LEU:O	1:B:238:SER:HB3	1.94	0.68
1:A:94:LEU:CD2	1:A:113:ARG:HD3	2.24	0.68
1:B:214:VAL:HG23	1:B:257:ARG:O	1.94	0.67
1:B:415:ARG:HD3	1:B:423:TRP:CZ2	2.30	0.67
1:B:493:CYS:O	1:B:494:LEU:HB2	1.93	0.67
1:B:430:GLU:O	1:B:430:GLU:HG2	1.95	0.67
1:A:45:ILE:HD12	1:A:46:GLN:N	2.08	0.66
1:B:395:TRP:HB3	1:B:409:CYS:HA	1.76	0.66
1:B:114:THR:O	1:B:114:THR:HG22	1.96	0.66
1:A:64:VAL:HA	1:A:90:ILE:HD11	1.78	0.66
1:B:209[B]:ARG:HD3	1:B:209[B]:ARG:N	2.10	0.66
1:A:32:LEU:N	1:A:32:LEU:HD12	2.11	0.66
1:B:394:ASN:O	1:B:409:CYS:HB3	1.96	0.66
1:A:314:LEU:HD23	1:A:314:LEU:N	2.11	0.66
1:A:43:GLU:HG3	1:A:219:MET:HG3	1.78	0.66
1:B:19:VAL:HG22	1:B:232:SER:HB3	1.77	0.65
1:A:379:GLN:HA	1:A:382:GLN:CG	2.27	0.65
1:B:202:LEU:HB3	1:B:209[B]:ARG:NH2	2.11	0.65
1:A:120:ILE:H	1:A:120:ILE:CD1	2.06	0.65
1:B:159:ARG:CZ	1:B:185:TYR:CE2	2.80	0.65
1:B:51:PHE:HD2	1:B:52:VAL:N	1.95	0.65
1:A:479:LEU:O	1:A:483:GLU:HB2	1.97	0.65
1:B:95:PHE:CE2	1:B:112:ILE:HD13	2.32	0.65
1:B:189:ARG:HD2	1:B:463:TRP:CH2	2.31	0.65
1:B:389:ILE:HD11	1:B:483:GLU:OE2	1.96	0.65
1:B:159:ARG:CZ	1:B:185:TYR:HE2	2.09	0.64
1:A:118:LEU:HD23	1:A:123:PHE:HB2	1.79	0.64
1:A:346:ILE:HG23	1:A:426:TRP:CZ3	2.32	0.64
1:B:31:THR:C	1:B:32:LEU:HD12	2.17	0.64
2:B:900[B]:BLA:HMA2	2:B:900[B]:BLA:CGA	2.28	0.64
1:B:159:ARG:NH1	1:B:185:TYR:HE2	1.96	0.64
1:B:454:LEU:O	1:B:455:THR:HG22	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG22	1:B:110:PHE:CD2	2.33	0.63
1:B:185:TYR:O	1:B:188:LEU:HB2	1.99	0.63
2:B:900[A]:BLA:HMB3	2:B:900[A]:BLA:CMA	2.28	0.63
2:B:900[B]:BLA:HMA1	2:B:900[B]:BLA:NB	2.13	0.63
1:B:215:ALA:HB3	1:B:257:ARG:HH12	1.63	0.63
1:A:190[B]:TYR:CE1	2:A:900[B]:BLA:HAB	2.34	0.63
1:B:286:TYR:HB3	1:B:287:PRO:HD3	1.79	0.63
1:A:33:ARG:HB3	1:A:39:LEU:CD1	2.27	0.63
1:B:19:VAL:CG2	1:B:232:SER:HB3	2.29	0.62
1:B:19:VAL:N	1:B:20:PRO:HD3	2.14	0.62
1:A:335:LEU:CD1	1:A:492:LEU:HD23	2.29	0.62
1:A:125:LEU:O	1:A:125:LEU:HD23	2.00	0.62
1:A:206:ASN:HB2	1:A:209[B]:ARG:NH2	2.15	0.62
1:A:188:LEU:HD22	1:A:190[B]:TYR:CZ	2.33	0.62
1:A:305:ARG:HH11	1:B:306:LEU:HD11	1.64	0.62
1:B:98:ILE:HG12	1:B:109:GLU:HB2	1.80	0.62
1:A:389:ILE:HD11	1:A:483:GLU:OE2	1.99	0.62
1:A:143:LEU:O	1:A:147:VAL:HG12	2.00	0.62
1:A:339:LEU:HD22	1:A:346:ILE:HD11	1.82	0.62
1:B:202:LEU:C	1:B:209[B]:ARG:NH2	2.53	0.61
1:A:162:ALA:HB3	1:A:175:ALA:HB3	1.82	0.61
1:B:90:ILE:HG22	1:B:91:GLY:N	2.14	0.61
1:B:376:ASN:O	1:B:379:GLN:HB3	1.99	0.61
2:B:900[A]:BLA:HMC1	2:B:900[A]:BLA:CBC	2.29	0.61
1:A:120:ILE:HD13	1:A:120:ILE:N	2.15	0.61
1:A:416:PHE:HE1	1:A:424:ILE:HG13	1.65	0.61
1:A:430:GLU:HG2	1:A:471:SER:HA	1.83	0.61
1:B:328:ARG:HD3	1:B:344:ASP:OD2	2.00	0.61
1:B:215:ALA:CB	1:B:257:ARG:HH12	2.14	0.61
1:A:22:ALA:O	1:A:242:SER:HB3	2.01	0.61
1:A:328:ARG:O	1:A:332:ALA:HB3	2.00	0.61
1:A:97:VAL:HG22	1:A:110:PHE:CD2	2.36	0.60
1:B:359:LEU:HD22	1:B:416:PHE:HE2	1.65	0.60
1:B:266:VAL:HG22	1:B:271:TRP:HB2	1.83	0.60
1:A:415:ARG:HD3	1:A:423:TRP:CZ2	2.37	0.60
1:B:43:GLU:HG3	1:B:219:MET:HG3	1.82	0.60
1:B:140:THR:HG23	1:B:164:ARG:NH2	2.17	0.59
1:B:409:CYS:SG	1:B:430:GLU:OE1	2.60	0.59
1:A:190[B]:TYR:N	1:A:190[B]:TYR:CD2	2.69	0.59
1:B:284:ILE:N	1:B:284:ILE:HD12	2.17	0.59
1:B:379:GLN:HA	1:B:382:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:900[B]:BLA:HMA1	2:B:900[B]:BLA:HB	1.66	0.59
1:A:294:ILE:O	1:A:298:VAL:HG23	2.03	0.59
1:B:90:ILE:CG2	1:B:91:GLY:H	2.16	0.59
1:B:341:HIS:O	1:B:345:GLY:N	2.36	0.59
1:A:134:VAL:HG22	1:A:143:LEU:HD21	1.85	0.59
1:A:191:PRO:HG2	1:A:453:ARG:HH22	1.67	0.59
1:A:359:LEU:HD13	1:A:422:GLY:HA3	1.83	0.59
