



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:49 AM GMT

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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

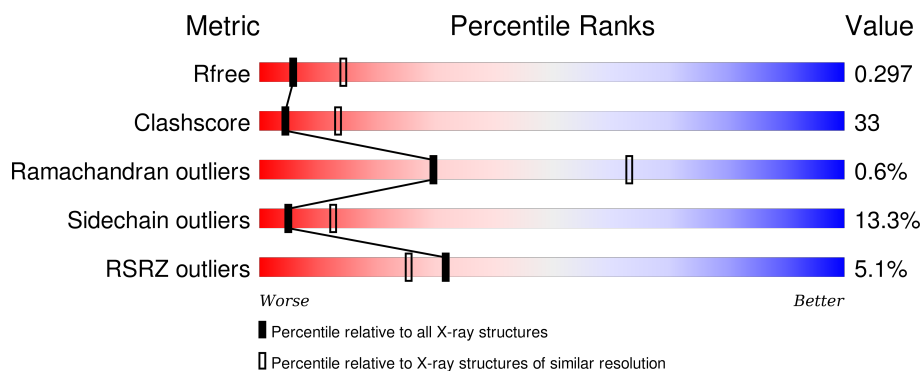
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	
1	B	505	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BLA	B	900[A]	-	-	-	X
2	BLA	B	900[B]	-	-	-	X

## 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.

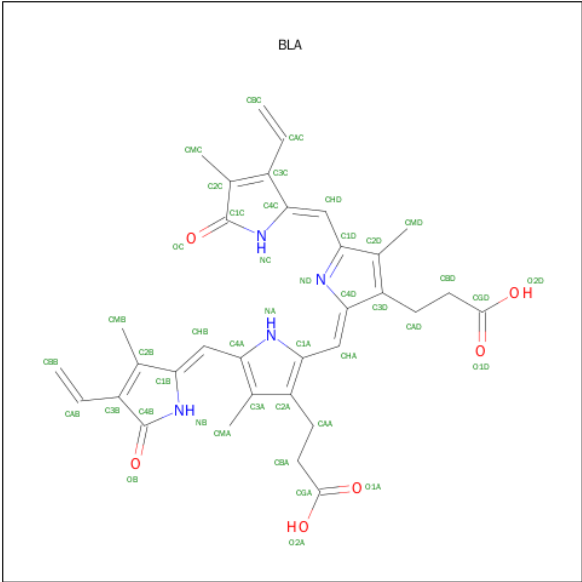
- Molecule 1 is a protein called Bacteriophytochrome.

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

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	GLN	ENGINEERED	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	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:  $C_{33}H_{34}N_4O_6$ ).



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		

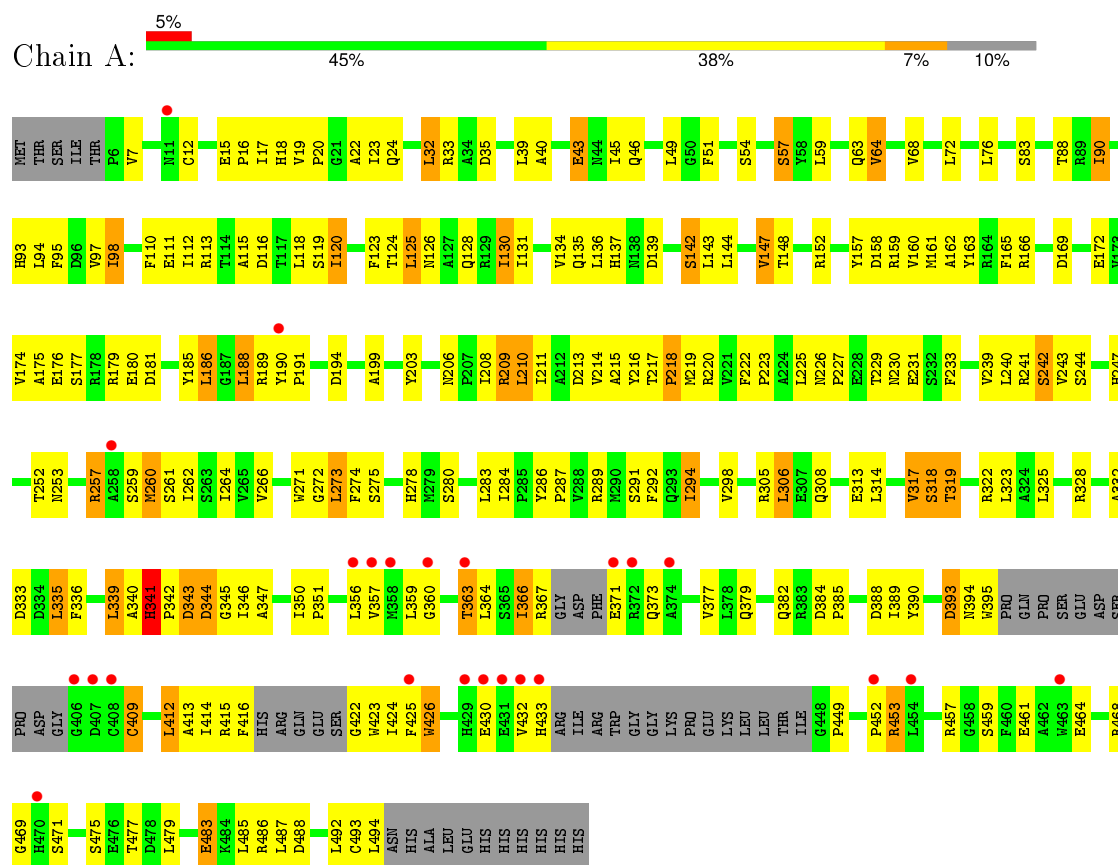
- Molecule 3 is water.

