



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:17 PM GMT

PDB ID : 4R70
Title : Crystal structure of bacteriophytochrome RpBphP3 from photosynthetic bacterium *R. palustris*
Authors : Yang, X.; Kuk, J.; Moffat, K.
Deposited on : 2014-08-26
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
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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

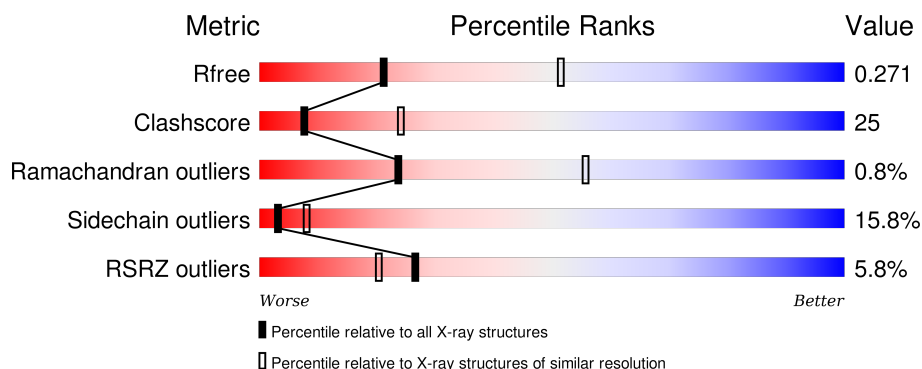
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

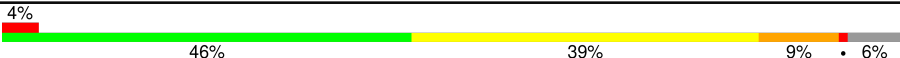
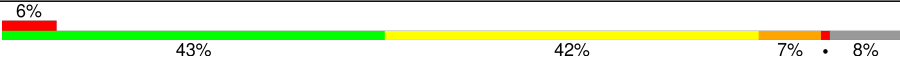
The reported resolution of this entry is 2.85 Å.

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 ≥ 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	529	 4% 46% 39% 9% • 6%
1	B	529	 6% 43% 42% 7% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7830 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.

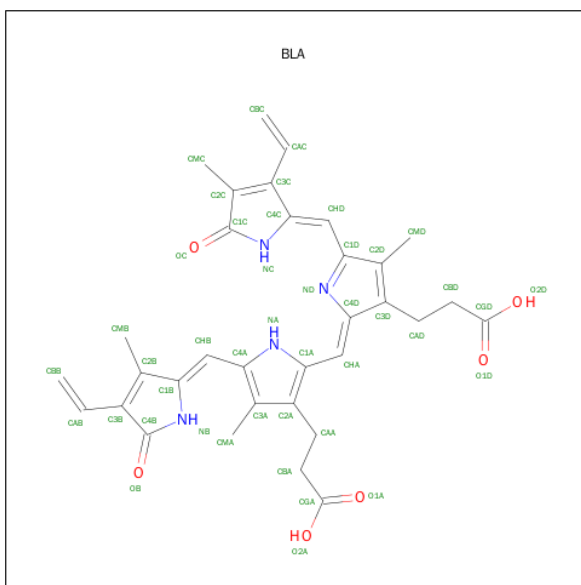
- Molecule 1 is a protein called Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	2	0
			3915	2467	715	719	14			
1	B	486	Total	C	N	O	S	0	0	0
			3806	2403	689	700	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	522	LEU	-	EXPRESSION TAG	UNP Q6N5G2
A	523	GLU	-	EXPRESSION TAG	UNP Q6N5G2
A	524	HIS	-	EXPRESSION TAG	UNP Q6N5G2
A	525	HIS	-	EXPRESSION TAG	UNP Q6N5G2
A	526	HIS	-	EXPRESSION TAG	UNP Q6N5G2
A	527	HIS	-	EXPRESSION TAG	UNP Q6N5G2
A	528	HIS	-	EXPRESSION TAG	UNP Q6N5G2
A	529	HIS	-	EXPRESSION TAG	UNP Q6N5G2
B	522	LEU	-	EXPRESSION TAG	UNP Q6N5G2
B	523	GLU	-	EXPRESSION TAG	UNP Q6N5G2
B	524	HIS	-	EXPRESSION TAG	UNP Q6N5G2
B	525	HIS	-	EXPRESSION TAG	UNP Q6N5G2
B	526	HIS	-	EXPRESSION TAG	UNP Q6N5G2
B	527	HIS	-	EXPRESSION TAG	UNP Q6N5G2
B	528	HIS	-	EXPRESSION TAG	UNP Q6N5G2
B	529	HIS	-	EXPRESSION TAG	UNP Q6N5G2

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0

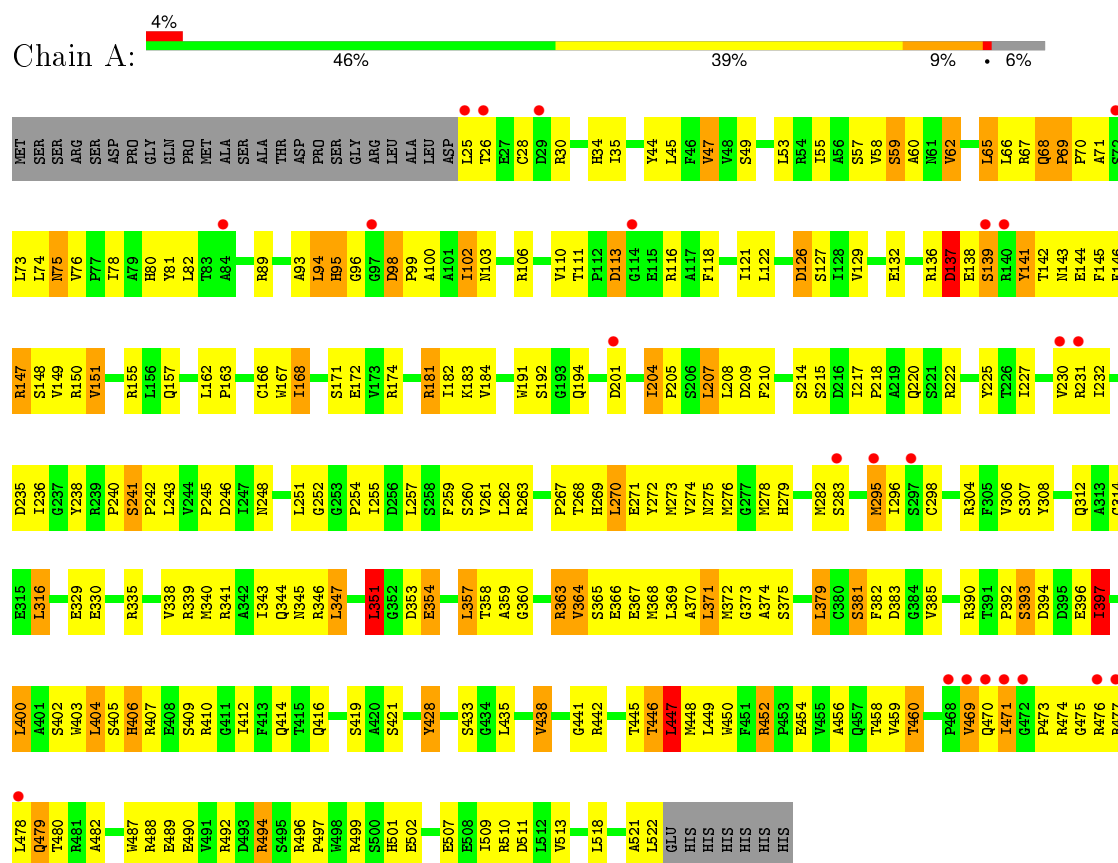
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	7	Total O 7 7	0	0