1:B:64:VAL:HG13	1:B:68:VAL:HB	1.85	0.59
1:B:158:ASP:OD1	1:B:278:HIS:HA	2.02	0.59
1:A:152:ARG:HB2	1:A:160:VAL:HG11	1.85	0.59
1:A:253:ASN:HD21	1:A:449:PRO:HB3	1.66	0.59
1:A:414:ILE:CG1	1:A:424:ILE:HB	2.33	0.59
1:B:45:ILE:HG22	1:B:49:LEU:HD12	1.83	0.59
1:B:493:CYS:O	1:B:494:LEU:CB	2.51	0.59
1:A:191:PRO:CD	1:A:453:ARG:HH22	2.16	0.59
1:A:203[B]:TYR:HA	1:A:209[B]:ARG:NH1	2.18	0.59
1:A:64:VAL:HA	1:A:90:ILE:CD1	2.32	0.58
1:B:161:MET:HE3	2:B:900[B]:BLA:HBB1	1.84	0.58
1:A:328:ARG:O	1:A:332:ALA:CB	2.50	0.58
2:B:900[B]:BLA:HMC1	2:B:900[B]:BLA:CBC	2.30	0.58
1:A:190[B]:TYR:CE1	2:A:900[B]:BLA:HMB1	2.39	0.58
1:A:359:LEU:HD12	1:A:360:GLY:H	1.68	0.58
1:B:359:LEU:HD13	1:B:422:GLY:CA	2.33	0.58
1:B:339:LEU:O	1:B:346:ILE:HG23	2.04	0.58
1:B:330:ARG:HB2	1:B:492:LEU:HD11	1.86	0.58
1:B:410:GLY:CA	1:B:474:TRP:HZ2	2.16	0.58
1:B:71:MET:O	1:B:74:GLU:HG2	2.04	0.57
1:B:261[A]:SER:HB2	1:B:273:LEU:HD13	1.86	0.57
1:A:294:ILE:HD11	1:B:294:ILE:CD1	2.29	0.57
1:B:468:ARG:HE	1:B:468:ARG:CA	2.14	0.57
1:A:273:LEU:C	1:A:273:LEU:HD12	2.25	0.57
1:A:253:ASN:ND2	1:A:449:PRO:HB3	2.20	0.57
1:A:390:TYR:HB3	1:A:413:ALA:HB3	1.86	0.57
1:A:393:ASP:O	1:A:394:ASN:CG	2.43	0.57
1:B:430:GLU:OE1	1:B:430:GLU:N	2.38	0.57
1:A:188:LEU:HD23	1:A:189:ARG:H	1.70	0.56
1:B:206:ASN:HB2	1:B:209[B]:ARG:NH2	2.20	0.56
1:A:199:ALA:HB1	1:A:203[B]:TYR:HE2	1.67	0.56
1:A:283:LEU:C	1:A:283:LEU:HD23	2.26	0.56
1:A:366:ILE:HG13	1:A:367:ARG:HG3	1.87	0.56
1:B:29:LEU:HD13	1:B:109:GLU:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HD11	1:B:454:LEU:HD21	1.86	0.56
1:B:298:VAL:O	1:B:302:ILE:HD13	2.06	0.56
1:B:157:TYR:HE1	1:B:284:ILE:CD1	2.17	0.56
1:B:209[B]:ARG:O	1:B:260:MET:HA	2.06	0.56
2:A:900[A]:BLA:HMA2	2:A:900[A]:BLA:O2A	2.06	0.56
1:B:354:GLY:HA2	1:B:367:ARG:HB2	1.87	0.56
1:B:206:ASN:HB2	1:B:209[B]:ARG:NE	2.20	0.55
1:B:346:ILE:O	1:B:426:TRP:HZ3	1.88	0.55
1:A:188:LEU:HD22	1:A:190[B]:TYR:CE2	2.42	0.55
1:A:366:ILE:HG13	1:A:367:ARG:N	2.19	0.55
1:A:379:GLN:CA	1:A:382:GLN:HG2	2.37	0.55
1:B:203[B]:TYR:CZ	2:B:900[B]:BLA:HAA1	2.41	0.55
1:A:163[B]:TYR:OH	1:A:190[B]:TYR:CD2	2.54	0.55
1:B:140:THR:HG23	1:B:164:ARG:HH22	1.71	0.55
1:A:340:ALA:O	1:A:342:PRO:N	2.40	0.55
1:A:211:ILE:HD13	1:A:243:VAL:HG21	1.87	0.55
1:A:426:TRP:N	1:A:426:TRP:CD1	2.75	0.55
1:A:134:VAL:HG12	1:A:135:GLN:HG3	1.88	0.54
1:A:214:VAL:HG23	1:A:257:ARG:C	2.28	0.54
1:B:45:ILE:HD12	1:B:46:GLN:H	1.72	0.54
1:B:432:VAL:HG22	1:B:468:ARG:NH2	2.23	0.54
1:A:339:LEU:O	1:A:345:GLY:HA2	2.08	0.54
1:A:98:ILE:HG21	1:A:286:TYR:CD1	2.43	0.54
1:B:72:LEU:O	1:B:76:LEU:HD13	2.08	0.54
1:B:319:THR:HG22	1:B:322:ARG:HH21	1.73	0.54
1:B:211:ILE:HB	1:B:259:SER:HB3	1.89	0.54
1:B:214:VAL:HG23	1:B:257:ARG:C	2.27	0.54
1:A:45:ILE:HB	1:A:51:PHE:CE1	2.42	0.54
1:B:17:ILE:HD13	2:B:900[B]:BLA:HAD1	1.88	0.54
1:B:202:LEU:O	1:B:209[B]:ARG:NH2	2.41	0.54
2:A:900[B]:BLA:OB	2:A:900[B]:BLA:HBB1	2.08	0.54
1:B:161:MET:HE3	2:B:900[B]:BLA:OB	2.07	0.54
1:B:188:LEU:HD23	1:B:189:ARG:H	1.72	0.54
1:A:203[B]:TYR:OH	2:A:900[B]:BLA:HAD2	2.07	0.53
1:A:19:VAL:N	1:A:20:PRO:HD3	2.23	0.53
1:A:325:LEU:C	1:A:325:LEU:HD13	2.29	0.53
1:B:60:THR:OG1	1:B:63:GLN:NE2	2.41	0.53
1:B:185:TYR:HD1	1:B:188:LEU:CD1	2.19	0.53
1:B:68:VAL:O	1:B:71:MET:HB3	2.08	0.53
1:B:189:ARG:HD2	1:B:463:TRP:CZ2	2.44	0.53
2:B:900[A]:BLA:HBC1	2:B:900[A]:BLA:CMC	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASP:CB	2:A:900[A]:BLA:HHB	2.31	0.53
2:A:900[A]:BLA:HMC1	2:A:900[A]:BLA:CBC	2.25	0.53
1:A:430:GLU:HG2	1:A:471:SER:CA	2.39	0.52
1:B:209[B]:ARG:N	1:B:209[B]:ARG:CD	2.72	0.52