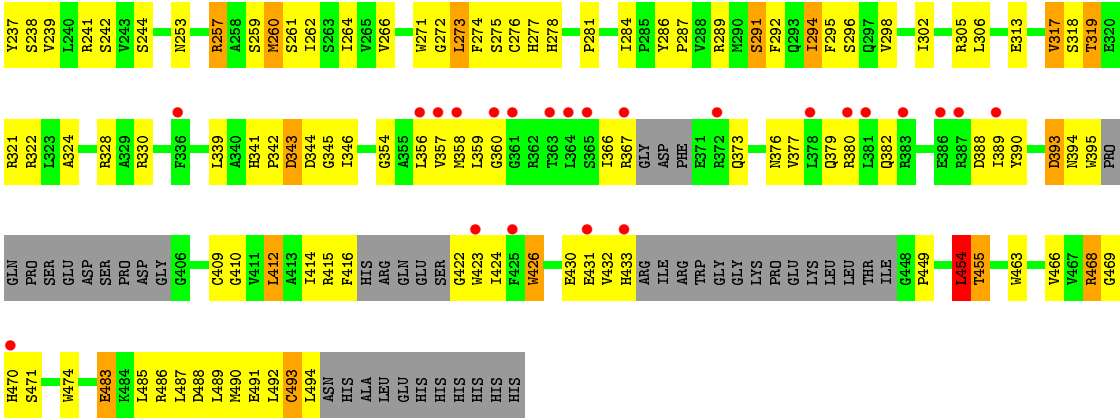
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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