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 (Light-regulated signal transduction histidine kinase), PhyB2





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.31Å 143.31Å 120.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.85 31.03 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.85) 98.1 (31.03-2.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.185 , 0.260 0.204 , 0.271	Depositor DCC
R_{free} test set	1682 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.3	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33567 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7830	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	1.11	7/4011 (0.2%)	1.22	14/5461 (0.3%)
1	B	1.11	10/3893 (0.3%)	1.16	11/5301 (0.2%)
All	All	1.11	17/7904 (0.2%)	1.20	25/10762 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	ALA	CA-CB	-7.80	1.36	1.52
1	A	298	CYS	CB-SG	-7.48	1.69	1.82
1	B	330	GLU	CD-OE2	7.15	1.33	1.25
1	A	184	VAL	CB-CG1	-7.12	1.38	1.52
1	B	327	VAL	CB-CG1	-6.66	1.38	1.52
1	B	508	GLU	CG-CD	6.57	1.61	1.51
1	B	165	ALA	CA-CB	-6.13	1.39	1.52
1	B	134	GLU	CG-CD	5.97	1.60	1.51
1	B	320	VAL	CB-CG2	-5.93	1.40	1.52
1	A	454	GLU	CG-CD	5.68	1.60	1.51
1	B	106	ARG	CG-CD	5.46	1.65	1.51
1	A	330	GLU	CG-CD	5.42	1.60	1.51
1	A	456	ALA	CA-CB	-5.34	1.41	1.52
1	A	507	GLU	CB-CG	5.20	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	ALA	CA-CB	-5.20	1.41	1.52
1	B	491	VAL	CB-CG1	-5.12	1.42	1.52
1	A	329	GLU	CG-CD	5.10	1.59	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ILE	CG1-CB-CG2	-9.61	90.26	111.40
1	A	207	LEU	CB-CG-CD2	-8.28	96.93	111.00
1	A	181	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	347	LEU	CB-CG-CD2	-7.70	97.92	111.00
1	A	166	CYS	CA-CB-SG	-6.89	101.60	114.00
1	A	447	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	B	404	LEU	CB-CG-CD2	-6.43	100.08	111.00
1	B	446	THR	N-CA-C	-6.41	93.70	111.00
1	A	235	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	351	LEU	CA-CB-CG	6.11	129.35	115.30
1	B	335	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	B	311	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	504	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	A	452	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	314	CYS	CA-CB-SG	-5.50	104.10	114.00
1	A	335	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	436	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	291	ARG	N-CA-C	-5.41	96.39	111.00
1	B	39	ILE	CB-CA-C	-5.35	100.90	111.60
1	B	65	LEU	CA-CB-CG	5.29	127.47	115.30
1	B	488	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	174	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	B	431	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	A	494	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	241	SER	C-N-CD	5.04	138.99	128.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASP	Peptide
1	A	141	TYR	Peptide
1	A	441	GLY	Peptide
1	A	49	SER	Peptide
1	B	141	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3915	0	3893	192	2
1	B	3806	0	3775	203	2
2	A	43	0	31	13	0
2	B	43	0	31	6	0
3	A	16	0	0	3	0
3	B	7	0	0	0	0
All	All	7830	0	7730	393	2

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 25.