1:B:261[B]:SER:HB2	1:B:273:LEU:HD13	1.92	0.52
1:A:395:TRP:CB	1:A:409:CYS:HA	2.39	0.52
1:A:157:TYR:HE1	1:A:284:ILE:CD1	2.22	0.52
1:A:247:HIS:ND1	3:A:506:HOH:O	2.34	0.52
1:B:194:ASP:HB3	2:B:900[A]:BLA:CHB	2.39	0.52
1:A:211:ILE:HB	1:A:259:SER:HB3	1.92	0.52
1:B:190[B]:TYR:CD1	2:B:900[B]:BLA:HMB1	2.44	0.52
1:A:206:ASN:HB2	1:A:209[B]:ARG:CZ	2.40	0.52
1:B:44:ASN:HB3	1:B:219:MET:HG2	1.92	0.51
1:B:172:GLU:HG2	1:B:174:VAL:HG12	1.92	0.51
1:A:98:ILE:HG21	1:A:286:TYR:CE1	2.44	0.51
1:A:409:CYS:SG	1:A:430:GLU:HG3	2.51	0.51
1:B:202:LEU:C	1:B:209[B]:ARG:HH21	2.11	0.51
1:B:393:ASP:HB2	1:B:394:ASN:OD1	2.11	0.51
1:A:124:THR:O	1:A:128:GLN:HG3	2.09	0.51
1:A:191:PRO:CG	1:A:453:ARG:HH22	2.23	0.51
1:B:176:GLU:HG2	1:B:177:SER:N	2.26	0.51
1:B:185:TYR:CD1	1:B:188:LEU:HD12	2.40	0.51
1:A:266:VAL:HG22	1:A:271:TRP:HB2	1.92	0.51
1:B:71:MET:CE	1:B:97:VAL:HG12	2.41	0.51
1:A:209[A]:ARG:NH1	1:A:209[A]:ARG:CG	2.64	0.51
1:B:59:LEU:HD22	1:B:59:LEU:N	2.23	0.51
1:B:239:VAL:HG11	1:B:289:ARG:NH2	2.25	0.51
2:B:900[B]:BLA:HBB1	2:B:900[B]:BLA:OB	2.09	0.51
1:A:24:GLN:HE21	1:A:243:VAL:HG23	1.75	0.51
1:A:213:ASP:O	1:A:216:TYR:HB3	2.11	0.51
1:A:284:ILE:HD12	1:A:284:ILE:N	2.25	0.51
1:A:134:VAL:HG13	1:A:134:VAL:O	2.11	0.50
1:A:159:ARG:NH2	1:A:185:TYR:HE2	2.08	0.50
1:A:215:ALA:HB3	1:A:257:ARG:HH22	1.76	0.50
1:B:291:SER:O	1:B:294:ILE:HG23	2.11	0.50
1:B:359:LEU:HD13	1:B:422:GLY:HA3	1.92	0.50
1:A:136:LEU:HB2	1:A:137:HIS:CE1	2.47	0.50
1:B:206:ASN:HD21	1:B:237:TYR:H	1.58	0.50
1:B:262:ILE:HD12	1:B:292:PHE:HB3	1.93	0.50
1:A:203[B]:TYR:HA	1:A:209[B]:ARG:HH11	1.77	0.50
1:A:373:GLN:O	1:A:377:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASP:HB3	1:A:486:ARG:NE	2.27	0.50
1:B:412:LEU:HD12	1:B:474:TRP:CE3	2.47	0.50
2:B:900[A]:BLA:HMD1	2:B:900[A]:BLA:HBD2	1.93	0.50
1:A:152:ARG:HB2	1:A:160:VAL:CG1	2.42	0.50
1:A:359:LEU:HD12	1:A:360:GLY:N	2.27	0.50
1:B:318:SER:O	1:B:321:ARG:HB2	2.11	0.50
1:A:209[B]:ARG:O	1:A:260:MET:HA	2.12	0.49
1:A:157:TYR:OH	1:A:260:MET:HB2	2.12	0.49
1:A:415:ARG:HB2	1:A:423:TRP:CH2	2.47	0.49
1:B:42:SER:HB2	1:B:44:ASN:OD1	2.11	0.49
1:A:415:ARG:HB2	1:A:423:TRP:CZ3	2.47	0.49
1:B:136:LEU:HB2	1:B:137:HIS:CE1	2.48	0.49
1:B:415:ARG:HB2	1:B:423:TRP:CZ3	2.47	0.49
1:B:181:ASP:N	1:B:181:ASP:OD1	2.45	0.49
1:B:430:GLU:HG3	1:B:468:ARG:O	2.12	0.49
1:A:172:GLU:HG2	1:A:174:VAL:CG1	2.42	0.49
1:B:67:GLU:OE1	1:B:88:THR:HA	2.12	0.49
1:B:236:SER:O	1:B:237:TYR:HB2	2.12	0.49
2:B:900[A]:BLA:HMB3	2:B:900[A]:BLA:HMA2	1.94	0.49
1:A:208:ILE:HA	1:A:261:SER:O	2.11	0.49
1:A:220:ARG:HE	1:A:222:PHE:HZ	1.58	0.49
1:B:51:PHE:CD1	1:B:63:GLN:CB	2.96	0.49
1:A:19:VAL:HG12	1:A:233:PHE:O	2.13	0.49
1:B:211:ILE:HB	1:B:259:SER:CB	2.43	0.49
1:A:305:ARG:HH11	1:B:306:LEU:CD1	2.26	0.49
1:B:143:LEU:O	1:B:147:VAL:HG12	2.13	0.49
2:B:900[A]:BLA:HMB3	2:B:900[A]:BLA:C3A	2.43	0.49
1:A:226:ASN:HB2	1:A:233:PHE:CZ	2.48	0.49
1:B:179:ARG:O	1:B:182:LEU:HG	2.12	0.49
1:B:262:ILE:HG22	1:B:296:SER:HB2	1.95	0.48
1:A:389:ILE:HG22	1:A:390:TYR:N	2.28	0.48
1:A:206:ASN:HB2	1:A:209[B]:ARG:HH22	1.77	0.48
1:A:356:LEU:HD13	1:A:357:VAL:N	2.29	0.48
1:A:159:ARG:NH2	1:A:185:TYR:CE2	2.82	0.48
1:A:225:LEU:HD21	1:A:230:ASN:O	2.14	0.48
1:B:48:LEU:HB3	1:B:49:LEU:HG	1.94	0.48
1:B:210:LEU:HD23	1:B:211:ILE:N	2.28	0.48
1:B:262:ILE:CG2	1:B:296:SER:HB2	2.44	0.48
1:A:12[A]:CYS:HB2	2:A:900[A]:BLA:HAC	1.85	0.48
1:B:54:SER:O	1:B:57:SER:HB3	2.14	0.48
1:B:201:ARG:HD2	1:B:201:ARG:HA	1.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ARG:NE	1:B:468:ARG:CA	2.68	0.48
1:A:115:ALA:HB1	1:A:116:ASP:OD1	2.14	0.48