#### • Molecule 1: Bacteriophytochrome





## 4 Data and refinement statistics

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)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.229 , 0.298 0.228 , 0.297	Depositor DCC
$R_{free}$ test set	1281 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.0	EDS
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 25918 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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:HHB	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:NH1	1:A:257:ARG:HG2	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
2:A:900[A]:BLA:HMA2	2:A:900[A]:BLA:HMB3	1.71	0.71
1:A:43:GLU:HG2	1:A:220:ARG:O	1.90	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:B:163[B]:TYR:OH	1:B:190[B]:TYR:HD2	1.74	0.70
1:A:363:THR:HG21	1:A:371:GLU:CB	2.22	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:B:19:VAL:HG13	1:B:19:VAL:O	1.93	0.69
1:A:94:LEU:HD22	1:A:113:ARG:HD3	1.75	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:B:235:LEU:O	1:B:238:SER:HB3	1.94	0.68
1:A:286:TYR:HB3	1:A:287:PRO:HD3	1.76	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:B:209[B]:ARG:HD3	1:B:209[B]:ARG:N	2.10	0.66
1:A:64:VAL:HA	1:A:90:ILE:HD11	1.78	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:N	1:A:314:LEU:HD23	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:B:202:LEU:HB3	1:B:209[B]:ARG:NH2	2.11	0.65
1:A:379:GLN:HA	1:A:382:GLN:CG	2.27	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:B:189:ARG:HD2	1:B:463:TRP:CH2	2.31	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: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:B:31:THR:C	1:B:32:LEU:HD12	2.17	0.64
1:A:346:ILE:HG23	1:A:426:TRP:CZ3	2.32	0.64
2:B:900[B]:BLA:CGA	2:B:900[B]:BLA:HMA2	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:185:TYR:O	1:B:188:LEU:HB2	1.99	0.63
1:B:97:VAL:HG22	1:B:110:PHE:CD2	2.33	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:N	1:B:20:PRO:HD3	2.14	0.62
1:B:19:VAL:CG2	1:B:232:SER:HB3	2.29	0.62
1:A:335:LEU:CD1	1:A:492:LEU:HD23	2.29	0.62
1:A:125:LEU:HD23	1:A:125:LEU:O	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:339:LEU:HD22	1:A:346:ILE:HD11	1.82	0.62
1:A:143:LEU:O	1:A:147:VAL:HG12	2.00	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
2:B:900[A]:BLA:HMC1	2:B:900[A]:BLA:CBC	2.29	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
1:A:120:ILE:HD13	1:A:120:ILE:N	2.15	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:A:416:PHE:HE1	1:A:424:ILE:HG13	1.65	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:B:43:GLU:HG3	1:B:219:MET:HG3	1.82	0.60
1:A:415:ARG:HD3	1:A:423:TRP:CZ2	2.37	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:CD2	1:A:190[B]:TYR:N	2.69	0.59
2:B:900[B]:BLA:HMA1	2:B:900[B]:BLA:HB	1.66	0.59
1:B:284:ILE:N	1:B:284:ILE:HD12	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLN:HA	1:B:382:GLN:HG2	1.84	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:B:64:VAL:HG13	1:B:68:VAL:HB	1.85	0.59
1:A:134:VAL:HG22	1:A:143:LEU:HD21	1.85	0.59
1:A:359:LEU:HD13	1:A:422:GLY:HA3	1.83	0.59
1:B:158:ASP:OD1	1:B:278:HIS:HA	2.02	0.59
1:A:191:PRO:HG2	1:A:453:ARG:HH22	1.67	0.59
1:A:414:ILE:CG1	1:A:424:ILE:HB	2.33	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:B:493:CYS:O	1:B:494:LEU:CB	2.51	0.59
1:B:45:ILE:HG22	1:B:49:LEU:HD12	1.83	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:B:161:MET:HE3	2:B:900[B]:BLA:HBB1	1.84	0.58
1:A:64:VAL:HA	1:A:90:ILE:CD1	2.32	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:B:359:LEU:HD13	1:B:422:GLY:CA	2.33	0.58
