



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:04 PM UTC

PDB ID : 4S21 / pdb_00004s21
Title : Crystal structure of the photosensory core module of bacteriophytochrome RPA3015 from *R. palustris*
Authors : Yang, X.; Stojkovi, E.A.; Ozarowski, W.B.; Moffat, K.
Deposited on : 2015-01-17
Resolution : 3.25 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

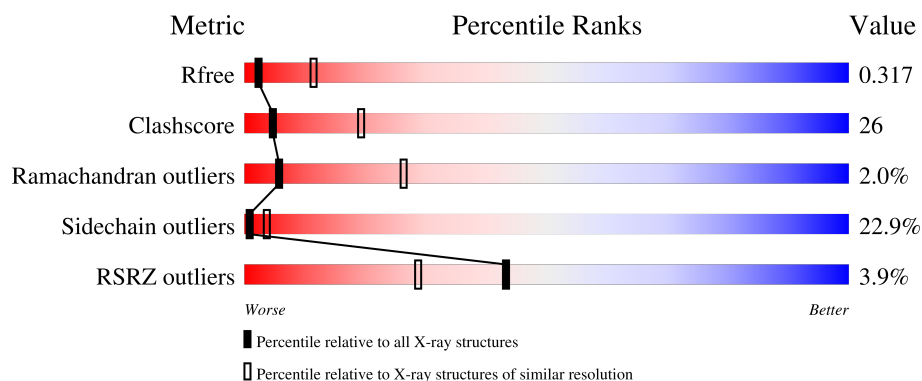
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	525	2% 41% 35% 13% 10%
1	B	525	4% 37% 39% 10% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7251 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	455	Total	C	N	O	S	0	0	0
			3525	2221	638	651	15			

There are 40 discrepancies between the modelled and reference sequences:

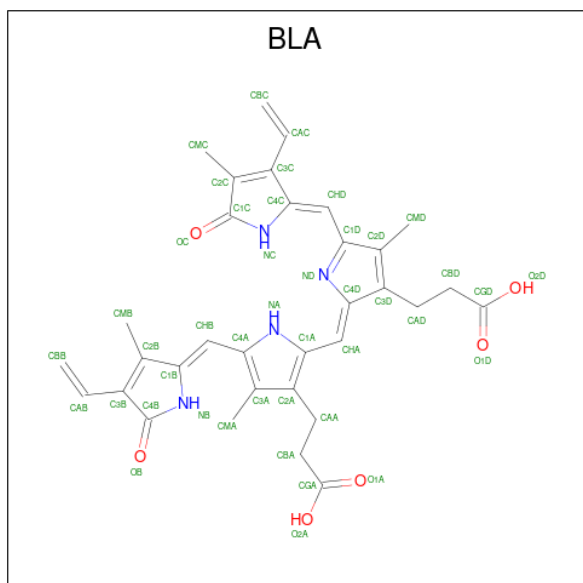
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q6N5G3
A	-18	GLY	-	expression tag	UNP Q6N5G3
A	-17	SER	-	expression tag	UNP Q6N5G3
A	-16	SER	-	expression tag	UNP Q6N5G3
A	-15	HIS	-	expression tag	UNP Q6N5G3
A	-14	HIS	-	expression tag	UNP Q6N5G3
A	-13	HIS	-	expression tag	UNP Q6N5G3
A	-12	HIS	-	expression tag	UNP Q6N5G3
A	-11	HIS	-	expression tag	UNP Q6N5G3
A	-10	HIS	-	expression tag	UNP Q6N5G3
A	-9	SER	-	expression tag	UNP Q6N5G3
A	-8	SER	-	expression tag	UNP Q6N5G3
A	-7	GLY	-	expression tag	UNP Q6N5G3
A	-6	LEU	-	expression tag	UNP Q6N5G3
A	-5	VAL	-	expression tag	UNP Q6N5G3
A	-4	PRO	-	expression tag	UNP Q6N5G3
A	-3	ARG	-	expression tag	UNP Q6N5G3
A	-2	GLY	-	expression tag	UNP Q6N5G3
A	-1	SER	-	expression tag	UNP Q6N5G3
A	0	HIS	-	expression tag	UNP Q6N5G3
B	-19	MET	-	expression tag	UNP Q6N5G3
B	-18	GLY	-	expression tag	UNP Q6N5G3
B	-17	SER	-	expression tag	UNP Q6N5G3
B	-16	SER	-	expression tag	UNP Q6N5G3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q6N5G3
B	-14	HIS	-	expression tag	UNP Q6N5G3
B	-13	HIS	-	expression tag	UNP Q6N5G3
B	-12	HIS	-	expression tag	UNP Q6N5G3
B	-11	HIS	-	expression tag	UNP Q6N5G3
B	-10	HIS	-	expression tag	UNP Q6N5G3
B	-9	SER	-	expression tag	UNP Q6N5G3
B	-8	SER	-	expression tag	UNP Q6N5G3
B	-7	GLY	-	expression tag	UNP Q6N5G3
B	-6	LEU	-	expression tag	UNP Q6N5G3
B	-5	VAL	-	expression tag	UNP Q6N5G3
B	-4	PRO	-	expression tag	UNP Q6N5G3
B	-3	ARG	-	expression tag	UNP Q6N5G3
B	-2	GLY	-	expression tag	UNP Q6N5G3
B	-1	SER	-	expression tag	UNP Q6N5G3
B	0	HIS	-	expression tag	UNP Q6N5G3

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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		

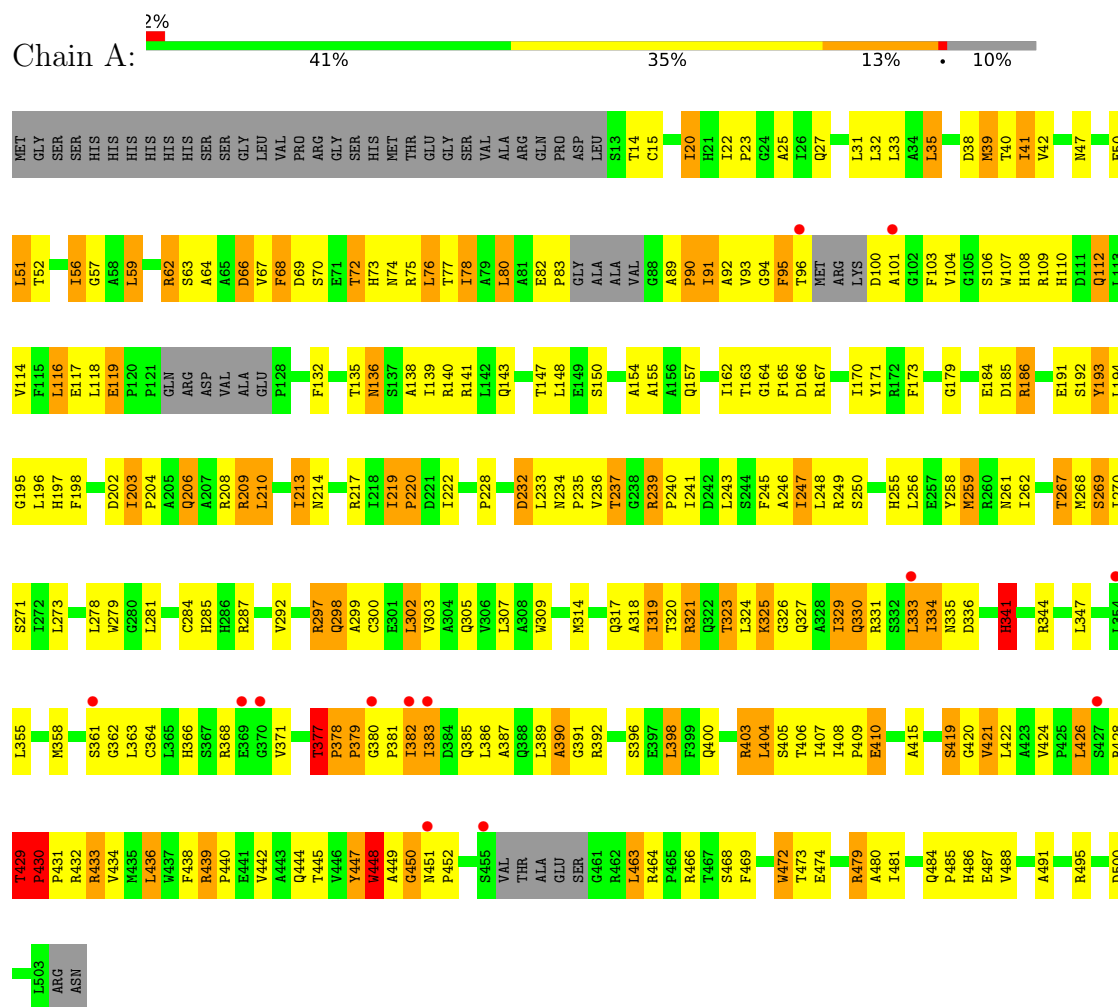
- Molecule 3 is water.

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

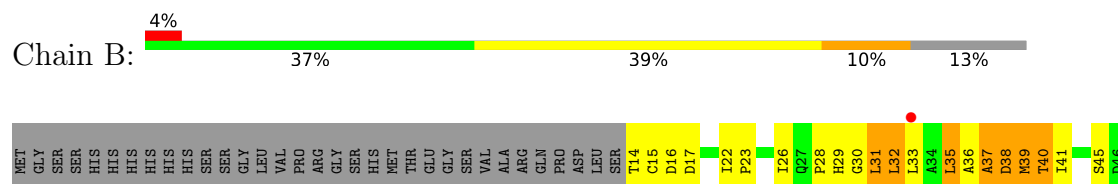
3 Residue-property plots

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



I481	A482	W483	Q484	P485	H486	E487	V488	A489	A490	A491	V492	E493	I494	R495	D496	L497	I498	I499	D500	V501	I502	LEU	ARG	ASN																																		
