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Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID : 3IBR
Title : Crystal Structure of P. aeruginosa Bacteriophytochrome Photosensory Core Module Mutant Q188L in the Mixed Pr/Pfr State
Authors : Yang, X.; Kuk, J.; Moffat, K.
Deposited on : 2009-07-16
Resolution : 2.97 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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.
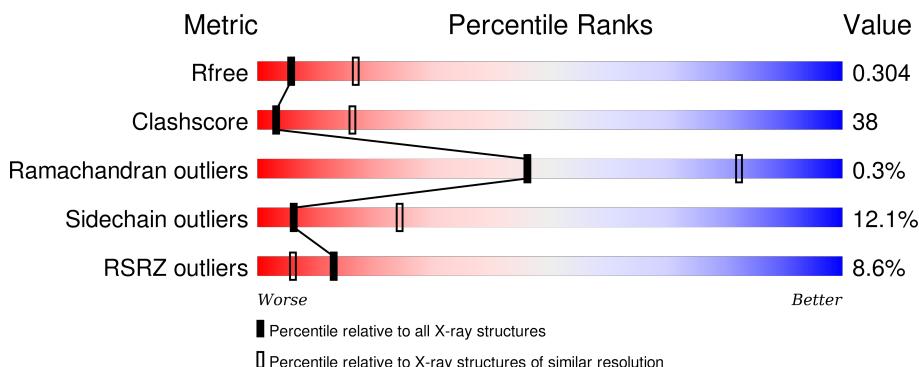
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 >=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 <=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	8% — 43% / 41% / 7% / 10%
1	B	505	8% — 39% / 45% / 6% / 10%
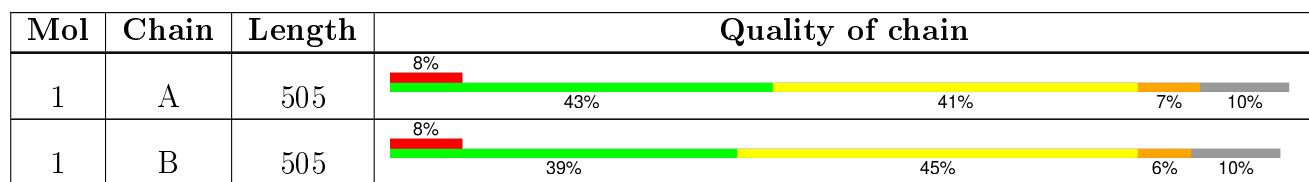
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7530 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	Se	0	6	0
			3666	2313	653	680	9	11			
1	B	457	Total	C	N	O	S	Se	0	9	0
			3690	2326	658	686	9	11			

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: $C_{33}H_{34}N_4O_6$).

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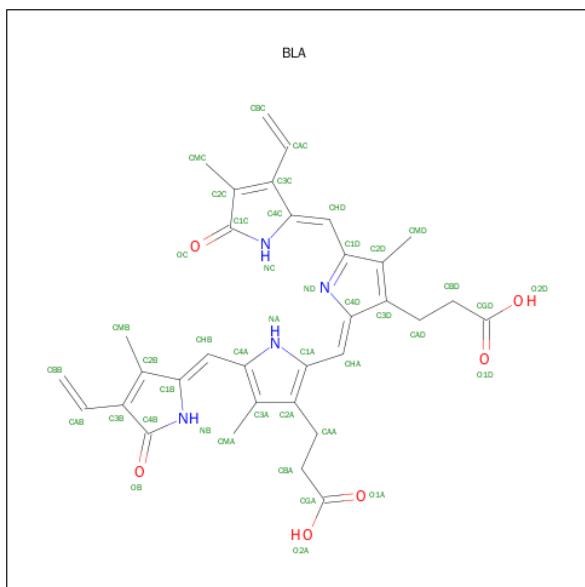
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			86	66	8	12		
2	B	1	Total	C	N	O	0	1
			86	66	8	12		

- 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
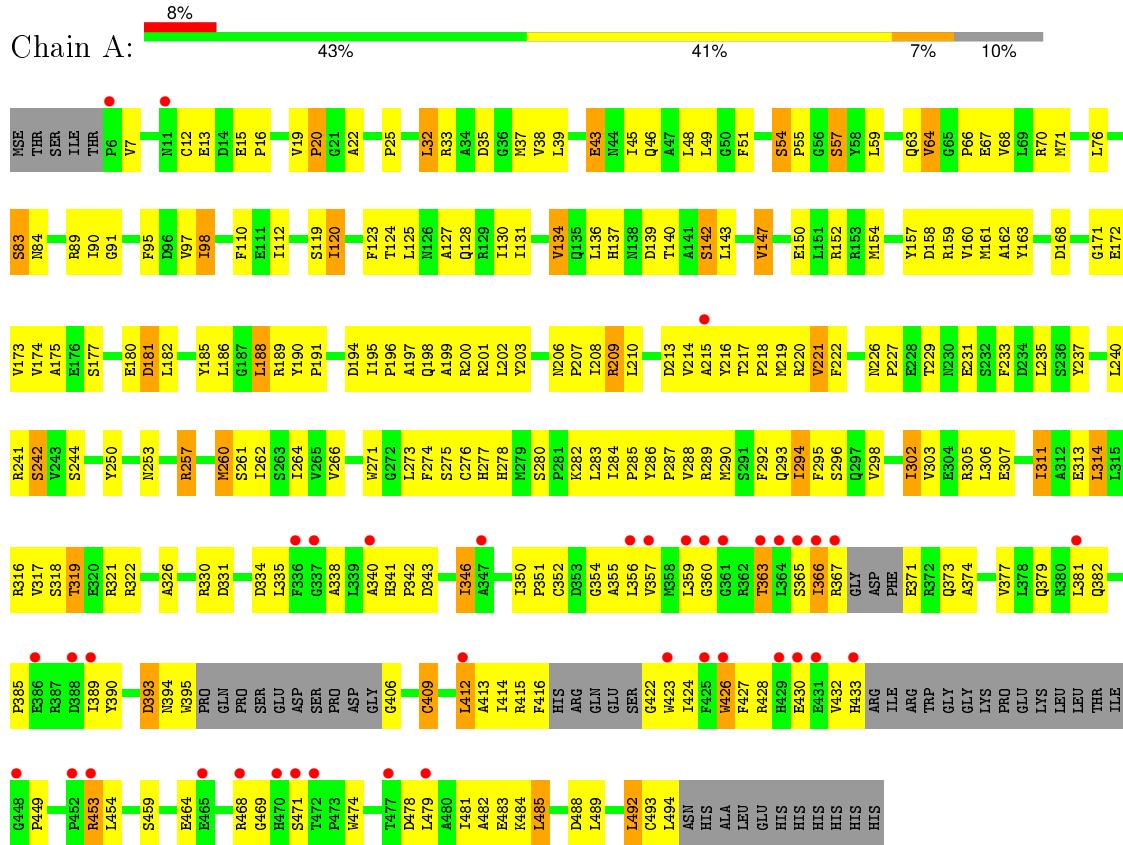
- Molecule 1: Bacteriophytochrome
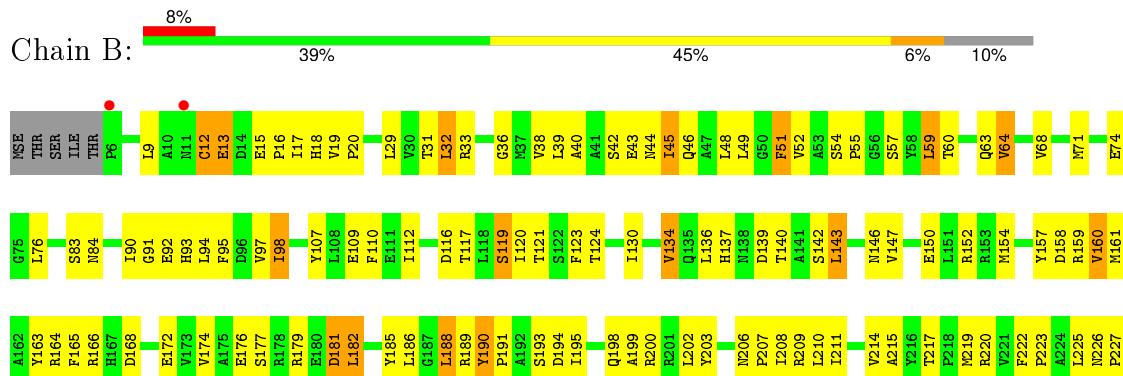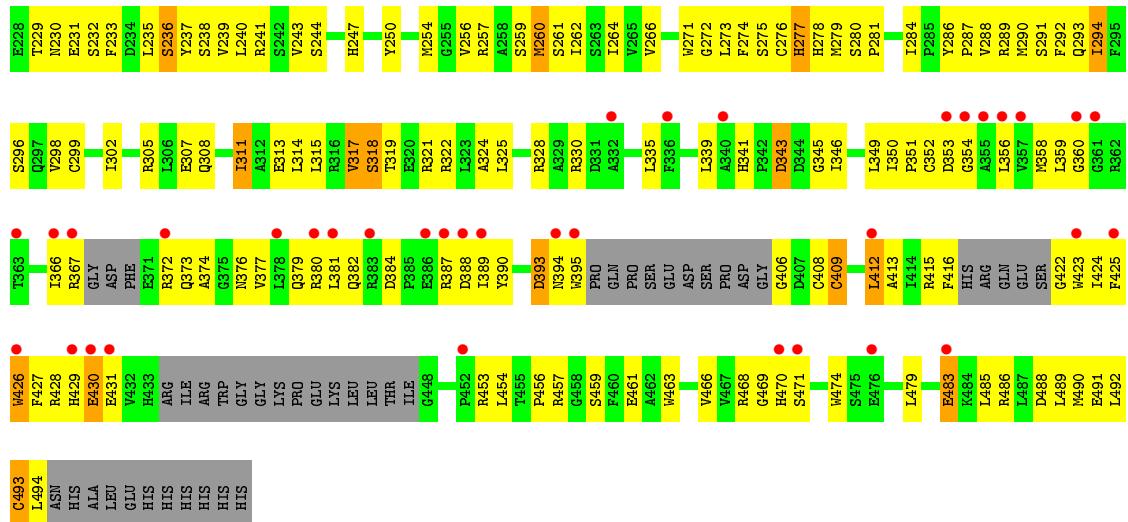
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	108.90Å 108.90Å 188.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.74 – 2.97 35.65 – 2.61	Depositor EDS
% Data completeness (in resolution range)	84.7 (37.74-2.97) 54.6 (35.65-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.04 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.233 , 0.307 0.235 , 0.304	Depositor DCC
R_{free} test set	1060 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	94.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.4	EDS
Estimated twinning fraction	0.430 for h,-h-k,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 20987 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7530	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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	0.37	0/3735	0.61	0/5050
1	B	0.36	0/3760	0.60	0/5084
All	All	0.36	0/7495	0.61	0/10134

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3666	0	3592	264	0
1	B	3690	0	3605	285	0
2	A	86	0	62	32	0
2	B	86	0	62	35	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
All	All	7530	0	7321	563	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 38.