1:A:359:LEU:HD12	1:A:360:GLY:H	1.68	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:CA	1:B:468:ARG:HE	2.14	0.57
1:A:273:LEU:HD12	1:A:273:LEU:C	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:B:430:GLU:N	1:B:430:GLU:OE1	2.38	0.57
1:A:393:ASP:O	1:A:394:ASN:CG	2.43	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:HD23	1:A:283:LEU:C	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:379:GLN:CA	1:A:382:GLN:HG2	2.37	0.55
1:A:366:ILE:HG13	1:A:367:ARG:N	2.19	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:B:17:ILE:HD13	2:B:900[B]:BLA:HAD1	1.88	0.54
1:A:45:ILE:HB	1:A:51:PHE:CE1	2.42	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:185:TYR:HD1	1:B:188:LEU:CD1	2.19	0.53
1:B:60:THR:OG1	1:B:63:GLN:NE2	2.41	0.53
1:B:189:ARG:HD2	1:B:463:TRP:CZ2	2.44	0.53
2:B:900[A]:BLA:CMC	2:B:900[A]:BLA:HBC1	2.33	0.53
1:B:68:VAL:O	1:B:71:MET:HB3	2.08	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:CBC	2:A:900[A]:BLA:HMC1	2.25	0.53
1:B:209[B]:ARG:N	1:B:209[B]:ARG:CD	2.72	0.52
1:A:430:GLU:HG2	1:A:471:SER:CA	2.39	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:B:393:ASP:HB2	1:B:394:ASN:OD1	2.11	0.51
1:B:202:LEU:C	1:B:209[B]:ARG:HH21	2.11	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:185:TYR:CD1	1:B:188:LEU:HD12	2.40	0.51
1:A:191:PRO:CG	1:A:453:ARG:HH22	2.23	0.51
1:A:124:THR:O	1:A:128:GLN:HG3	2.09	0.51
1:B:176:GLU:HG2	1:B:177:SER:N	2.26	0.51
1:B:71:MET:CE	1:B:97:VAL:HG12	2.41	0.51
1:A:266:VAL:HG22	1:A:271:TRP:HB2	1.92	0.51
1:A:209[A]:ARG:NH1	1:A:209[A]:ARG:CG	2.64	0.51
2:B:900[B]:BLA:OB	2:B:900[B]:BLA:HBB1	2.09	0.51
1:B:239:VAL:HG11	1:B:289:ARG:NH2	2.25	0.51
1:B:59:LEU:HD22	1:B:59:LEU:N	2.23	0.51
1:A:24:GLN:HE21	1:A:243:VAL:HG23	1.75	0.51
1:A:284:ILE:N	1:A:284:ILE:HD12	2.25	0.51
1:A:213:ASP:O	1:A:216:TYR:HB3	2.11	0.51
1:A:159:ARG:NH2	1:A:185:TYR:HE2	2.08	0.50
1:A:134:VAL:HG13	1:A:134:VAL:O	2.11	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:B:206:ASN:HD21	1:B:237:TYR:H	1.58	0.50
1:A:136:LEU:HB2	1:A:137:HIS:CE1	2.47	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
2:B:900[A]:BLA:HBD2	2:B:900[A]:BLA:HMD1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LEU:HD12	1:B:474:TRP:CE3	2.47	0.50
1:A:388:ASP:HB3	1:A:486:ARG:NE	2.27	0.50
1:A:373:GLN:O	1:A:377:VAL:HG23	2.11	0.50
1:A:359:LEU:HD12	1:A:360:GLY:N	2.27	0.50
1:A:152:ARG:HB2	1:A:160:VAL:CG1	2.42	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:B:42:SER:HB2	1:B:44:ASN:OD1	2.11	0.49
1:A:415:ARG:HB2	1:A:423:TRP:CH2	2.47	0.49
1:B:415:ARG:HB2	1:B:423:TRP:CZ3	2.47	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:430:GLU:HG3	1:B:468:ARG:O	2.12	0.49
1:B:181:ASP:N	1:B:181:ASP:OD1	2.45	0.49
2:B:900[A]:BLA:HMA2	2:B:900[A]:BLA:HMB3	1.94	0.49
1:B:236:SER:O	1:B:237:TYR:HB2	2.12	0.49
1:B:67:GLU:OE1	1:B:88:THR:HA	2.12	0.49
1:A:172:GLU:HG2	1:A:174:VAL:CG1	2.42	0.49
1:A:208:ILE:HA	1:A:261:SER:O	2.11	0.49
1:B:51:PHE:CD1	1:B:63:GLN:CB	2.96	0.49
1:A:220:ARG:HE	1:A:222:PHE:HZ	1.58	0.49
1:B:211:ILE:HB	1:B:259:SER:CB	2.43	0.49
1:A:19:VAL:HG12	1:A:233:PHE:O	2.13	0.49
2:B:900[A]:BLA:HMB3	2:B:900[A]:BLA:C3A	2.43	0.49
1:B:143:LEU:O	1:B:147:VAL:HG12	2.13	0.49
1:A:305:ARG:HH11	1:B:306:LEU:CD1	2.26	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:B:210:LEU:HD23	1:B:211:ILE:N	2.28	0.48
1:A:159:ARG:NH2	1:A:185:TYR:CE2	2.82	0.48
1:B:48:LEU:HB3	1:B:49:LEU:HG	1.94	0.48
1:B:262:ILE:CG2	1:B:296:SER:HB2	2.44	0.48
1:A:225:LEU:HD21	1:A:230:ASN:O	2.14	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:HA	1:B:201:ARG:HD2	1.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ARG:CA	1:B:468:ARG:NE	2.68	0.48