E410	A415	S419	G420	V421	L422	A423	V424	P425	L426	S427	R428	T429	P430	P431	R432	R433	V434	M435	L436	W437	F438	R439	P440	E441	V442	A443	Q444	A449	G450	N451	P452	D453	K454	S455	VAL	THR	ALA	GLU	SER	GLY	ARG	LEU	ARG	PRO	R466	T467	S468	F469	W472	T476	H477	G478	R479	A480				
R344	L347	A348	S351	E352	A353	L354	L355	E356	L357	M358	S361	G362	L363	C364	L365	H366	S367	R368	E369	G370	V371	I372	T373	I374	G375	Q376	T377	P378	P379	I382	I383	D384	Q385	L386	A387	Q388	L389	A390	G391	R392	S393	G394	L398	F399	Q400	T401	D402	R403	L404	S405	T406	I407	I408	P409				
T267	M268	S269	I270	R274	L278	W279	G280	L281	H285	H286	R287	K288	Y291	E301	L302	Q305	V306	L307	A308	W309	Q310	I311	G312	V313	M314	E315	E316	Q317	A318	I319	T320	R321	Q322	T323	L324	K325	G326	I329	Q330	R331	S332	L333	N335	D336	I337	E338	Q339	L340	H341	D342	M343							
Y193	L196	H197	F198	S201	D202	I203	P204	A205	Q206	A207	R208	R209	L210	Y211	M214	V215	V216	R217	I218	I219	P220	D221	I222	M223	Y224	V227	T230	P231	D232	L233	N234	R239	P240	I241	D242	L243	I247	L248	R249	S252	P253	L256	M259	R260	N261	I262	G263	M264										
L116	E117	L118	E119	P120	P121	GLN	ARG	ASP	VAL	ALA	GLU	PRO	GLN	LEU	G61	R62	S63	A64	A65	D66	V67	F68	D69	S70	E71	T72	H73	N74	R75	L76	T77	I78	A79	L80	A81	E82	P83	GLY	GLY	ALA	ALA	VAL	GLY	ALA	P90	I91	A92	V93	GLY	PHE	T96	R98	K99	D100	H110	D111	V114	F115

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	175.36Å 175.36Å 96.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.89 – 3.25 39.89 – 3.25	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.89-3.25) 73.7 (39.89-3.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.262 , 0.316 0.271 , 0.317	Depositor DCC
R_{free} test set	1340 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	108.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 127.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.107 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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	0.45	0/3716	1.00	21/5057 (0.4%)
1	B	0.44	0/3598	1.05	15/4893 (0.3%)
All	All	0.45	0/7314	1.03	36/9950 (0.4%)

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	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	HIS	N-CA-C	-8.98	101.57	111.36
1	B	427	SER	N-CA-C	8.62	124.43	112.45
1	A	377	THR	CA-C-N	8.02	128.64	120.38
1	A	377	THR	C-N-CA	8.02	128.64	120.38
1	A	464	ARG	CA-C-N	7.86	128.01	120.31
1	A	464	ARG	C-N-CA	7.86	128.01	120.31
1	B	48	LEU	CA-C-N	-7.52	111.96	119.56
1	B	48	LEU	C-N-CA	-7.52	111.96	119.56
1	A	390	ALA	N-CA-C	7.48	119.13	110.97
1	A	429	THR	CA-C-N	7.08	127.68	120.38
1	A	429	THR	C-N-CA	7.08	127.68	120.38
1	B	484	GLN	CA-C-N	-6.59	112.80	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	GLN	C-N-CA	-6.59	112.80	120.12
1	A	450	GLY	CA-C-O	-6.31	117.91	122.45
1	A	334	ILE	N-CA-C	-6.09	105.79	111.45