All (393) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLY:O	1:B:100:ALA:N	2.00	0.95
1:B:217:ILE:HG22	1:B:222:ARG:HG2	1.46	0.94
1:A:149:VAL:HG21	1:B:338:VAL:HG11	1.52	0.92
1:B:265:VAL:HG13	1:B:270:LEU:HD11	1.53	0.90
1:A:351:LEU:HD11	1:A:357:LEU:HD12	1.55	0.87
1:A:98:ASP:N	1:A:98:ASP:OD2	2.12	0.80
1:A:132:GLU:HB3	1:A:262:LEU:HD22	1.65	0.79
1:B:267:PRO:HA	1:B:270:LEU:HD22	1.63	0.79
1:A:220:GLN:OE1	1:A:220:GLN:N	2.18	0.76
1:A:138:GLU:HB2	1:A:141:TYR:CE2	2.21	0.76
1:B:441:GLY:HA3	1:B:444:SER:HB2	1.68	0.76
1:B:415:THR:OG1	1:B:416:GLN:N	2.16	0.75
1:A:65:LEU:HD13	1:A:66:LEU:HG	1.67	0.74
2:A:900:BLA:HMA1	2:A:900:BLA:NB	2.03	0.74
1:B:419:SER:HA	1:B:422:PHE:O	1.87	0.74
1:A:98:ASP:OD1	1:B:348:LEU:HG	1.87	0.73
1:B:176:ILE:HD12	1:B:310:VAL:HG13	1.71	0.73
1:A:144:GLU:HA	1:A:147:ARG:HH12	1.54	0.73
1:B:269:HIS:O	1:B:272:TYR:HB3	1.89	0.72
1:B:385:VAL:HG11	1:B:397:ILE:HD11	1.71	0.72
1:B:62:VAL:HG13	1:B:65:LEU:HD11	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:SER:OG	1:B:366:GLU:N	2.23	0.71
1:A:181:ARG:HE	1:A:183:LYS:HZ2	1.37	0.71
2:A:900:BLA:ND	3:A:1014:HOH:O	2.24	0.71
1:B:117:ALA:HB3	1:B:136:ARG:CZ	2.22	0.70
1:A:181:ARG:HE	1:A:183:LYS:NZ	1.90	0.69
1:A:201:ASP:HB3	1:A:204:ILE:HD13	1.75	0.69
1:A:476:ARG:HE	1:A:478:LEU:HG	1.58	0.69
1:B:460:THR:HG21	1:B:488:ARG:HH21	1.57	0.69
1:B:92:HIS:O	1:B:96:GLY:N	2.26	0.69
1:A:71:ALA:HA	1:A:74:LEU:HG	1.75	0.68
1:A:144:GLU:HA	1:A:147:ARG:NH1	2.09	0.68
1:A:60:ALA:HB2	1:A:242:PRO:HD2	1.74	0.68
1:B:266:SER:O	1:B:270:LEU:HD13	1.93	0.68
1:A:392:PRO:HB3	1:A:396:GLU:HG3	1.75	0.67
1:A:379:LEU:HD23	1:A:448:MET:HG3	1.77	0.67
1:A:400:LEU:HD11	1:A:435:LEU:HD22	1.76	0.67
1:A:66:LEU:O	1:A:68:GLN:N	2.28	0.66
1:B:510:ARG:NH1	1:B:511:ASP:OD1	2.27	0.66
1:B:381:SER:HB3	1:B:383:ASP:H	1.61	0.66
1:B:155:ARG:HH12	1:B:175:ARG:HH12	1.44	0.66
1:B:398:GLN:O	1:B:402:SER:OG	2.14	0.66
1:A:26:THR:O	1:A:30:ARG:HG3	1.96	0.66
1:B:483:SER:HB3	1:B:485:GLU:OE1	1.94	0.65
1:A:268:THR:OG1	1:A:478:LEU:HB2	1.97	0.65
1:A:207:LEU:HD21	1:A:276:MET:CE	2.27	0.65
1:A:347:LEU:HD22	1:A:351:LEU:HD23	1.78	0.65
1:A:509:ILE:O	1:A:513:VAL:HG23	1.96	0.65
1:A:136:ARG:NH1	1:A:139:SER:OG	2.30	0.65
1:A:268:THR:HG21	2:A:900:BLA:HAC	1.80	0.64
1:A:473:PRO:HD3	1:A:479:GLN:HE22	1.62	0.64
1:A:73:LEU:O	1:A:76:VAL:HG13	1.96	0.64
1:A:142:THR:HG23	1:A:145:PHE:H	1.61	0.63
1:B:462:GLY:HA3	1:B:481:ARG:HH21	1.63	0.63
1:B:208:LEU:HG	1:B:208:LEU:O	1.96	0.63
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.63	0.63
1:A:381:SER:HB3	1:A:383:ASP:H	1.64	0.63
1:B:236:ILE:HD13	1:B:278:MET:O	1.99	0.63
1:B:147:ARG:O	1:B:151:VAL:HG13	1.99	0.63
1:B:404:LEU:O	1:B:407:ARG:NH1	2.31	0.63
1:A:272:TYR:HB2	1:A:480:THR:HG21	1.80	0.62
1:B:217:ILE:CG2	1:B:222:ARG:HG2	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HB2	1:A:141:TYR:CZ	2.34	0.62
1:A:225:TYR:OH	2:A:900:BLA:HAD2	1.99	0.62
1:B:462:GLY:HA3	1:B:481:ARG:NH2	2.14	0.62
1:B:65:LEU:HD13	1:B:66:LEU:HG	1.82	0.62
1:A:347:LEU:CD2	1:A:351:LEU:HD23	2.29	0.62
1:A:351:LEU:O	1:A:351:LEU:HD12	1.99	0.62
1:B:272:TYR:N	1:B:480:THR:HG21	2.15	0.62
1:B:385:VAL:HG23	1:B:398:GLN:NE2	2.15	0.61
1:B:354:GLU:OE1	1:B:356:GLY:N	2.30	0.61
1:B:65:LEU:CD1	1:B:66:LEU:HG	2.30	0.61
1:A:412:ILE:CD1	1:A:438:VAL:HB	2.31	0.61
1:B:268:THR:HG21	2:B:900:BLA:HAC	1.83	0.61
1:B:381:SER:HA	1:B:446:THR:HG22	1.81	0.61
1:B:185:TYR:CZ	1:B:193:GLY:HA3	2.36	0.61
1:B:73:LEU:HD21	1:B:81:TYR:OH	2.01	0.60
1:B:73:LEU:HD12	1:B:76:VAL:HG21	1.83	0.60
1:B:464:ASP:HB3	1:B:466:HIS:CE1	2.36	0.60
1:B:452:ARG:NH1	1:B:497:PRO:O	2.33	0.60
1:A:57:SER:HB2	1:A:245:PRO:HD2	1.83	0.59
1:A:65:LEU:CD1	1:A:66:LEU:HG	2.32	0.59
1:A:448:MET:HE1	1:A:513:VAL:HG21	1.83	0.59
1:B:132:GLU:HB3	1:B:262:LEU:HD12	1.84	0.59
1:A:343:ILE:HD12	1:A:371:LEU:HD12	1.85	0.59
1:A:238:TYR:CE2	1:A:270:LEU:HD21	2.38	0.58
1:B:27:GLU:OE1	1:B:477:ARG:HD2	2.03	0.58
1:A:448:MET:CE	1:A:513:VAL:HG21	2.34	0.58
1:A:338:VAL:HG21	1:B:149:VAL:HG21	1.86	0.58
1:B:52:ASP:OD1	1:B:52:ASP:N	2.33	0.58
1:A:445:THR:HB	1:A:446:THR:HG22	1.85	0.58
1:A:113:ASP:N	1:A:113:ASP:OD1	2.37	0.57
1:B:102:ILE:HD13	1:B:102:ILE:H	1.69	0.57
1:A:207:LEU:HD21	1:A:276:MET:HE3	1.87	0.57
1:B:347:LEU:HD23	1:B:364:VAL:HG21	1.86	0.57
1:A:476:ARG:HE	1:A:478:LEU:CG	2.18	0.57
1:B:58:VAL:HG22	1:B:62:VAL:HG21	1.87	0.57
1:A:55:ILE:O	1:A:75:ASN:N	2.34	0.57
1:A:487:TRP:CZ3	1:A:489:GLU:HB2	2.40	0.57
1:B:245:PRO:HG2	1:B:247:ILE:HG12	1.87	0.57
1:B:46:PHE:CD1	1:B:58:VAL:HG23	2.40	0.56
1:B:59:SER:O	1:B:62:VAL:HG23	2.05	0.56
1:A:358:THR:OG1	1:A:359:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:TRP:HZ3	1:A:489:GLU:HB2	1.71	0.56
1:A:283:SER:HB2	1:A:295:MET:CE	2.36	0.56
2:A:900:BLA:NC	3:A:1014:HOH:O	2.21	0.56
1:B:400:LEU:O	1:B:404:LEU:HD22	2.05	0.56
1:A:155:ARG:NH1	1:A:172:GLU:OE2	2.38	0.56
1:B:218:PRO:HB2	1:B:220:GLN:OE1	2.06	0.56
1:B:410:ARG:HE	1:B:443:ALA:HB1	1.70	0.56
1:B:426:GLU:O	1:B:429:SER:HB2	2.06	0.56
1:B:375:SER:HB3	1:B:390:ARG:HB2	1.88	0.56
1:B:198:GLU:OE2	1:B:206:SER:OG	2.12	0.56
1:B:248:ASN:OD1	1:B:251:LEU:N	2.28	0.56
1:A:269:HIS:O	1:A:272:TYR:HB3	2.06	0.55
1:B:278:MET:HG3	1:B:299:HIS:HB3	1.87	0.55
1:B:217:ILE:HD11	2:B:900:BLA:C4A	2.36	0.55
1:A:143:ASN:O	1:A:147:ARG:NH1	2.40	0.55
1:A:460:THR:HB	1:A:488:ARG:HG2	1.88	0.55
1:A:257:LEU:HB3	1:A:260:SER:HB3	1.87	0.54
1:A:45:LEU:HD22	1:A:243:LEU:HD22	1.89	0.54
1:A:142:THR:HG23	1:A:144:GLU:N	2.22	0.54
1:A:341:ARG:CZ	1:B:101:ALA:HB1	2.36	0.54
1:A:268:THR:HG23	1:A:478:LEU:O	2.07	0.54
1:A:345:ASN:O	1:A:346:ARG:C	2.46	0.54
1:A:94:LEU:HG	1:A:95:HIS:ND1	2.23	0.54
1:A:248:ASN:O	1:A:252:GLY:N	2.35	0.54
1:A:447:LEU:HD13	1:A:449:LEU:HD21	1.88	0.54
1:A:268:THR:HG21	2:A:900:BLA:CAC	2.38	0.54
1:A:393:SER:O	1:A:397:ILE:HG13	2.07	0.54
1:B:372:MET:HG3	1:B:450:TRP:CE3	2.42	0.54