1:A:191:PRO:HD2	1:A:453:ARG:HH22	1.78	0.48
1:A:40:ALA:HB2	1:A:223:PRO:HD2	1.96	0.47
2:A:900[B]:BLA:O2A	2:A:900[B]:BLA:HMA2	2.13	0.47
1:B:134:VAL:HA	1:B:143:LEU:CD2	2.40	0.47
1:B:489:LEU:C	1:B:491:GLU:N	2.68	0.47
1:B:489:LEU:C	1:B:491:GLU:H	2.18	0.47
1:A:339:LEU:HD22	1:A:346:ILE:CD1	2.44	0.47
1:B:163[A]:TYR:OH	1:B:275:SER:HB3	2.14	0.47
1:B:343:ASP:C	1:B:345:GLY:H	2.16	0.47
1:A:314:LEU:O	1:A:318:SER:HB3	2.15	0.47
1:B:161:MET:CE	2:B:900[B]:BLA:HBB1	2.45	0.47
1:B:210:LEU:HD23	1:B:210:LEU:C	2.35	0.47
1:B:216:TYR:CE2	1:B:218:PRO:HG3	2.50	0.47
1:A:158:ASP:HB2	1:A:278:HIS:HA	1.97	0.47
1:B:324:ALA:HB1	1:B:328:ARG:CZ	2.45	0.47
1:B:430:GLU:HB3	1:B:471:SER:HA	1.96	0.47
1:A:409:CYS:SG	1:A:430:GLU:CD	2.93	0.47
1:B:157:TYR:CG	1:B:276:CYS:HB3	2.50	0.47
1:A:24:GLN:NE2	1:A:243:VAL:HG23	2.30	0.46
1:A:395:TRP:HB3	1:A:409:CYS:HA	1.96	0.46
1:B:42:SER:O	1:B:45:ILE:HG13	2.15	0.46
1:A:179:ARG:NH1	1:A:181:ASP:OD2	2.45	0.46
1:A:209[B]:ARG:CG	1:A:261:SER:HB2	2.40	0.46
1:A:414:ILE:HG12	1:A:424:ILE:HB	1.95	0.46
1:B:377:VAL:HG22	1:B:395:TRP:CH2	2.49	0.46
1:B:190[B]:TYR:OH	2:B:900[B]:BLA:HAB	2.14	0.46
1:B:454:LEU:O	1:B:455:THR:CG2	2.62	0.46
1:A:115:ALA:HB1	1:A:116:ASP:HA	1.97	0.46
1:A:313:GLU:O	1:A:317:VAL:HG13	2.16	0.46
1:A:464:GLU:O	1:A:468:ARG:HG3	2.15	0.46
1:A:206:ASN:HB2	1:A:209[B]:ARG:NH1	2.30	0.46
1:B:90:ILE:CG2	1:B:91:GLY:N	2.77	0.46
1:B:157:TYR:OH	1:B:259:SER:O	2.32	0.46
1:B:356:LEU:HD13	1:B:357:VAL:N	2.31	0.46
1:B:415:ARG:HB2	1:B:423:TRP:CZ2	2.51	0.46
1:A:209[B]:ARG:HE	1:A:209[B]:ARG:HB3	1.26	0.46
1:B:179:ARG:HD2	1:B:181:ASP:OD2	2.16	0.46
1:B:432:VAL:HG22	1:B:468:ARG:HH22	1.80	0.46
1:B:432:VAL:O	1:B:433:HIS:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PHE:CD1	1:A:272:GLY:HA2	2.51	0.46
1:A:143:LEU:HD12	1:A:144:LEU:HD23	1.97	0.46
1:A:210:LEU:HD11	1:A:284:ILE:H	1.81	0.46
1:B:32:LEU:HD12	1:B:32:LEU:N	2.31	0.46
1:B:341:HIS:O	1:B:343:ASP:N	2.49	0.46
1:A:394:ASN:HA	1:A:469:GLY:O	2.15	0.45
1:B:83:SER:O	1:B:84:ASN:HB2	2.14	0.45
1:B:359:LEU:HD22	1:B:416:PHE:CE2	2.49	0.45
1:B:7:VAL:HG23	1:B:7:VAL:O	2.16	0.45
1:B:19:VAL:O	1:B:19:VAL:CG1	2.64	0.45
1:A:359:LEU:HD22	1:A:416:PHE:HE2	1.80	0.45
1:B:226:ASN:HB2	1:B:233:PHE:CZ	2.51	0.45
1:B:51:PHE:CD2	1:B:52:VAL:N	2.79	0.45
1:B:71:MET:HE3	1:B:97:VAL:HG12	1.97	0.45
1:B:261[A]:SER:HB2	1:B:273:LEU:CD1	2.46	0.45
1:B:466:VAL:O	1:B:470:HIS:CD2	2.70	0.45
1:A:18:HIS:C	1:A:20:PRO:HD3	2.37	0.45
1:A:416:PHE:CE1	1:A:424:ILE:HG13	2.49	0.45
1:A:139:ASP:HB3	1:A:142:SER:OG	2.17	0.45
1:A:341:HIS:O	1:A:344:ASP:N	2.36	0.45
1:B:346:ILE:HB	1:B:426:TRP:CH2	2.52	0.45
1:A:159:ARG:CZ	1:A:185:TYR:CE2	2.89	0.45
1:B:388:ASP:HB3	1:B:486:ARG:HE	1.81	0.45
1:A:98:ILE:H	1:A:98:ILE:HG12	1.70	0.45
1:A:432:VAL:O	1:A:433:HIS:CB	2.65	0.45
1:B:8:THR:H	1:B:11:ASN:HB2	1.82	0.45
1:B:209[A]:ARG:O	1:B:260:MET:HA	2.17	0.45
1:A:49:LEU:HD22	1:A:90:ILE:HG21	1.98	0.45
1:A:350:ILE:HG23	1:A:351:PRO:HD2	1.99	0.45
1:A:492:LEU:N	1:A:492:LEU:CD1	2.80	0.45
1:A:33:ARG:HG3	1:A:35:ASP:OD1	2.17	0.44
1:B:163[B]:TYR:O	1:B:272:GLY:HA2	2.16	0.44
1:A:49:LEU:HD13	1:A:51:PHE:HE2	1.82	0.44
1:B:217:THR:HA	1:B:218:PRO:HD3	1.65	0.44
1:B:235:LEU:HB2	1:B:241:ARG:HD3	1.99	0.44
1:A:314:LEU:HD23	1:A:314:LEU:H	1.80	0.44
1:A:148:THR:O	1:A:160:VAL:HG11	2.18	0.44
1:A:163[A]:TYR:OH	1:A:275:SER:HB3	2.18	0.44
1:A:199:ALA:O	1:A:203[B]:TYR:CD2	2.71	0.44
1:B:373:GLN:NE2	1:B:395:TRP:CD1	2.85	0.44
1:B:393:ASP:CB	1:B:394:ASN:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:HD12	1:A:292:PHE:HB3	2.00	0.43
1:B:273:LEU:HD12	1:B:274:PHE:O	2.18	0.43