1	B	37	ALA	N-CA-C	6.06	117.97	111.36
1	A	430	PRO	N-CA-C	5.92	117.92	110.70
1	B	70	SER	N-CA-C	-5.91	105.82	114.39
1	A	119	GLU	CA-C-N	5.70	126.25	120.38
1	A	119	GLU	C-N-CA	5.70	126.25	120.38
1	A	89	ALA	C-N-CD	-5.66	108.14	120.60
1	B	50	GLU	N-CA-C	5.63	117.28	111.03
1	A	378	PRO	CA-C-N	5.58	126.81	119.84
1	A	378	PRO	C-N-CA	5.58	126.81	119.84
1	A	424	VAL	N-CA-C	5.54	113.93	107.89
1	B	424	VAL	CA-C-N	-5.37	114.39	119.76
1	B	424	VAL	C-N-CA	-5.37	114.39	119.76
1	B	430	PRO	CA-C-N	5.23	139.55	127.00
1	B	430	PRO	C-N-CA	5.23	139.55	127.00
1	B	178	SER	N-CA-C	-5.22	103.79	110.53
1	A	203	ILE	CA-C-N	5.21	125.21	120.21
1	A	203	ILE	C-N-CA	5.21	125.21	120.21
1	A	68	PHE	N-CA-C	5.15	118.03	109.94
1	B	394	GLY	N-CA-C	-5.08	106.64	112.73
1	A	27	GLN	CA-C-N	5.00	124.78	119.28
1	A	27	GLN	C-N-CA	5.00	124.78	119.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	HIS	Peptide
1	A	448	TRP	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	190	0
1	B	3525	0	3507	185	0
2	A	43	0	31	7	0
2	B	43	0	31	6	0
3	A	1	0	0	1	0
All	All	7251	0	7194	373	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 26.

All (373) 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:322:GLN:HG3	1:B:486:HIS:HA	1.50	0.94
1:A:75:ARG:NH2	1:A:92:ALA:O	2.06	0.88
1:B:202:ASP:OD1	1:B:466:ARG:NH2	2.10	0.83
1:A:141:ARG:HH21	1:A:154:ALA:HA	1.48	0.79
2:A:900:BLA:ND	3:A:1001:HOH:O	2.16	0.79
1:B:274:ARG:NH1	1:B:308:ALA:O	2.17	0.77
1:A:20:ILE:O	1:A:249:ARG:NH1	2.15	0.77
1:A:140:ARG:HA	1:A:143:GLN:HG3	1.65	0.77
1:B:415:ALA:O	1:B:419:SER:OG	2.01	0.76
1:B:76:LEU:HG	1:B:91:ILE:HG12	1.68	0.76
1:B:331:ARG:HA	1:B:334:ILE:HD12	1.68	0.75
1:B:439:ARG:NH2	1:B:482:ALA:O	2.18	0.75
1:B:160:ARG:NH1	1:B:187:CYS:SG	2.60	0.75
1:B:261:ASN:ND2	1:B:466:ARG:O	2.20	0.74
1:A:70:SER:O	1:A:74:ASN:ND2	2.21	0.73
1:A:368:ARG:HD3	1:A:432:ARG:HB3	1.69	0.72
1:A:214:ASN:O	1:A:217:ARG:NH1	2.22	0.72
1:B:430:PRO:HA	1:B:432:ARG:HB2	1.71	0.72
1:A:331:ARG:O	1:A:335:ASN:ND2	2.22	0.71
1:A:109:ARG:HG2	1:A:114:VAL:HG22	1.71	0.71
1:B:449:ALA:HB1	1:B:469:PHE:HB3	1.72	0.71
1:B:319:ILE:O	1:B:322:GLN:NE2	2.22	0.71
1:A:202:ASP:HB3	2:A:900:BLA:HHB	1.73	0.71
1:A:309:TRP:CH2	1:B:309:TRP:HB3	2.27	0.70
1:A:66:ASP:OD1	1:A:66:ASP:N	2.21	0.70
1:B:337:ILE:HG12	1:B:347:LEU:HA	1.73	0.70
1:B:404:LEU:HD11	1:B:421:VAL:HB	1.73	0.70
1:A:439:ARG:NH1	1:A:487:GLU:OE2	2.23	0.70
1:B:211:TYR:OH	2:B:900:BLA:HAD2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PRO:HD2	1:A:243:LEU:HD12	1.74	0.69
1:A:436:LEU:HD13	1:A:438:PHE:HE1	1.57	0.69
1:B:36:ALA:HB3	1:B:40:THR:HG23	1.73	0.69
1:B:485:PRO:HA	1:B:488:VAL:HB	1.74	0.68
1:B:325:LYS:N	1:B:326:GLY:HA3	2.09	0.68
1:B:338:GLU:HA	1:B:340:LEU:HD12	1.76	0.68
1:B:352:GLU:HA	1:B:355:LEU:HD12	1.75	0.68
1:B:334:ILE:HD13	1:B:497:LEU:HD12	1.74	0.67
1:A:403:ARG:HG2	1:A:479:ARG:HG2	1.75	0.67
1:A:68:PHE:HA	1:A:95:PHE:HB2	1.77	0.67