All (563) 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:363:THR:HG21	1:A:371:GLU:HB2	1.27	1.16
1:A:194:ASP:HB3	2:A:900[A]:BLA:HHB	1.34	1.05
2:B:900[A]:BLA:HMC1	2:B:900[A]:BLA:HBC1	1.33	1.04
1:A:209[A]:ARG:HH11	1:A:209[A]:ARG:HG2	1.27	1.00
1:B:182:LEU:HD13	1:B:279:MSE:HE3	1.41	1.00
1:B:206:ASN:HB2	1:B:209[B]:ARG:CZ	1.92	0.99
1:B:229:THR:HG23	1:B:231:GLU:H	1.26	0.96
2:A:900[A]:BLA:HMC1	2:A:900[A]:BLA:HBC1	1.46	0.95
2:B:900[A]:BLA:HBD2	2:B:900[A]:BLA:HMD1	1.48	0.95
1:A:206:ASN:HB2	1:A:209[B]:ARG:HH22	1.32	0.94
1:B:206:ASN:HB2	1:B:209[B]:ARG:NH2	1.80	0.94
1:A:203[B]:TYR:HA	1:A:209[B]:ARG:NH1	1.83	0.94
1:A:188:LEU:HD13	1:A:190[B]:TYR:OH	1.67	0.94
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.35	0.90
1:A:90:ILE:HG22	1:A:91:GLY:H	1.35	0.90
1:B:33:ARG:HB3	1:B:39:LEU:HD11	1.51	0.90
2:A:900[A]:BLA:CMA	2:A:900[A]:BLA:HMB3	2.06	0.86
1:A:363:THR:HG21	1:A:371:GLU:CB	2.05	0.86
1:B:20:PRO:HD2	1:B:235:LEU:HD12	1.59	0.85
1:B:210:LEU:HD12	1:B:289:ARG:HD3	1.59	0.85
1:B:208:ILE:C	1:B:209[B]:ARG:HD3	1.97	0.84
1:A:194:ASP:HB3	2:A:900[A]:BLA:CHB	2.07	0.84
1:A:25:PRO:HB3	1:A:219:MSE:HE2	1.59	0.83
1:B:194[A]:ASP:HB3	2:B:900[A]:BLA:HHB	1.61	0.82
1:B:134:VAL:HA	1:B:143:LEU:HD21	1.62	0.81
1:A:209[B]:ARG:HG2	1:A:261:SER:HB2	1.62	0.81
1:B:188:LEU:HD22	1:B:190[B]:TYR:CE2	2.15	0.80
1:B:416:PHE:HE1	1:B:424:ILE:HG13	1.45	0.80
1:B:209[B]:ARG:HD3	1:B:209[B]:ARG:N	1.97	0.80
1:B:95:PHE:CE2	1:B:112:ILE:HD13	2.18	0.79
1:A:203[B]:TYR:CD1	1:A:209[B]:ARG:HD3	2.18	0.78
1:A:199:ALA:HB1	1:A:203[B]:TYR:CE2	2.19	0.78
1:A:206:ASN:HB2	1:A:209[B]:ARG:NH2	1.99	0.77
1:A:203[B]:TYR:CZ	2:A:900[B]:BLA:HAA1	2.19	0.77
1:B:161:MSE:HE1	2:B:900[B]:BLA:HBB1	1.66	0.77
1:A:335:LEU:HD13	1:A:492:LEU:HD23	1.65	0.77
1:B:266:VAL:HG22	1:B:271:TRP:HB2	1.65	0.77
1:A:123:PHE:HE2	1:B:123:PHE:CE2	2.02	0.77
1:B:185:TYR:HD1	1:B:188:LEU:HD12	1.49	0.77
1:A:416:PHE:HE1	1:A:424:ILE:HG13	1.48	0.77
2:A:900[A]:BLA:HMA2	2:A:900[A]:BLA:HMB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HD12	1:B:46:GLN:H	1.50	0.76
1:B:163[B]:TYR:OH	1:B:190[B]:TYR:CD2	2.39	0.76
1:A:220:ARG:HE	1:A:222:PHE:HZ	1.33	0.76
1:B:415:ARG:HD3	1:B:423:TRP:CZ2	2.20	0.76
1:B:29:LEU:HD13	1:B:109:GLU:HG2	1.67	0.76
1:A:194:ASP:CB	2:A:900[A]:BLA:HHB	2.15	0.76
1:B:64:VAL:HG13	1:B:68:VAL:HB	1.67	0.75
1:A:493:CYS:O	1:A:494:LEU:HB2	1.86	0.75
2:A:900[A]:BLA:HMD1	2:A:900[A]:BLA:HBD2	1.67	0.75
1:B:203[B]:TYR:OH	2:B:900[B]:BLA:HAA1	1.86	0.75
1:B:19:VAL:CG2	1:B:232:SER:HB3	2.17	0.74
1:A:90:ILE:HG22	1:A:91:GLY:N	2.02	0.74
1:A:95:PHE:CE2	1:A:112:ILE:HD13	2.22	0.74
1:B:206:ASN:HD21	1:B:237:TYR:H	1.32	0.74
1:B:493:CYS:O	1:B:494:LEU:HB2	1.85	0.74
1:A:188:LEU:HD23	1:A:189:ARG:H	1.51	0.74
1:A:302:ILE:HG23	1:B:305:ARG:HH12	1.52	0.74
1:A:415:ARG:HD3	1:A:423:TRP:CZ2	2.23	0.73
1:A:123:PHE:CE2	1:B:123:PHE:CE2	2.76	0.73
1:A:191:PRO:HD2	1:A:453:ARG:HH22	1.53	0.73
1:A:123:PHE:HE2	1:B:123:PHE:HE2	1.36	0.73
1:B:140:THR:HG23	1:B:164:ARG:NH2	2.03	0.73
1:A:190[B]:TYR:CD1	2:A:900[B]:BLA:HMB1	2.23	0.72
1:A:314:LEU:N	1:A:314:LEU:HD23	2.04	0.72
1:B:415:ARG:HB2	1:B:423:TRP:CH2	2.24	0.72
1:B:19:VAL:HG21	1:B:232:SER:HB3	1.71	0.72
1:B:194[A]:ASP:HB3	2:B:900[A]:BLA:CHB	2.19	0.72
1:A:203[B]:TYR:OH	2:A:900[B]:BLA:HHA	1.89	0.72
1:B:488:ASP:O	1:B:491:GLU:HB3	1.90	0.72
1:A:90:ILE:CG2	1:A:91:GLY:H	2.03	0.72
1:A:414:ILE:CG1	1:A:424:ILE:HB	2.20	0.71
1:A:98:ILE:HG21	1:A:286:TYR:CD1	2.25	0.71
1:B:90:ILE:HG22	1:B:91:GLY:H	1.54	0.71
1:A:257:ARG:NH1	1:A:257:ARG:HG2	1.97	0.71
1:A:359:LEU:HD13	1:A:422:GLY:HA3	1.73	0.71
1:B:390:TYR:HB3	1:B:413:ALA:HB3	1.73	0.71
1:B:376:ASN:O	1:B:379:GLN:HB3	1.90	0.71
1:B:430:GLU:HG2	1:B:471:SER:CA	2.21	0.70
1:A:390:TYR:HB3	1:A:413:ALA:HB3	1.74	0.70
1:B:19:VAL:N	1:B:20:PRO:HD3	2.07	0.70
1:B:209[A]:ARG:NH1	1:B:241:ARG:NH1	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203[B]:TYR:OH	2:A:900[B]:BLA:HAA1	1.91	0.70
1:A:190[B]:TYR:CD2	1:A:190[B]:TYR:N	2.60	0.69
1:A:209[A]:ARG:HH11	1:A:209[A]:ARG:CG	2.04	0.69
1:A:190[B]:TYR:CE1	2:A:900[B]:BLA:HAB	2.28	0.69
2:B:900[B]:BLA:HMA1	2:B:900[B]:BLA:NB	2.07	0.69
1:B:341:HIS:O	1:B:345:GLY:N	2.26	0.69
1:B:150:GLU:O	1:B:154:MSE:HG3	1.93	0.68
1:B:188:LEU:HD11	1:B:190[B]:TYR:OH	1.93	0.68
1:A:33:ARG:HB3	1:A:39:LEU:HD11	1.75	0.68
1:A:43:GLU:HG2	1:A:220:ARG:O	1.94	0.68
1:A:98:ILE:HG21	1:A:286:TYR:CE1	2.29	0.68
1:A:64:VAL:HG13	1:A:68:VAL:HB	1.75	0.67
1:A:346:ILE:HG23	1:A:426:TRP:CZ3	2.29	0.67
1:A:124:THR:O	1:A:128:GLN:HG3	1.92	0.67
1:A:379:GLN:HA	1:A:382:GLN:CG	2.24	0.67
1:B:211:ILE:HB	1:B:259:SER:HB3	1.75	0.67
1:A:294:ILE:O	1:A:298:VAL:HG23	1.94	0.67
1:A:363:THR:CG2	1:A:371:GLU:HB2	2.17	0.67
1:A:209[A]:ARG:HG2	1:A:209[A]:ARG:NH1	2.06	0.67
1:B:209[B]:ARG:N	1:B:209[B]:ARG:CD	2.57	0.66
1:A:350:ILE:HG23	1:A:351:PRO:HD2	1.77	0.66
1:B:430:GLU:HG2	1:B:471:SER:HA	1.76	0.66
1:B:59:LEU:H	1:B:59:LEU:HD22	1.60	0.66