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.14	0.43
1:A:306:LEU:HD13	1:B:305:ARG:HH11	1.81	0.43
1:A:359:LEU:HD13	1:A:422:GLY:CA	2.46	0.43
1:B:12[B]:CYS:HB2	2:B:900[B]:BLA:HAC	1.35	0.43
1:A:54:SER:O	1:A:57:SER:HB3	2.17	0.43
1:A:95:PHE:CE2	1:A:112:ILE:HD13	2.53	0.43
1:A:243:VAL:HG12	1:A:244:SER:O	2.18	0.43
2:B:900[A]:BLA:HBB1	2:B:900[A]:BLA:OB	2.18	0.43
1:A:123:PHE:CE2	1:B:123:PHE:HE2	2.15	0.43
1:A:134:VAL:O	1:A:134:VAL:CG1	2.66	0.43
1:A:188:LEU:HD23	1:A:189:ARG:N	2.33	0.43
1:A:214:VAL:HG23	1:A:257:ARG:O	2.19	0.43
1:A:273:LEU:HD12	1:A:273:LEU:O	2.18	0.43
1:A:336:PHE:O	1:A:340:ALA:HB2	2.19	0.43
1:B:388:ASP:HB3	1:B:486:ARG:NE	2.34	0.42
1:A:161:MET:O	1:A:274:PHE:HA	2.18	0.42
1:A:15:GLU:HA	1:A:16:PRO:HD3	1.75	0.42
1:A:217:THR:HA	1:A:218:PRO:HD3	1.75	0.42
1:A:394:ASN:O	1:A:395:TRP:C	2.57	0.42
1:B:38:VAL:O	1:B:55:PRO:HA	2.18	0.42
1:B:98:ILE:HG12	1:B:98:ILE:O	2.18	0.42
1:A:341:HIS:C	1:A:343:ASP:H	2.20	0.42
2:A:900[A]:BLA:HMB3	2:A:900[A]:BLA:C3A	2.49	0.42
1:A:17:ILE:HD11	1:A:199:ALA:N	2.33	0.42
1:A:390:TYR:O	1:A:412:LEU:HD23	2.19	0.42
1:A:453:ARG:HH21	1:A:459:SER:CB	2.32	0.42
1:B:313:GLU:O	1:B:317:VAL:HG13	2.19	0.42
1:B:454:LEU:C	1:B:455:THR:CG2	2.87	0.42
2:B:900[B]:BLA:HBC1	2:B:900[B]:BLA:CMC	2.35	0.42
1:A:363:THR:CG2	1:A:371:GLU:HB2	2.38	0.42
1:A:90:ILE:O	1:A:93:HIS:O	2.38	0.42
1:A:222:PHE:HA	1:A:223:PRO:C	2.40	0.42
1:B:124:THR:O	1:B:128:GLN:HG3	2.18	0.42
1:B:414:ILE:HB	1:B:486:ARG:HB2	2.02	0.42
1:A:130:ILE:CG2	1:A:131:ILE:N	2.82	0.42
1:A:384:ASP:N	1:A:385:PRO:HD3	2.34	0.42
1:A:457:ARG:O	1:A:461:GLU:HG3	2.20	0.42
1:B:15:GLU:HA	1:B:16:PRO:HD3	1.83	0.42
1:B:359:LEU:HD12	1:B:360:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:HIS:C	1:A:343:ASP:N	2.73	0.42
1:B:100:HIS:CE1	1:B:107:TYR:HB2	2.55	0.42
1:B:253:ASN:ND2	1:B:449:PRO:HB3	2.35	0.42
1:B:358:MET:O	1:B:422:GLY:HA2	2.19	0.42
1:A:32:LEU:N	1:A:32:LEU:CD1	2.82	0.41
1:A:166:ARG:O	1:A:169:ASP:N	2.52	0.41
1:A:423:TRP:HB3	1:A:425:PHE:CE1	2.55	0.41
1:B:491:GLU:HG3	1:B:492:LEU:HD12	2.01	0.41
1:A:226:ASN:HA	1:A:227:PRO:HD3	1.82	0.41
1:B:213:ASP:O	1:B:216:TYR:HB3	2.21	0.41
1:A:49:LEU:HB2	1:A:51:PHE:CE2	2.55	0.41
1:A:160:VAL:CG1	1:A:177:SER:HB3	2.50	0.41
1:A:191:PRO:HG2	1:A:453:ARG:NH2	2.32	0.41
1:A:226:ASN:HB2	1:A:233:PHE:CE1	2.56	0.41
1:A:342:PRO:HG2	1:A:343:ASP:OD2	2.19	0.41
1:B:292:PHE:HA	1:B:295:PHE:HB3	2.01	0.41
1:A:328:ARG:O	1:A:332:ALA:HB2	2.20	0.41
1:B:157:TYR:CE1	1:B:284:ILE:CD1	2.96	0.41
1:B:209[A]:ARG:NH1	1:B:241:ARG:HH12	2.19	0.41
1:B:257:ARG:HH11	1:B:257:ARG:HG2	1.86	0.41
1:B:264:ILE:HB	1:B:272:GLY:O	2.21	0.41
1:A:240:LEU:O	1:A:241:ARG:C	2.58	0.41
1:B:130:ILE:HD12	1:B:295:PHE:CE1	2.56	0.41
1:B:133:GLN:HG3	1:B:150:GLU:HG2	2.02	0.41
1:B:215:ALA:HB3	1:B:257:ARG:NH1	2.34	0.41
1:B:390:TYR:O	1:B:412:LEU:HD23	2.20	0.41
1:A:163[A]:TYR:CZ	1:A:275:SER:HB3	2.55	0.41
1:A:185:TYR:O	1:A:186:LEU:C	2.59	0.41
1:B:19:VAL:HG23	1:B:233:PHE:O	2.21	0.41
1:B:188:LEU:HD23	1:B:189:ARG:N	2.35	0.41
1:B:190[B]:TYR:CZ	2:B:900[B]:BLA:HMB1	2.56	0.41
1:A:216:TYR:CE2	1:A:218:PRO:HG3	2.56	0.41
1:B:59:LEU:H	1:B:59:LEU:CD2	2.27	0.41
1:B:210:LEU:C	1:B:210:LEU:CD2	2.88	0.41
1:A:336:PHE:HZ	1:A:364:LEU:HB2	1.86	0.41
1:A:239:VAL:HG11	1:A:289:ARG:NH2	2.35	0.40
1:A:176:GLU:HG2	1:A:177:SER:N	2.36	0.40
1:A:264:ILE:HD11	1:A:274:PHE:CE1	2.55	0.40
1:A:346:ILE:HG22	1:A:347:ALA:N	2.35	0.40
1:A:366:ILE:CG1	1:A:367:ARG:HG3	2.49	0.40
1:B:373:GLN:O	1:B:377:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:THR:O	1:A:323:LEU:HG	2.21	0.40