1:A:191:PRO:HD2	1:A:453:ARG:HH22	1.78	0.48
1:A:115:ALA:HB1	1:A:116:ASP:OD1	2.14	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:H	2.18	0.47
1:B:489:LEU:C	1:B:491:GLU:N	2.68	0.47
1:B:163[A]:TYR:OH	1:B:275:SER:HB3	2.14	0.47
1:A:339:LEU:HD22	1:A:346:ILE:CD1	2.44	0.47
1:B:343:ASP:C	1:B:345:GLY:H	2.16	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:A:314:LEU:O	1:A:318:SER:HB3	2.15	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:B:157:TYR:CG	1:B:276:CYS:HB3	2.50	0.47
1:A:409:CYS:SG	1:A:430:GLU:CD	2.93	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:209[B]:ARG:CG	1:A:261:SER:HB2	2.40	0.46
1:B:377:VAL:HG22	1:B:395:TRP:CH2	2.49	0.46
1:A:414:ILE:HG12	1:A:424:ILE:HB	1.95	0.46
1:A:179:ARG:NH1	1:A:181:ASP:OD2	2.45	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:157:TYR:OH	1:B:259:SER:O	2.32	0.46
1:B:90:ILE:CG2	1:B:91:GLY:N	2.77	0.46
1:B:415:ARG:HB2	1:B:423:TRP:CZ2	2.51	0.46
1:B:356:LEU:HD13	1:B:357:VAL:N	2.31	0.46
1:A:209[B]:ARG:HB3	1:A:209[B]:ARG:HE	1.26	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
1:B:179:ARG:HD2	1:B:181:ASP:OD2	2.16	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:210:LEU:HD11	1:A:284:ILE:H	1.81	0.46
1:B:32:LEU:N	1:B:32:LEU:HD12	2.31	0.46
1:A:143:LEU:HD12	1:A:144:LEU:HD23	1.97	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:19:VAL:CG1	1:B:19:VAL:O	2.64	0.45
1:B:7:VAL:O	1:B:7:VAL:HG23	2.16	0.45
1:B:226:ASN:HB2	1:B:233:PHE:CZ	2.51	0.45
1:A:359:LEU:HD22	1:A:416:PHE:HE2	1.80	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:416:PHE:CE1	1:A:424:ILE:HG13	2.49	0.45
1:A:18:HIS:C	1:A:20:PRO:HD3	2.37	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:139:ASP:HB3	1:A:142:SER:OG	2.17	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:B:209[A]:ARG:O	1:B:260:MET:HA	2.17	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:A:49:LEU:HD22	1:A:90:ILE:HG21	1.98	0.45
1:A:492:LEU:N	1:A:492:LEU:CD1	2.80	0.45
1:A:350:ILE:HG23	1:A:351:PRO:HD2	1.99	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:H	1:A:314:LEU:HD23	1.80	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
1:A:148:THR:O	1:A:160:VAL:HG11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LEU:HD12	1:B:274:PHE:O	2.18	0.43
1:A:262:ILE:HD12	1:A:292:PHE:HB3	2.00	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:B:12[B]:CYS:HB2	2:B:900[B]:BLA:HAC	1.35	0.43
1:A:359:LEU:HD13	1:A:422:GLY:CA	2.46	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: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:123:PHE:CE2	1:B:123:PHE:HE2	2.15	0.43
1:A:134:VAL:CG1	1:A:134:VAL:O	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:336:PHE:O	1:A:340:ALA:HB2	2.19	0.43
1:A:273:LEU:O	1:A:273:LEU:HD12	2.18	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:394:ASN:O	1:A:395:TRP:C	2.57	0.42
1:B:98:ILE:O	1:B:98:ILE:HG12	2.18	0.42
1:A:217:THR:HA	1:A:218:PRO:HD3	1.75	0.42
1:B:38:VAL:O	1:B:55:PRO:HA	2.18	0.42
1:A:15:GLU:HA	1:A:16:PRO:HD3	1.75	0.42
2:A:900[A]:BLA:HMB3	2:A:900[A]:BLA:C3A	2.49	0.42
1:A:341:HIS:C	1:A:343:ASP:H	2.20	0.42
1:A:17:ILE:HD11	1:A:199:ALA:N	2.33	0.42
2:B:900[B]:BLA:HBC1	2:B:900[B]:BLA:CMC	2.35	0.42
1:A:390:TYR:O	1:A:412:LEU:HD23	2.19	0.42
1:B:454:LEU:C	1:B:455:THR:CG2	2.87	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: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:414:ILE:HB	1:B:486:ARG:HB2	2.02	0.42
1:B:124:THR:O	1:B:128:GLN:HG3	2.18	0.42
1:B:359:LEU:HD12	1:B:360:GLY:H	1.84	0.42
1:A:384:ASP:N	1:A:385:PRO:HD3	2.34	0.42
1:A:130:ILE:CG2	1:A:131:ILE:N	2.82	0.42
1:B:15:GLU:HA	1:B:16:PRO:HD3	1.83	0.42
1:A:457:ARG:O	1:A:461:GLU:HG3	2.20	0.42