1:A:139:ASP:HB3	1:A:142:SER:OG	1.95	0.66
1:A:45:ILE:HB	1:A:51:PHE:CE1	2.30	0.66
1:B:190[B]:TYR:CE1	2:B:900[B]:BLA:HMB1	2.31	0.66
1:B:335:LEU:HD13	1:B:492:LEU:HD23	1.76	0.66
1:B:136:LEU:HB2	1:B:137:HIS:CE1	2.30	0.66
1:A:22:ALA:O	1:A:242:SER:HB3	1.96	0.65
1:A:379:GLN:HA	1:A:382:GLN:HG2	1.79	0.65
1:B:43:GLU:HG3	1:B:219:MSE:HG3	1.77	0.65
1:B:209[A]:ARG:O	1:B:260:MSE:HA	1.97	0.65
1:A:159:ARG:CZ	1:A:185:TYR:HE2	2.09	0.65
1:A:294:ILE:HD11	1:B:294:ILE:CD1	2.26	0.65
1:B:9:LEU:HD11	1:B:454:LEU:HD21	1.78	0.65
1:A:157:TYR:CZ	1:A:260:MSE:HB2	2.31	0.65
1:B:134:VAL:HG13	1:B:302:ILE:HG21	1.79	0.65
1:B:32:LEU:HD12	1:B:32:LEU:N	2.11	0.64
1:A:33:ARG:HB3	1:A:39:LEU:CD1	2.26	0.64
1:A:216:TYR:CE2	1:A:218:PRO:HG3	2.32	0.64
1:A:209[B]:ARG:CG	1:A:261:SER:HB2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:HIS:C	1:B:20:PRO:HD3	2.18	0.64
1:B:68:VAL:O	1:B:71:MSE:HB3	1.98	0.64
1:B:359:LEU:HD13	1:B:422:GLY:CA	2.27	0.64
2:A:900[B]:BLA:NB	2:A:900[B]:BLA:HMA1	2.12	0.64
1:A:191:PRO:CD	1:A:453:ARG:HH22	2.09	0.64
1:A:314:LEU:H	1:A:314:LEU:HD23	1.61	0.64
1:A:152:ARG:HB2	1:A:160:VAL:HG11	1.78	0.64
1:A:359:LEU:HD22	1:A:416:PHE:HE2	1.62	0.64
1:B:202:LEU:O	1:B:209[B]:ARG:NH2	2.30	0.64
1:B:359:LEU:HD22	1:B:416:PHE:HE2	1.60	0.64
1:B:493:CYS:O	1:B:494:LEU:CB	2.46	0.64
1:B:140:THR:HG23	1:B:164:ARG:HH22	1.63	0.63
1:B:90:ILE:CG2	1:B:91:GLY:H	2.11	0.63
1:B:479:LEU:O	1:B:483:GLU:HB2	1.99	0.63
1:A:83:SER:O	1:A:84:ASN:HB2	1.98	0.63
1:A:359:LEU:HD13	1:A:422:GLY:CA	2.28	0.63
1:B:319:THR:HG22	1:B:322:ARG:HH21	1.63	0.63
1:A:199:ALA:HB1	1:A:203[B]:TYR:HE2	1.58	0.63
1:B:377:VAL:HG22	1:B:395:TRP:CH2	2.33	0.63
1:B:190[B]:TYR:CZ	2:B:900[B]:BLA:HAB	2.34	0.63
1:A:283:LEU:C	1:A:283:LEU:HD23	2.19	0.63
1:A:335:LEU:CD1	1:A:492:LEU:HD23	2.27	0.63
1:B:163[B]:TYR:OH	1:B:190[B]:TYR:HD2	1.81	0.62
1:B:172:GLU:HG2	1:B:174:VAL:HG12	1.81	0.62
1:A:49:LEU:HD21	1:A:95:PHE:CE1	2.35	0.62
1:B:90:ILE:HG22	1:B:91:GLY:N	2.13	0.62
1:B:235:LEU:O	1:B:241:ARG:HD3	1.99	0.62
1:A:416:PHE:CE1	1:A:424:ILE:HG13	2.33	0.62
1:A:389:ILE:HD11	1:A:483:GLU:OE2	1.99	0.62
1:A:354:GLY:HA2	1:A:367:ARG:HB2	1.82	0.61
2:B:900[B]:BLA:HMA1	2:B:900[B]:BLA:HB	1.65	0.61
1:B:307:GLU:O	1:B:311:ILE:HG23	2.00	0.61
2:B:900[B]:BLA:CGA	2:B:900[B]:BLA:HMA2	2.31	0.61
1:B:209[B]:ARG:O	1:B:260:MSE:HA	2.00	0.61
1:A:203[B]:TYR:HA	1:A:209[B]:ARG:HH12	1.60	0.61
1:B:208:ILE:C	1:B:209[B]:ARG:CD	2.67	0.61
1:B:339:LEU:O	1:B:346:ILE:HG23	2.00	0.61
1:A:453:ARG:HH21	1:A:459:SER:CB	2.13	0.61
1:B:32:LEU:HD23	1:B:36:GLY:O	2.01	0.61
1:B:165:PHE:CD1	1:B:272:GLY:HA2	2.36	0.61
1:B:235:LEU:O	1:B:238:SER:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HD22	1:B:305:ARG:NH1	2.16	0.60
1:A:206:ASN:CB	1:A:209[B]:ARG:NH2	2.64	0.60
1:B:12[A]:CYS:SG	1:B:13:GLU:N	2.73	0.60
1:A:414:ILE:HG12	1:A:424:ILE:HB	1.82	0.60
1:A:359:LEU:HD12	1:A:360:GLY:H	1.66	0.60
1:A:294:ILE:HD11	1:B:294:ILE:HD11	1.82	0.60
1:A:203[B]:TYR:HD1	1:A:209[B]:ARG:HD3	1.64	0.60
1:B:202:LEU:C	1:B:209[B]:ARG:NH2	2.54	0.60
1:B:38:VAL:O	1:B:55:PRO:HA	2.01	0.60
1:A:319:THR:HG22	1:A:322:ARG:HH21	1.65	0.60
2:A:900[B]:BLA:HB	2:A:900[B]:BLA:HMA1	1.66	0.60
2:B:900[B]:BLA:OB	2:B:900[B]:BLA:HBB1	2.00	0.60
1:A:366:ILE:HG13	1:A:367:ARG:HG3	1.83	0.60
1:B:394:ASN:CB	1:B:469:GLY:O	2.49	0.60
1:B:48:LEU:HB3	1:B:49:LEU:HG	1.83	0.59
1:B:257:ARG:HD2	1:B:281:PRO:HD3	1.83	0.59
1:B:318:SER:O	1:B:321:ARG:HB2	2.02	0.59
1:B:203[B]:TYR:OH	2:B:900[B]:BLA:HHA	2.02	0.59
1:B:408:CYS:SG	1:B:429:HIS:HB3	2.43	0.59
2:A:900[A]:BLA:CBC	2:A:900[A]:BLA:HMC1	2.28	0.59
1:A:206:ASN:HD21	1:A:237:TYR:HA	1.68	0.59
1:B:239:VAL:HG11	1:B:289:ARG:NH2	2.18	0.59
1:B:163[A]:TYR:OH	1:B:275:SER:HB3	2.01	0.59
1:B:134:VAL:HA	1:B:143:LEU:CD2	2.30	0.59
1:A:307:GLU:O	1:A:311:ILE:HG23	2.02	0.59
1:B:395:TRP:HB3	1:B:409:CYS:HA	1.85	0.58
1:B:457:ARG:O	1:B:461:GLU:HG3	2.02	0.58
1:A:49:LEU:HB2	1:A:51:PHE:CE2	2.38	0.58
1:A:33:ARG:HG3	1:A:35:ASP:OD1	2.02	0.58
1:A:426:TRP:CD1	1:A:426:TRP:N	2.71	0.58
1:A:253:ASN:ND2	1:A:449:PRO:HB3	2.17	0.58
1:A:371:GLU:O	1:A:374:ALA:HB3	2.03	0.58
2:B:900[A]:BLA:HMB3	2:B:900[A]:BLA:CMA	2.33	0.58
1:A:157:TYR:OH	1:A:260:MSE:HB2	2.02	0.58
2:B:900[A]:BLA:HMC1	2:B:900[A]:BLA:CBC	2.22	0.58
1:B:346:ILE:O	1:B:426:TRP:HZ3	1.87	0.58
1:B:379:GLN:HA	1:B:382:GLN:HG2	1.85	0.58
1:B:159:ARG:NH1	1:B:185:TYR:HE2	2.01	0.58
1:A:479:LEU:O	1:A:483:GLU:HB2	2.04	0.58
1:B:313:GLU:O	1:B:317:VAL:HG13	2.04	0.58
1:A:197:ALA:O	1:A:201:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:MSE:HE1	1:B:97:VAL:HG12	1.85	0.57
1:B:290:MSE:HE1	1:B:293:GLN:OE1	2.03	0.57
1:B:209[A]:ARG:NH1	1:B:241:ARG:HH12	2.01	0.57
1:A:159:ARG:HD2	1:A:161:MSE:HE2	1.85	0.57
1:B:247[B]:HIS:CE1	2:B:900[B]:BLA:C1A	2.88	0.57
1:B:314:LEU:N	1:B:314:LEU:HD23	2.19	0.57
1:B:210:LEU:HD23	1:B:211:ILE:N	2.20	0.57
1:A:181:ASP:N	1:A:181:ASP:OD1	2.38	0.57
1:A:214:VAL:HG23	1:A:257:ARG:C	2.25	0.56
