



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:19 AM UTC

PDB ID : 4R6L / pdb_00004r6l
Title : Crystal structure of bacteriophytochrome RpBphP2 from photosynthetic bacterium *R. palustris*
Authors : Yang, X.; Stojkovic, E.; Ozarowski, W.; Kuk, J.; Davydova, E.; Moffat, K.
Deposited on : 2014-08-25
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

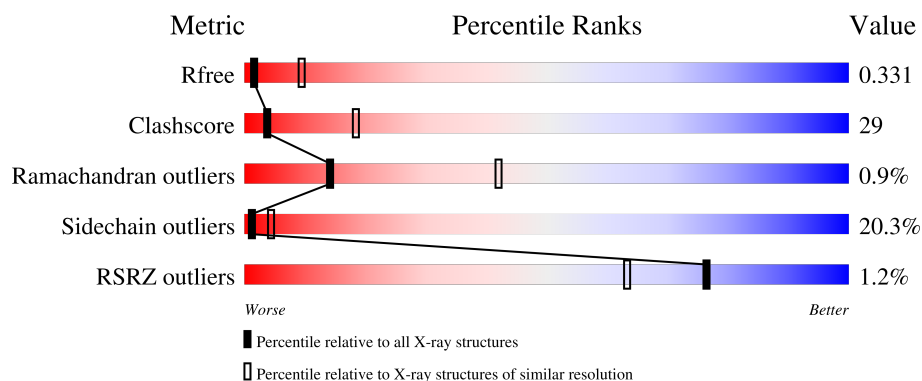
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	 40% 38% 12% 9%
1	B	519	 34% 37% 15% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7198 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), PhyB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3639	2295	659	671	14			
1	B	448	Total	C	N	O	S	0	0	0
			3473	2191	627	641	14			

There are 26 discrepancies between the modelled and reference sequences:

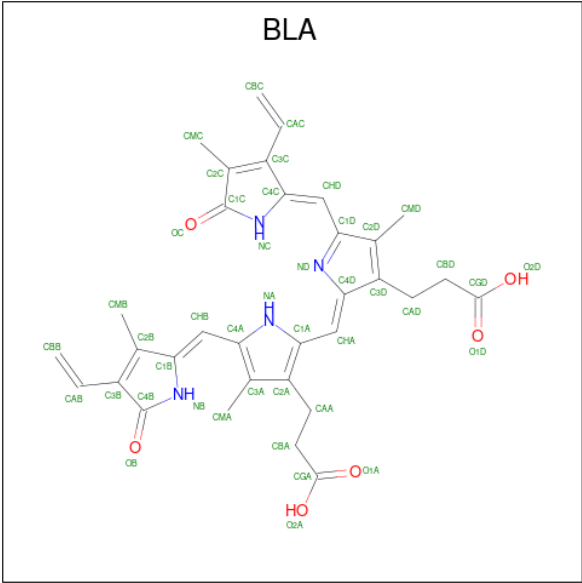
Chain	Residue	Modelled	Actual	Comment	Reference
A	507	LYS	-	expression tag	UNP Q6N5G3
A	508	LEU	-	expression tag	UNP Q6N5G3
A	509	ALA	-	expression tag	UNP Q6N5G3
A	510	ALA	-	expression tag	UNP Q6N5G3
A	511	ALA	-	expression tag	UNP Q6N5G3
A	512	LEU	-	expression tag	UNP Q6N5G3
A	513	GLU	-	expression tag	UNP Q6N5G3
A	514	HIS	-	expression tag	UNP Q6N5G3
A	515	HIS	-	expression tag	UNP Q6N5G3
A	516	HIS	-	expression tag	UNP Q6N5G3
A	517	HIS	-	expression tag	UNP Q6N5G3
A	518	HIS	-	expression tag	UNP Q6N5G3
A	519	HIS	-	expression tag	UNP Q6N5G3
B	507	LYS	-	expression tag	UNP Q6N5G3
B	508	LEU	-	expression tag	UNP Q6N5G3
B	509	ALA	-	expression tag	UNP Q6N5G3
B	510	ALA	-	expression tag	UNP Q6N5G3
B	511	ALA	-	expression tag	UNP Q6N5G3
B	512	LEU	-	expression tag	UNP Q6N5G3
B	513	GLU	-	expression tag	UNP Q6N5G3
B	514	HIS	-	expression tag	UNP Q6N5G3
B	515	HIS	-	expression tag	UNP Q6N5G3
B	516	HIS	-	expression tag	UNP Q6N5G3
B	517	HIS	-	expression tag	UNP Q6N5G3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	518	HIS	-	expression tag	UNP Q6N5G3
B	519	HIS	-	expression tag	UNP Q6N5G3

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: C₃₃H₃₄N₄O₆).