1:A:379:GLN:O	1:A:379:GLN:CG	2.69	0.40
1:B:244:SER:HB3	2:B:900[A]:BLA:HMD2	2.03	0.40
1:A:45:ILE:H	1:A:45:ILE:HG13	1.69	0.40
1:A:210:LEU:HD23	1:A:259:SER:O	2.21	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	453/505 (90%)	415 (92%)	35 (8%)	3 (1%)	22	50
1	B	454/505 (90%)	411 (90%)	41 (9%)	2 (0%)	34	62
All	All	907/1010 (90%)	826 (91%)	76 (8%)	5 (1%)	25	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	454	LEU
1	A	341	HIS
1	A	218	PRO
1	A	452	PRO
1	B	342	PRO

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

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/431 (91%)	339 (86%)	55 (14%)	3	9
1	B	395/431 (92%)	346 (88%)	49 (12%)	4	12
All	All	789/862 (92%)	685 (87%)	104 (13%)	4	10

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	23	ILE
1	A	32	LEU
1	A	43	GLU
1	A	57	SER
1	A	59	LEU
1	A	64	VAL
1	A	83	SER
1	A	88	THR
1	A	98	ILE
1	A	111	GLU
1	A	119	SER
1	A	120	ILE
1	A	125	LEU
1	A	126	ASN
1	A	130	ILE
1	A	142	SER
1	A	147	VAL
1	A	180	GLU
1	A	186	LEU
1	A	188	LEU
1	A	209[A]	ARG
1	A	209[B]	ARG
1	A	210	LEU
1	A	242	SER
1	A	252	THR
1	A	257	ARG
1	A	260	MET
1	A	273	LEU
1	A	280	SER
1	A	291	SER
1	A	294	ILE
1	A	306	LEU
1	A	308	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	317	VAL
1	A	318	SER
1	A	319	THR
1	A	333	ASP
1	A	335	LEU
1	A	341	HIS
1	A	343	ASP
1	A	344	ASP
1	A	363	THR
1	A	366	ILE
1	A	393	ASP
1	A	409	CYS
1	A	412	LEU
1	A	426	TRP
1	A	453	ARG
1	A	475	SER
1	A	477	THR
1	A	483	GLU
1	A	485	LEU
1	A	487	LEU
1	A	488	ASP
1	B	13	GLU
1	B	32	LEU
1	B	45	ILE
1	B	51	PHE
1	B	59	LEU
1	B	64	VAL
1	B	76	LEU
1	B	86	VAL
1	B	98	ILE
1	B	113	ARG
1	B	119	SER
1	B	125	LEU
1	B	130	ILE
1	B	134	VAL
1	B	146	ASN
1	B	147	VAL
1	B	160	VAL
1	B	179	ARG
1	B	181	ASP
1	B	182	LEU
1	B	186	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	188	LEU
1	B	198	GLN
1	B	221	VAL
1	B	236	SER
1	B	242	SER
1	B	257	ARG
1	B	260	MET
1	B	273	LEU
1	B	277	HIS
1	B	291	SER
1	B	294	ILE
1	B	317	VAL
1	B	319	THR
1	B	343	ASP
1	B	366	ILE
1	B	380	ARG
1	B	393	ASP
1	B	412	LEU
1	B	426	TRP
1	B	431	GLU
1	B	454	LEU
1	B	455	THR
1	B	468	ARG
1	B	483	GLU
1	B	485	LEU
1	B	487	LEU
1	B	490	MET
1	B	493	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	24	GLN
1	A	26	HIS
1	A	138	ASN
1	A	373	GLN
1	B	308	GLN
1	B	373	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](#)

4 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	BLA	B	900[B]	1	36,46,46	3.02	18 (50%)	47,67,67	1.42	8 (17%)
2	BLA	B	900[A]	1	36,46,46	3.01	18 (50%)	47,67,67	1.70	9 (19%)
2	BLA	A	900[B]	1	36,46,46	2.99	18 (50%)	47,67,67	1.64	10 (21%)
2	BLA	A	900[A]	1	36,46,46	3.03	18 (50%)	47,67,67	1.64	7 (14%)

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	BLA	B	900[B]	1	-	2/22/74/74	0/4/4/4
2	BLA	B	900[A]	1	-	8/22/74/74	0/4/4/4
2	BLA	A	900[B]	1	-	1/22/74/74	0/4/4/4
2	BLA	A	900[A]	1	-	5/22/74/74	0/4/4/4

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900[A]	BLA	CHB-C1B	9.11	1.53	1.34
2	B	900[A]	BLA	CHB-C1B	8.76	1.52	1.34
2	B	900[B]	BLA	CHB-C1B	8.37	1.51	1.34
2	A	900[B]	BLA	CHB-C1B	8.21	1.51	1.34
2	B	900[A]	BLA	CHD-C4C	6.55	1.53	1.38
2	B	900[B]	BLA	CHD-C4C	6.49	1.53	1.38
2	A	900[A]	BLA	CHD-C4C	6.47	1.53	1.38
2	A	900[B]	BLA	CHD-C4C	6.34	1.53	1.38
2	A	900[B]	BLA	CHD-C1D	5.62	1.53	1.40
2	B	900[B]	BLA	CHD-C1D	5.49	1.53	1.40
2	B	900[A]	BLA	CHD-C1D	5.45	1.53	1.40
2	A	900[B]	BLA	CHA-C4D	5.33	1.39	1.35
2	A	900[A]	BLA	CHD-C1D	5.26	1.52	1.40
2	A	900[A]	BLA	CHA-C4D	5.11	1.39	1.35
2	B	900[A]	BLA	CHA-C4D	4.88	1.39	1.35
2	B	900[A]	BLA	CBC-CAC	4.82	1.54	1.30
2	A	900[A]	BLA	CBC-CAC	4.79	1.54	1.30