1:A:217:ARG:NH2	1:A:269:SER:OG	2.23	0.67
1:A:479:ARG:HG3	1:A:479:ARG:HH21	1.59	0.66
1:A:366:HIS:HE2	1:A:383:ILE:HG23	1.59	0.66
1:A:107:TRP:HB3	1:A:116:LEU:HD23	1.77	0.66
1:B:159:VAL:HA	1:B:162:ILE:HG12	1.79	0.65
1:A:39:MET:SD	1:A:39:MET:N	2.69	0.65
1:B:165:PHE:HA	1:B:286:HIS:HD2	1.61	0.65
1:A:157:GLN:NE2	1:A:185:ASP:OD1	2.30	0.65
1:B:425:PRO:HA	1:B:434:VAL:HG22	1.78	0.65
1:B:351:SER:O	1:B:355:LEU:N	2.27	0.64
1:A:449:ALA:HB1	1:A:469:PHE:HD1	1.63	0.64
1:A:80:LEU:HD21	1:A:114:VAL:HG11	1.80	0.63
1:B:218:ILE:HG13	1:B:268:MET:HB2	1.80	0.63
1:B:421:VAL:HG22	1:B:438:PHE:HB3	1.80	0.63
1:A:206:GLN:HA	1:A:209:ARG:HD2	1.81	0.62
1:A:472:TRP:C	1:A:472:TRP:CD1	2.77	0.62
1:A:42:VAL:HG11	1:A:235:PRO:HD3	1.80	0.62
1:B:232:ASP:HA	1:B:241:ILE:HG12	1.81	0.62
1:A:406:THR:HB	1:A:407:ILE:HD12	1.82	0.62
1:B:67:VAL:HG12	1:B:73:HIS:HB2	1.81	0.62
1:B:391:GLY:HA3	1:B:432:ARG:HD3	1.80	0.62
1:A:219:ILE:HD11	1:A:222:ILE:HG22	1.82	0.62
1:A:404:LEU:HD11	1:A:421:VAL:HB	1.81	0.62
1:A:426:LEU:HD13	1:A:495:ARG:HD2	1.81	0.62
1:B:36:ALA:N	1:B:40:THR:O	2.32	0.61
1:A:186:ARG:NH2	1:A:192:SER:HB2	2.14	0.61
1:A:271:SER:HA	1:A:281:LEU:HD12	1.81	0.61
1:A:132:PHE:O	1:A:135:THR:OG1	2.16	0.60
1:A:117:GLU:HB3	1:A:248:LEU:HD12	1.83	0.60
1:A:232:ASP:O	1:A:240:PRO:HA	2.01	0.60
1:A:333:LEU:HA	1:A:336:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ALA:O	1:A:419:SER:OG	2.16	0.60
1:B:40:THR:HA	1:B:64:ALA:H	1.66	0.59
1:A:14:THR:HB	1:A:463:LEU:HD21	1.84	0.59
1:A:270:ILE:HD11	1:A:300:CYS:HB3	1.85	0.59
1:A:112:GLN:HB2	1:A:236:VAL:HG11	1.83	0.59
1:A:166:ASP:OD2	1:A:287:ARG:NH1	2.36	0.59
1:A:485:PRO:HA	1:A:488:VAL:HB	1.84	0.59
1:B:31:LEU:HB2	1:B:48:LEU:HD23	1.85	0.59
1:B:347:LEU:O	1:B:351:SER:N	2.36	0.59
1:A:203:ILE:HG22	1:A:208:ARG:HG3	1.84	0.58
1:A:422:LEU:HD11	1:A:488:VAL:HG22	1.84	0.58
1:A:355:LEU:HD22	1:A:362:GLY:HA2	1.86	0.58
1:B:216:VAL:HG23	1:B:270:ILE:HG13	1.86	0.58
1:B:33:LEU:HG	1:B:48:LEU:HD21	1.85	0.58
1:B:306:VAL:HA	1:B:309:TRP:NE1	2.18	0.58
1:B:64:ALA:O	1:B:66:ASP:N	2.37	0.58
1:A:450:GLY:HA2	1:A:451:ASN:HB2	1.85	0.58
1:A:324:LEU:O	1:A:327:GLN:HB2	2.03	0.57
1:B:451:ASN:C	1:B:453:ASP:H	2.12	0.57
1:B:348:ALA:HA	1:B:351:SER:HB3	1.86	0.57
1:B:324:LEU:C	1:B:326:GLY:HA3	2.30	0.57
1:A:403:ARG:CG	1:A:479:ARG:HG2	2.34	0.56
1:A:163:THR:O	1:A:165:PHE:N	2.39	0.56
1:A:94:GLY:HA2	1:A:101:ALA:O	2.06	0.56
1:B:274:ARG:HD3	1:B:279:TRP:CD1	2.41	0.56
1:A:104:VAL:HB	1:A:119:GLU:HB3	1.88	0.56
1:A:47:ASN:O	1:A:50:GLU:HG2	2.05	0.56
1:B:441:GLU:OE1	1:B:441:GLU:N	2.32	0.56
1:A:155:ALA:HB2	1:A:307:LEU:HD13	1.88	0.56
1:B:163:THR:HG21	1:B:268:MET:HE1	1.87	0.55
1:B:378:PRO:HG2	1:B:382:ILE:HG13	1.88	0.55
1:A:171:TYR:CZ	1:A:179:GLY:HA3	2.41	0.55
1:B:334:ILE:O	1:B:338:GLU:N	2.38	0.55
1:B:26:ILE:HG21	1:B:32:LEU:HD23	1.89	0.55
1:B:402:ASP:OD2	1:B:403:ARG:NH1	2.40	0.55
1:A:377:THR:HG23	1:A:382:ILE:HD12	1.89	0.55
1:A:382:ILE:O	1:A:386:LEU:HB2	2.08	0.55