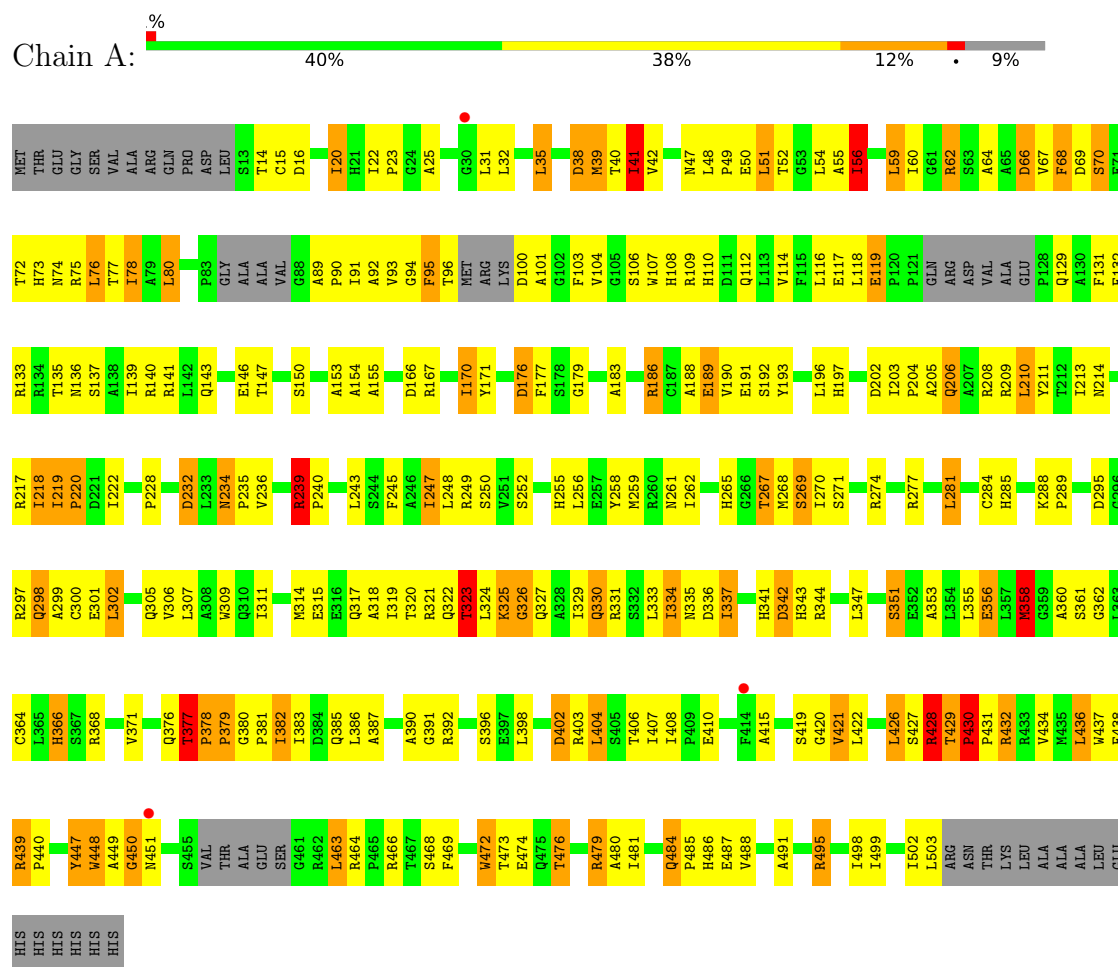


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		

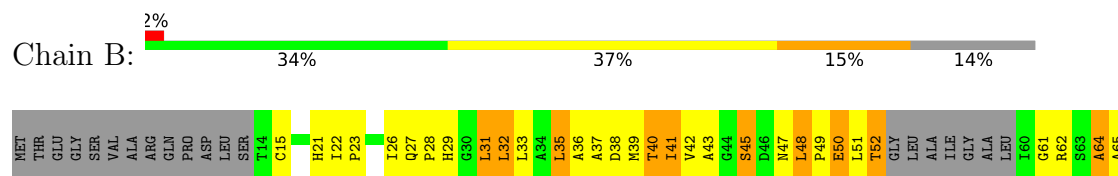
3 Residue-property plots

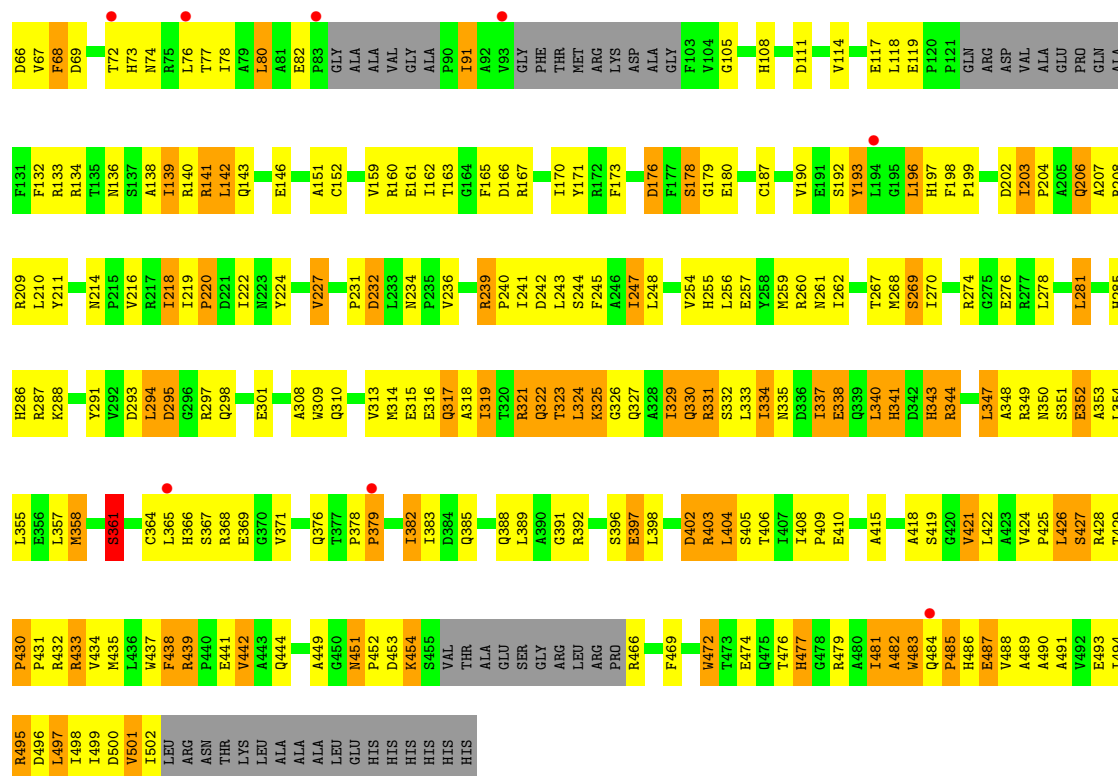
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB1



- Molecule 1: Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB1





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	174.40 Å 174.40 Å 95.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.02 – 3.40 49.02 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.02-3.40) 95.5 (49.02-3.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.268 , 0.322 0.278 , 0.331	Depositor DCC
R_{free} test set	1121 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	114.4	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 114.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.105 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7198	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	1/3716 (0.0%)	1.24	40/5057 (0.8%)
1	B	0.59	0/3546	1.28	39/4825 (0.8%)
All	All	0.57	1/7262 (0.0%)	1.26	79/9882 (0.8%)

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	1
1	B	0	3
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	PRO	CA-C	5.50	1.57	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	HIS	N-CA-C	-11.57	97.29	111.40
1	A	239	ARG	N-CA-C	10.72	120.68	108.25
1	B	427	SER	N-CA-C	10.36	124.04	111.40
1	A	377	THR	CA-C-N	9.69	130.36	120.38
1	A	377	THR	C-N-CA	9.69	130.36	120.38
1	A	378	PRO	CA-C-N	9.43	131.62	119.84
1	A	378	PRO	C-N-CA	9.43	131.62	119.84
1	B	50	GLU	N-CA-C	8.85	120.69	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ILE	N-CA-C	-8.41	102.62	110.53
1	A	464	ARG	CA-C-N	7.95	127.90	120.03
1	A	464	ARG	C-N-CA	7.95	127.90	120.03
1	A	334	ILE	N-CA-C	-7.60	104.45	111.67
1	B	482	ALA	N-CA-C	7.32	120.80	109.60
1	B	484	GLN	CA-C-N	-7.12	112.84	119.82
1	B	484	GLN	C-N-CA	-7.12	112.84	119.82
1	B	64	ALA	N-CA-C	7.07	122.16	112.90
1	B	37	ALA	N-CA-C	6.95	119.45	111.11
1	A	119	GLU	CA-C-N	6.90	127.49	120.38
1	A	119	GLU	C-N-CA	6.90	127.49	120.38
1	A	323	THR	N-CA-C	-6.90	104.12	112.54
1	A	428	ARG	N-CA-C	-6.62	100.51	110.24
1	A	68	PHE	N-CA-C	6.61	119.06	110.53
1	B	454	LYS	N-CA-C	6.60	120.15	110.59
1	B	426	LEU	N-CA-C	-6.59	97.78	108.52
1	B	334	ILE	N-CA-C	-6.50	105.50	111.67
1	A	41	ILE	N-CA-C	-6.48	100.34	108.89
1	B	325	LYS	N-CA-C	6.36	119.97	112.72
1	B	347	LEU	N-CA-C	6.23	117.74	111.07
1	A	427	SER	N-CA-C	6.17	117.92	108.42
1	A	48	LEU	CA-C-N	-6.07	112.60	119.28
1	A	48	LEU	C-N-CA	-6.07	112.60	119.28
1	B	48	LEU	N-CA-C	6.04	123.16	109.81
1	B	236	VAL	N-CA-C	5.99	116.16	110.53
1	A	358	MET	N-CA-C	-5.96	104.39	112.26
1	A	342	ASP	N-CA-C	-5.90	100.08	109.23
1	B	41	ILE	N-CA-C	5.89	117.06	108.58
1	A	40	THR	N-CA-C	-5.86	99.64	108.96
1	A	70	SER	N-CA-C	-5.81	106.36	113.50
1	A	434	VAL	N-CA-C	5.81	116.48	108.12
1	B	501	VAL	N-CA-C	5.76	116.41	110.82
1	B	294	LEU	N-CA-C	5.69	117.17	110.97
1	B	485	PRO	N-CA-C	5.66	121.28	113.98
1	B	424	VAL	CA-C-N	-5.64	114.16	120.14
1	B	424	VAL	C-N-CA	-5.64	114.16	120.14
1	A	89	ALA	C-N-CD	-5.63	108.21	120.60
1	A	322	GLN	N-CA-C	-5.62	105.54	112.90
1	A	450	GLY	CA-C-O	-5.61	118.09	122.52
1	A	476	THR	N-CA-C	5.55	118.28	109.24
1	B	82	GLU	N-CA-C	5.54	122.06	109.81
1	B	428	ARG	N-CA-C	5.53	118.36	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	SER	N-CA-C	-5.50	105.38	111.71
1	B	338	GLU	N-CA-C	-5.46	106.65	113.15
1	B	361	SER	N-CA-C	-5.43	105.44	111.36
1	B	352	GLU	N-CA-C	-5.42	106.37	112.87
1	B	178	SER	N-CA-C	-5.41	103.55	110.53
1	A	402	ASP	N-CA-C	-5.34	106.61	113.23
1	A	56	ILE	N-CA-C	5.28	116.01	110.62
1	A	430	PRO	N-CA-C	5.28	117.15	110.70
1	A	247	ILE	N-CA-C	-5.21	105.93	113.07
1	A	176	ASP	N-CA-C	5.21	118.73	112.38
1	A	429	THR	CA-C-N	5.20	125.74	120.38
1	A	429	THR	C-N-CA	5.20	125.74	120.38
1	B	430	PRO	CA-C-N	5.19	139.46	127.00
1	B	430	PRO	C-N-CA	5.19	139.46	127.00
1	A	41	ILE	CB-CA-C	5.16	117.86	111.15
1	B	318	ALA	N-CA-C	-5.12	105.78	112.23
1	B	301	GLU	N-CA-C	5.09	116.51	111.07
1	B	433	ARG	N-CA-C	-5.08	102.33	109.96
1	A	337	ILE	N-CA-C	-5.08	107.48	113.42
1	A	239	ARG	CB-CA-C	-5.07	102.11	109.97
1	A	326	GLY	N-CA-C	-5.07	106.95	115.62
1	A	153	ALA	N-CA-C	-5.06	107.05	113.18
1	B	439	ARG	CA-C-N	-5.06	115.57	120.98
1	B	439	ARG	C-N-CA	-5.06	115.57	120.98
1	B	42	VAL	N-CA-C	5.04	119.83	109.34
1	A	379	PRO	N-CA-C	5.02	122.82	112.47
1	B	208	ARG	N-CA-C	5.01	116.83	111.36
1	B	343	HIS	N-CA-C	5.01	119.46	112.90
1	B	337	ILE	N-CA-C	-5.00	107.57	113.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	HIS	Peptide
1	B	38	ASP	Peptide
1	B	426	LEU	Peptide
1	B	68	PHE	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	3639	0	3625	198	0
1	B	3473	0	3453	225	0
2	A	43	0	31	3	0
2	B	43	0	31	4	0
All	All	7198	0	7140	413	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 29.