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:SER:HB3	2:B:900[A]:BLA:HMD2	2.03	0.40
1:A:379:GLN:O	1:A:379:GLN:CG	2.69	0.40
1:A:319:THR:O	1:A:323:LEU:HG	2.21	0.40
1:A:210:LEU:HD23	1:A:259:SER:O	2.21	0.40
1:A:45:ILE:H	1:A:45:ILE:HG13	1.69	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%)	26	59
1	B	454/505 (90%)	411 (90%)	41 (9%)	2 (0%)	39	71
All	All	907/1010 (90%)	826 (91%)	76 (8%)	5 (1%)	30	63

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%)	4	11
1	B	395/431 (92%)	346 (88%)	49 (12%)	6	15
All	All	789/862 (92%)	685 (87%)	104 (13%)	5	13

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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
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 ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	900[A]	1	35,46,46	2.90	16 (45%)	43,67,67	1.33	5 (11%)
2	BLA	A	900[B]	1	35,46,46	2.86	17 (48%)	43,67,67	1.54	7 (16%)
2	BLA	B	900[A]	1	35,46,46	2.89	17 (48%)	43,67,67	1.46	8 (18%)
2	BLA	B	900[B]	1	35,46,46	2.89	16 (45%)	43,67,67	1.25	5 (11%)