2	B	900[B]	BLA	CBC-CAC	4.79	1.54	1.30
2	A	900[B]	BLA	CBC-CAC	4.69	1.53	1.30
2	B	900[B]	BLA	CHA-C4D	4.63	1.39	1.35
2	B	900[B]	BLA	C4D-C3D	-4.44	1.38	1.45
2	A	900[B]	BLA	C4D-C3D	-4.08	1.39	1.45
2	A	900[A]	BLA	C4D-C3D	-3.84	1.39	1.45
2	B	900[A]	BLA	C4D-C3D	-3.70	1.39	1.45
2	B	900[B]	BLA	C1D-C2D	-3.69	1.37	1.45
2	A	900[B]	BLA	C1D-C2D	-3.59	1.38	1.45
2	A	900[A]	BLA	C1D-C2D	-3.54	1.38	1.45
2	B	900[B]	BLA	C1C-C2C	-3.48	1.38	1.47
2	A	900[A]	BLA	C1C-C2C	-3.48	1.38	1.47
2	A	900[B]	BLA	C1B-C2B	-3.47	1.38	1.45
2	A	900[B]	BLA	C1C-C2C	-3.46	1.38	1.47
2	B	900[B]	BLA	C1B-C2B	-3.43	1.38	1.45
2	B	900[A]	BLA	C1D-C2D	-3.43	1.38	1.45
2	B	900[A]	BLA	C1C-C2C	-3.39	1.38	1.47
2	B	900[B]	BLA	C3C-C4C	-3.12	1.40	1.45
2	A	900[A]	BLA	C4A-CHB	3.08	1.53	1.41
2	A	900[B]	BLA	C3B-C4B	-3.07	1.38	1.47
2	A	900[A]	BLA	CAB-C3B	-3.07	1.39	1.47
2	B	900[B]	BLA	C3B-C4B	-3.03	1.38	1.47
2	B	900[A]	BLA	C4A-CHB	3.03	1.52	1.41
2	B	900[B]	BLA	CAB-C3B	-3.02	1.39	1.47
2	A	900[B]	BLA	CAB-C3B	-3.01	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900[A]	BLA	CAB-C3B	-3.01	1.39	1.47
2	A	900[A]	BLA	C3B-C4B	-2.93	1.39	1.47
2	B	900[A]	BLA	C3B-C4B	-2.93	1.39	1.47
2	B	900[B]	BLA	C4A-CHB	2.89	1.52	1.41
2	A	900[B]	BLA	C3C-C4C	-2.86	1.40	1.45
2	B	900[A]	BLA	C1B-C2B	-2.84	1.40	1.45
2	A	900[A]	BLA	C3C-C4C	-2.84	1.40	1.45
2	B	900[A]	BLA	C3C-C4C	-2.81	1.40	1.45
2	A	900[A]	BLA	C1B-C2B	-2.75	1.40	1.45
2	B	900[B]	BLA	CAC-C3C	2.74	1.54	1.47
2	B	900[A]	BLA	CAC-C3C	2.72	1.54	1.47
2	A	900[A]	BLA	CAC-C3C	2.66	1.54	1.47
2	A	900[B]	BLA	C4A-CHB	2.57	1.51	1.41
2	A	900[B]	BLA	CAC-C3C	2.50	1.54	1.47
2	A	900[A]	BLA	C1C-NC	-2.44	1.32	1.38
2	B	900[A]	BLA	C1C-NC	-2.42	1.32	1.38
2	A	900[B]	BLA	C1C-NC	-2.41	1.32	1.38
2	A	900[B]	BLA	C4C-NC	-2.36	1.33	1.37
2	B	900[A]	BLA	C4C-NC	-2.33	1.33	1.37
2	B	900[A]	BLA	C4D-ND	-2.26	1.33	1.38
2	A	900[A]	BLA	C4C-NC	-2.24	1.34	1.37
2	A	900[A]	BLA	C4D-ND	-2.22	1.33	1.38
2	B	900[B]	BLA	C4C-NC	-2.20	1.34	1.37
2	A	900[B]	BLA	C1B-NB	-2.16	1.34	1.37
2	B	900[B]	BLA	C4D-ND	-2.16	1.33	1.38
2	B	900[B]	BLA	C1C-NC	-2.14	1.33	1.38
2	A	900[B]	BLA	C4D-ND	-2.11	1.34	1.38
2	B	900[A]	BLA	C1B-NB	-2.10	1.34	1.37
2	B	900[B]	BLA	C1B-NB	-2.08	1.34	1.37
2	A	900[A]	BLA	C1B-NB	-2.03	1.34	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900[A]	BLA	C1A-CHA-C4D	-6.22	121.38	128.81
2	B	900[A]	BLA	C1A-CHA-C4D	-5.45	122.30	128.81
2	A	900[B]	BLA	C4C-CHD-C1D	-5.12	115.57	128.08
2	A	900[A]	BLA	CMB-C2B-C1B	3.48	128.51	124.17
2	B	900[A]	BLA	C4C-CHD-C1D	-3.41	119.75	128.08
2	B	900[A]	BLA	CBA-CAA-C2A	3.27	118.53	112.49
2	A	900[A]	BLA	C4C-CHD-C1D	-3.19	120.28	128.08
2	B	900[A]	BLA	C3B-C4B-NB	3.13	109.72	106.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900[B]	BLA	C1A-CHA-C4D	-3.09	125.11	128.81
2	A	900[B]	BLA	CBC-CAC-C3C	-3.03	112.56	127.62
2	A	900[B]	BLA	C3B-C4B-NB	2.95	109.52	106.19
2	B	900[B]	BLA	C3B-C4B-NB	2.88	109.44	106.19
2	A	900[B]	BLA	CBA-CAA-C2A	2.74	117.54	112.49
2	B	900[A]	BLA	CMB-C2B-C1B	2.63	127.45	124.17
2	B	900[A]	BLA	CBC-CAC-C3C	-2.60	114.68	127.62
2	A	900[B]	BLA	CHA-C4D-ND	2.60	132.43	128.83
2	A	900[A]	BLA	CBC-CAC-C3C	-2.58	114.79	127.62
2	B	900[B]	BLA	CHA-C4D-ND	2.55	132.36	128.83
2	B	900[B]	BLA	CBC-CAC-C3C	-2.52	115.07	127.62
2	B	900[A]	BLA	CAD-C3D-C4D	2.47	129.38	125.01
2	B	900[B]	BLA	CHA-C4D-C3D	-2.47	119.62	125.32
2	B	900[B]	BLA	CBA-CAA-C2A	2.46	117.03	112.49
2	A	900[A]	BLA	C3B-C4B-NB	2.42	108.93	106.19
2	A	900[B]	BLA	CHA-C4D-C3D	-2.40	119.78	125.32
2	A	900[B]	BLA	CHD-C4C-NC	-2.39	120.94	126.06