1:B:74:LEU:O	1:B:76:VAL:HG23	2.07	0.53
1:B:73:LEU:HD11	1:B:81:TYR:OH	2.08	0.53
1:A:477:ARG:O	1:A:477:ARG:HG2	2.08	0.53
1:B:50:GLU:HA	1:B:53:LEU:HD23	1.90	0.53
1:B:283:SER:HA	1:B:296:ILE:O	2.08	0.53
1:A:81:TYR:O	1:A:110:VAL:HG12	2.09	0.53
1:A:238:TYR:O	1:A:240:PRO:HD3	2.09	0.53
1:B:231:ARG:NH1	1:B:285:SER:OG	2.38	0.53
1:B:415:THR:OG1	1:B:417:GLN:N	2.38	0.52
1:A:147:ARG:HB2	1:A:147:ARG:HH11	1.73	0.52
1:B:50:GLU:O	1:B:53:LEU:N	2.42	0.52
1:A:354:GLU:OE1	1:A:363:ARG:HD3	2.09	0.52
1:B:414:GLN:HG2	1:B:415:THR:N	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:O	1:A:351:LEU:HB3	2.10	0.52
2:B:900:BLA:HMA1	2:B:900:BLA:NB	2.24	0.52
1:A:385:VAL:HG11	1:A:397:ILE:CD1	2.39	0.52
1:B:439:PRO:HA	1:B:447:LEU:HD22	1.91	0.52
1:B:439:PRO:HA	1:B:447:LEU:CD2	2.39	0.52
1:B:448:MET:CE	1:B:513:VAL:HG11	2.40	0.52
1:B:400:LEU:HD11	1:B:435:LEU:HD22	1.93	0.51
1:B:200:ARG:HD2	1:B:204:ILE:O	2.10	0.51
1:B:231:ARG:HH12	1:B:285:SER:HG	1.56	0.51
1:A:490:GLU:HG2	1:A:492:ARG:CZ	2.40	0.51
1:B:265:VAL:CG1	1:B:270:LEU:HD11	2.35	0.51
1:A:360:GLY:O	1:A:364:VAL:HG12	2.09	0.51
1:A:103:ASN:ND2	1:A:121:ILE:HG23	2.25	0.51
1:B:385:VAL:HG11	1:B:397:ILE:CD1	2.39	0.51
1:A:490:GLU:HG2	1:A:492:ARG:NH2	2.26	0.51
1:B:267:PRO:O	1:B:270:LEU:HB2	2.11	0.50
1:A:89:ARG:HA	1:B:353:ASP:OD2	2.11	0.50
1:B:243:LEU:HD13	1:B:255:ILE:HD12	1.93	0.50
1:A:217:ILE:O	1:A:222:ARG:NH1	2.42	0.50
1:B:201:ASP:HB3	1:B:204:ILE:HD13	1.91	0.50
1:A:25:LEU:N	1:A:477:ARG:NH1	2.60	0.50
1:B:99:PRO:HD2	1:B:101:ALA:HB3	1.93	0.50
1:A:316:LEU:HD22	1:B:338:VAL:HG13	1.94	0.50
1:B:369:LEU:HD22	1:B:374:ALA:O	2.12	0.50
1:B:283:SER:HB2	1:B:295:MET:HE2	1.93	0.50
1:A:471:ILE:HD11	1:A:475:GLY:HA2	1.93	0.50
1:A:137:ASP:CB	1:A:307:SER:HB3	2.42	0.50
1:A:341:ARG:O	1:A:344:GLN:HB3	2.11	0.50
1:A:73:LEU:HD12	1:A:73:LEU:O	2.12	0.50
2:A:900:BLA:HMA1	2:A:900:BLA:HB	1.74	0.50
1:A:490:GLU:HG2	1:A:492:ARG:NH1	2.26	0.50
1:A:69:PRO:CB	1:A:70:PRO:HD2	2.42	0.50
1:B:238:TYR:HE1	1:B:264:SER:HG	1.56	0.50
1:A:102:ILE:HG12	1:A:103:ASN:N	2.27	0.50
1:B:116:ARG:NH1	1:B:136:ARG:HH21	2.09	0.50
1:B:510:ARG:NH1	1:B:510:ARG:HG2	2.27	0.50
1:A:470:GLN:HG3	1:A:479:GLN:HB3	1.94	0.49
1:B:200:ARG:HD3	1:B:206:SER:OG	2.11	0.49
1:A:59:SER:HA	1:A:243:LEU:HD23	1.93	0.49
1:B:81:TYR:C	1:B:110:VAL:HG12	2.33	0.49
1:B:36:PRO:HG2	1:B:38:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG13	1:B:59:SER:N	2.28	0.49
1:A:111:THR:HG23	1:A:113:ASP:O	2.11	0.49
1:B:499:ARG:N	1:B:502:GLU:OE1	2.32	0.49
1:B:412:ILE:H	1:B:412:ILE:HD13	1.77	0.49
1:A:273:MET:HA	1:A:273:MET:HE2	1.95	0.49
1:A:416:GLN:OE1	1:A:497:PRO:HA	2.12	0.49
1:B:431:ILE:C	1:B:431:ILE:HD12	2.33	0.49
1:B:468:PRO:HA	1:B:481:ARG:HD2	1.95	0.49
1:B:379:LEU:HD12	1:B:447:LEU:O	2.12	0.49
1:A:116:ARG:HB3	1:A:118:PHE:HE2	1.76	0.49
1:A:55:ILE:HD11	1:A:78:ILE:HG13	1.93	0.49
1:A:236:ILE:HG12	1:A:279:HIS:HA	1.94	0.49
1:B:74:LEU:HD21	1:B:244:VAL:O	2.13	0.48
1:B:62:VAL:HA	1:B:65:LEU:HG	1.95	0.48
1:B:385:VAL:HG23	1:B:398:GLN:HE21	1.76	0.48
1:A:394:ASP:HA	1:A:397:ILE:HD11	1.94	0.48
1:B:63:GLU:HG3	1:B:68:GLN:O	2.14	0.48
1:B:125:HIS:O	1:B:128:ILE:HG13	2.13	0.48
1:B:56:ALA:HB1	1:B:249:PRO:HG3	1.95	0.48
1:B:397:ILE:HG12	1:B:398:GLN:N	2.29	0.48
1:A:181:ARG:HG2	1:A:183:LYS:HZ2	1.78	0.48
1:A:106:ARG:HH22	1:A:136:ARG:CZ	2.27	0.48
1:B:379:LEU:HA	1:B:447:LEU:O	2.14	0.48
1:B:481:ARG:NH1	1:B:484:PHE:HE1	2.12	0.47
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.72	0.47
1:A:95:HIS:ND1	1:A:95:HIS:N	2.59	0.47
1:A:271:GLU:O	1:A:275[A]:ASN:ND2	2.38	0.47
1:B:375:SER:O	1:B:390:ARG:N	2.43	0.47
1:A:402:SER:O	1:A:403:TRP:C	2.53	0.47
1:B:207:LEU:HD12	1:B:210:PHE:CD1	2.49	0.47
1:A:62:VAL:O	1:A:65:LEU:HD12	2.14	0.47
2:A:900:BLA:HMA2	2:A:900:BLA:CGA	2.45	0.47
1:A:397:ILE:HG13	1:A:397:ILE:H	1.47	0.47
1:B:478:LEU:HG	1:B:479:GLN:H	1.79	0.47
1:A:353:ASP:OD2	1:B:89:ARG:HG3	2.14	0.47
1:B:340:MET:O	1:B:344:GLN:HG3	2.15	0.47
1:A:162:LEU:HB3	1:A:163:PRO:HD3	1.96	0.47
1:A:396:GLU:HB2	1:A:428:TYR:CE1	2.50	0.47
1:A:75:ASN:ND2	1:A:75:ASN:O	2.47	0.47
1:A:204:ILE:HG23	1:A:205:PRO:HD2	1.97	0.46
1:A:126:ASP:OD2	1:A:251:LEU:HD12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:HG21	1:A:62:VAL:HG21	1.97	0.46
1:A:473:PRO:HD2	1:A:476:ARG:HH12	1.81	0.46
1:B:272:TYR:O	1:B:275:ASN:HB2	2.16	0.46
1:B:116:ARG:HD2	1:B:116:ARG:HA	1.45	0.46
1:B:117:ALA:HB3	1:B:136:ARG:NH2	2.31	0.46
1:A:267:PRO:HA	1:A:270:LEU:HB2	1.97	0.46
1:B:245:PRO:CG	1:B:247:ILE:HG12	2.44	0.46
1:B:418:LEU:HD12	1:B:418:LEU:HA	1.56	0.46
1:A:392:PRO:CB	1:A:396:GLU:HG3	2.43	0.46
1:B:174:ARG:HB2	1:B:182:ILE:HG12	1.97	0.46
1:A:44:TYR:HE2	1:A:118:PHE:CE1	2.33	0.46
1:B:58:VAL:HG22	1:B:59:SER:H	1.81	0.46
1:B:510:ARG:HG2	1:B:511:ASP:N	2.31	0.46
1:B:294:GLY:C	1:B:295:MET:HG2	2.34	0.46
1:A:157:GLN:OE1	1:B:335:ARG:NH1	2.48	0.46
1:B:302:THR:OG1	1:B:303:PRO:O	2.33	0.46
1:B:33:ILE:HD13	1:B:220:GLN:HG2	1.97	0.46
1:A:499:ARG:O	1:A:502:GLU:N	2.39	0.46
1:A:400:LEU:HD11	1:A:435:LEU:CD2	2.45	0.46
1:B:213:PRO:HD2	1:B:216:ASP:OD1	2.16	0.46
1:B:123:HIS:CE1	1:B:259:PHE:HB2	2.51	0.46
1:A:366:GLU:O	1:A:370:ALA:N	2.41	0.46
1:B:81:TYR:O	1:B:110:VAL:HG12	2.15	0.46
1:A:58:VAL:HG22	1:A:59:SER:H	1.79	0.46
1:A:343:ILE:O	1:A:347:LEU:HB2	2.16	0.45
1:B:369:LEU:O	1:B:372:MET:O	2.34	0.45
1:A:59:SER:CA	1:A:243:LEU:HD23	2.45	0.45
1:A:473:PRO:O	1:A:476:ARG:NH1	2.49	0.45
1:A:476:ARG:NE	1:A:478:LEU:HG	2.28	0.45
1:B:44:TYR:CE2	1:B:65:LEU:HD23	2.51	0.45
1:A:227:ILE:HD12	1:A:259:PHE:HZ	1.82	0.45
1:A:308:TYR:CE2	1:A:312:GLN:NE2	2.83	0.45
1:B:436:LEU:HA	1:B:436:LEU:HD12	1.51	0.45
1:B:385:VAL:HG21	1:B:397:ILE:HD11	1.97	0.45
1:B:381:SER:HB3	1:B:383:ASP:OD1	2.17	0.45
1:A:47:VAL:CG1	1:A:57:SER:HB3	2.46	0.45
1:A:167:TRP:HE3	1:A:168:ILE:HG12	1.82	0.45