All (413) 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:202:ASP:OD1	1:B:466:ARG:NH2	1.95	1.00
1:B:274:ARG:NH1	1:B:308:ALA:O	1.99	0.94
1:A:75:ARG:NH2	1:A:92:ALA:O	2.01	0.94
1:B:330:GLN:NE2	1:B:493:GLU:OE2	2.01	0.93
1:B:451:ASN:OD1	1:B:453:ASP:N	2.05	0.90
1:B:322:GLN:HG3	1:B:486:HIS:HA	1.53	0.88
1:B:338:GLU:HA	1:B:340:LEU:HD12	1.61	0.82
1:A:288:LYS:HD2	1:A:289:PRO:HD2	1.60	0.82
1:A:141:ARG:HH21	1:A:154:ALA:HA	1.45	0.80
1:B:163:THR:HG21	1:B:268:MET:HE1	1.62	0.80
1:B:483:TRP:HA	1:B:487:GLU:OE2	1.82	0.79
1:A:415:ALA:O	1:A:419:SER:OG	2.01	0.78
1:A:485:PRO:HA	1:A:488:VAL:HB	1.64	0.78
1:B:50:GLU:HG3	1:B:51:LEU:HG	1.65	0.78
1:B:430:PRO:HA	1:B:432:ARG:HB2	1.65	0.78
1:B:404:LEU:HD11	1:B:421:VAL:HB	1.66	0.78
1:A:270:ILE:HD11	1:A:300:CYS:HB3	1.64	0.78
1:A:66:ASP:OD1	1:A:66:ASP:N	2.14	0.77
1:A:219:ILE:HD11	1:A:222:ILE:HG22	1.66	0.77
1:A:214:ASN:O	1:A:217:ARG:NH1	2.18	0.77
1:A:476:THR:OG1	1:A:479:ARG:NH2	2.18	0.77
1:B:76:LEU:HG	1:B:91:ILE:HG12	1.66	0.76
1:A:439:ARG:NH1	1:A:487:GLU:OE2	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ARG:NH2	1:B:482:ALA:O	2.19	0.75
1:B:415:ALA:O	1:B:419:SER:OG	2.05	0.75
1:A:20:ILE:O	1:A:249:ARG:NH1	2.19	0.75
1:B:402:ASP:OD1	1:B:402:ASP:N	2.20	0.74
1:A:117:GLU:HB3	1:A:248:LEU:HD12	1.70	0.73
1:B:67:VAL:HG12	1:B:68:PHE:H	1.53	0.72
1:B:319:ILE:O	1:B:322:GLN:NE2	2.23	0.72
1:B:337:ILE:HG12	1:B:347:LEU:HA	1.71	0.72
1:A:368:ARG:HD3	1:A:432:ARG:HB3	1.72	0.71
1:B:485:PRO:HA	1:B:488:VAL:HB	1.72	0.71
1:B:261:ASN:ND2	1:B:466:ARG:O	2.23	0.71
1:A:70:SER:O	1:A:74:ASN:ND2	2.24	0.71
1:B:348:ALA:HA	1:B:351:SER:HB3	1.73	0.71
1:A:217:ARG:NH2	1:A:269:SER:OG	2.23	0.70
1:B:67:VAL:HB	1:B:73:HIS:HB2	1.73	0.70
1:A:484:GLN:HG3	1:A:486:HIS:HB3	1.73	0.70
1:B:36:ALA:HB3	1:B:40:THR:HG23	1.74	0.70
1:B:352:GLU:HA	1:B:355:LEU:HD12	1.73	0.70
1:A:333:LEU:HA	1:A:336:ASP:HB2	1.73	0.69
1:A:23:PRO:HD2	1:A:243:LEU:HD12	1.74	0.69
1:A:140:ARG:HA	1:A:143:GLN:HG3	1.75	0.69
1:B:232:ASP:HA	1:B:241:ILE:HG12	1.75	0.68
1:B:324:LEU:C	1:B:326:GLY:HA3	2.19	0.67
1:B:421:VAL:HG22	1:B:438:PHE:HB3	1.76	0.67
1:A:14:THR:HB	1:A:463:LEU:HD21	1.77	0.66
1:B:206:GLN:OE1	1:B:207:ALA:N	2.28	0.66
1:B:319:ILE:HD11	1:B:485:PRO:HG2	1.78	0.66
1:A:472:TRP:C	1:A:472:TRP:CD1	2.73	0.66
1:B:337:ILE:HD13	1:B:347:LEU:HD23	1.75	0.66
1:A:39:MET:SD	1:A:39:MET:N	2.69	0.66
1:A:314:MET:HA	1:A:317:GLN:HG2	1.77	0.66
1:B:391:GLY:HA3	1:B:432:ARG:HD3	1.77	0.66
1:B:176:ASP:OD1	1:B:176:ASP:N	2.27	0.65
1:A:361:SER:HB2	1:A:440:PRO:HD3	1.78	0.64
1:B:136:ASN:C	1:B:136:ASN:HD22	2.06	0.64
1:A:404:LEU:HD11	1:A:421:VAL:HB	1.80	0.63
1:B:485:PRO:O	1:B:489:ALA:N	2.28	0.63
1:B:449:ALA:HB1	1:B:469:PHE:HB3	1.81	0.63
1:A:382:ILE:O	1:A:386:LEU:HB2	1.97	0.62
1:A:429:THR:HG22	1:A:432:ARG:NH2	2.14	0.62
1:B:23:PRO:HD2	1:B:243:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ARG:HH11	1:B:344:ARG:HB2	1.65	0.62
1:B:495:ARG:NE	1:B:496:ASP:OD1	2.33	0.62
1:B:331:ARG:HA	1:B:334:ILE:HD12	1.81	0.62
1:A:129:GLN:NE2	1:B:295:ASP:OD2	2.32	0.61
1:B:36:ALA:N	1:B:40:THR:O	2.28	0.61
1:A:211:TYR:OH	2:A:900:BLA:HAD2	2.00	0.61
1:A:135:THR:HG21	1:B:132:PHE:CE2	2.36	0.61
1:B:77:THR:HA	1:B:80:LEU:HD23	1.81	0.61
1:B:165:PHE:HA	1:B:286:HIS:HD2	1.66	0.61
1:B:218:ILE:HG13	1:B:268:MET:HB2	1.83	0.61
1:A:103:PHE:HD2	1:A:118:LEU:HB3	1.63	0.61
1:B:454:LYS:HA	1:B:466:ARG:HD3	1.83	0.61
1:B:334:ILE:O	1:B:338:GLU:N	2.34	0.60
1:B:242:ASP:OD1	1:B:244:SER:OG	2.18	0.60
1:A:96:THR:HG1	1:A:100:ASP:N	1.99	0.60
1:A:476:THR:OG1	1:A:479:ARG:HD2	2.00	0.60
1:A:42:VAL:HG11	1:A:235:PRO:HD3	1.82	0.60
1:A:166:ASP:HB3	1:A:190:VAL:HG21	1.84	0.60
1:A:422:LEU:HB3	1:A:437:TRP:HB2	1.82	0.60
1:A:331:ARG:O	1:A:335:ASN:ND2	2.29	0.60
1:B:425:PRO:HA	1:B:434:VAL:HG22	1.83	0.59
1:B:67:VAL:CG1	1:B:68:PHE:H	2.16	0.59
1:B:211:TYR:OH	2:B:900:BLA:HAD2	2.01	0.59
1:A:343:HIS:CD2	1:A:344:ARG:HG2	2.38	0.59
1:A:450:GLY:HA2	1:A:451:ASN:HB2	1.85	0.59
1:B:439:ARG:NH1	1:B:487:GLU:OE1	2.36	0.59
1:B:449:ALA:O	1:B:469:PHE:HD1	1.86	0.59
1:B:490:ALA:O	1:B:494:ILE:HG13	2.03	0.59
1:A:403:ARG:HD3	1:A:479:ARG:CZ	2.33	0.58
1:A:203:ILE:HG22	1:A:208:ARG:HG3	1.84	0.58
1:B:15:CYS:SG	1:B:204:PRO:HB3	2.43	0.58
1:B:343:HIS:O	1:B:347:LEU:N	2.22	0.58
1:A:54:LEU:HB2	1:A:59:LEU:HD13	1.84	0.58
1:A:368:ARG:NH2	1:A:431:PRO:HA	2.18	0.58
1:B:73:HIS:O	1:B:77:THR:HG23	2.04	0.58
1:A:132:PHE:O	1:A:135:THR:OG1	2.18	0.58
1:B:41:ILE:HD13	1:B:62:ARG:NH2	2.19	0.58
1:B:403:ARG:HB3	1:B:406:THR:OG1	2.03	0.58
1:B:419:SER:OG	1:B:441:GLU:HB3	2.04	0.58
1:B:498:ILE:O	1:B:501:VAL:HB	2.03	0.58
1:A:377:THR:HG23	1:A:382:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB2	1:A:307:LEU:HD13	1.86	0.58
1:B:365:LEU:O	1:B:371:VAL:HA	2.04	0.58
1:A:380:GLY:H	1:A:381:PRO:HD2	1.68	0.57
1:B:491:ALA:HA	1:B:494:ILE:HD12	1.86	0.57
1:A:35:LEU:HD22	1:A:41:ILE:HG22	1.86	0.57
1:A:355:LEU:O	1:A:360:ALA:N	2.35	0.57
1:A:355:LEU:HD22	1:A:362:GLY:HA2	1.85	0.57
1:B:32:LEU:O	1:B:45:SER:HB3	2.04	0.57
1:B:74:ASN:O	1:B:78:ILE:HG13	2.05	0.57
1:A:382:ILE:HA	1:A:386:LEU:HD12	1.86	0.57
1:B:41:ILE:HD13	1:B:62:ARG:HH21	1.70	0.57
1:A:186:ARG:HH11	1:A:186:ARG:CG	2.18	0.57
1:A:259:MET:HE3	1:A:262:ILE:HG21	1.86	0.57
1:A:366:HIS:HE2	1:A:383:ILE:HG23	1.69	0.56
1:B:28:PRO:HD2	1:B:224:TYR:HD2	1.69	0.56
1:A:15:CYS:O	1:A:206:GLN:NE2	2.39	0.56
1:A:472:TRP:C	1:A:472:TRP:HD1	2.11	0.56
1:A:93:VAL:O	1:A:103:PHE:HB2	2.06	0.56
1:A:366:HIS:NE2	1:A:383:ILE:HG23	2.20	0.56
1:A:385:GLN:O	1:A:408:ILE:HD11	2.06	0.55
1:B:497:LEU:O	1:B:501:VAL:HG23	2.05	0.55
1:A:205:ALA:O	1:A:209:ARG:HG3	2.06	0.55
1:B:45:SER:O	1:B:49:PRO:HD3	2.06	0.55
1:B:64:ALA:C	1:B:66:ASP:H	2.14	0.55
1:B:216:VAL:HG23	1:B:270:ILE:HG13	1.89	0.55
1:B:325:LYS:N	1:B:326:GLY:HA3	2.22	0.55
1:B:330:GLN:HE21	1:B:497:LEU:HD21	1.72	0.55
1:A:403:ARG:HD3	1:A:479:ARG:HG3	1.89	0.55
1:A:94:GLY:HA2	1:A:101:ALA:O	2.06	0.55
1:B:26:ILE:HG21	1:B:32:LEU:HD23	1.89	0.55
1:A:406:THR:HB	1:A:407:ILE:HD12	1.89	0.55
1:B:35:LEU:HA	1:B:41:ILE:HA	1.89	0.55
1:B:64:ALA:C	1:B:66:ASP:N	2.65	0.54
1:B:39:MET:C	1:B:64:ALA:HB3	2.32	0.54
1:B:351:SER:HA	1:B:354:LEU:HG	1.90	0.54