1:B:402:ASP:OD1	1:B:402:ASP:N	2.30	0.55
1:B:439:ARG:NH2	1:B:481:ILE:O	2.35	0.55
1:A:500:ASP:HB3	1:B:428:ARG:HB2	1.88	0.54
1:A:382:ILE:HD11	1:A:438:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:HD22	1:B:99:LYS:HZ1	1.72	0.54
1:A:259:MET:HE3	1:A:262:ILE:HG21	1.89	0.54
1:B:138:ALA:O	1:B:142:LEU:HB2	2.08	0.54
1:B:403:ARG:CD	1:B:479:ARG:HG2	2.37	0.54
1:A:93:VAL:O	1:A:103:PHE:HB2	2.07	0.54
1:A:366:HIS:NE2	1:A:383:ILE:HG23	2.22	0.54
1:A:387:ALA:HA	1:A:390:ALA:HB2	1.88	0.54
1:B:454:LYS:HG2	1:B:466:ARG:HD3	1.90	0.54
1:A:366:HIS:HB3	1:A:434:VAL:HB	1.90	0.54
1:A:358:MET:HE1	1:A:491:ALA:HB2	1.89	0.53
1:B:305:GLN:O	1:B:309:TRP:CD1	2.62	0.53
1:A:403:ARG:HD3	1:A:479:ARG:CZ	2.38	0.53
1:B:23:PRO:HD2	1:B:243:LEU:HD12	1.90	0.53
1:A:96:THR:HG1	1:A:100:ASP:N	2.06	0.53
1:A:148:LEU:HA	1:A:314:MET:HE1	1.90	0.53
1:A:479:ARG:HH21	1:A:479:ARG:CG	2.21	0.53
1:B:498:ILE:O	1:B:501:VAL:N	2.38	0.53
1:A:472:TRP:C	1:A:472:TRP:HD1	2.17	0.53
1:B:152:CYS:HB3	1:B:170:ILE:HG21	1.91	0.53
1:A:51:LEU:HD23	1:A:95:PHE:HZ	1.74	0.53
1:A:217:ARG:HH21	1:A:269:SER:HG	1.56	0.53
1:A:358:MET:HE3	1:A:487:GLU:O	2.09	0.53
1:B:31:LEU:CB	1:B:48:LEU:HB3	2.39	0.53
1:A:448:TRP:CD1	1:A:448:TRP:N	2.78	0.52
1:A:198:PHE:CD2	2:A:900:BLA:HAB	2.44	0.52
1:A:361:SER:HB2	1:A:440:PRO:HD3	1.92	0.52
1:A:366:HIS:HE1	1:A:368:ARG:HA	1.74	0.52
1:A:320:THR:O	1:A:323:THR:HG22	2.09	0.52
1:A:378:PRO:HG2	1:A:382:ILE:HG13	1.92	0.52
1:B:41:ILE:HG13	1:B:64:ALA:HB2	1.92	0.52
1:B:167:ARG:HB3	1:B:285:HIS:HB2	1.92	0.52
1:B:408:ILE:O	1:B:408:ILE:HG13	2.10	0.52
1:A:255:HIS:NE2	2:A:900:BLA:HBA1	2.25	0.51
1:B:371:VAL:HG11	1:B:383:ILE:HG12	1.92	0.51
1:A:380:GLY:H	1:A:381:PRO:HD2	1.74	0.51
1:B:500:ASP:C	1:B:502:ILE:H	2.18	0.51
1:B:450:GLY:HA2	1:B:472:TRP:HB3	1.93	0.51
1:A:255:HIS:O	1:A:258:TYR:HB3	2.10	0.51
1:B:32:LEU:O	1:B:45:SER:HB3	2.10	0.51
1:A:103:PHE:HD1	1:A:118:LEU:HB3	1.74	0.51
1:A:135:THR:O	1:A:139:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASP:HB3	1:B:205:ALA:HB3	1.93	0.51
1:B:369:GLU:N	1:B:369:GLU:OE2	2.44	0.51
1:A:331:ARG:HA	1:A:334:ILE:HD12	1.92	0.50
1:A:426:LEU:HB3	1:A:433:ARG:HB2	1.92	0.50
1:B:28:PRO:HD2	1:B:224:TYR:HB2	1.94	0.50
1:B:259:MET:HA	1:B:262:ILE:HG22	1.92	0.50
1:B:206:GLN:HA	1:B:209:ARG:NE	2.26	0.50
1:A:219:ILE:O	1:A:219:ILE:HG13	2.09	0.50
1:A:318:ALA:HA	1:A:321:ARG:HD3	1.92	0.50
1:B:41:ILE:HD13	1:B:62:ARG:HH21	1.77	0.50
1:A:297:ARG:HA	1:A:300:CYS:HB2	1.93	0.50
1:B:302:LEU:O	1:B:306:VAL:HG23	2.12	0.50
1:B:358:MET:HE1	1:B:491:ALA:HB2	1.94	0.50
1:A:314:MET:HA	1:A:317:GLN:HG2	1.93	0.50
1:B:210:LEU:O	1:B:214:ASN:N	2.39	0.50
1:B:30:GLY:O	1:B:47:ASN:ND2	2.45	0.50
1:B:249:ARG:HH22	2:B:900:BLA:CGD	2.24	0.49
1:A:309:TRP:CE3	1:A:309:TRP:HA	2.46	0.49
1:A:329:ILE:O	1:A:329:ILE:HG13	2.10	0.49
1:B:40:THR:HA	1:B:64:ALA:N	2.26	0.49
1:B:173:PHE:HE2	1:B:278:LEU:HG	1.77	0.49
1:A:62:ARG:HG3	1:A:62:ARG:HH11	1.76	0.49