1:A:100:ALA:HA	1:A:102:ILE:HD13	1.99	0.45
1:A:47:VAL:HA	1:A:129:VAL:O	2.16	0.45
1:B:396:GLU:O	1:B:399:ALA:HB3	2.17	0.45
1:B:145:PHE:O	1:B:148:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:CG2	1:A:145:PHE:H	2.27	0.45
1:B:40:GLN:HB2	1:B:42:HIS:CE1	2.51	0.45
1:B:142:THR:OG1	1:B:143:ASN:N	2.49	0.45
1:A:66:LEU:C	1:A:68:GLN:H	2.20	0.45
1:A:150:ARG:HG3	1:B:335:ARG:O	2.17	0.44
1:B:211:HIS:CD2	1:B:459:VAL:HG23	2.51	0.44
1:B:113:ASP:OD1	1:B:114:GLY:N	2.50	0.44
1:B:44:TYR:CD1	1:B:61:ASN:ND2	2.85	0.44
1:B:50:GLU:O	1:B:51:THR:C	2.56	0.44
1:A:341:ARG:NH1	1:B:101:ALA:HB1	2.33	0.44
1:A:232:ILE:HD12	1:A:282:MET:HE2	2.00	0.44
1:B:118:PHE:CE1	1:B:133:LEU:HB3	2.53	0.44
1:B:98:ASP:HA	1:B:99:PRO:HA	1.62	0.44
1:A:276:MET:HE2	3:A:1007:HOH:O	2.17	0.44
1:A:81:TYR:CD2	1:A:81:TYR:N	2.84	0.44
1:A:369:LEU:HD22	1:A:374:ALA:O	2.16	0.44
1:B:448:MET:HB2	1:B:448:MET:HE3	1.78	0.44
1:A:236:ILE:HD13	1:A:278:MET:O	2.18	0.44
1:B:35:ILE:O	1:B:37:GLY:N	2.51	0.44
1:A:393:SER:CB	1:A:396:GLU:HG2	2.47	0.44
1:A:283:SER:HB2	1:A:295:MET:HE1	2.00	0.44
1:A:448:MET:HB2	1:A:448:MET:HE2	1.67	0.44
1:B:403:TRP:CE3	1:B:404:LEU:HD13	2.53	0.44
1:B:464:ASP:N	1:B:464:ASP:OD1	2.51	0.44
1:A:295:MET:HB3	1:A:295:MET:HE2	1.48	0.44
1:A:232:ILE:HB	1:A:282:MET:HG3	1.99	0.44
1:B:491:VAL:O	1:B:491:VAL:HG13	2.18	0.44
1:B:416:GLN:HE21	1:B:497:PRO:HA	1.83	0.44
1:A:55:ILE:HD12	1:A:73:LEU:HD11	2.00	0.44
1:A:146:PHE:CD2	1:B:339:ARG:HG2	2.52	0.44
1:A:191:TRP:O	1:A:214:SER:HA	2.18	0.44
2:B:900:BLA:HMA2	2:B:900:BLA:CGA	2.48	0.43
1:A:102:ILE:HG22	1:B:348:LEU:HD11	2.00	0.43
1:A:269:HIS:CE1	2:A:900:BLA:C1A	3.00	0.43
1:B:383:ASP:N	1:B:383:ASP:OD1	2.52	0.43
1:A:390:ARG:HD3	1:A:390:ARG:HA	1.68	0.43
1:B:248:ASN:O	1:B:252:GLY:HA2	2.19	0.43
1:B:181:ARG:HE	1:B:183:LYS:HZ2	1.65	0.43
1:A:402:SER:O	1:A:405:SER:N	2.51	0.43
1:A:53:LEU:O	1:A:78:ILE:HG22	2.18	0.43
1:B:448:MET:HE2	1:B:513:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HB2	1:B:131:LEU:HD12	2.00	0.43
1:B:198:GLU:OE1	1:B:207:LEU:N	2.50	0.43
1:A:167:TRP:CE3	1:A:168:ILE:HG12	2.53	0.43
1:A:510:ARG:NE	1:A:511:ASP:OD1	2.51	0.43
1:B:285:SER:HB3	1:B:292:LEU:HD11	2.01	0.43
1:A:137:ASP:HB3	1:A:307:SER:HB3	2.01	0.43
1:A:236:ILE:HD12	1:A:274:VAL:HG22	1.99	0.43
1:A:406:HIS:O	1:A:407:ARG:C	2.56	0.43
1:B:181:ARG:HE	1:B:183:LYS:NZ	2.16	0.43
1:B:403:TRP:HE3	1:B:404:LEU:HD13	1.83	0.43
1:B:431:ILE:HD12	1:B:432:ALA:N	2.34	0.43
1:A:347:LEU:CD2	1:A:364:VAL:HG21	2.49	0.43
1:B:406:HIS:O	1:B:407:ARG:C	2.56	0.43
1:A:275[B]:ASN:HD21	1:A:482:ALA:HA	1.84	0.43
1:A:246:ASP:OD2	1:A:254:PRO:HA	2.19	0.43
1:A:263:ARG:NH2	2:A:900:BLA:O1D	2.45	0.43
1:B:155:ARG:NH1	1:B:172:GLU:OE2	2.52	0.43
1:A:208:LEU:O	1:A:209:ASP:HB2	2.19	0.42
1:A:34:HIS:CD2	1:A:35:ILE:HG23	2.54	0.42
1:B:39:ILE:HD12	1:B:40:GLN:C	2.40	0.42
1:B:272:TYR:CE2	1:B:484:PHE:HZ	2.37	0.42
1:B:478:LEU:CG	1:B:479:GLN:H	2.31	0.42
1:B:281:ALA:HA	1:B:298:CYS:O	2.19	0.42
1:A:182:ILE:HG23	1:A:182:ILE:HD12	1.79	0.42
1:B:272:TYR:CD1	1:B:273:MET:HE2	2.55	0.42
1:B:231:ARG:NH2	1:B:295:MET:HE1	2.34	0.42
1:A:518:LEU:HA	1:A:518:LEU:HD23	1.61	0.42
1:B:62:VAL:O	1:B:65:LEU:HD12	2.20	0.42
1:B:481:ARG:NH1	1:B:484:PHE:CE1	2.88	0.42
1:B:180:ASP:HB3	1:B:204:ILE:HG12	2.02	0.42
1:A:132:GLU:OE2	1:A:260:SER:OG	2.20	0.42
1:B:452:ARG:NH2	1:B:502:GLU:OE2	2.52	0.42
2:A:900:BLA:HHA	2:A:900:BLA:HAD2	1.85	0.42
1:B:390:ARG:HD3	1:B:390:ARG:HA	1.81	0.42
1:A:217:ILE:HA	1:A:218:PRO:HD2	1.81	0.42
1:B:56:ALA:CB	1:B:249:PRO:HG3	2.49	0.42
1:B:361:LEU:HA	1:B:361:LEU:HD23	1.80	0.42
1:B:515:ASP:O	1:B:518:LEU:HB2	2.20	0.42
1:A:372:MET:HG3	1:A:450:TRP:CZ3	2.55	0.42
1:A:373:GLY:O	1:A:452:ARG:NE	2.48	0.42
2:B:900:BLA:HMA2	2:B:900:BLA:O1A	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:900:BLA:HB	2:A:900:BLA:CMA	2.33	0.42
1:A:147:ARG:O	1:A:151:VAL:HG13	2.20	0.42
1:B:460:THR:HG21	1:B:488:ARG:NH2	2.29	0.42
1:B:229:PRO:C	1:B:231:ARG:HH11	2.23	0.42
1:B:56:ALA:O	1:B:57:SER:OG	2.36	0.42
1:A:365:SER:OG	1:A:366:GLU:N	2.53	0.42
1:A:93:ALA:C	1:A:96:GLY:H	2.22	0.42
1:A:521:ALA:C	1:A:522:LEU:HG	2.39	0.42
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.88	0.41
1:A:58:VAL:O	1:A:243:LEU:HA	2.21	0.41
1:B:44:TYR:CD2	1:B:65:LEU:HD23	2.55	0.41
1:A:400:LEU:HD22	1:A:404:LEU:HD22	2.02	0.41
1:A:44:TYR:CE2	1:A:65:LEU:HD23	2.55	0.41
1:B:86:SER:HA	1:B:89:ARG:NH2	2.34	0.41
1:B:344:GLN:HA	1:B:347:LEU:HD12	2.02	0.41
1:B:394:ASP:HA	1:B:397:ILE:CD1	2.51	0.41
1:B:94:LEU:HA	1:B:94:LEU:HD23	1.65	0.41
1:B:344:GLN:O	1:B:348:LEU:HB2	2.20	0.41
1:A:59:SER:HB2	1:A:241:SER:OG	2.20	0.41
1:B:208:LEU:O	1:B:208:LEU:CG	2.66	0.41
1:A:409:SER:O	1:A:410:ARG:HD3	2.21	0.41
1:B:99:PRO:O	1:B:100:ALA:C	2.59	0.41
1:B:266:SER:HB3	2:B:900:BLA:HBD2	2.03	0.41
1:A:255:ILE:HG22	1:A:257:LEU:HG	2.03	0.41
1:A:210:PHE:N	1:A:210:PHE:CD2	2.88	0.41
1:B:324:GLN:HA	1:B:327:VAL:HG13	2.01	0.41
1:A:94:LEU:HG	1:A:95:HIS:CE1	2.56	0.41
1:B:391:THR:OG1	1:B:392:PRO:O	2.38	0.41
1:B:413:PHE:CG	1:B:414:GLN:N	2.88	0.41
1:A:403:TRP:CE3	1:A:404:LEU:HD13	2.56	0.41
1:A:347:LEU:HG	1:A:364:VAL:HG21	2.03	0.40
1:B:369:LEU:HA	1:B:369:LEU:HD23	1.72	0.40
1:A:283:SER:HA	1:A:296:ILE:O	2.20	0.40
1:B:248:ASN:ND2	1:B:251:LEU:HB2	2.35	0.40
1:B:279:HIS:HB2	1:B:301:LEU:O	2.20	0.40
2:A:900:BLA:HMA1	2:A:900:BLA:C1B	2.52	0.40
1:B:131:LEU:HG	1:B:132:GLU:N	2.34	0.40
1:B:102:ILE:HG12	1:B:103:ASN:N	2.35	0.40
1:A:496:ARG:HA	1:A:497:PRO:HD3	1.85	0.40
1:A:412:ILE:HD13	1:A:412:ILE:HA	1.84	0.40
1:B:132:GLU:HB3	1:B:262:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LEU:HD13	1:B:255:ILE:CD1	2.50	0.40
1:A:98:ASP:OD1	1:B:348:LEU:CG	2.62	0.40
1:A:338:VAL:O	1:A:339:ARG:C	2.59	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:NE	1:B:98:ASP:OD1[6_555]	1.99	0.21
1:A:390:ARG:NH2	1:B:458:THR:OG1[3_564]	2.06	0.14