1:A:387:ALA:HA	1:A:390:ALA:HB2	1.89	0.54
1:B:68:PHE:HB2	1:B:72:THR:OG1	2.07	0.54
1:A:429:THR:HB	1:A:430:PRO:HD2	1.90	0.54
1:A:47:ASN:O	1:A:50:GLU:HG2	2.08	0.54
1:B:32:LEU:HD13	1:B:117:GLU:HG2	1.90	0.54
1:B:67:VAL:HG12	1:B:68:PHE:N	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ILE:HG22	1:B:383:ILE:HG13	1.89	0.54
1:A:234:ASN:HB2	1:A:239:ARG:HB2	1.89	0.54
1:A:324:LEU:O	1:A:327:GLN:HB2	2.07	0.54
1:A:218:ILE:HG13	1:A:268:MET:HB2	1.88	0.53
1:A:222:ILE:HB	1:A:256:LEU:HD22	1.89	0.53
1:A:298:GLN:HA	1:B:140:ARG:NH2	2.23	0.53
1:A:259:MET:HE2	1:A:267:THR:HG21	1.90	0.53
1:A:429:THR:HG22	1:A:432:ARG:CZ	2.37	0.53
1:B:138:ALA:O	1:B:142:LEU:HB2	2.08	0.53
1:A:135:THR:O	1:A:139:ILE:N	2.42	0.53
1:A:326:GLY:O	1:A:330:GLN:HB3	2.08	0.53
1:A:353:ALA:O	1:A:356:GLU:HG3	2.08	0.53
1:A:382:ILE:HD11	1:A:438:PHE:CZ	2.43	0.53
1:A:426:LEU:HD13	1:A:495:ARG:HD2	1.90	0.53
1:B:324:LEU:O	1:B:327:GLN:N	2.42	0.53
1:B:404:LEU:HD13	1:B:418:ALA:O	2.08	0.53
1:A:68:PHE:HA	1:A:95:PHE:HB2	1.90	0.53
1:A:436:LEU:HD13	1:A:438:PHE:HE1	1.73	0.53
1:A:270:ILE:CD1	1:A:300:CYS:HB3	2.38	0.53
1:A:331:ARG:HA	1:A:334:ILE:HD12	1.90	0.53
1:B:331:ARG:O	1:B:335:ASN:ND2	2.40	0.53
1:A:104:VAL:HB	1:A:119:GLU:HB3	1.90	0.52
1:A:391:GLY:O	1:A:392:ARG:HG2	2.09	0.52
1:A:74:ASN:O	1:A:77:THR:OG1	2.23	0.52
1:A:23:PRO:HB2	1:A:250:SER:HB3	1.92	0.52
1:B:134:ARG:NH2	1:B:161:GLU:O	2.41	0.52
1:B:347:LEU:O	1:B:351:SER:N	2.43	0.52
1:B:358:MET:HE1	1:B:491:ALA:HB2	1.92	0.52
1:A:109:ARG:HG2	1:A:114:VAL:HG22	1.92	0.52
1:A:107:TRP:HB3	1:A:116:LEU:HD23	1.91	0.51
1:A:358:MET:HE1	1:A:491:ALA:HB2	1.92	0.51
1:B:348:ALA:HA	1:B:351:SER:CB	2.39	0.51
1:A:210:LEU:O	1:A:214:ASN:N	2.34	0.51
1:B:171:TYR:OH	1:B:198:PHE:HB2	2.10	0.51
1:A:135:THR:O	1:A:139:ILE:HG13	2.11	0.51
1:A:197:HIS:HB3	1:A:448:TRP:CE3	2.45	0.51
1:A:271:SER:HA	1:A:281:LEU:HD12	1.92	0.51
1:B:232:ASP:O	1:B:240:PRO:HA	2.10	0.51
1:A:41:ILE:HD12	1:A:41:ILE:O	2.11	0.51
1:A:327:GLN:O	1:A:330:GLN:NE2	2.43	0.51
1:B:31:LEU:CB	1:B:48:LEU:HB3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:VAL:HA	1:B:162:ILE:HG12	1.93	0.51
1:A:15:CYS:HB3	1:A:204:PRO:HB3	1.91	0.51
1:A:448:TRP:CD1	1:A:448:TRP:N	2.79	0.51
1:B:72:THR:O	1:B:76:LEU:HD22	2.11	0.51
1:B:152:CYS:HB3	1:B:170:ILE:HG21	1.92	0.50
1:B:354:LEU:HA	1:B:357:LEU:HG	1.92	0.50
1:B:403:ARG:HD2	1:B:479:ARG:HG2	1.93	0.50
1:B:29:HIS:CG	1:B:291:TYR:HE2	2.30	0.50
1:B:210:LEU:O	1:B:214:ASN:N	2.39	0.50
1:A:358:MET:HE3	1:A:487:GLU:O	2.12	0.50
1:A:301:GLU:OE1	1:B:140:ARG:NE	2.44	0.50
1:B:493:GLU:O	1:B:497:LEU:HD22	2.12	0.50
1:A:74:ASN:O	1:A:78:ILE:HG22	2.11	0.50
1:A:320:THR:O	1:A:323:THR:HG22	2.12	0.50
1:B:39:MET:O	1:B:64:ALA:HB3	2.12	0.50
1:B:442:VAL:HB	1:B:481:ILE:HG22	1.94	0.50
1:B:421:VAL:CG2	1:B:438:PHE:HB3	2.41	0.50
1:A:255:HIS:HD1	1:A:258:TYR:HD2	1.59	0.50
1:B:371:VAL:HG11	1:B:383:ILE:HG12	1.93	0.50
1:A:259:MET:HE1	1:A:285:HIS:NE2	2.27	0.49
1:A:402:ASP:O	1:A:480:ALA:N	2.40	0.49
1:A:171:TYR:CZ	1:A:179:GLY:HA3	2.46	0.49
1:B:66:ASP:CG	1:B:66:ASP:O	2.54	0.49
1:B:167:ARG:HB3	1:B:285:HIS:HB2	1.94	0.49
1:B:173:PHE:CE2	1:B:278:LEU:HG	2.47	0.49
1:B:40:THR:HA	1:B:64:ALA:H	1.77	0.49
1:A:403:ARG:HG3	1:A:479:ARG:HG3	1.94	0.49
1:A:56:ILE:O	1:A:60:ILE:HG12	2.13	0.49
1:B:43:ALA:HB1	1:B:231:PRO:HD2	1.94	0.49
1:B:422:LEU:HD23	1:B:437:TRP:CE3	2.47	0.49
1:A:188:ALA:O	1:A:189:GLU:HG3	2.13	0.49
1:B:108:HIS:CD2	1:B:245:PHE:HB2	2.48	0.49
1:A:49:PRO:HG3	1:A:55:ALA:HA	1.93	0.49
1:A:108:HIS:NE2	1:A:245:PHE:HB2	2.28	0.48
1:B:47:ASN:HA	1:B:227:VAL:HG11	1.94	0.48
1:A:80:LEU:O	1:A:109:ARG:NH2	2.43	0.48
1:A:403:ARG:HD3	1:A:479:ARG:NE	2.28	0.48
1:B:27:GLN:HG2	1:B:224:TYR:CE2	2.48	0.48
1:B:72:THR:O	1:B:76:LEU:HB2	2.13	0.48
1:A:449:ALA:HB1	1:A:469:PHE:HD1	1.78	0.48
1:B:40:THR:HA	1:B:64:ALA:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASP:HB2	1:B:286:HIS:HA	1.95	0.48
1:B:408:ILE:O	1:B:408:ILE:HG13	2.13	0.48
1:B:454:LYS:HG2	1:B:466:ARG:NH1	2.28	0.48
1:B:173:PHE:HE2	1:B:278:LEU:HG	1.78	0.48
1:A:311:ILE:O	1:A:315:GLU:HB2	2.14	0.48
1:A:366:HIS:HE1	1:A:368:ARG:HA	1.78	0.48
1:B:495:ARG:O	1:B:499:ILE:HG13	2.13	0.48
1:A:403:ARG:HE	1:A:403:ARG:HB2	1.56	0.48
1:B:45:SER:O	1:B:48:LEU:HG	2.14	0.47
1:B:139:ILE:O	1:B:143:GLN:HG3	2.14	0.47
1:B:335:ASN:HA	1:B:338:GLU:HB3	1.96	0.47
1:B:269:SER:OG	2:B:900:BLA:O2A	2.22	0.47
1:A:32:LEU:HD13	1:A:117:GLU:HG2	1.95	0.47
1:B:429:THR:HA	1:B:432:ARG:HE	1.79	0.47
1:A:20:ILE:HD13	1:A:20:ILE:HA	1.70	0.47
1:B:41:ILE:HD12	1:B:64:ALA:HA	1.95	0.47
1:B:67:VAL:HB	1:B:73:HIS:CB	2.43	0.47
1:B:67:VAL:HB	1:B:73:HIS:CG	2.49	0.47
1:B:141:ARG:HG2	1:B:141:ARG:HH11	1.80	0.47
1:B:369:GLU:OE2	1:B:369:GLU:N	2.48	0.47
1:A:42:VAL:HG11	1:A:235:PRO:CD	2.45	0.47
1:A:186:ARG:HH11	1:A:186:ARG:HG3	1.79	0.47
1:A:297:ARG:HA	1:A:300:CYS:HB2	1.97	0.47
1:A:337:ILE:HG12	1:A:343:HIS:HA	1.95	0.47
1:B:31:LEU:O	1:B:118:LEU:HB2	2.14	0.47
1:B:141:ARG:HH11	1:B:141:ARG:CG	2.27	0.47
1:B:293:ASP:O	1:B:297:ARG:HG3	2.14	0.47
1:B:435:MET:HE1	1:B:498:ILE:HD12	1.96	0.47
1:B:451:ASN:OD1	1:B:451:ASN:C	2.58	0.47
1:A:41:ILE:HD12	1:A:41:ILE:C	2.40	0.47
1:B:222:ILE:O	1:B:256:LEU:HD22	2.14	0.47
1:A:176:ASP:O	1:A:177:PHE:HB2	2.14	0.47
1:A:112:GLN:HB2	1:A:236:VAL:HG11	1.95	0.46
1:A:49:PRO:HA	1:A:54:LEU:O	2.15	0.46
1:A:249:ARG:HH22	2:A:900:BLA:CGD	2.29	0.46
1:B:378:PRO:HA	1:B:379:PRO:HD3	1.60	0.46
1:A:95:PHE:C	1:A:95:PHE:CD1	2.94	0.46
1:A:305:GLN:NE2	1:B:143:GLN:OE1	2.49	0.46
1:B:203:ILE:N	1:B:203:ILE:HD12	2.30	0.46
1:A:51:LEU:HD23	1:A:95:PHE:CZ	2.51	0.46
1:A:62:ARG:HD2	1:A:62:ARG:HA	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:SER:OG	1:B:439:ARG:HA	2.16	0.46
1:A:103:PHE:CD2	1:A:118:LEU:HB3	2.48	0.46
1:B:141:ARG:HG2	1:B:141:ARG:NH1	2.31	0.46
1:B:477:HIS:ND1	1:B:477:HIS:N	2.61	0.46
1:A:25:ALA:HA	1:A:228:PRO:HA	1.97	0.46
1:A:284:CYS:O	1:A:285:HIS:HD2	1.98	0.46
1:B:21:HIS:C	1:B:23:PRO:HD3	2.41	0.46
1:B:31:LEU:HB3	1:B:48:LEU:HB3	1.98	0.46
1:B:179:GLY:O	1:B:197:HIS:HA	2.16	0.45
1:B:321:ARG:O	1:B:321:ARG:HG2	2.16	0.45
1:B:378:PRO:HG2	1:B:382:ILE:HG13	1.97	0.45