1:A:327:GLN:O	1:A:330:GLN:NE2	2.45	0.49
1:A:197:HIS:HB3	1:A:448:TRP:CE3	2.47	0.49
1:B:319:ILE:HD11	1:B:485:PRO:HG2	1.93	0.49
1:B:331:ARG:O	1:B:335:ASN:ND2	2.38	0.49
1:B:435:MET:HE1	1:B:498:ILE:HD12	1.93	0.49
1:B:72:THR:HA	1:B:76:LEU:HD13	1.94	0.49
2:A:900:BLA:NB	2:A:900:BLA:CMA	2.75	0.49
1:A:51:LEU:HD23	1:A:95:PHE:CZ	2.47	0.49
1:A:141:ARG:HE	1:A:154:ALA:HB1	1.78	0.49
1:A:184:GLU:OE2	1:A:192:SER:OG	2.22	0.49
1:A:268:MET:HE1	1:A:292:VAL:HG21	1.95	0.49
1:B:333:LEU:HA	1:B:336:ASP:HB2	1.95	0.49
1:B:495:ARG:HA	1:B:498:ILE:HB	1.94	0.49
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.78	0.48
1:B:501:VAL:HG12	1:B:501:VAL:O	2.12	0.48
1:A:186:ARG:HH21	1:A:192:SER:HB2	1.78	0.48
1:A:206:GLN:O	1:A:210:LEU:HD23	2.13	0.48
1:A:33:LEU:HB3	1:A:35:LEU:HD21	1.95	0.48
1:A:341:HIS:ND1	1:A:341:HIS:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD23	1:A:91:ILE:HD13	1.95	0.48
1:B:403:ARG:HD2	1:B:479:ARG:HG2	1.95	0.48
1:B:173:PHE:CE2	1:B:278:LEU:HG	2.49	0.48
1:B:403:ARG:HB3	1:B:406:THR:OG1	2.13	0.48
1:B:72:THR:O	1:B:76:LEU:HD22	2.13	0.48
1:B:382:ILE:HG22	1:B:383:ILE:HG13	1.95	0.48
1:B:432:ARG:O	1:B:434:VAL:HG23	2.14	0.48
1:A:222:ILE:HB	1:A:256:LEU:HD22	1.95	0.47
1:B:159:VAL:HG23	1:B:168:VAL:HG11	1.95	0.47
1:B:230:THR:HA	1:B:231:PRO:HA	1.67	0.47
1:A:197:HIS:O	1:A:448:TRP:HB3	2.14	0.47
1:B:491:ALA:O	1:B:494:ILE:HB	2.15	0.47
1:A:173:PHE:HB2	1:A:279:TRP:O	2.14	0.47
1:B:50:GLU:HG3	1:B:51:LEU:HG	1.96	0.47
1:B:365:LEU:HD12	1:B:372:ILE:HB	1.95	0.47
1:B:137:SER:HA	1:B:140:ARG:HD2	1.96	0.47
1:A:259:MET:SD	1:A:267:THR:HG21	2.54	0.47
1:A:368:ARG:CZ	1:A:431:PRO:HA	2.44	0.47
1:A:385:GLN:O	1:A:408:ILE:HD11	2.13	0.47
1:B:253:PRO:HA	1:B:256:LEU:HB2	1.95	0.47
1:B:490:ALA:O	1:B:494:ILE:HG13	2.14	0.47
1:B:429:THR:HA	1:B:432:ARG:HE	1.80	0.47
1:A:62:ARG:HH11	1:A:62:ARG:CG	2.27	0.46
1:A:69:ASP:HB2	1:A:94:GLY:O	2.16	0.46
1:B:368:ARG:CZ	1:B:431:PRO:HB3	2.45	0.46
1:A:319:ILE:HD12	1:A:319:ILE:HA	1.73	0.46
1:A:368:ARG:NH2	1:A:431:PRO:HA	2.29	0.46
1:B:166:ASP:HB2	1:B:286:HIS:HA	1.97	0.46
1:B:171:TYR:CZ	1:B:179:GLY:HA3	2.50	0.46
1:B:31:LEU:HB3	1:B:48:LEU:HB3	1.97	0.46
1:A:23:PRO:HB2	1:A:250:SER:HB3	1.96	0.46
1:A:194:LEU:HD12	1:A:195:GLY:H	1.80	0.46
1:B:32:LEU:HB2	1:B:117:GLU:HA	1.97	0.46
1:B:316:GLU:HA	1:B:319:ILE:HB	1.97	0.46
1:A:20:ILE:HD13	1:A:20:ILE:HA	1.68	0.46
1:A:162:ILE:HD11	1:A:300:CYS:SG	2.56	0.46
1:A:284:CYS:O	1:A:285:HIS:HD2	1.99	0.46
1:B:29:HIS:CG	1:B:291:TYR:HE1	2.33	0.46
1:B:309:TRP:O	1:B:313:VAL:N	2.48	0.46
1:A:193:TYR:HE2	1:A:262:ILE:HD11	1.81	0.46
1:A:258:TYR:O	1:A:261:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:H	1:A:325:LYS:HG3	1.41	0.46
1:A:368:ARG:NH1	1:A:430:PRO:HA	2.31	0.46
1:B:206:GLN:OE1	1:B:207:ALA:N	2.48	0.46
1:B:117:GLU:OE2	1:B:247:ILE:N	2.47	0.45
1:B:357:LEU:HB2	1:B:358:MET:HG2	1.97	0.45
1:A:463:LEU:H	1:A:463:LEU:HG	1.48	0.45
1:A:56:ILE:HD12	1:A:57:GLY:H	1.81	0.45