1:B:98:ILE:O	1:B:98:ILE:HG12	2.04	0.56
1:B:209[A]:ARG:HH12	1:B:241:ARG:HH12	1.52	0.56
1:A:43:GLU:HG3	1:A:219:MSE:HG3	1.87	0.56
1:B:286:TYR:HB3	1:B:287:PRO:HD3	1.86	0.56
1:A:203[B]:TYR:OH	2:A:900[B]:BLA:HAD2	2.06	0.56
1:B:359:LEU:HD13	1:B:422:GLY:HA3	1.87	0.56
1:A:366:ILE:HG13	1:A:367:ARG:N	2.21	0.56
1:A:190[B]:TYR:CE1	2:A:900[B]:BLA:HMB1	2.40	0.56
1:B:181:ASP:N	1:B:181:ASP:OD1	2.38	0.56
1:B:209[A]:ARG:HG2	1:B:209[A]:ARG:HH11	1.70	0.56
1:B:260:MSE:CE	1:B:289:ARG:HG2	2.36	0.56
1:A:282:LYS:HE3	1:A:284:ILE:HD11	1.88	0.56
1:B:158:ASP:OD1	1:B:278:HIS:HA	2.06	0.56
1:A:20:PRO:HD2	1:A:235:LEU:HD12	1.86	0.56
1:A:159:ARG:NH2	1:A:185:TYR:HE2	2.03	0.56
1:A:19:VAL:HG23	1:A:19:VAL:O	2.06	0.56
1:B:260:MSE:HE3	1:B:284:ILE:HB	1.87	0.56
1:B:206:ASN:CB	1:B:209[B]:ARG:CZ	2.77	0.55
1:B:179:ARG:O	1:B:182:LEU:HG	2.07	0.55
1:B:389:ILE:HD11	1:B:483:GLU:OE2	2.05	0.55
1:B:189:ARG:HD3	1:B:463:TRP:CZ2	2.42	0.55
1:B:29:LEU:HD11	1:B:107:TYR:HB3	1.88	0.55
1:A:226:ASN:HB2	1:A:233:PHE:CZ	2.41	0.55
1:A:190[B]:TYR:CZ	2:A:900[B]:BLA:HAB	2.40	0.55
1:B:393:ASP:HB2	1:B:394:ASN:OD1	2.06	0.55
1:B:193:SER:O	2:B:900[B]:BLA:HBC1	2.07	0.55
1:B:33:ARG:CB	1:B:39:LEU:HD11	2.32	0.55
1:B:261[A]:SER:HB2	1:B:273:LEU:HD13	1.89	0.55
1:B:394:ASN:HB3	1:B:469:GLY:O	2.06	0.55
1:A:359:LEU:HD12	1:A:360:GLY:N	2.23	0.54
1:A:124:THR:HG21	1:B:290:MSE:HE3	1.87	0.54
1:A:373:GLN:NE2	1:A:406:GLY:HA3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLU:HG2	1:A:471:SER:HA	1.89	0.54
1:A:341:HIS:C	1:A:343:ASP:H	2.11	0.54
1:A:235:LEU:O	1:A:241:ARG:HD3	2.06	0.54
1:B:430:GLU:OE1	1:B:468:ARG:O	2.24	0.54
1:B:42:SER:O	1:B:45:ILE:HG13	2.07	0.54
1:A:49:LEU:HD21	1:A:95:PHE:CZ	2.42	0.54
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.15	0.53
1:A:393:ASP:HA	1:A:409:CYS:O	2.08	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:CH2	2.42	0.53
2:B:900[A]:BLA:HMB3	2:B:900[A]:BLA:C3A	2.38	0.53
1:A:45:ILE:HD12	1:A:46:GLN:N	2.24	0.53
1:A:66:PRO:HD2	1:A:67:GLU:HG3	1.90	0.53
1:B:415:ARG:HB2	1:B:423:TRP:CZ2	2.44	0.53
1:A:54:SER:O	1:A:57:SER:HB3	2.09	0.53
1:A:464:GLU:O	1:A:468:ARG:HG3	2.09	0.53
1:B:203[B]:TYR:CZ	2:B:900[B]:BLA:HAA1	2.44	0.53
1:A:38:VAL:O	1:A:55:PRO:HA	2.09	0.53
1:B:225:LEU:HD21	1:B:230:ASN:HA	1.90	0.52
1:B:152:ARG:HB2	1:B:160:VAL:HG11	1.91	0.52
1:B:188:LEU:HD13	1:B:190[B]:TYR:CE2	2.44	0.52
1:A:393:ASP:O	1:A:394:ASN:CG	2.48	0.52
1:A:250[B]:TYR:CD1	2:A:900[B]:BLA:OC	2.63	0.52
1:B:266:VAL:HG21	1:B:271:TRP:CD1	2.44	0.52
1:B:90:ILE:CG2	1:B:91:GLY:N	2.72	0.52
1:B:188:LEU:CD1	1:B:190[B]:TYR:OH	2.56	0.52
1:B:415:ARG:HB2	1:B:423:TRP:CZ3	2.44	0.52
1:B:214:VAL:HG23	1:B:257:ARG:O	2.10	0.52
1:B:244:SER:HB3	2:B:900[A]:BLA:HMD2	1.91	0.52
1:A:287:PRO:HB3	1:B:120:ILE:HD13	1.91	0.52
1:A:159:ARG:NH2	1:A:185:TYR:CE2	2.78	0.52
1:B:190[B]:TYR:CD1	2:B:900[B]:BLA:HMB1	2.45	0.52
1:A:390:TYR:O	1:A:412:LEU:HD23	2.09	0.51
1:B:381:LEU:HD11	1:B:390:TYR:HB2	1.92	0.51
1:B:321:ARG:HB3	1:B:349:LEU:CD2	2.41	0.51
1:A:206:ASN:O	1:A:209[B]:ARG:NH1	2.43	0.51
1:B:19:VAL:HG23	1:B:233:PHE:O	2.10	0.51
1:B:359:LEU:HD12	1:B:360:GLY:H	1.75	0.51
1:B:19:VAL:HG22	1:B:232:SER:HB3	1.91	0.51
1:A:306:LEU:HD22	1:B:305:ARG:HH12	1.74	0.51
1:A:350:ILE:HD13	1:A:478:ASP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG23	1:B:257:ARG:C	2.31	0.51
2:A:900[B]:BLA:HB	2:A:900[B]:BLA:CMA	2.23	0.51
1:B:359:LEU:HD22	1:B:416:PHE:CE2	2.43	0.51
1:A:49:LEU:HD22	1:A:90:ILE:HG21	1.93	0.51
1:B:394:ASN:CG	1:B:469:GLY:O	2.49	0.51
1:A:190[B]:TYR:N	1:A:190[B]:TYR:HD2	2.05	0.51
1:B:209[A]:ARG:NH1	2:B:900[A]:BLA:O1D	2.43	0.51
1:B:453:ARG:O	1:B:453:ARG:HG2	2.04	0.51
1:A:203[B]:TYR:CE1	1:A:209[B]:ARG:HD3	2.46	0.51
2:A:900[A]:BLA:HMB3	2:A:900[A]:BLA:C3A	2.41	0.51
2:B:900[B]:BLA:HB	2:B:900[B]:BLA:CMA	2.24	0.51
1:A:306:LEU:HD13	1:B:305:ARG:NH1	2.26	0.51
1:B:165:PHE:CE1	1:B:272:GLY:HA2	2.46	0.51
1:A:136:LEU:HB2	1:A:137:HIS:CE1	2.46	0.51
1:B:188:LEU:HD13	1:B:190[B]:TYR:HE2	1.75	0.50
1:A:319:THR:HG22	1:A:322:ARG:NH2	2.26	0.50
1:A:226:ASN:HB2	1:A:233:PHE:CE1	2.46	0.50
1:A:394:ASN:O	1:A:395:TRP:C	2.50	0.50
1:B:161:MSE:HE3	1:B:163[A]:TYR:OH	2.12	0.50
1:B:188:LEU:CD2	1:B:190[B]:TYR:CE2	2.93	0.50
1:A:203[B]:TYR:HA	1:A:209[B]:ARG:HH11	1.71	0.50
1:B:203[B]:TYR:OH	2:B:900[B]:BLA:HAD2	2.11	0.50
1:A:264:ILE:HD11	1:A:274:PHE:CE1	2.47	0.50
1:B:262:ILE:CG2	1:B:296:SER:HB2	2.42	0.50
1:A:350:ILE:HD11	1:A:481:ILE:HB	1.94	0.50
1:A:159:ARG:HB3	1:A:277:HIS:HB2	1.93	0.50
1:B:31:THR:C	1:B:32:LEU:HD12	2.32	0.50
1:A:423:TRP:O	1:A:424:ILE:HG13	2.11	0.49
1:B:166:ARG:HB2	1:B:168:ASP:OD1	2.11	0.49
2:A:900[A]:BLA:CMC	2:A:900[A]:BLA:HBC1	2.30	0.49
1:B:19:VAL:HG13	1:B:19:VAL:O	2.12	0.49
1:A:120:ILE:N	1:A:120:ILE:HD13	2.27	0.49
1:A:97:VAL:HG22	1:A:110:PHE:CD2	2.47	0.49
1:A:214:VAL:HG23	1:A:257:ARG:O	2.12	0.49
1:B:412:LEU:HB3	1:B:426:TRP:HD1	1.77	0.49
1:A:326:ALA:O	1:A:330:ARG:HB3	2.12	0.49