1:A:429:THR:CB	1:A:430:PRO:HD2	2.46	0.45
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.70	0.45
1:A:447:TYR:HB3	1:A:473:THR:HG22	1.98	0.45
1:B:180:GLU:HA	1:B:196:LEU:O	2.15	0.45
1:A:428:ARG:HD3	1:A:428:ARG:HA	1.74	0.45
1:B:117:GLU:OE2	1:B:247:ILE:N	2.46	0.45
1:B:192:SER:C	1:B:193:TYR:HD1	2.25	0.45
1:B:232:ASP:HA	1:B:241:ILE:CG1	2.45	0.45
1:B:295:ASP:HA	1:B:298:GLN:OE1	2.17	0.45
1:B:385:GLN:NE2	1:B:410:GLU:OE2	2.35	0.45
1:A:274:ARG:HD2	1:A:311:ILE:HG22	1.98	0.45
1:B:220:PRO:HG2	1:B:291:TYR:CE2	2.52	0.45
1:A:299:ALA:O	1:A:302:LEU:HB3	2.17	0.44
1:B:351:SER:O	1:B:355:LEU:N	2.43	0.44
1:A:20:ILE:HD11	1:A:252:SER:HB2	2.00	0.44
1:B:314:MET:HA	1:B:317:GLN:HE22	1.82	0.44
1:B:33:LEU:HG	1:B:48:LEU:CD2	2.47	0.44
1:B:494:ILE:HA	1:B:497:LEU:HD22	1.99	0.44
1:A:16:ASP:HB3	1:A:205:ALA:HB3	1.98	0.44
1:A:342:ASP:OD1	1:A:344:ARG:HG3	2.18	0.44
1:B:28:PRO:HA	1:B:47:ASN:ND2	2.33	0.44
1:B:160:ARG:NH1	1:B:187:CYS:SG	2.90	0.44
1:B:366:HIS:HB3	1:B:434:VAL:O	2.18	0.44
1:A:325:LYS:H	1:A:325:LYS:HG3	1.51	0.44
1:B:451:ASN:HA	1:B:452:PRO:HD3	1.77	0.44
1:A:52:THR:HG21	1:A:67:VAL:HG13	1.99	0.44
1:A:69:ASP:HB2	1:A:94:GLY:O	2.18	0.44
1:A:285:HIS:NE2	2:A:900:BLA:OB	2.51	0.44
1:A:404:LEU:N	1:A:419:SER:O	2.51	0.44
1:A:93:VAL:HG12	1:A:95:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:HE1	1:B:132:PHE:CD1	2.36	0.43
1:B:357:LEU:HB2	1:B:358:MET:HG2	2.00	0.43
1:B:397:GLU:HA	1:B:397:GLU:OE1	2.18	0.43
1:B:136:ASN:HA	1:B:139:ILE:HG12	1.99	0.43
1:B:142:LEU:HD21	1:B:151:ALA:O	2.19	0.43
1:B:28:PRO:HD2	1:B:224:TYR:HB2	1.98	0.43
1:B:35:LEU:HG	1:B:114:VAL:HB	2.00	0.43
1:A:219:ILE:O	1:A:219:ILE:HG13	2.16	0.43
1:A:309:TRP:CD1	1:B:309:TRP:CD2	3.07	0.43
1:B:163:THR:C	1:B:165:PHE:H	2.26	0.43
1:B:322:GLN:HG2	1:B:323:THR:N	2.30	0.43
1:A:298:GLN:O	1:B:136:ASN:OD1	2.37	0.43
1:A:378:PRO:O	1:A:382:ILE:HD12	2.18	0.43
1:B:259:MET:HA	1:B:262:ILE:HG22	2.00	0.43
1:A:51:LEU:HD23	1:A:95:PHE:HZ	1.84	0.43
1:A:167:ARG:HH21	1:A:190:VAL:CG1	2.31	0.43
1:A:318:ALA:HB1	1:A:486:HIS:CD2	2.54	0.43
1:B:28:PRO:HD2	1:B:224:TYR:CD2	2.50	0.43
1:B:472:TRP:CH2	1:B:474:GLU:HG3	2.53	0.43
1:A:222:ILE:HG23	1:A:265:HIS:O	2.19	0.43
1:A:466:ARG:NH2	1:A:469:PHE:HE1	2.16	0.43
1:A:495:ARG:O	1:A:499:ILE:HG13	2.18	0.43
1:B:199:PRO:HG2	1:B:466:ARG:NH2	2.33	0.43
1:B:310:GLN:O	1:B:313:VAL:HB	2.18	0.43
1:B:378:PRO:O	1:B:382:ILE:HD12	2.18	0.43
1:B:62:ARG:NH1	1:B:62:ARG:HB2	2.33	0.42
1:A:306:VAL:O	1:A:309:TRP:HB3	2.19	0.42
1:A:351:SER:O	1:A:355:LEU:HG	2.19	0.42
1:B:202:ASP:HA	2:B:900:BLA:C1C	2.50	0.42
1:B:234:ASN:N	1:B:239:ARG:O	2.35	0.42
1:B:48:LEU:O	1:B:52:THR:HG23	2.19	0.42
1:B:67:VAL:CG1	1:B:68:PHE:N	2.80	0.42
1:B:351:SER:C	1:B:353:ALA:N	2.77	0.42
1:A:73:HIS:O	1:A:77:THR:HG23	2.19	0.42
1:A:186:ARG:NE	1:A:192:SER:HB2	2.34	0.42
1:A:202:ASP:O	1:A:203:ILE:HG13	2.19	0.42
1:B:388:GLN:HB3	1:B:392:ARG:NH1	2.35	0.42
1:A:219:ILE:HA	1:A:220:PRO:HD3	1.76	0.42
1:A:420:GLY:HA3	1:A:480:ALA:HB2	2.01	0.42
1:A:295:ASP:OD1	1:B:133:ARG:HG2	2.19	0.42
1:A:68:PHE:HB3	1:A:72:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:HIS:ND1	1:A:366:HIS:C	2.77	0.42
1:B:33:LEU:HG	1:B:48:LEU:HD21	2.02	0.42
1:A:330:GLN:HB3	1:A:330:GLN:HE21	1.61	0.42
1:B:132:PHE:CD1	1:B:132:PHE:C	2.98	0.42
1:B:368:ARG:CZ	1:B:431:PRO:HB3	2.49	0.42
1:A:484:GLN:HG3	1:A:486:HIS:CB	2.46	0.42
1:B:276:GLU:HG2	1:B:276:GLU:O	2.20	0.42
1:B:294:LEU:HA	1:B:297:ARG:CZ	2.50	0.42
1:A:202:ASP:OD2	1:A:466:ARG:NH2	2.48	0.41
1:A:422:LEU:HD11	1:A:488:VAL:HG22	2.00	0.41
1:B:254:VAL:O	1:B:257:GLU:HB3	2.19	0.41
1:B:330:GLN:O	1:B:334:ILE:HG13	2.19	0.41
1:B:343:HIS:HB2	1:B:347:LEU:HD12	2.02	0.41
1:B:134:ARG:H	1:B:134:ARG:HG3	1.53	0.41
1:B:278:LEU:HD11	1:B:281:LEU:HD12	2.02	0.41
1:A:20:ILE:HG23	1:A:249:ARG:NH1	2.34	0.41
1:B:315:GLU:O	1:B:319:ILE:HD13	2.20	0.41
1:A:69:ASP:HB2	1:A:72:THR:HG22	2.02	0.41
1:A:353:ALA:HA	1:A:356:GLU:HG3	2.01	0.41
1:B:47:ASN:HB2	1:B:227:VAL:HB	2.02	0.41
1:B:67:VAL:O	1:B:69:ASP:HA	2.21	0.41
1:B:91:ILE:HG22	1:B:105:GLY:O	2.20	0.41
1:A:38:ASP:OD1	1:A:38:ASP:N	2.53	0.41
1:A:197:HIS:O	1:A:448:TRP:HB3	2.21	0.41
1:B:405:SER:O	1:B:409:PRO:HA	2.20	0.41
1:A:117:GLU:OE2	1:A:248:LEU:HB2	2.21	0.41
1:A:210:LEU:HA	1:A:213:ILE:HG12	2.02	0.41
1:B:451:ASN:OD1	1:B:453:ASP:HB2	2.20	0.41
1:B:487:GLU:O	1:B:490:ALA:HB3	2.21	0.41
1:A:32:LEU:HD12	1:A:116:LEU:O	2.21	0.41
1:A:56:ILE:H	1:A:56:ILE:HG13	1.41	0.41
1:A:498:ILE:O	1:A:502:ILE:HG13	2.21	0.41
1:B:314:MET:HA	1:B:317:GLN:NE2	2.36	0.41
1:B:367:SER:HA	1:B:433:ARG:HG2	2.02	0.41
1:A:366:HIS:CE1	1:A:368:ARG:HA	2.56	0.41
1:B:31:LEU:HB2	1:B:48:LEU:HB3	2.01	0.41
1:B:65:ALA:HA	1:B:73:HIS:CD2	2.56	0.41
1:A:170:ILE:HG23	1:A:183:ALA:HB3	2.02	0.41
1:A:232:ASP:O	1:A:240:PRO:HA	2.21	0.41
1:A:258:TYR:O	1:A:261:ASN:HB2	2.20	0.41
1:A:495:ARG:HD2	1:A:495:ARG:HH11	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HB2	1:B:117:GLU:HA	2.03	0.41
1:B:193:TYR:N	1:B:193:TYR:CD1	2.89	0.41
1:B:316:GLU:HA	1:B:319:ILE:HB	2.03	0.41
1:B:358:MET:HE3	1:B:358:MET:HB3	1.84	0.41
1:B:430:PRO:HB2	1:B:431:PRO:CA	2.51	0.41
1:B:349:ARG:HG2	1:B:350:ASN:OD1	2.21	0.41
1:A:72:THR:O	1:A:76:LEU:HG	2.21	0.40
1:A:205:ALA:HB1	1:A:209:ARG:CZ	2.51	0.40
1:A:402:ASP:OD2	1:A:479:ARG:HG2	2.21	0.40
1:B:219:ILE:HD11	1:B:224:TYR:CE1	2.56	0.40
1:A:277:ARG:HD2	1:A:277:ARG:HA	1.89	0.40
1:A:305:GLN:HG2	1:B:143:GLN:HE22	1.85	0.40
1:A:437:TRP:CD1	1:A:437:TRP:N	2.89	0.40
1:A:108:HIS:HD2	1:A:110:HIS:HB2	1.85	0.40
1:A:463:LEU:H	1:A:463:LEU:HG	1.63	0.40
1:B:255:HIS:HE1	2:B:900:BLA:O1A	2.04	0.40
1:B:329:ILE:O	1:B:332:SER:HB3	2.21	0.40
1:B:344:ARG:HB2	1:B:344:ARG:NH1	2.35	0.40
1:A:39:MET:HB3	1:A:64:ALA:HB2	2.03	0.40
1:B:190:VAL:HG22	1:B:287:ARG:HD3	2.03	0.40
1:B:403:ARG:CD	1:B:479:ARG:HG2	2.51	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	463/519 (89%)	429 (93%)	30 (6%)	4 (1%)	14	42
1	B	436/519 (84%)	398 (91%)	34 (8%)	4 (1%)	14	42
All	All	899/1038 (87%)	827 (92%)	64 (7%)	8 (1%)	14	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	379	PRO
1	A	430	PRO
1	B	111	ASP
1	B	379	PRO
1	A	220	PRO
1	B	220	PRO
1	B	61	GLY