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	498/529 (94%)	449 (90%)	45 (9%)	4 (1%)	24	56
1	B	480/529 (91%)	440 (92%)	36 (8%)	4 (1%)	24	56
All	All	978/1058 (92%)	889 (91%)	81 (8%)	8 (1%)	24	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	B	70	PRO
1	A	67	ARG
1	B	100	ALA
1	A	69	PRO
1	B	99	PRO
1	A	469	VAL
1	B	35	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	421/445 (95%)	350 (83%)	71 (17%)	2	6
1	B	409/445 (92%)	349 (85%)	60 (15%)	4	10
All	All	830/890 (93%)	699 (84%)	131 (16%)	3	8

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	CYS
1	A	47	VAL
1	A	59	SER
1	A	62	VAL
1	A	65	LEU
1	A	68	GLN
1	A	75	ASN
1	A	80	HIS
1	A	82	LEU
1	A	94	LEU
1	A	95	HIS
1	A	98	ASP
1	A	102	ILE
1	A	113	ASP
1	A	122	LEU
1	A	126	ASP
1	A	127	SER
1	A	137	ASP
1	A	139	SER
1	A	147	ARG
1	A	148	SER
1	A	151	VAL
1	A	168	ILE
1	A	171	SER
1	A	192	SER
1	A	194	GLN
1	A	204	ILE