1:B:159:ARG:CZ	1:B:185:TYR:CE2	2.96	0.49
1:B:40:ALA:HB2	1:B:223:PRO:HD2	1.95	0.49
1:A:32:LEU:N	1:A:32:LEU:HD12	2.28	0.49
1:B:428:ARG:HG3	1:B:474:TRP:CH2	2.48	0.49
1:B:64:VAL:HG13	1:B:68:VAL:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:N	1:A:284:ILE:HD12	2.28	0.49
1:B:373:GLN:HG2	1:B:406:GLY:HA3	1.94	0.49
1:A:381:LEU:HD21	1:A:390:TYR:CD1	2.47	0.49
2:A:900[B]:BLA:NC	2:A:900[B]:BLA:ND	2.61	0.48
1:B:430:GLU:HG2	1:B:471:SER:HB3	1.95	0.48
1:B:373:GLN:CG	1:B:406:GLY:HA3	2.42	0.48
1:A:150:GLU:HA	1:A:150:GLU:OE2	2.13	0.48
1:B:353:ASP:O	1:B:367:ARG:HB3	2.13	0.48
1:A:286:TYR:HB3	1:A:287:PRO:HD3	1.94	0.48
1:A:163[A]:TYR:CD2	1:A:173:VAL:HG22	2.48	0.48
1:B:207:PRO:HG2	1:B:293:GLN:HG3	1.95	0.48
1:B:239:VAL:HG11	1:B:289:ARG:HH21	1.77	0.48
1:B:43:GLU:HG2	1:B:220:ARG:O	2.12	0.48
1:A:209[A]:ARG:NH1	1:A:209[A]:ARG:CG	2.67	0.48
1:B:261[B]:SER:HB2	1:B:273:LEU:HD13	1.96	0.48
1:B:211:ILE:HB	1:B:259:SER:CB	2.44	0.48
1:A:45:ILE:HD12	1:A:46:GLN:H	1.79	0.48
1:A:355:ALA:O	1:A:366:ILE:HG23	2.13	0.48
1:A:430:GLU:HG2	1:A:471:SER:CA	2.44	0.48
1:A:306:LEU:HD13	1:B:305:ARG:HH11	1.78	0.48
1:A:15:GLU:O	1:A:198:GLN:OE1	2.31	0.48
1:B:202:LEU:HD21	1:B:236:SER:HB3	1.94	0.48
1:B:254:MSE:HE1	1:B:277:HIS:CD2	2.48	0.48
1:B:264:ILE:HB	1:B:272:GLY:O	2.13	0.48
1:A:152:ARG:HB2	1:A:160:VAL:CG1	2.44	0.47
1:A:71:MSE:HE1	1:A:97:VAL:HG12	1.96	0.47
1:A:158:ASP:HB2	1:A:278:HIS:HA	1.96	0.47
1:B:430:GLU:HG2	1:B:471:SER:CB	2.45	0.47
1:A:395:TRP:HB3	1:A:409:CYS:HA	1.97	0.47
1:B:352:CYS:HB2	1:B:427:PHE:O	2.13	0.47
1:A:338:ALA:C	1:A:340:ALA:H	2.17	0.47
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.71	0.47
1:B:157:TYR:CG	1:B:276:CYS:HB3	2.49	0.47
1:A:330:ARG:HG2	1:A:331:ASP:OD1	2.14	0.47
1:B:152:ARG:HD2	1:B:160:VAL:HG12	1.96	0.47
1:A:12[A]:CYS:HB2	2:A:900[A]:BLA:HAC	1.80	0.47
1:B:45:ILE:HG22	1:B:49:LEU:HD12	1.97	0.47
1:B:51:PHE:HD2	1:B:52:VAL:H	1.62	0.47
1:B:116:ASP:CG	1:B:117:THR:N	2.68	0.47
1:A:209[A]:ARG:CZ	1:A:241:ARG:NH1	2.78	0.47
1:A:163[B]:TYR:OH	1:A:190[B]:TYR:CD2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ASN:HB2	1:B:233:PHE:CZ	2.50	0.47
1:A:16:PRO:HA	1:A:198:GLN:OE1	2.15	0.47
1:A:484:LYS:O	1:A:488:ASP:OD2	2.33	0.47
2:B:900[A]:BLA:C2B	2:B:900[A]:BLA:HMA1	2.45	0.47
1:A:48:LEU:C	1:A:49:LEU:HG	2.33	0.47
1:A:350:ILE:CG2	1:A:351:PRO:HD2	2.44	0.47
1:A:160:VAL:CG1	1:A:177:SER:HB3	2.45	0.47
1:A:152:ARG:HD2	1:A:177:SER:O	2.15	0.47
1:A:198:GLN:O	1:A:202:LEU:HB2	2.15	0.47
1:B:388:ASP:HA	1:B:415:ARG:HB3	1.96	0.47
1:B:59:LEU:HD22	1:B:59:LEU:N	2.28	0.47
1:A:341:HIS:O	1:A:343:ASP:N	2.47	0.47
1:A:194:ASP:OD2	2:A:900[A]:BLA:NB	2.39	0.46
1:A:213:ASP:O	1:A:216:TYR:HB3	2.14	0.46
1:A:70:ARG:HH12	1:B:116:ASP:CG	2.18	0.46
1:B:159:ARG:CZ	1:B:185:TYR:HE2	2.28	0.46
1:B:226:ASN:HB3	1:B:229:THR:HG22	1.97	0.46
1:A:33:ARG:NH1	1:A:37:MSE:SE	2.98	0.46
1:A:294:ILE:CG2	1:B:124:THR:HG23	2.46	0.46
1:B:189:ARG:CD	1:B:463:TRP:CH2	2.98	0.46
1:B:71:MSE:O	1:B:74:GLU:HG2	2.16	0.46
1:B:394:ASN:O	1:B:409:CYS:HB3	2.16	0.46
1:A:395:TRP:CB	1:A:409:CYS:HA	2.45	0.46
1:B:354:GLY:HA2	1:B:367:ARG:HB2	1.97	0.46
1:A:163[A]:TYR:CE1	1:A:275:SER:HB2	2.50	0.46
1:B:163[A]:TYR:CE1	1:B:275:SER:HB2	2.51	0.46
1:B:12[B]:CYS:HB2	2:B:900[B]:BLA:HAC	1.54	0.46
1:A:250[A]:TYR:CD2	1:A:454:LEU:HB3	2.51	0.46
1:B:19:VAL:N	1:B:20:PRO:CD	2.76	0.46
1:A:262:ILE:HD12	1:A:292:PHE:HB3	1.98	0.46
1:B:51:PHE:CD1	1:B:63:GLN:HB2	2.50	0.46
1:B:359:LEU:HD12	1:B:360:GLY:N	2.31	0.46
1:A:196:PRO:HG2	2:A:900[B]:BLA:HMD3	1.98	0.45
2:A:900[B]:BLA:OB	2:A:900[B]:BLA:HBB1	2.15	0.45
1:A:157:TYR:CG	1:A:276:CYS:HB3	2.51	0.45
1:B:346:ILE:HD12	1:B:424:ILE:HG23	1.98	0.45
1:A:66:PRO:HD2	1:A:67:GLU:H	1.81	0.45
1:B:152:ARG:HG3	1:B:157:TYR:O	2.17	0.45
1:B:54:SER:O	1:B:57:SER:HB3	2.15	0.45
1:A:356:LEU:HD13	1:A:357:VAL:N	2.32	0.45
1:B:346:ILE:HG13	1:B:426:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:O	1:A:154:MSE:HG3	2.17	0.45
1:B:195:ILE:O	1:B:200:ARG:NH2	2.49	0.45
1:A:171:GLY:O	1:A:189:ARG:HA	2.17	0.45
1:A:415:ARG:HB2	1:A:423:TRP:CZ3	2.51	0.45
1:B:273:LEU:HD12	1:B:274:PHE:C	2.36	0.45
1:A:229:THR:HG23	1:A:231:GLU:H	1.82	0.45
1:B:211:ILE:HG12	1:B:243:VAL:HG21	1.99	0.45
1:A:382:GLN:O	1:A:385:PRO:HG3	2.17	0.45
1:A:373:GLN:O	1:A:377:VAL:HG23	2.17	0.45
1:B:356:LEU:HB3	1:B:425:PHE:HB2	1.99	0.45
1:A:305:ARG:NH2	1:B:137:HIS:O	2.50	0.45
1:A:485:LEU:HD23	1:A:485:LEU:HA	1.79	0.45
1:B:38:VAL:HG23	1:B:57:SER:O	2.17	0.45
1:B:185:TYR:CD1	1:B:188:LEU:HD12	2.39	0.44
1:B:261[B]:SER:HB3	2:B:900[B]:BLA:O2A	2.17	0.44
1:A:229:THR:C	1:A:231:GLU:H	2.21	0.44
1:A:290:MSE:HE1	1:A:293:GLN:OE1	2.16	0.44
1:B:134:VAL:CG1	1:B:302:ILE:HG12	2.47	0.44
1:A:162:ALA:HB3	1:A:175:ALA:HB3	1.99	0.44
1:A:221:VAL:CG2	1:A:221:VAL:O	2.64	0.44
1:B:51:PHE:CD1	1:B:63:GLN:CB	3.01	0.44
1:B:466:VAL:O	1:B:470:HIS:CD2	2.71	0.44
2:B:900[A]:BLA:CMD	2:B:900[A]:BLA:HBD2	2.31	0.44