1:B:68:PHE:HB2	1:B:72:THR:OG1	2.17	0.45
1:A:135:THR:O	1:A:139:ILE:N	2.46	0.45
1:A:74:ASN:O	1:A:78:ILE:HG22	2.16	0.45
1:B:419:SER:OG	1:B:441:GLU:HB3	2.16	0.45
1:A:20:ILE:HG23	1:A:249:ARG:NH1	2.31	0.45
1:A:398:LEU:HD22	1:A:398:LEU:HA	1.80	0.45
1:A:76:LEU:O	1:A:80:LEU:HD12	2.17	0.45
1:B:67:VAL:HG13	1:B:68:PHE:H	1.81	0.45
1:B:278:LEU:HD11	1:B:281:LEU:HD12	1.98	0.45
1:A:219:ILE:HA	1:A:220:PRO:HD3	1.78	0.44
1:A:299:ALA:O	1:A:302:LEU:HB3	2.17	0.44
1:A:326:GLY:O	1:A:330:GLN:HB3	2.18	0.44
1:A:330:GLN:HB3	1:A:330:GLN:HE21	1.59	0.44
1:A:382:ILE:HA	1:A:386:LEU:HD12	1.98	0.44
1:A:447:TYR:HD2	1:A:473:THR:HG22	1.82	0.44
1:A:245:PHE:CD2	1:A:245:PHE:N	2.86	0.44
1:B:35:LEU:HA	1:B:41:ILE:HA	2.00	0.44
1:B:330:GLN:HG2	1:B:334:ILE:HD11	1.99	0.44
1:B:441:GLU:H	1:B:441:GLU:CD	2.23	0.44
1:A:90:PRO:HG2	1:B:133:ARG:HH11	1.83	0.44
1:A:108:HIS:HD2	1:A:110:HIS:HB2	1.82	0.44
1:A:420:GLY:HA3	1:A:480:ALA:HB2	2.00	0.44
1:B:132:PHE:O	1:B:135:THR:OG1	2.30	0.44
1:A:309:TRP:HA	1:A:309:TRP:HE3	1.82	0.44
1:B:239:ARG:HE	1:B:239:ARG:HB2	1.38	0.44
1:B:382:ILE:O	1:B:386:LEU:HB2	2.18	0.44
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.85	0.44
1:B:134:ARG:NH2	1:B:161:GLU:O	2.51	0.43
1:B:309:TRP:CD1	1:B:309:TRP:N	2.86	0.43
1:B:491:ALA:HA	1:B:494:ILE:HD12	2.00	0.43
1:A:136:ASN:HA	1:A:139:ILE:HB	2.00	0.43
1:B:35:LEU:HG	1:B:114:VAL:HB	2.00	0.43
1:B:134:ARG:H	1:B:134:ARG:HG3	1.57	0.43
1:B:201:SER:O	2:B:900:BLA:HBC1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HG21	1:A:67:VAL:HG13	2.00	0.43
1:B:60:ILE:HG22	1:B:61:GLY:N	2.33	0.43
1:A:466:ARG:NH2	1:A:469:PHE:HE1	2.16	0.43
2:A:900:BLA:HB	2:A:900:BLA:HMA2	1.84	0.43
1:B:343:HIS:O	1:B:347:LEU:N	2.32	0.43
1:B:309:TRP:CD1	1:B:309:TRP:H	2.36	0.43
1:A:439:ARG:HH12	1:A:487:GLU:CD	2.27	0.43
1:B:354:LEU:HA	1:B:357:LEU:HG	2.00	0.43
1:B:365:LEU:HB2	1:B:372:ILE:HB	1.99	0.43
1:A:73:HIS:O	1:A:77:THR:HG23	2.18	0.43
1:B:82:GLU:N	1:B:83:PRO:HD3	2.32	0.43
1:B:494:ILE:O	1:B:498:ILE:HG13	2.18	0.43
1:A:25:ALA:HA	1:A:228:PRO:HA	2.00	0.43
1:B:35:LEU:HB3	1:B:41:ILE:HG12	2.01	0.43
1:A:62:ARG:HG3	1:A:62:ARG:NH1	2.34	0.43
1:A:408:ILE:HG22	1:A:410:GLU:HG2	2.00	0.43
1:B:385:GLN:NE2	1:B:410:GLU:OE2	2.32	0.43
1:B:378:PRO:HA	1:B:379:PRO:HD3	1.57	0.42
1:B:14:THR:HA	1:B:17:ASP:OD2	2.20	0.42
1:B:15:CYS:SG	1:B:204:PRO:HB3	2.59	0.42
1:B:171:TYR:OH	1:B:198:PHE:HB2	2.18	0.42
1:B:234:ASN:HB2	1:B:239:ARG:O	2.19	0.42
1:B:365:LEU:O	1:B:371:VAL:HA	2.18	0.42
1:A:245:PHE:N	1:A:245:PHE:HD2	2.17	0.42
1:B:39:MET:C	1:B:64:ALA:HB3	2.44	0.42
1:B:424:VAL:HG11	1:B:495:ARG:HG2	2.01	0.42
1:A:68:PHE:HB3	1:A:72:THR:CG2	2.49	0.42
1:A:259:MET:HE2	1:A:259:MET:HB3	1.86	0.42
1:A:391:GLY:O	1:A:392:ARG:HG2	2.20	0.42
1:A:436:LEU:HD13	1:A:438:PHE:CE1	2.47	0.42
1:B:286:HIS:ND1	1:B:288:LYS:O	2.53	0.42
1:A:82:GLU:HA	1:A:83:PRO:HD3	1.91	0.42
1:A:203:ILE:HA	1:A:204:PRO:HD2	1.92	0.42