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Mol	Chain	Res	Type
1	A	215	SER
1	A	230	VAL
1	A	231	ARG
1	A	261	VAL
1	A	270	LEU
1	A	295	MET
1	A	304	ARG
1	A	306	VAL
1	A	316	LEU
1	A	340	MET
1	A	351	LEU
1	A	354	GLU
1	A	357	LEU
1	A	363	ARG
1	A	364	VAL
1	A	367	GLU
1	A	368	MET
1	A	371	LEU
1	A	375	SER
1	A	379	LEU
1	A	381	SER
1	A	382	PHE
1	A	393	SER
1	A	397	ILE
1	A	400	LEU
1	A	404	LEU
1	A	406	HIS
1	A	414	GLN
1	A	419	SER
1	A	421	SER
1	A	428	TYR
1	A	433	SER
1	A	438	VAL
1	A	446	THR
1	A	447	LEU
1	A	458	THR
1	A	459	VAL
1	A	460	THR
1	A	469	VAL
1	A	471	ILE
1	A	474	ARG
1	A	479	GLN

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Mol	Chain	Res	Type
1	A	494	ARG
1	A	501	HIS
1	B	51	THR
1	B	58	VAL
1	B	65	LEU
1	B	68	GLN
1	B	75	ASN
1	B	80	HIS
1	B	82	LEU
1	B	86	SER
1	B	94	LEU
1	B	95	HIS
1	B	102	ILE
1	B	111	THR
1	B	116	ARG
1	B	124	ARG
1	B	126	ASP
1	B	168	ILE
1	B	171	SER
1	B	176	ILE
1	B	192	SER
1	B	202	SER
1	B	204	ILE
1	B	206	SER
1	B	214	SER
1	B	227	ILE
1	B	231	ARG
1	B	239	ARG
1	B	241	SER
1	B	247	ILE
1	B	274	VAL
1	B	276	MET
1	B	295	MET
1	B	302	THR
1	B	319	GLN
1	B	328	LEU
1	B	338	VAL
1	B	341	ARG
1	B	357	LEU
1	B	358	THR
1	B	364	VAL
1	B	367	GLU

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Mol	Chain	Res	Type
1	B	368	MET
1	B	371	LEU
1	B	381	SER
1	B	391	THR
1	B	397	ILE
1	B	400	LEU
1	B	404	LEU
1	B	412	ILE
1	B	414	GLN
1	B	421	SER
1	B	438	VAL
1	B	446	THR
1	B	459	VAL
1	B	460	THR
1	B	469	VAL
1	B	479	GLN
1	B	493	ASP
1	B	494	ARG
1	B	510	ARG
1	B	516	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	A	501	HIS
1	B	42	HIS
1	B	211	HIS
1	B	269	HIS
1	B	344	GLN
1	B	398	GLN
1	B	416	GLN
1	B	501	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BLA	A	900	1	36,46,46	3.08	17 (47%)	45,67,67	1.89	14 (31%)
2	BLA	B	900	1	36,46,46	3.09	16 (44%)	45,67,67	2.14	15 (33%)