2:B:900[A]:BLA:HMA2	2:B:900[A]:BLA:HMB3	1.98	0.44
1:B:266:VAL:HG21	1:B:271:TRP:HD1	1.82	0.44
1:A:199:ALA:O	1:A:203[B]:TYR:CD2	2.71	0.44
1:A:314:LEU:CD2	1:A:314:LEU:N	2.76	0.44
1:B:341:HIS:O	1:B:343:ASP:N	2.50	0.44
1:B:225:LEU:O	1:B:227:PRO:HD3	2.18	0.44
1:B:119:SER:C	1:B:121:THR:N	2.71	0.44
1:A:313:GLU:O	1:A:317:VAL:HG13	2.17	0.44
1:A:127:ALA:O	1:A:131:ILE:HG13	2.17	0.44
1:A:208:ILE:HA	1:A:261:SER:O	2.18	0.44
1:A:379:GLN:O	1:A:379:GLN:HG2	2.16	0.44
1:A:51:PHE:HB3	1:A:63:GLN:HG2	1.98	0.44
1:A:416:PHE:O	1:A:416:PHE:CD2	2.70	0.44
1:B:379:GLN:HA	1:B:382:GLN:CG	2.47	0.44
1:A:253:ASN:HD21	1:A:449:PRO:HB3	1.83	0.44
1:A:454:LEU:HD23	1:A:454:LEU:N	2.33	0.43
1:B:409:CYS:HB2	1:B:430:GLU:OE2	2.18	0.43
1:B:202:LEU:CD2	1:B:236:SER:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ILE:CD1	1:B:424:ILE:HG23	2.48	0.43
1:A:147:VAL:HG21	1:A:295:PHE:HZ	1.83	0.43
1:B:217:THR:HG23	1:B:217:THR:O	2.17	0.43
1:B:350:ILE:HG23	1:B:351:PRO:HD2	2.00	0.43
1:A:432:VAL:O	1:A:433:HIS:CB	2.66	0.43
2:A:900[A]:BLA:NA	3:A:506:HOH:O	2.36	0.43
1:B:453:ARG:O	1:B:453:ARG:CG	2.64	0.43
1:B:217:THR:O	1:B:217:THR:CG2	2.66	0.43
1:A:266:VAL:HG22	1:A:271:TRP:HB2	2.00	0.43
1:B:298:VAL:O	1:B:302:ILE:HD13	2.18	0.43
1:B:330:ARG:HB2	1:B:492:LEU:HD11	1.99	0.43
1:A:134:VAL:CG1	1:A:134:VAL:O	2.67	0.43
1:A:250[B]:TYR:CE1	2:A:900[B]:BLA:OC	2.72	0.43
1:A:64:VAL:HG13	1:A:64:VAL:O	2.18	0.43
1:A:294:ILE:HD11	1:B:294:ILE:HD13	1.99	0.43
1:A:215:ALA:HB3	1:A:257:ARG:HH12	1.84	0.43
1:B:315:LEU:HA	1:B:315:LEU:HD12	1.83	0.43
1:A:428:ARG:NE	1:A:474:TRP:CZ3	2.86	0.43
1:B:17:ILE:HD11	1:B:199:ALA:HA	2.00	0.43
1:B:17:ILE:HD13	2:B:900[B]:BLA:HAD1	2.00	0.43
1:A:188:LEU:HB3	1:A:190[B]:TYR:CE2	2.53	0.43
1:A:240:LEU:O	1:A:241:ARG:C	2.57	0.43
1:B:159:ARG:HB3	1:B:277:HIS:HB2	2.00	0.43
1:B:298:VAL:HG12	1:B:299:CYS:N	2.32	0.43
1:B:45:ILE:HG13	1:B:45:ILE:H	1.64	0.43
1:A:313:GLU:O	1:A:316:ARG:N	2.45	0.43
1:A:273:LEU:C	1:A:273:LEU:HD12	2.39	0.43
1:B:250[B]:TYR:CE1	2:B:900[B]:BLA:OC	2.72	0.42
1:B:190[B]:TYR:CD1	1:B:459:SER:HB2	2.54	0.42
1:A:160:VAL:HG12	1:A:177:SER:O	2.18	0.42
1:B:262:ILE:HD12	1:B:292:PHE:HB3	2.00	0.42
1:B:273:LEU:HD12	1:B:273:LEU:C	2.39	0.42
1:B:284:ILE:CG2	1:B:288:VAL:HB	2.49	0.42
1:A:389:ILE:HG22	1:A:390:TYR:N	2.34	0.42
1:B:262:ILE:HG22	1:B:296:SER:HB2	2.00	0.42
1:B:190[B]:TYR:HD1	1:B:194[B]:ASP:OD1	2.03	0.42
1:A:416:PHE:HE1	1:A:424:ILE:CG1	2.24	0.42
1:A:172:GLU:HG2	1:A:174:VAL:CG1	2.49	0.42
1:B:325:LEU:HD11	1:B:339:LEU:HD23	2.01	0.42
1:A:283:LEU:C	1:A:283:LEU:CD2	2.88	0.42
1:A:134:VAL:HA	1:A:143:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLU:HA	1:B:16:PRO:HD3	1.89	0.42
1:B:388:ASP:HB3	1:B:486:ARG:HE	1.85	0.42
1:B:97:VAL:HG22	1:B:110:PHE:CD2	2.54	0.42
1:A:302:ILE:HG22	1:A:303:VAL:N	2.35	0.42
1:B:358:MSE:O	1:B:423:TRP:N	2.46	0.42
1:B:139:ASP:HB3	1:B:142:SER:OG	2.19	0.42
1:A:188:LEU:CD2	1:A:189:ARG:H	2.26	0.42
1:B:209[A]:ARG:NH1	1:B:209[A]:ARG:HG2	2.32	0.42
1:A:414:ILE:HG21	1:A:482:ALA:O	2.19	0.42
1:B:284:ILE:N	1:B:284:ILE:HD12	2.34	0.42
1:A:284:ILE:HA	1:A:285:PRO:HD3	1.94	0.42
1:B:254:MSE:HE2	1:B:256:VAL:HG21	2.02	0.42
1:A:172:GLU:HG2	1:A:174:VAL:HG12	2.02	0.42
1:A:195:ILE:HB	1:A:200:ARG:NH2	2.34	0.42
1:B:83:SER:O	1:B:84:ASN:HB2	2.19	0.42
1:B:308:GLN:O	1:B:311:ILE:HD13	2.19	0.42
1:B:54:SER:HA	1:B:55:PRO:HD3	1.87	0.42
1:B:176:GLU:HG2	1:B:177:SER:N	2.34	0.42
1:A:288:VAL:O	1:A:289:ARG:C	2.58	0.42
1:A:492:LEU:N	1:A:492:LEU:CD1	2.83	0.41
1:A:293:GLN:O	1:A:296:SER:HB3	2.20	0.41
1:B:384:ASP:OD1	1:B:387:ARG:HG2	2.20	0.41
1:A:352:CYS:HB2	1:A:427:PHE:O	2.20	0.41
1:A:180:GLU:C	1:A:182:LEU:H	2.22	0.41
2:A:900[A]:BLA:HBB1	2:A:900[A]:BLA:OB	2.19	0.41
1:B:190[A]:TYR:N	1:B:190[A]:TYR:CD1	2.87	0.41
1:A:415:ARG:HB2	1:A:423:TRP:CH2	2.55	0.41
1:B:339:LEU:HD21	1:B:489:LEU:HD21	2.01	0.41
1:A:481:ILE:O	1:A:485:LEU:HB2	2.21	0.41
1:B:373:GLN:HE21	1:B:406:GLY:CA	2.34	0.41
1:B:372:ARG:C	1:B:374:ALA:N	2.74	0.41
1:B:12[A]:CYS:SG	1:B:13:GLU:HG3	2.61	0.41
1:A:306:LEU:HD13	1:B:305:ARG:HD3	2.03	0.41
1:A:168:ASP:N	1:A:168:ASP:OD1	2.44	0.41
2:B:900[A]:BLA:CMC	2:B:900[A]:BLA:HBC1	2.21	0.41
1:A:25:PRO:HB3	1:A:219:MSE:CE	2.41	0.41
1:B:222:PHE:HA	1:B:223:PRO:C	2.40	0.41
2:B:900[A]:BLA:HMA1	2:B:900[A]:BLA:C1B	2.51	0.41
1:A:15:GLU:HA	1:A:16:PRO:HD3	1.94	0.41
1:B:92:GLU:HB3	1:B:93:HIS:NE2	2.35	0.41
1:A:394:ASN:HA	1:A:469:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:HA	1:A:207:PRO:HD3	1.94	0.41
1:B:240:LEU:O	1:B:241:ARG:C	2.59	0.41
1:B:254:MSE:HE1	1:B:277:HIS:HD2	1.86	0.41
1:B:335:LEU:CD1	1:B:492:LEU:HD23	2.46	0.41
1:A:394:ASN:C	1:A:394:ASN:OD1	2.59	0.41
1:B:324:ALA:HB1	1:B:328:ARG:CZ	2.51	0.41
1:A:39:LEU:HD22	1:A:227:PRO:HD2	2.03	0.41
1:B:188:LEU:HD23	1:B:189:ARG:N	2.36	0.41
1:B:266:VAL:CG2	1:B:271:TRP:CD1	3.04	0.41
1:A:98:ILE:CG2	1:A:286:TYR:CE1	3.03	0.41
1:B:215:ALA:H	1:B:257:ARG:HH12	1.68	0.41