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

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900[B]	BLA	C4D-C3D	-4.04	1.38	1.45
2	A	900[B]	BLA	C4D-C3D	-3.71	1.39	1.45
2	B	900[B]	BLA	C1D-C2D	-3.57	1.37	1.45
2	A	900[A]	BLA	C4D-C3D	-3.49	1.39	1.45
2	A	900[B]	BLA	C1D-C2D	-3.47	1.38	1.45
2	A	900[A]	BLA	C1D-C2D	-3.42	1.38	1.45
2	B	900[A]	BLA	C4D-C3D	-3.36	1.39	1.45
2	B	900[A]	BLA	C1D-C2D	-3.32	1.38	1.45
2	A	900[B]	BLA	C1B-C2B	-3.29	1.38	1.45
2	B	900[B]	BLA	C1B-C2B	-3.26	1.38	1.45
2	B	900[B]	BLA	C1C-C2C	-3.15	1.38	1.47
2	A	900[A]	BLA	C1C-C2C	-3.15	1.38	1.47
2	A	900[B]	BLA	C1C-C2C	-3.13	1.38	1.47
2	B	900[A]	BLA	C1C-C2C	-3.07	1.38	1.47
2	A	900[B]	BLA	C3B-C4B	-2.86	1.38	1.47
2	B	900[B]	BLA	C3B-C4B	-2.83	1.38	1.47
2	A	900[A]	BLA	CAB-C3B	-2.82	1.39	1.47
2	B	900[B]	BLA	CAB-C3B	-2.77	1.39	1.47
2	A	900[B]	BLA	CAB-C3B	-2.77	1.39	1.47
2	B	900[A]	BLA	CAB-C3B	-2.77	1.39	1.47
2	A	900[A]	BLA	C3B-C4B	-2.73	1.39	1.47
2	B	900[A]	BLA	C3B-C4B	-2.72	1.39	1.47
2	B	900[A]	BLA	C1B-C2B	-2.70	1.40	1.45
2	A	900[A]	BLA	C1B-C2B	-2.60	1.40	1.45
2	A	900[B]	BLA	C4C-NC	-2.31	1.33	1.37
2	B	900[A]	BLA	C4C-NC	-2.27	1.33	1.37
2	A	900[A]	BLA	C1C-NC	-2.25	1.32	1.37
2	B	900[A]	BLA	C1C-NC	-2.22	1.32	1.37
2	A	900[B]	BLA	C1C-NC	-2.22	1.32	1.37
2	A	900[A]	BLA	C4C-NC	-2.19	1.34	1.37
2	B	900[A]	BLA	C4D-ND	-2.16	1.33	1.38
2	B	900[B]	BLA	C4C-NC	-2.15	1.34	1.37
2	A	900[A]	BLA	C4D-ND	-2.12	1.33	1.38
2	A	900[B]	BLA	C1B-NB	-2.11	1.34	1.37
2	B	900[B]	BLA	C4D-ND	-2.06	1.33	1.38
2	B	900[A]	BLA	C1B-NB	-2.06	1.34	1.37
2	B	900[B]	BLA	C1B-NB	-2.03	1.34	1.37
2	A	900[B]	BLA	C4D-ND	-2.01	1.34	1.38
2	A	900[B]	BLA	CAC-C3C	2.14	1.54	1.47
2	A	900[A]	BLA	CAC-C3C	2.29	1.54	1.47
2	B	900[A]	BLA	CAC-C3C	2.34	1.54	1.47
2	B	900[B]	BLA	CAC-C3C	2.36	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900[B]	BLA	C4A-CHB	2.84	1.51	1.40
2	B	900[B]	BLA	C4A-CHB	3.17	1.52	1.40
2	B	900[A]	BLA	C4A-CHB	3.32	1.52	1.40
2	A	900[A]	BLA	C4A-CHB	3.37	1.53	1.40
2	B	900[B]	BLA	CHA-C4D	4.40	1.39	1.35
2	B	900[A]	BLA	CHA-C4D	4.64	1.39	1.35
2	A	900[B]	BLA	CBC-CAC	4.69	1.53	1.30
2	B	900[B]	BLA	CBC-CAC	4.79	1.54	1.30
2	A	900[A]	BLA	CBC-CAC	4.79	1.54	1.30
2	B	900[A]	BLA	CBC-CAC	4.82	1.54	1.30
2	A	900[A]	BLA	CHA-C4D	4.86	1.39	1.35
2	A	900[A]	BLA	CHD-C1D	4.95	1.52	1.40
2	A	900[B]	BLA	CHA-C4D	5.06	1.39	1.35
2	B	900[A]	BLA	CHD-C1D	5.13	1.53	1.40
2	B	900[B]	BLA	CHD-C1D	5.17	1.53	1.40
2	A	900[B]	BLA	CHD-C1D	5.29	1.53	1.40
2	A	900[B]	BLA	CHD-C4C	6.44	1.53	1.37
2	A	900[A]	BLA	CHD-C4C	6.58	1.53	1.37
2	B	900[B]	BLA	CHD-C4C	6.59	1.53	1.37
2	B	900[A]	BLA	CHD-C4C	6.65	1.53	1.37
2	A	900[B]	BLA	CHB-C1B	7.63	1.51	1.34
2	B	900[B]	BLA	CHB-C1B	7.79	1.51	1.34
2	B	900[A]	BLA	CHB-C1B	8.15	1.52	1.34
2	A	900[A]	BLA	CHB-C1B	8.47	1.53	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900[B]	BLA	C4C-CHD-C1D	-4.83	115.57	128.06
2	B	900[A]	BLA	C4C-CHD-C1D	-3.21	119.75	128.06
2	A	900[A]	BLA	C4C-CHD-C1D	-3.01	120.28	128.06
2	A	900[B]	BLA	CBC-CAC-C3C	-2.85	112.56	127.01
2	B	900[B]	BLA	CHA-C4D-C3D	-2.53	119.62	125.55
2	A	900[B]	BLA	CHA-C4D-C3D	-2.46	119.78	125.55
2	B	900[A]	BLA	CBC-CAC-C3C	-2.43	114.68	127.01
2	A	900[B]	BLA	CHD-C4C-NC	-2.41	120.94	126.16
2	A	900[A]	BLA	CBC-CAC-C3C	-2.41	114.79	127.01
2	B	900[B]	BLA	CBC-CAC-C3C	-2.35	115.07	127.01
2	B	900[A]	BLA	CAA-C2A-C1A	-2.05	124.78	127.01
2	A	900[A]	BLA	C4D-ND-C1D	2.05	110.56	106.51
2	B	900[B]	BLA	CHA-C4D-ND	2.07	132.36	128.67
2	B	900[A]	BLA	C1D-C2D-C3D	2.09	109.00	106.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900[A]	BLA	CAD-C3D-C4D	2.09	128.79	125.06
2	A	900[B]	BLA	CHA-C4D-ND	2.10	132.43	128.67
2	B	900[B]	BLA	C4D-ND-C1D	2.12	110.70	106.51
2	B	900[A]	BLA	C4D-ND-C1D	2.15	110.77	106.51
2	A	900[B]	BLA	C4D-ND-C1D	2.25	110.95	106.51
2	B	900[A]	BLA	CAD-C3D-C4D	2.42	129.38	125.06
2	B	900[A]	BLA	CMB-C2B-C1B	2.44	127.45	124.20
2	B	900[B]	BLA	CBA-CAA-C2A	2.51	117.03	112.53
2	A	900[B]	BLA	CBA-CAA-C2A	2.80	117.54	112.53
2	A	900[A]	BLA	CMB-C2B-C1B	3.24	128.51	124.20
2	B	900[A]	BLA	CBA-CAA-C2A	3.35	118.53	112.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900[A]	BLA	C4A-CHB-C1B-NB
2	A	900[A]	BLA	C4A-CHB-C1B-NB