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	1	-	0/22/74/74	0/4/4/4
2	BLA	B	900	1	-	0/22/74/74	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C1C-C2C	-4.35	1.35	1.47
2	B	900	BLA	C1D-C2D	-4.05	1.36	1.45
2	A	900	BLA	C4D-C3D	-3.94	1.38	1.45
2	B	900	BLA	C1C-C2C	-3.45	1.37	1.47
2	A	900	BLA	C1B-C2B	-3.40	1.38	1.45
2	B	900	BLA	CAB-C3B	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C1D-C2D	-3.12	1.38	1.45
2	A	900	BLA	C1B-NB	-3.11	1.32	1.37
2	B	900	BLA	C1B-C2B	-2.93	1.39	1.45
2	A	900	BLA	CAB-C3B	-2.92	1.39	1.47
2	B	900	BLA	C3C-C4C	-2.85	1.41	1.45
2	A	900	BLA	C3B-C4B	-2.85	1.38	1.47
2	B	900	BLA	C4D-C3D	-2.82	1.40	1.45
2	B	900	BLA	C1B-NB	-2.71	1.33	1.37
2	A	900	BLA	C3C-C4C	-2.64	1.41	1.45
2	A	900	BLA	C4C-NC	-2.45	1.33	1.37
2	B	900	BLA	C3B-C4B	-2.43	1.39	1.47
2	A	900	BLA	C4B-NB	-2.04	1.33	1.37
2	A	900	BLA	CAC-C3C	2.07	1.53	1.47
2	B	900	BLA	CAC-C3C	2.34	1.54	1.47
2	A	900	BLA	C4A-CHB	2.85	1.51	1.40
2	B	900	BLA	CMA-C3A	2.92	1.57	1.51
2	B	900	BLA	C4A-CHB	2.98	1.51	1.40
2	A	900	BLA	CBC-CAC	4.60	1.52	1.30
2	B	900	BLA	CBC-CAC	4.72	1.53	1.30
2	A	900	BLA	CHD-C1D	5.95	1.55	1.40
2	B	900	BLA	CHD-C1D	6.22	1.55	1.40
2	B	900	BLA	CHB-C1B	6.49	1.47	1.34
2	A	900	BLA	CHB-C1B	6.68	1.47	1.34
2	A	900	BLA	CHD-C4C	7.16	1.54	1.37
2	A	900	BLA	CHA-C4D	7.59	1.42	1.35
2	B	900	BLA	CHA-C4D	7.59	1.42	1.35
2	B	900	BLA	CHD-C4C	7.86	1.56	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	CHA-C4D-C3D	-3.76	116.92	125.48
2	A	900	BLA	C3A-C4A-NA	-3.70	104.23	110.29
2	A	900	BLA	CBC-CAC-C3C	-3.52	108.92	127.70
2	B	900	BLA	CAD-CBD-CGD	-3.49	106.00	112.78
2	B	900	BLA	CHA-C4D-C3D	-3.37	117.81	125.48
2	B	900	BLA	CHD-C1D-C2D	-3.28	116.87	124.71
2	B	900	BLA	C1B-NB-C4B	-3.15	106.17	110.73
2	B	900	BLA	CBC-CAC-C3C	-2.61	113.73	127.70
2	A	900	BLA	C2D-C1D-ND	-2.59	104.99	110.65
2	A	900	BLA	CAD-CBD-CGD	-2.39	108.13	112.78
2	B	900	BLA	CHD-C4C-C3C	-2.35	121.84	128.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	C3A-C4A-NA	-2.33	106.48	110.29
2	A	900	BLA	C3D-C4D-ND	-2.29	106.50	109.98
2	A	900	BLA	CMB-C2B-C3B	-2.23	123.24	128.58
2	B	900	BLA	C4C-CHD-C1D	-2.12	122.69	128.03
2	A	900	BLA	CAB-C3B-C4B	2.06	129.51	123.58
2	B	900	BLA	CAB-C3B-C4B	2.28	130.15	123.58
2	A	900	BLA	C1D-C2D-C3D	2.47	109.29	106.43
2	A	900	BLA	CAC-C3C-C4C	2.60	130.11	123.67
2	B	900	BLA	CHA-C4D-ND	2.61	133.34	128.71
2	B	900	BLA	C2B-C1B-NB	2.88	111.00	106.94
2	B	900	BLA	CBA-CAA-C2A	2.94	117.67	112.49
2	B	900	BLA	C1D-C2D-C3D	3.01	109.91	106.43
2	A	900	BLA	C4D-ND-C1D	3.27	112.72	106.50
2	A	900	BLA	CMB-C2B-C1B	3.56	128.85	124.20
2	A	900	BLA	CHD-C1D-ND	3.57	131.55	124.89
2	B	900	BLA	CMB-C2B-C1B	3.78	129.12	124.20
2	A	900	BLA	CHA-C4D-ND	4.08	135.95	128.71
2	B	900	BLA	CHD-C1D-ND	6.13	136.33	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	13	0
2	B	900	BLA	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	498/529 (94%)	-0.17	23 (4%)	36 30	61, 107, 181, 236	0
1	B	486/529 (91%)	0.10	34 (6%)	19 13	65, 132, 200, 232	0
All	All	984/1058 (93%)	-0.04	57 (5%)	26 20	61, 119, 194, 236	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	ARG	6.4
1	B	355	GLN	5.3
1	A	114	GLY	5.1
1	B	353	ASP	4.9
1	A	476	ARG	4.8
1	A	283	SER	4.5
1	A	471	ILE	4.3
1	B	113	ASP	4.0
1	A	25	LEU	3.8
1	A	470	GLN	3.7
1	A	478	LEU	3.7
1	B	114	GLY	3.4
1	A	84	ALA	3.3
1	B	67	ARG	3.3
1	B	110	VAL	3.1
1	B	252	GLY	3.1
1	A	26	THR	3.1
1	B	520	ARG	3.0
1	B	283	SER	3.0
1	A	231	ARG	2.9
1	B	116	ARG	2.9
1	B	467	LYS	2.8
1	B	289	ASP	2.8
1	A	97	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	428	TYR	2.8
1	B	297	SER	2.8
1	B	382	PHE	2.7
1	B	478	LEU	2.7
1	A	29	ASP	2.7
1	B	479	GLN	2.7
1	B	521	ALA	2.6
1	B	239	ARG	2.6
1	A	469	VAL	2.5
1	B	477	ARG	2.5
1	B	111	THR	2.5
1	B	108	ASP	2.4
1	A	140	ARG	2.4
1	B	256	ASP	2.4
1	B	84	ALA	2.4
1	B	115	GLU	2.4
1	A	201	ASP	2.3
1	B	251	LEU	2.3
1	A	72	SER	2.2
1	A	139	SER	2.2
1	A	297	SER	2.2
1	B	423	PRO	2.2
1	A	295	MET	2.2
1	A	472	GLY	2.2
1	A	230	VAL	2.2
1	B	427	VAL	2.2
1	B	298	CYS	2.2
1	B	27	GLU	2.1
1	B	469	VAL	2.1
1	B	80	HIS	2.1
1	A	468	PRO	2.1
1	B	136	ARG	2.0
1	B	354	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
2	BLA	B	900	43/43	0.87	0.32	0.84	108,145,171,175	0
2	BLA	A	900	43/43	0.90	0.32	0.79	82,104,136,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.