1:B:161:MSE:HE1	2:B:900[B]:BLA:OB	2.21	0.40
1:B:44:ASN:HB3	1:B:219:MSE:HG2	2.03	0.40
1:A:157:TYR:CE1	1:A:284:ILE:HD11	2.56	0.40
1:A:321:ARG:O	1:A:322:ARG:C	2.60	0.40
1:A:409:CYS:SG	1:A:430:GLU:CD	2.99	0.40
1:B:166:ARG:HD3	1:B:166:ARG:HA	1.90	0.40
1:A:261:SER:HA	1:A:274:PHE:O	2.21	0.40
1:B:51:PHE:HD2	1:B:52:VAL:N	2.18	0.40
2:A:900[A]:BLA:CMD	2:A:900[A]:BLA:HBD2	2.46	0.40
1:B:163[B]:TYR:CE1	1:B:172:GLU:C	2.95	0.40
1:A:379:GLN:HA	1:A:382:GLN:HG3	2.03	0.40
1:A:217:THR:HA	1:A:218:PRO:HD3	1.65	0.40
1:B:163[A]:TYR:OH	1:B:275:SER:CB	2.68	0.40
1:B:191:PRO:HD2	1:B:194[A]:ASP:CG	2.42	0.40
2:B:900[A]:BLA:HBB1	2:B:900[A]:BLA:OB	2.20	0.40
1:B:116:ASP:CG	1:B:117:THR:H	2.24	0.40
1:A:189:ARG:C	1:A:190[B]:TYR:CD2	2.95	0.40
1:A:244:SER:HB3	2:A:900[A]:BLA:HMD2	2.03	0.40
1:A:19:VAL:HG12	1:A:233:PHE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	409 (90%)	42 (9%)	2 (0%)	39	79
1	B	456/505 (90%)	403 (88%)	52 (11%)	1 (0%)	52	87
All	All	909/1010 (90%)	812 (89%)	94 (10%)	3 (0%)	46	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	456	PRO
1	A	342	PRO
1	A	20	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	394/419 (94%)	344 (87%)	50 (13%)	5	22
1	B	397/419 (95%)	350 (88%)	47 (12%)	6	25
All	All	791/838 (94%)	694 (88%)	97 (12%)	6	23

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	GLU
1	A	32	LEU
1	A	43	GLU
1	A	54	SER
1	A	57	SER
1	A	59	LEU
1	A	64	VAL
1	A	76	LEU
1	A	83	SER

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Mol	Chain	Res	Type
1	A	89	ARG
1	A	98	ILE
1	A	119	SER
1	A	120	ILE
1	A	125	LEU
1	A	130	ILE
1	A	134	VAL
1	A	140	THR
1	A	142	SER
1	A	147	VAL
1	A	181	ASP
1	A	186	LEU
1	A	188	LEU
1	A	209[A]	ARG
1	A	209[B]	ARG
1	A	210	LEU
1	A	221	VAL
1	A	242	SER
1	A	257	ARG
1	A	260	MSE
1	A	280	SER
1	A	294	ILE
1	A	302	ILE
1	A	311	ILE
1	A	314	LEU
1	A	318	SER
1	A	319	THR
1	A	334	ASP
1	A	346	ILE
1	A	363	THR
1	A	365	SER
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	485	LEU
1	A	489	LEU
1	A	492	LEU
1	B	12[A]	CYS
1	B	12[B]	CYS

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Mol	Chain	Res	Type
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	94	LEU
1	B	98	ILE
1	B	119	SER
1	B	130	ILE
1	B	134	VAL
1	B	143	LEU
1	B	146	ASN
1	B	147	VAL
1	B	160	VAL
1	B	181	ASP
1	B	182	LEU
1	B	186	LEU
1	B	188	LEU
1	B	190[A]	TYR
1	B	190[B]	TYR
1	B	198	GLN
1	B	236	SER
1	B	260	MSE
1	B	277	HIS
1	B	280	SER
1	B	291	SER
1	B	294	ILE
1	B	311	ILE
1	B	317	VAL
1	B	318	SER
1	B	343	ASP
1	B	366	ILE
1	B	380	ARG
1	B	393	ASP
1	B	409	CYS
1	B	412	LEU
1	B	426	TRP
1	B	430	GLU
1	B	431	GLU
1	B	483	GLU

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Mol	Chain	Res	Type
1	B	485	LEU
1	B	490	MSE
1	B	493	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	167	HIS
1	A	206	ASN
1	A	373	GLN
1	B	135	GLN
1	B	206	ASN
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 carbohydrates 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	A	900[A]	-	35,46,46	3.00	13 (37%)	43,67,67	1.63	9 (20%)
2	BLA	A	900[B]	-	35,46,46	3.02	16 (45%)	43,67,67	1.89	9 (20%)
2	BLA	B	900[A]	-	35,46,46	2.89	15 (42%)	43,67,67	1.72	8 (18%)
2	BLA	B	900[B]	-	35,46,46	3.07	14 (40%)	43,67,67	1.84	10 (23%)

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

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900[B]	BLA	C4D-C3D	-3.67	1.39	1.45
2	B	900[B]	BLA	C4D-C3D	-3.56	1.39	1.45
2	A	900[A]	BLA	C4D-C3D	-3.52	1.39	1.45
2	B	900[B]	BLA	C1B-C2B	-3.51	1.38	1.45
2	A	900[B]	BLA	C1B-C2B	-3.48	1.38	1.45
2	A	900[B]	BLA	C1D-C2D	-3.38	1.38	1.45
2	B	900[B]	BLA	C1D-C2D	-3.33	1.38	1.45
2	B	900[B]	BLA	C1C-C2C	-3.23	1.38	1.47
2	A	900[A]	BLA	C1D-C2D	-3.19	1.38	1.45
2	B	900[A]	BLA	C4D-C3D	-3.16	1.40	1.45
2	B	900[B]	BLA	C3B-C4B	-3.15	1.37	1.47
2	B	900[A]	BLA	C1C-C2C	-3.14	1.38	1.47
2	A	900[A]	BLA	C1C-C2C	-3.05	1.38	1.47
2	B	900[A]	BLA	C1D-C2D	-3.03	1.39	1.45
2	A	900[B]	BLA	C1C-C2C	-2.99	1.38	1.47
2	B	900[B]	BLA	CAB-C3B	-2.84	1.39	1.47
2	B	900[A]	BLA	C1B-C2B	-2.84	1.39	1.45
2	A	900[A]	BLA	C3B-C4B	-2.81	1.38	1.47
2	A	900[B]	BLA	C3B-C4B	-2.81	1.38	1.47
2	B	900[A]	BLA	CAB-C3B	-2.78	1.39	1.47
2	A	900[B]	BLA	CAB-C3B	-2.70	1.39	1.47
2	A	900[A]	BLA	C1B-C2B	-2.68	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900[A]	BLA	CAB-C3B	-2.59	1.39	1.47
2	B	900[A]	BLA	C3B-C4B	-2.59	1.39	1.47
2	A	900[B]	BLA	C4C-NC	-2.29	1.33	1.37
2	A	900[B]	BLA	C1C-NC	-2.19	1.32	1.37
2	B	900[A]	BLA	C4C-NC	-2.15	1.34	1.37
2	B	900[B]	BLA	C1B-NB	-2.06	1.34	1.37
2	A	900[B]	BLA	C1B-NB	-2.02	1.34	1.37
2	B	900[A]	BLA	C1C-NC	-2.02	1.33	1.37
2	B	900[B]	BLA	CAC-C3C	2.07	1.54	1.47
2	B	900[A]	BLA	CAC-C3C	2.17	1.54	1.47
2	A	900[B]	BLA	CAC-C3C	2.25	1.54	1.47
2	A	900[A]	BLA	CAC-C3C	2.43	1.55	1.47
2	B	900[B]	BLA	C4A-CHB	3.26	1.52	1.40
2	A	900[B]	BLA	C4A-CHB	3.39	1.53	1.40
2	A	900[A]	BLA	C4A-CHB	3.76	1.54	1.40
2	B	900[A]	BLA	C4A-CHB	3.84	1.54	1.40
2	B	900[A]	BLA	CBC-CAC	4.64	1.53	1.30