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	382/418 (91%)	303 (79%)	79 (21%)	1	4
1	B	368/418 (88%)	295 (80%)	73 (20%)	1	5
All	All	750/836 (90%)	598 (80%)	152 (20%)	1	4

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	22	ILE
1	A	31	LEU
1	A	35	LEU
1	A	38	ASP
1	A	39	MET
1	A	41	ILE
1	A	51	LEU
1	A	56	ILE
1	A	59	LEU
1	A	62	ARG
1	A	66	ASP
1	A	76	LEU
1	A	78	ILE
1	A	80	LEU

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Mol	Chain	Res	Type
1	A	91	ILE
1	A	95	PHE
1	A	106	SER
1	A	133	ARG
1	A	136	ASN
1	A	146	GLU
1	A	147	THR
1	A	150	SER
1	A	170	ILE
1	A	186	ARG
1	A	189	GLU
1	A	191	GLU
1	A	193	TYR
1	A	196	LEU
1	A	206	GLN
1	A	210	LEU
1	A	218	ILE
1	A	219	ILE
1	A	232	ASP
1	A	234	ASN
1	A	239	ARG
1	A	247	ILE
1	A	267	THR
1	A	269	SER
1	A	281	LEU
1	A	298	GLN
1	A	302	LEU
1	A	319	ILE
1	A	321	ARG
1	A	323	THR
1	A	325	LYS
1	A	329	ILE
1	A	330	GLN
1	A	347	LEU
1	A	351	SER
1	A	356	GLU
1	A	358	MET
1	A	364	CYS
1	A	366	HIS
1	A	371	VAL
1	A	376	GLN
1	A	377	THR

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Mol	Chain	Res	Type
1	A	382	ILE
1	A	396	SER
1	A	398	LEU
1	A	404	LEU
1	A	410	GLU
1	A	421	VAL
1	A	426	LEU
1	A	428	ARG
1	A	432	ARG
1	A	436	LEU
1	A	439	ARG
1	A	447	TYR
1	A	448	TRP
1	A	463	LEU
1	A	468	SER
1	A	472	TRP
1	A	474	GLU
1	A	479	ARG
1	A	481	ILE
1	A	484	GLN
1	A	495	ARG
1	A	503	LEU
1	B	22	ILE
1	B	31	LEU
1	B	32	LEU
1	B	35	LEU
1	B	40	THR
1	B	45	SER
1	B	52	THR
1	B	80	LEU
1	B	91	ILE
1	B	119	GLU
1	B	141	ARG
1	B	142	LEU
1	B	146	GLU
1	B	176	ASP
1	B	178	SER
1	B	193	TYR
1	B	196	LEU
1	B	203	ILE
1	B	206	GLN
1	B	209	ARG

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Mol	Chain	Res	Type
1	B	218	ILE
1	B	227	VAL
1	B	232	ASP
1	B	239	ARG
1	B	247	ILE
1	B	248	LEU
1	B	260	ARG
1	B	267	THR
1	B	269	SER
1	B	281	LEU
1	B	288	LYS
1	B	295	ASP
1	B	317	GLN
1	B	319	ILE
1	B	321	ARG
1	B	322	GLN
1	B	323	THR
1	B	324	LEU
1	B	329	ILE
1	B	330	GLN
1	B	331	ARG
1	B	333	LEU
1	B	340	LEU
1	B	341	HIS
1	B	344	ARG
1	B	358	MET
1	B	361	SER
1	B	364	CYS
1	B	376	GLN
1	B	382	ILE
1	B	389	LEU
1	B	396	SER
1	B	397	GLU
1	B	398	LEU
1	B	402	ASP
1	B	403	ARG
1	B	404	LEU
1	B	421	VAL
1	B	427	SER
1	B	438	PHE
1	B	442	VAL
1	B	444	GLN

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Mol	Chain	Res	Type
1	B	451	ASN
1	B	472	TRP
1	B	476	THR
1	B	477	HIS
1	B	481	ILE
1	B	483	TRP
1	B	487	GLU
1	B	495	ARG
1	B	497	LEU
1	B	500	ASP
1	B	502	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	305	GLN
1	A	330	GLN
1	A	385	GLN
1	A	486	HIS
1	B	27	GLN
1	B	29	HIS
1	B	136	ASN
1	B	143	GLN
1	B	327	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	46,46,46	2.68	14 (30%)	66,67,67	1.91	15 (22%)
2	BLA	B	900	1	46,46,46	2.69	14 (30%)	66,67,67	1.95	19 (28%)