There are no ring outliers.

4 monomers are involved in 49 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	457/505 (90%)	-0.06	24 (5%)	30	24	63, 120, 219, 317	0
1	B	457/505 (90%)	-0.11	23 (5%)	32	26	62, 119, 230, 373	0
All	All	914/1010 (90%)	-0.08	47 (5%)	32	25	62, 119, 223, 373	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	ARG	9.6
1	A	452	PRO	8.2
1	A	431	GLU	8.2
1	A	433	HIS	7.0
1	B	360	GLY	6.6
1	B	381	LEU	6.3
1	B	361	GLY	6.3
1	A	363	THR	5.4
1	A	374	ALA	4.3
1	B	363	THR	4.3
1	A	406	GLY	3.8
1	A	430	GLU	3.8
1	B	372	ARG	3.7
1	B	356	LEU	3.7
1	B	378	LEU	3.7
1	B	336	PHE	3.6
1	A	371	GLU	3.4
1	A	258	ALA	3.3
1	B	383	ARG	3.2
1	B	364	LEU	3.2
1	B	367	ARG	3.2
1	B	425	PHE	3.1
1	A	358	MET	3.1
1	B	358	MET	3.1

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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	B	386	GLU	2.7
1	A	454	LEU	2.7
1	A	408	CYS	2.6
1	A	463	TRP	2.6
1	B	357	VAL	2.5
1	B	387	ARG	2.5
1	B	380	ARG	2.5
1	A	360	GLY	2.5
1	A	190[A]	TYR	2.4
1	A	425	PHE	2.4
1	A	407	ASP	2.4
1	A	429	HIS	2.4
1	A	470	HIS	2.3
1	A	357	VAL	2.3
1	B	389	ILE	2.2
1	B	431	GLU	2.2
1	A	11	ASN	2.2
1	B	365	SER	2.1
1	B	423	TRP	2.1
1	A	432	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BLA	B	900[B]	43/43	0.91	0.31	2.07	79,114,146,176	43
2	BLA	B	900[A]	43/43	0.91	0.31	2.05	85,123,149,164	43
2	BLA	A	900[B]	43/43	0.89	0.30	1.31	85,127,170,173	43
2	BLA	A	900[A]	43/43	0.89	0.30	1.27	92,130,170,177	43

## 6.5 Other polymers [i](#)

There are no such residues in this entry.