2	A	900[B]	BLA	C4D-ND-C1D	2.36	110.95	106.51
2	B	900[A]	BLA	C4D-ND-C1D	2.26	110.77	106.51
2	B	900[B]	BLA	C4D-ND-C1D	2.23	110.70	106.51
2	B	900[A]	BLA	C1D-C2D-C3D	2.17	109.00	106.51
2	A	900[A]	BLA	C4D-ND-C1D	2.15	110.56	106.51
2	A	900[A]	BLA	CAD-C3D-C4D	2.14	128.79	125.01
2	A	900[B]	BLA	CAC-C3C-C4C	2.12	129.70	123.54
2	A	900[B]	BLA	C1A-CHA-C4D	-2.06	126.34	128.81
2	B	900[B]	BLA	CAD-CBD-CGD	-2.03	109.27	112.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900[A]	BLA	NB-C1B-CHB-C4A
2	A	900[A]	BLA	C2B-C1B-CHB-C4A
2	A	900[B]	BLA	C3A-C4A-CHB-C1B
2	B	900[A]	BLA	NA-C4A-CHB-C1B
2	B	900[A]	BLA	C3A-C4A-CHB-C1B
2	B	900[A]	BLA	NB-C1B-CHB-C4A
2	B	900[A]	BLA	C2B-C1B-CHB-C4A
2	B	900[B]	BLA	NA-C4A-CHB-C1B
2	B	900[B]	BLA	C3A-C4A-CHB-C1B
2	B	900[A]	BLA	C3C-C4C-CHD-C1D
2	B	900[A]	BLA	NC-C4C-CHD-C1D

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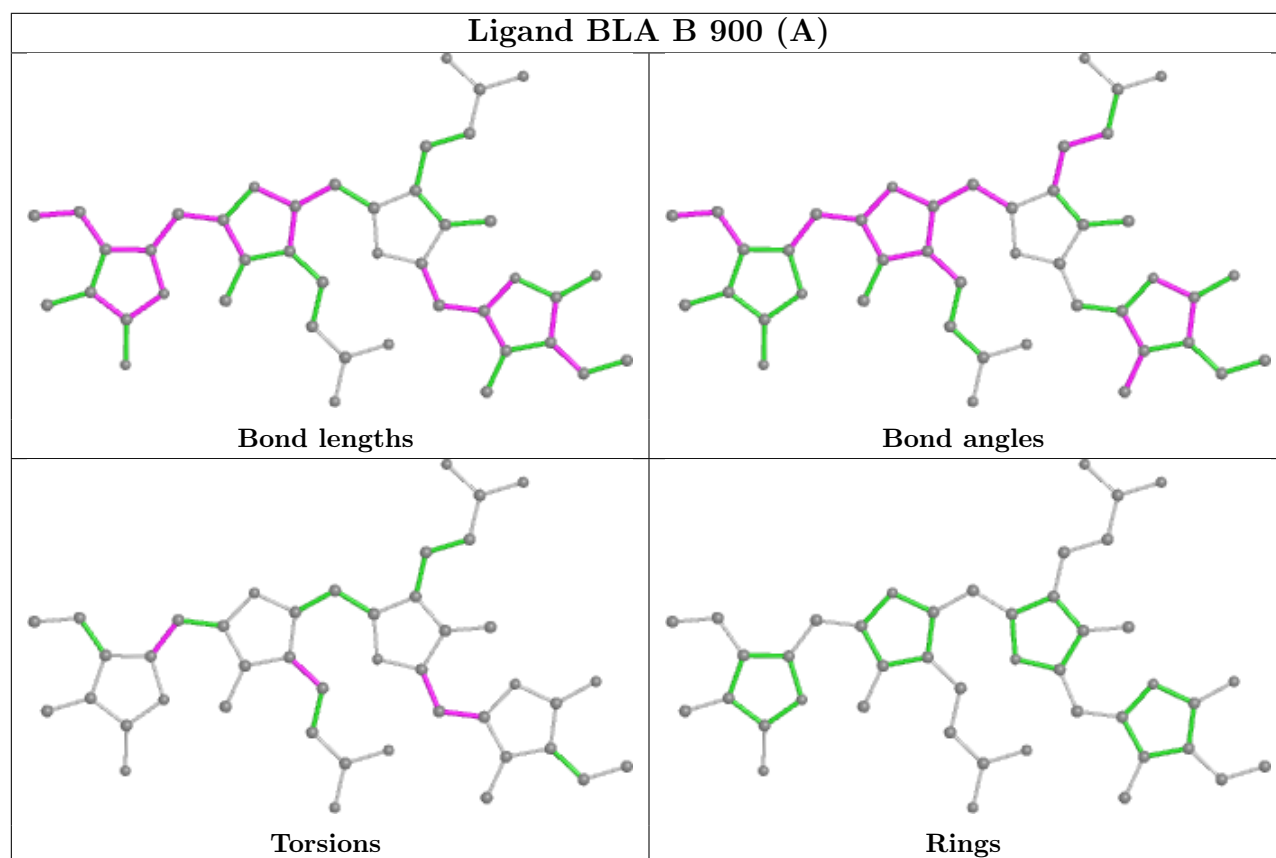
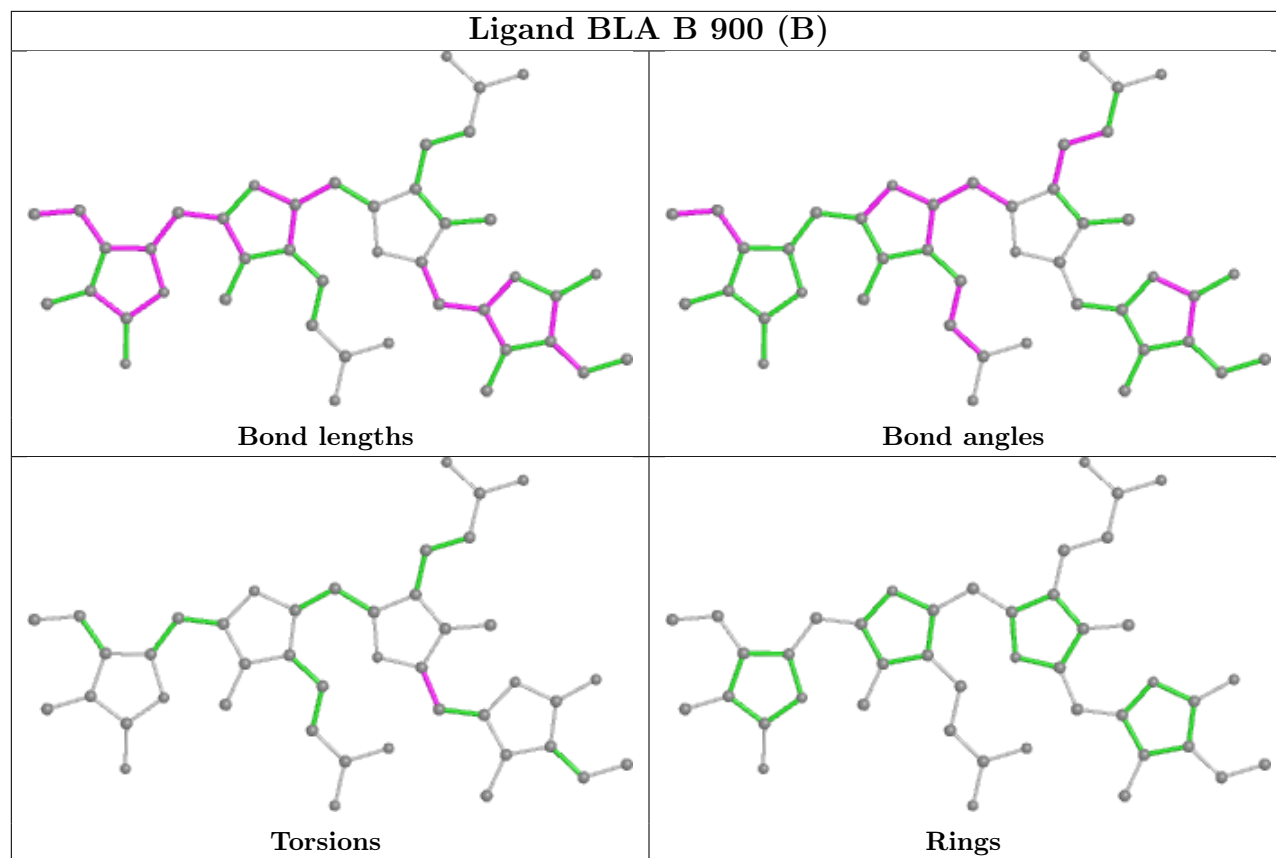
Mol	Chain	Res	Type	Atoms
2	A	900[A]	BLA	NC-C4C-CHD-C1D
2	A	900[A]	BLA	C3C-C4C-CHD-C1D
2	B	900[A]	BLA	C2D-C3D-CAD-CBD
2	B	900[A]	BLA	C4D-C3D-CAD-CBD
2	A	900[A]	BLA	C2D-C3D-CAD-CBD

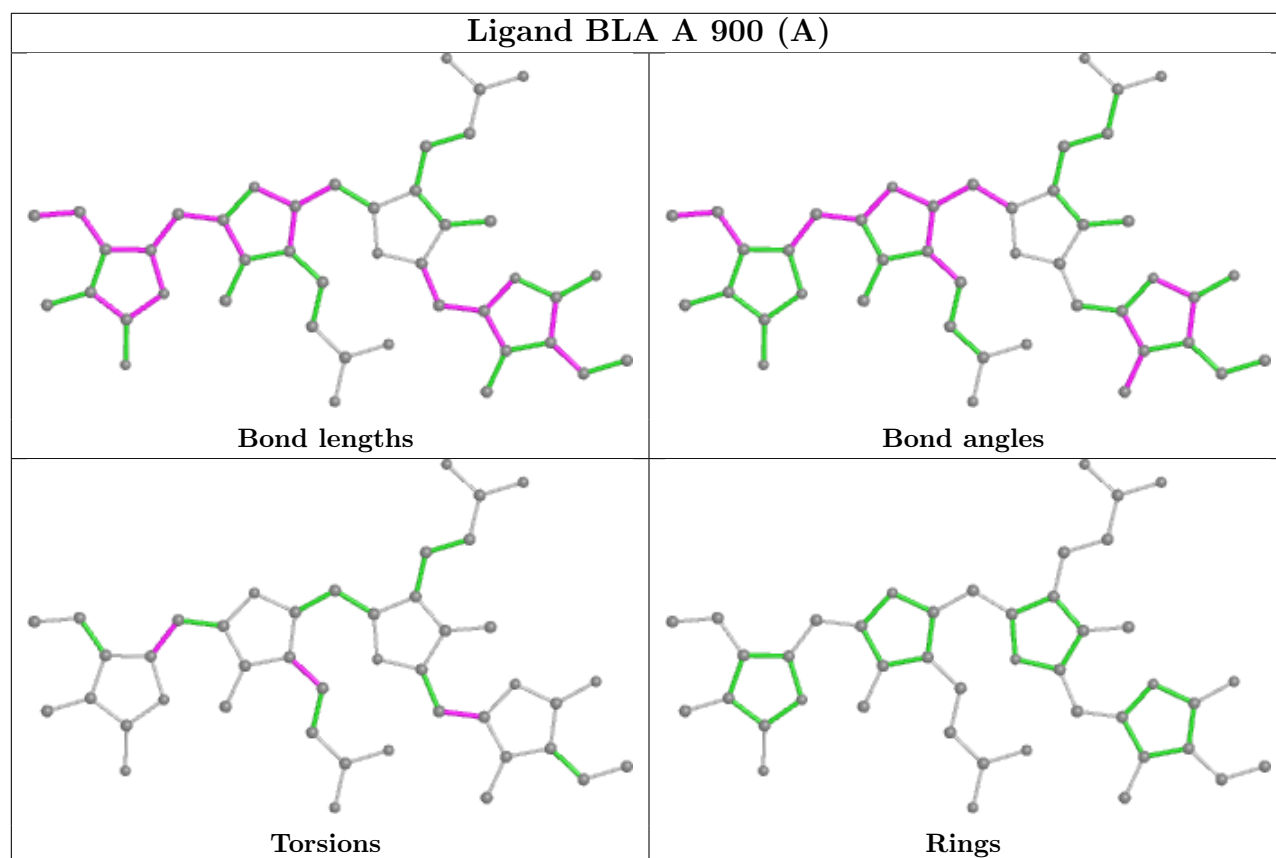
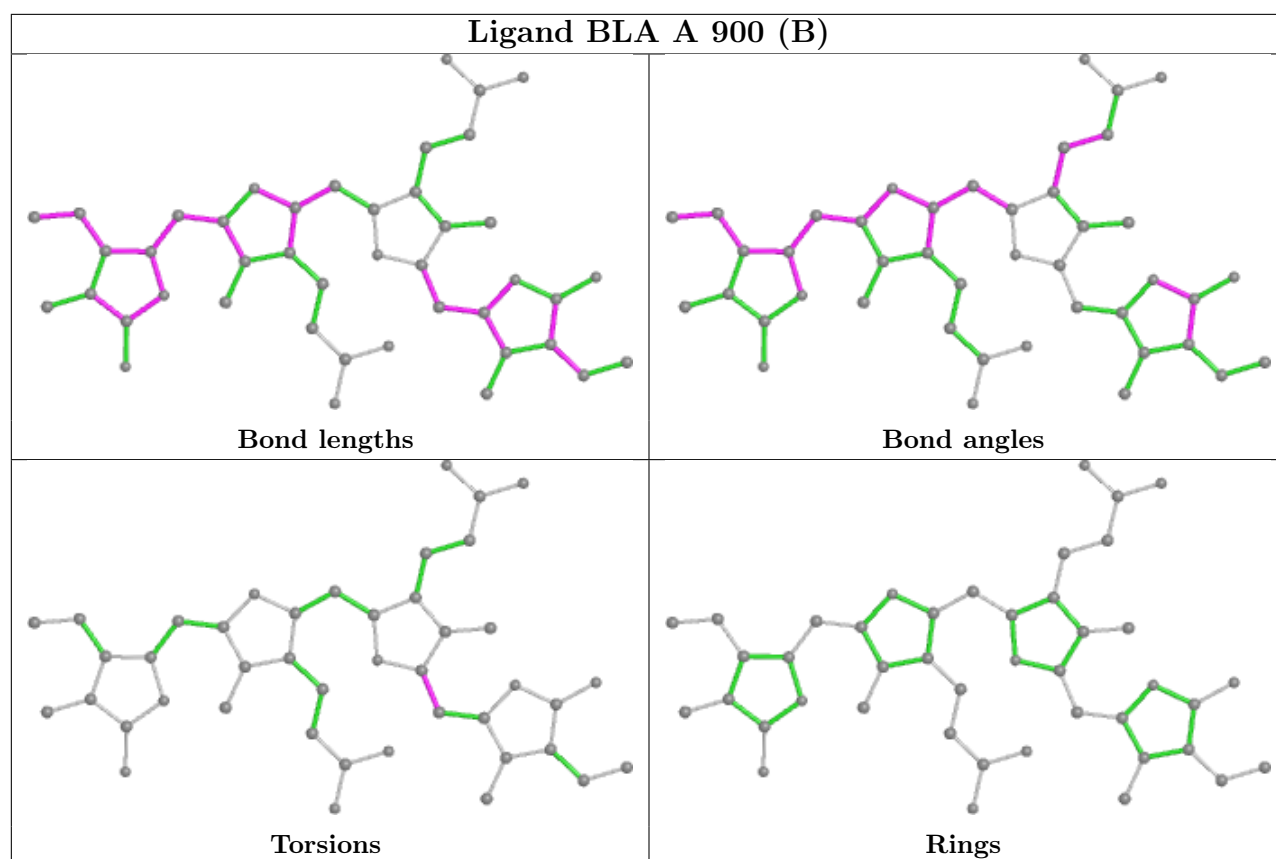
There are no ring outliers.

4 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900[B]	BLA	20	0
2	B	900[A]	BLA	11	0
2	A	900[B]	BLA	9	0
2	A	900[A]	BLA	9	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

### 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	457/505 (90%)	-0.07	24 (5%) 26 22	63, 120, 219, 317	0
1	B	457/505 (90%)	-0.11	23 (5%) 28 24	62, 119, 230, 373	0
All	All	914/1010 (90%)	-0.09	47 (5%) 28 23	62, 119, 222, 373	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	ARG	10.0
1	A	431	GLU	8.0
1	A	452	PRO	7.9
1	A	433	HIS	6.9
1	B	360	GLY	6.5
1	B	361	GLY	6.2
1	B	381	LEU	6.2
1	A	363	THR	5.2
1	A	374	ALA	4.4
1	B	363	THR	4.1
1	B	372	ARG	3.9
1	A	406	GLY	3.8
1	A	430	GLU	3.7
1	B	356	LEU	3.6
1	B	378	LEU	3.6
1	B	336	PHE	3.6
1	B	383	ARG	3.3
1	A	258	ALA	3.3
1	B	367	ARG	3.3
1	A	371	GLU	3.3
1	B	364	LEU	3.1
1	B	425	PHE	3.1
1	A	358	MET	3.0
1	B	358	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	356	LEU	3.0
1	B	433	HIS	2.9
1	B	470	HIS	2.9
1	A	454	LEU	2.7
1	B	386	GLU	2.7
1	B	387	ARG	2.6
1	B	380	ARG	2.6
1	A	408	CYS	2.5
1	A	463	TRP	2.5
1	B	357	VAL	2.5
1	A	360	GLY	2.4
1	A	190[A]	TYR	2.4
1	A	425	PHE	2.3
1	A	429	HIS	2.3
1	A	470	HIS	2.3
1	A	407	ASP	2.3
1	A	357	VAL	2.3
1	B	389	ILE	2.2
1	B	431	GLU	2.1
1	B	365	SER	2.1
1	A	11	ASN	2.1
1	A	432	VAL	2.0
1	B	423	TRP	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](#)

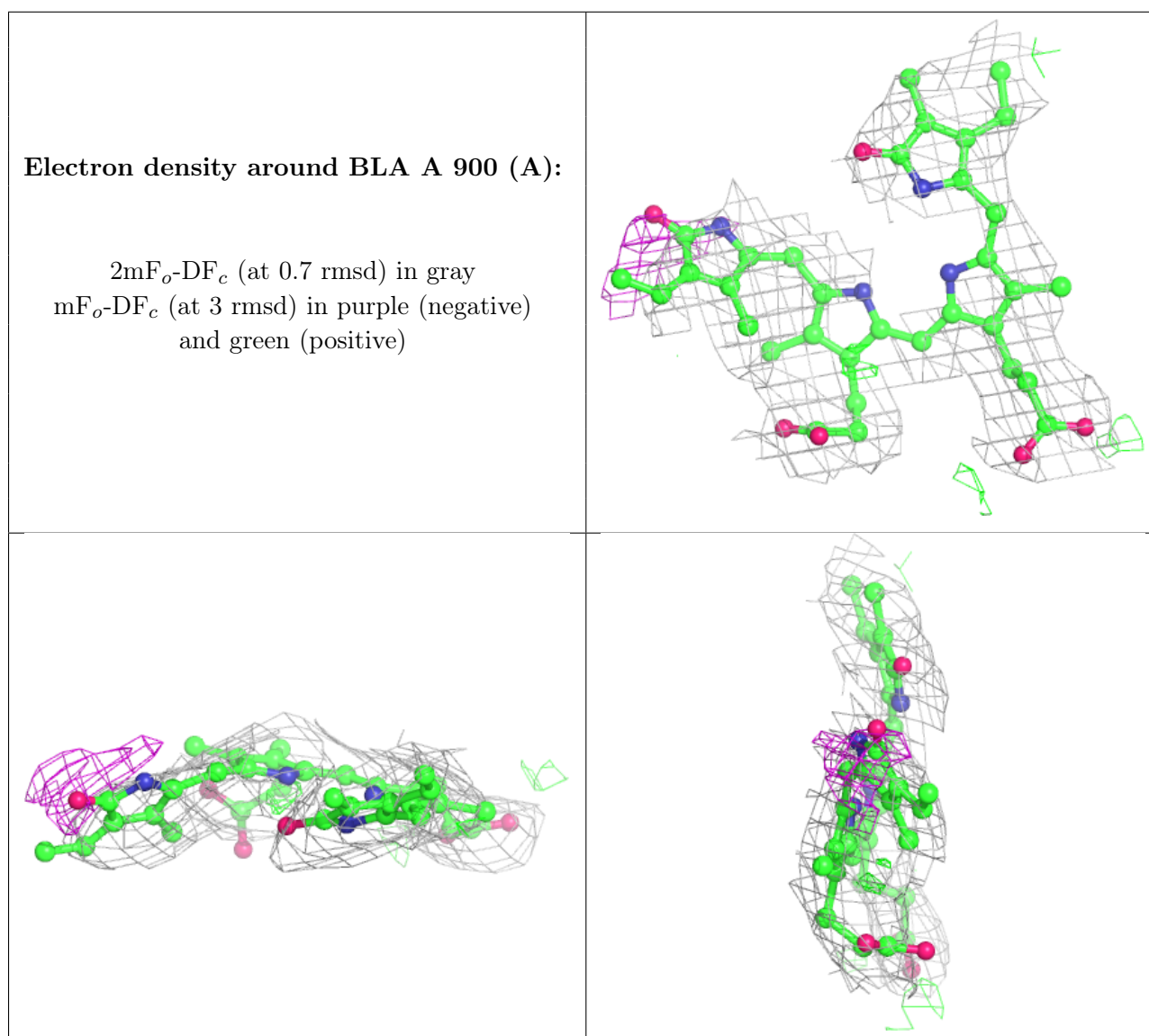
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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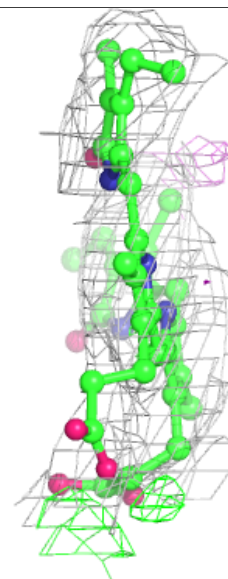
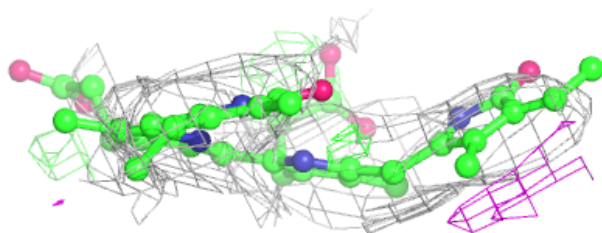
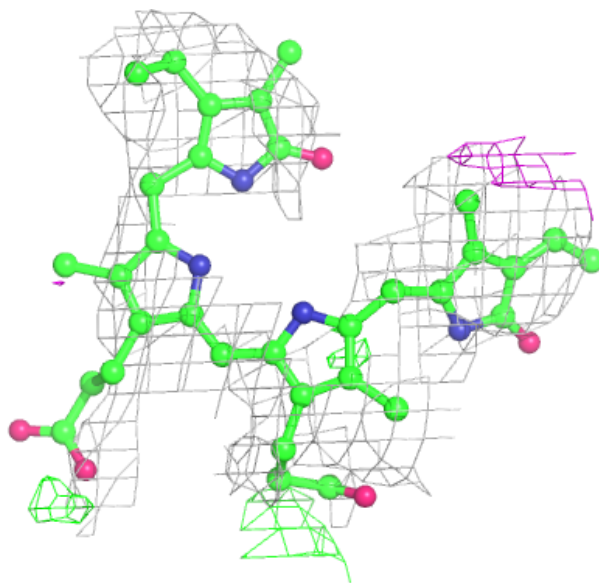
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BLA	A	900[A]	43/43	0.89	0.30	92,130,170,177	43
2	BLA	A	900[B]	43/43	0.89	0.30	85,127,170,173	43
2	BLA	B	900[A]	43/43	0.91	0.31	85,123,149,164	43
2	BLA	B	900[B]	43/43	0.91	0.31	79,114,146,176	43

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.



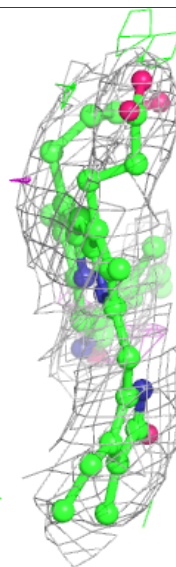
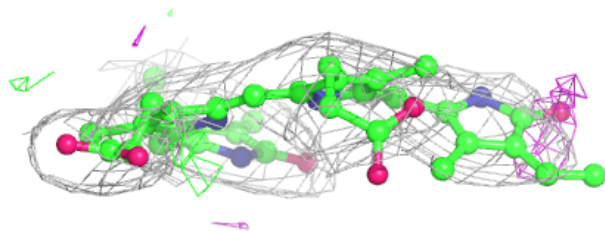
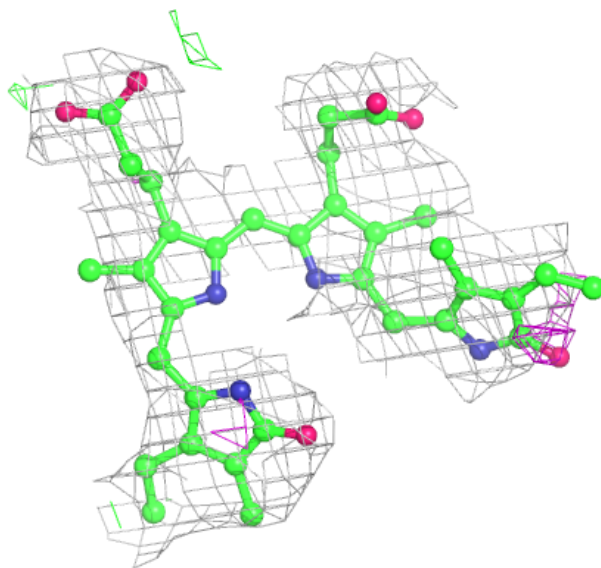
**Electron density around BLA A 900 (B):**

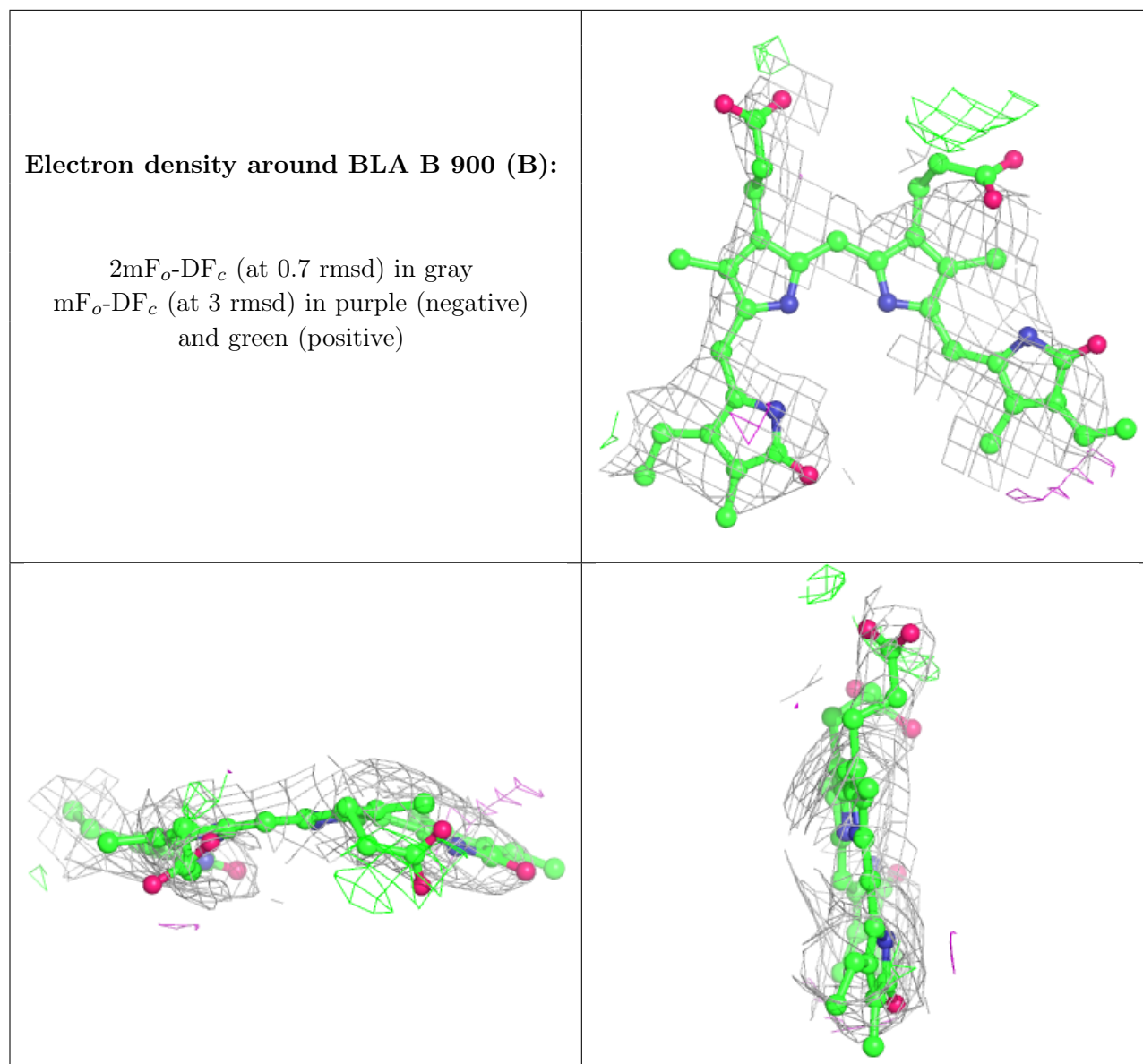
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BLA B 900 (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.