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	-	8/26/74/74	0/4/4/4
2	BLA	B	900	1	-	12/26/74/74	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	CHD-C4C	6.83	1.54	1.37
2	A	900	BLA	CHB-C4A	6.75	1.55	1.40
2	B	900	BLA	CHD-C4C	6.67	1.53	1.37
2	A	900	BLA	CHB-C1B	6.55	1.53	1.37
2	B	900	BLA	CHB-C1B	6.50	1.53	1.37
2	B	900	BLA	CHB-C4A	6.26	1.54	1.40
2	A	900	BLA	CHD-C1D	6.18	1.54	1.40
2	B	900	BLA	CHD-C1D	5.69	1.53	1.40
2	A	900	BLA	CBC-CAC	4.93	1.54	1.30
2	B	900	BLA	CBC-CAC	4.88	1.53	1.30
2	A	900	BLA	C1C-C2C	-4.17	1.38	1.48
2	B	900	BLA	C4D-C3D	-4.09	1.39	1.45
2	B	900	BLA	C1C-C2C	-4.07	1.38	1.48
2	B	900	BLA	C1D-C2D	-4.03	1.37	1.45
2	B	900	BLA	C1B-C2B	-3.31	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C1D-C2D	-3.28	1.38	1.45
2	B	900	BLA	C3C-C4C	-3.24	1.39	1.45
2	A	900	BLA	C1B-C2B	-3.14	1.39	1.45
2	A	900	BLA	CAB-C3B	-3.00	1.39	1.47
2	A	900	BLA	C3C-C4C	-2.93	1.40	1.45
2	B	900	BLA	CAC-C3C	2.90	1.55	1.47
2	B	900	BLA	CAB-C3B	-2.83	1.39	1.47
2	A	900	BLA	CAC-C3C	2.73	1.54	1.47
2	A	900	BLA	C4A-NA	-2.58	1.33	1.37
2	B	900	BLA	C1A-NA	-2.56	1.33	1.37
2	A	900	BLA	C4D-C3D	-2.40	1.42	1.45
2	B	900	BLA	C4A-NA	-2.38	1.33	1.37
2	A	900	BLA	C1B-NB	-2.07	1.34	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C4A-CHB-C1B	-5.86	113.95	130.82
2	B	900	BLA	C4A-CHB-C1B	-5.43	115.19	130.82
2	A	900	BLA	CHA-C4D-ND	5.33	135.79	124.60
2	B	900	BLA	C1A-CHA-C4D	-4.67	118.03	128.22
2	B	900	BLA	CHD-C1D-ND	4.64	134.99	124.95
2	A	900	BLA	C1A-CHA-C4D	-4.51	118.37	128.22
2	A	900	BLA	C4C-CHD-C1D	-4.20	117.75	128.06
2	B	900	BLA	CAD-C3D-C4D	3.99	132.03	125.02
2	A	900	BLA	CHA-C4D-C3D	-3.69	116.88	125.40
2	B	900	BLA	CHD-C4C-C3C	-3.53	117.86	127.94
2	A	900	BLA	CHD-C1D-ND	3.27	132.03	124.95
2	B	900	BLA	C1D-C2D-C3D	3.14	110.04	106.48
2	A	900	BLA	CMA-C3A-C4A	3.03	130.03	125.62
2	B	900	BLA	CHA-C4D-ND	3.01	130.92	124.60
2	B	900	BLA	CHD-C4C-NC	2.91	132.25	126.06
2	A	900	BLA	C1D-C2D-C3D	2.87	109.74	106.48
2	A	900	BLA	CAD-CBD-CGD	-2.59	106.79	113.67
2	B	900	BLA	C4C-NC-C1C	-2.57	107.51	110.66
2	A	900	BLA	C3D-C4D-ND	-2.51	106.48	110.04
2	B	900	BLA	CAD-C3D-C2D	-2.48	123.21	127.87
2	B	900	BLA	C3B-C4B-NB	2.48	109.25	106.13
2	B	900	BLA	CMA-C3A-C4A	2.47	129.21	125.62
2	B	900	BLA	CHD-C1D-C2D	-2.37	118.79	124.87
2	A	900	BLA	CBC-CAC-C3C	-2.31	116.00	127.53
2	A	900	BLA	C4D-ND-C1D	2.27	110.69	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	CHA-C1A-C2A	-2.25	122.38	127.22
2	B	900	BLA	CBC-CAC-C3C	-2.25	116.31	127.53
2	A	900	BLA	C3B-C4B-NB	2.20	108.89	106.13
2	B	900	BLA	C4D-ND-C1D	2.18	110.53	106.52
2	A	900	BLA	CHA-C1A-C2A	-2.14	122.61	127.22
2	B	900	BLA	CHB-C4A-C3A	2.13	132.75	127.53
2	B	900	BLA	CHA-C4D-C3D	-2.12	120.50	125.40
2	B	900	BLA	O1D-CGD-CBD	-2.05	116.59	123.09
2	A	900	BLA	CHB-C4A-C3A	2.01	132.45	127.53

There are no chirality outliers.

All (20) torsion outliers are listed below:

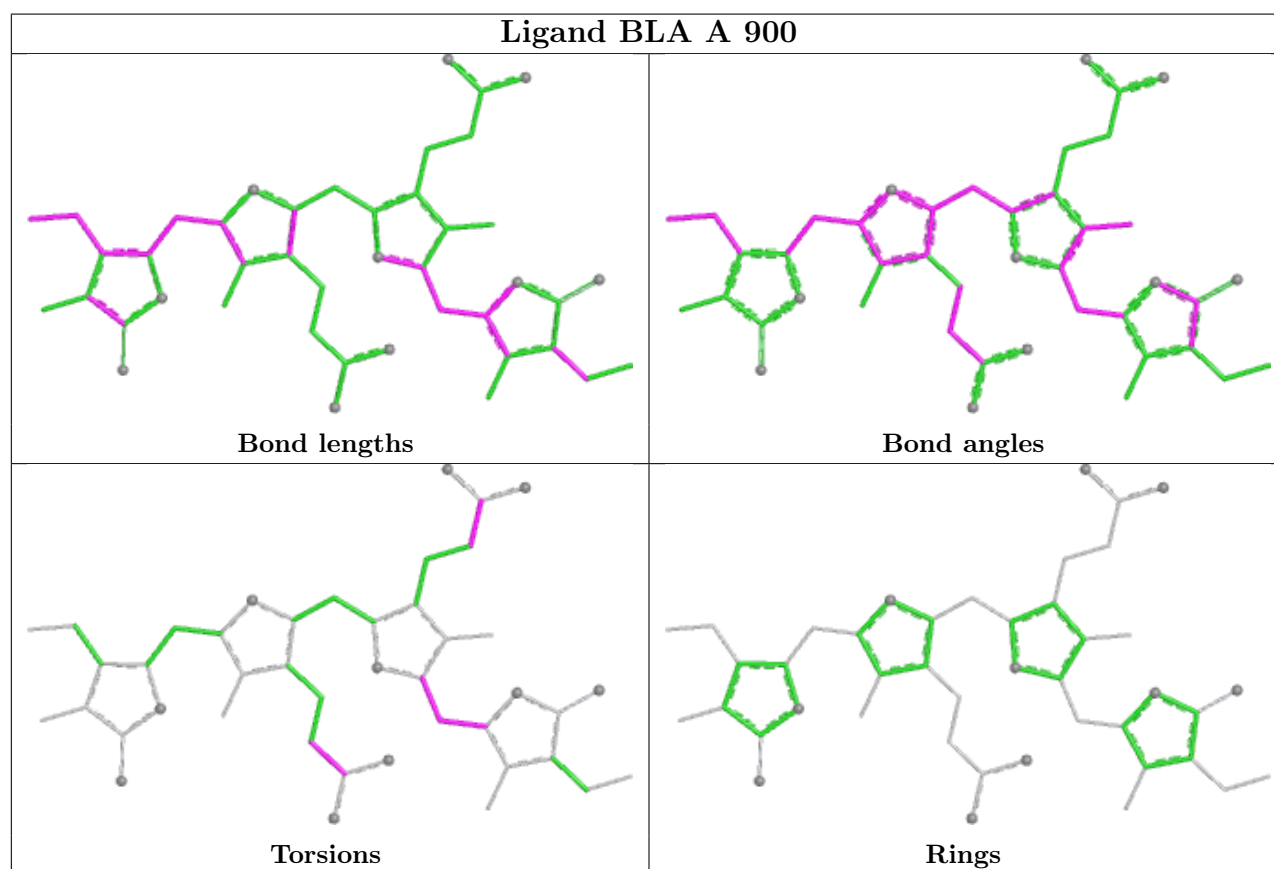
Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	C2B-C1B-CHB-C4A
2	B	900	BLA	NC-C4C-CHD-C1D
2	B	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	C3C-C4C-CHD-C1D
2	A	900	BLA	CAA-CBA-CGA-O1A
2	A	900	BLA	CAA-CBA-CGA-O2A
2	A	900	BLA	CAD-CBD-CGD-O2D
2	B	900	BLA	C4C-C3C-CAC-CBC
2	B	900	BLA	CAA-CBA-CGA-O2A
2	A	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAA-CBA-CGA-O1A
2	B	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	C2B-C1B-CHB-C4A