2	A	900[B]	BLA	CBC-CAC	4.71	1.53	1.30
2	B	900[B]	BLA	CBC-CAC	4.75	1.53	1.30
2	A	900[A]	BLA	CBC-CAC	4.75	1.53	1.30
2	B	900[A]	BLA	CHA-C4D	5.08	1.39	1.35
2	B	900[A]	BLA	CHD-C1D	5.14	1.53	1.40
2	A	900[A]	BLA	CHA-C4D	5.18	1.39	1.35
2	A	900[A]	BLA	CHD-C1D	5.48	1.54	1.40
2	A	900[B]	BLA	CHD-C1D	5.58	1.54	1.40
2	B	900[B]	BLA	CHD-C1D	6.16	1.55	1.40
2	B	900[A]	BLA	CHD-C4C	6.46	1.53	1.37
2	A	900[B]	BLA	CHD-C4C	6.55	1.53	1.37
2	A	900[B]	BLA	CHA-C4D	6.60	1.40	1.35
2	B	900[B]	BLA	CHA-C4D	6.95	1.41	1.35
2	A	900[A]	BLA	CHD-C4C	7.08	1.54	1.37
2	B	900[B]	BLA	CHD-C4C	7.09	1.54	1.37
2	B	900[B]	BLA	CHB-C1B	8.14	1.52	1.34
2	B	900[A]	BLA	CHB-C1B	8.32	1.53	1.34
2	A	900[B]	BLA	CHB-C1B	8.39	1.53	1.34
2	A	900[A]	BLA	CHB-C1B	8.84	1.54	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900[B]	BLA	C4C-CHD-C1D	-7.22	109.39	128.06
2	B	900[A]	BLA	C4C-CHD-C1D	-5.99	112.58	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900[A]	BLA	C4C-CHD-C1D	-5.66	113.41	128.06
2	B	900[B]	BLA	CHA-C4D-C3D	-3.81	116.61	125.55
2	A	900[B]	BLA	CHB-C1B-C2B	-3.45	119.80	126.94
2	B	900[B]	BLA	CHB-C1B-C2B	-3.41	119.88	126.94
2	A	900[B]	BLA	CHA-C4D-C3D	-3.25	117.92	125.55
2	B	900[A]	BLA	CAA-C2A-C1A	-3.09	123.65	127.01
2	B	900[B]	BLA	CBC-CAC-C3C	-3.05	111.56	127.01
2	B	900[A]	BLA	CHA-C4D-C3D	-2.79	119.00	125.55
2	B	900[B]	BLA	C4C-CHD-C1D	-2.66	121.18	128.06
2	B	900[A]	BLA	C3A-C4A-NA	-2.62	106.00	110.29
2	B	900[A]	BLA	CBC-CAC-C3C	-2.61	113.74	127.01
2	A	900[B]	BLA	CBC-CAC-C3C	-2.59	113.88	127.01
2	B	900[B]	BLA	OB-C4B-C3B	-2.58	123.38	129.82
2	A	900[A]	BLA	C3A-C4A-NA	-2.51	106.18	110.29
2	A	900[A]	BLA	CHA-C4D-C3D	-2.48	119.72	125.55
2	A	900[A]	BLA	CBC-CAC-C3C	-2.46	114.50	127.01
2	A	900[A]	BLA	CHB-C1B-NB	-2.30	122.36	130.87
2	A	900[A]	BLA	CAA-C2A-C1A	-2.17	124.65	127.01
2	A	900[B]	BLA	OB-C4B-C3B	-2.12	124.52	129.82
2	B	900[B]	BLA	C2D-C1D-ND	-2.11	105.73	110.55
2	A	900[B]	BLA	C3A-C4A-NA	-2.05	106.93	110.29
2	B	900[B]	BLA	C4D-ND-C1D	2.01	110.50	106.51
2	A	900[B]	BLA	CHD-C1D-ND	2.02	128.75	124.91
2	A	900[A]	BLA	C4D-ND-C1D	2.04	110.56	106.51
2	B	900[A]	BLA	C1D-C2D-C3D	2.12	109.04	106.50
2	A	900[A]	BLA	C1D-C2D-C3D	2.34	109.30	106.50
2	B	900[A]	BLA	CMB-C2B-C1B	2.48	127.50	124.20
2	A	900[A]	BLA	CMB-C2B-C1B	3.13	128.36	124.20
2	A	900[B]	BLA	CHA-C4D-ND	3.16	134.32	128.67
2	B	900[B]	BLA	C1D-C2D-C3D	3.37	110.55	106.50
2	B	900[A]	BLA	CBA-CAA-C2A	3.44	118.69	112.53
2	A	900[B]	BLA	CBA-CAA-C2A	3.63	119.04	112.53
2	B	900[B]	BLA	CHA-C4D-ND	3.74	135.35	128.67
2	B	900[B]	BLA	CHD-C1D-ND	4.55	133.57	124.91

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 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900[A]	BLA	16	0
2	A	900[B]	BLA	16	0
2	B	900[A]	BLA	15	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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^2)	Q<0.9
1	A	446/505 (88%)	0.25	39 (8%)	13	6	60, 115, 249, 498	0
1	B	446/505 (88%)	0.20	38 (8%)	13	6	52, 113, 268, 462	0
All	All	892/1010 (88%)	0.23	77 (8%)	13	6	52, 114, 258, 498	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	THR	23.4
1	A	430	GLU	19.1
1	A	471	SER	14.5
1	B	389	ILE	13.8
1	A	360	GLY	11.7
1	A	452	PRO	11.6
1	A	431	GLU	11.6
1	A	389	ILE	8.0
1	B	353	ASP	7.7
1	B	360	GLY	7.2
1	B	426	TRP	7.0
1	B	361	GLY	6.8
1	B	430	GLU	6.7
1	B	412	LEU	6.6
1	A	357	VAL	6.3
1	A	366	ILE	6.2
1	A	367	ARG	6.0
1	B	332	ALA	5.7
1	A	361	GLY	5.6
1	B	383	ARG	5.6
1	B	372	ARG	5.5
1	A	336	PHE	5.5
1	B	378	LEU	5.3
1	B	366	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	363	THR	4.7
1	A	364	LEU	4.6
1	A	479	LEU	4.5
1	B	336	PHE	4.4
1	A	388	ASP	4.3
1	A	412	LEU	4.3
1	A	470	HIS	4.2
1	A	423	TRP	4.1
1	B	387	ARG	4.0
1	B	425	PHE	3.9
1	A	468	ARG	3.8
1	B	356	LEU	3.7
1	B	471	SER	3.7
1	A	356	LEU	3.6
1	A	11	ASN	3.5
1	B	395	TRP	3.4
1	A	426	TRP	3.4
1	B	470	HIS	3.3
1	A	477	THR	3.3
1	B	380	ARG	3.2
1	A	425	PHE	3.2
1	A	6	PRO	3.1
1	B	431	GLU	3.1
1	A	337	GLY	3.1
1	B	381	LEU	3.0
1	A	448	GLY	3.0
1	A	359	LEU	3.0
1	A	215	ALA	3.0
1	B	476	GLU	2.9
1	B	452	PRO	2.8
1	A	386	GLU	2.8
1	A	453	ARG	2.8
1	B	423	TRP	2.8
1	B	357	VAL	2.8
1	B	367	ARG	2.8
1	B	340	ALA	2.8
1	A	429	HIS	2.7
1	B	355	ALA	2.7
1	A	381	LEU	2.6
1	A	472	THR	2.5
1	A	365	SER	2.4
1	B	429	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	354	GLY	2.3
1	A	347	ALA	2.3
1	A	340	ALA	2.2
1	B	6	PRO	2.2
1	B	388	ASP	2.2
1	B	11	ASN	2.2
1	A	465	GLU	2.1
1	B	386	GLU	2.1
1	B	483	GLU	2.1
1	A	433	HIS	2.0
1	B	394	ASN	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, 95th 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(Å^2)	Q<0.9
2	BLA	A	900[B]	43/43	0.90	0.32	1.68	69,122,152,156	43
2	BLA	B	900[B]	43/43	0.92	0.27	1.68	63,100,136,157	43
2	BLA	A	900[A]	43/43	0.90	0.32	1.67	104,133,154,159	43
2	BLA	B	900[A]	43/43	0.92	0.27	1.59	85,111,135,158	43

6.5 Other polymers (i)

There are no such residues in this entry.