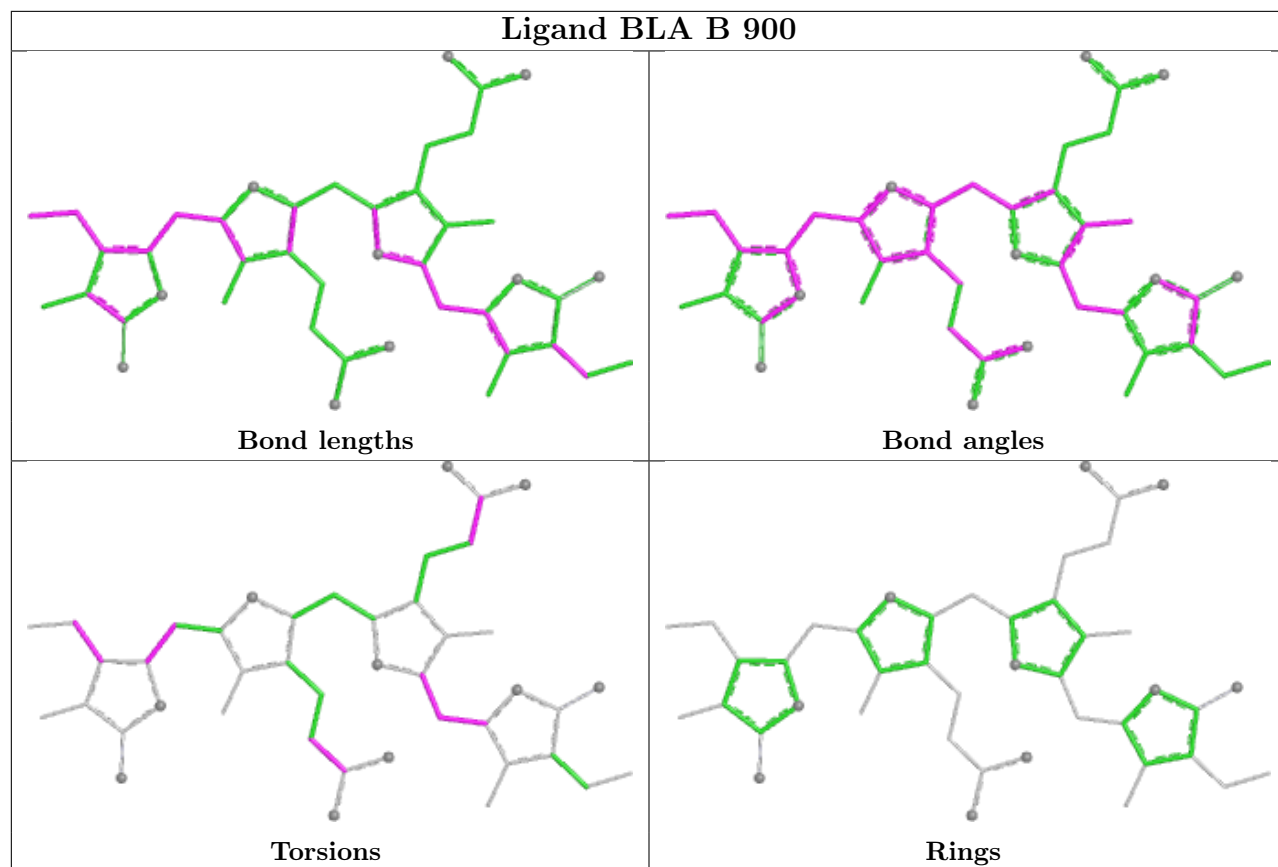
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	3	0
2	B	900	BLA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	473/519 (91%)	-0.18	3 (0%) 85 75	93, 131, 185, 270	0
1	B	448/519 (86%)	-0.01	8 (1%) 67 53	119, 172, 245, 344	0
All	All	921/1038 (88%)	-0.09	11 (1%) 76 63	93, 149, 232, 344	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	LEU	2.9
1	A	451	ASN	2.6
1	A	414	PHE	2.6
1	B	93	VAL	2.6
1	A	30	GLY	2.5
1	B	72	THR	2.4
1	B	379	PRO	2.3
1	B	365	LEU	2.2
1	B	484	GLN	2.2
1	B	83	PRO	2.1
1	B	194	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

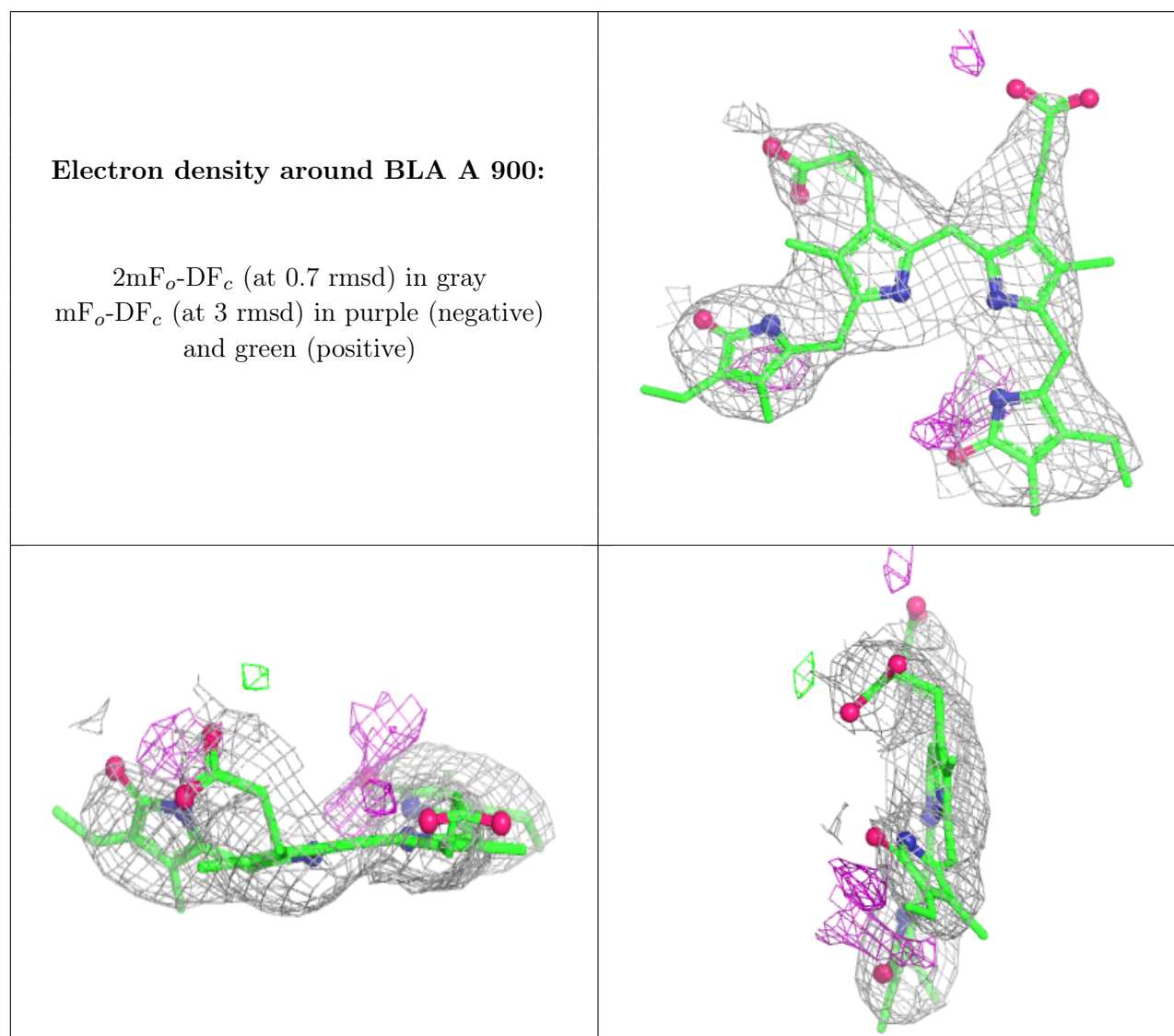
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

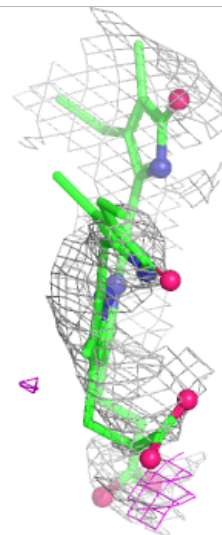
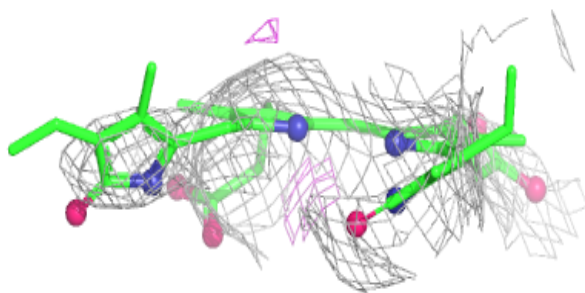
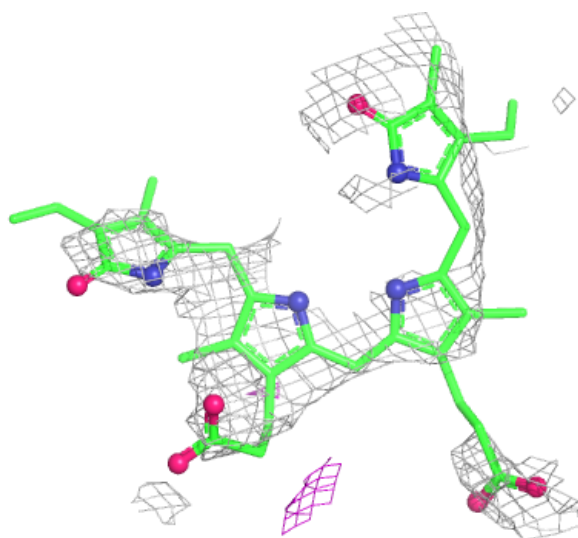
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BLA	A	900	43/43	0.92	0.14	90,114,146,153	0
2	BLA	B	900	43/43	0.93	0.14	140,153,180,212	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around BLA B 900:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.