1:A:318:ALA:HB1	1:A:486:HIS:NE2	2.34	0.42
1:B:314:MET:HA	1:B:317:GLN:CD	2.44	0.42
1:A:210:LEU:HA	1:A:213:ILE:HG12	2.01	0.42
1:A:379:PRO:HB2	1:A:380:GLY:H	1.65	0.42
1:B:73:HIS:O	1:B:77:THR:HG23	2.19	0.42
1:B:270:ILE:HG21	1:B:301:GLU:HA	2.02	0.42
1:A:32:LEU:HD13	1:A:117:GLU:HG2	2.00	0.42
1:A:72:THR:O	1:A:76:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:CB	1:A:430:PRO:HD2	2.49	0.42
1:B:307:LEU:HG	1:B:311:ILE:HG13	2.01	0.42
1:B:485:PRO:O	1:B:489:ALA:N	2.52	0.42
1:A:309:TRP:CZ2	1:B:309:TRP:HB3	2.55	0.42
1:B:489:ALA:O	1:B:493:GLU:HB2	2.20	0.42
1:A:405:SER:O	1:A:409:PRO:HA	2.20	0.41
1:B:252:SER:HB2	2:B:900:BLA:HBD2	2.02	0.41
1:B:368:ARG:H	1:B:368:ARG:HG3	1.73	0.41
1:A:298:GLN:O	1:B:136:ASN:ND2	2.53	0.41
2:A:900:BLA:CMA	2:A:900:BLA:HB	2.33	0.41
1:B:426:LEU:O	1:B:432:ARG:HA	2.20	0.41
1:B:428:ARG:NH2	1:B:431:PRO:HD3	2.35	0.41
1:B:388:GLN:O	1:B:392:ARG:HG3	2.20	0.41
1:A:68:PHE:HB3	1:A:72:THR:HG22	2.02	0.41
1:A:203:ILE:CG2	1:A:208:ARG:HG3	2.48	0.41
1:A:243:LEU:O	1:A:249:ARG:HD2	2.20	0.41
1:B:37:ALA:O	1:B:39:MET:HG2	2.20	0.41
1:B:217:ARG:HG3	2:B:900:BLA:HBA2	2.03	0.41
1:B:262:ILE:HG23	1:B:264:MET:H	1.85	0.41
1:B:319:ILE:HD12	1:B:319:ILE:HA	1.85	0.41
1:B:386:LEU:HA	1:B:389:LEU:HB3	2.02	0.41
1:A:246:ALA:HB3	1:A:249:ARG:HB3	2.02	0.41
1:A:451:ASN:N	1:A:452:PRO:HD3	2.35	0.41
1:B:176:ASP:OD1	1:B:176:ASP:N	2.52	0.41
1:A:192:SER:C	1:A:193:TYR:HD1	2.29	0.41
1:A:210:LEU:O	1:A:214:ASN:N	2.31	0.41
1:A:258:TYR:C	1:A:258:TYR:CD2	2.99	0.41
1:A:302:LEU:O	1:A:305:GLN:HB2	2.21	0.41
1:A:404:LEU:N	1:A:419:SER:O	2.53	0.41
1:B:202:ASP:HA	2:B:900:BLA:C1C	2.51	0.41
1:A:434:VAL:HG12	1:A:436:LEU:HG	2.03	0.41
1:A:380:GLY:N	1:A:381:PRO:HD2	2.35	0.41
1:B:41:ILE:HD13	1:B:62:ARG:NH2	2.36	0.41
1:B:286:HIS:HD1	1:B:288:LYS:H	1.69	0.41
1:B:386:LEU:HA	1:B:386:LEU:HD23	1.90	0.41
1:A:41:ILE:HD11	1:A:59:LEU:HB3	2.02	0.41
1:A:366:HIS:ND1	1:A:366:HIS:C	2.79	0.41
1:B:222:ILE:O	1:B:256:LEU:HD22	2.20	0.41
1:B:363:LEU:HG	1:B:374:ILE:HB	2.03	0.41
1:A:39:MET:HB3	1:A:64:ALA:HB2	2.03	0.41
1:A:247:ILE:H	1:A:247:ILE:HG13	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ILE:HG22	1:B:61:GLY:H	1.86	0.40
1:B:222:ILE:HD13	1:B:259:MET:HB2	2.03	0.40
1:A:138:ALA:HA	1:A:141:ARG:HB3	2.03	0.40
1:A:428:ARG:HH12	1:B:497:LEU:HD11	1.85	0.40
1:B:74:ASN:O	1:B:78:ILE:HG13	2.21	0.40
1:B:204:PRO:O	1:B:208:ARG:HG3	2.21	0.40
1:B:340:LEU:HD21	1:B:343:HIS:HB3	2.03	0.40
1:A:141:ARG:NH2	1:A:154:ALA:HA	2.27	0.40
1:A:186:ARG:HH11	1:A:186:ARG:HG2	1.87	0.40
1:A:479:ARG:CG	1:A:479:ARG:NH2	2.85	0.40
1:B:259:MET:HE1	1:B:285:HIS:NE2	2.37	0.40
1:B:422:LEU:HD23	1:B:437:TRP:CE3	2.57	0.40
1:A:237:THR:OG1	1:A:239:ARG:HD2	2.22	0.40
1:A:429:THR:HG22	1:A:432:ARG:CZ	2.51	0.40
1:B:110:HIS:HB3	1:B:115:PHE:CE2	2.56	0.40
1:B:498:ILE:O	1:B:500:ASP:N	2.55	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	463/525 (88%)	418 (90%)	38 (8%)	7 (2%)	8	32
1	B	443/525 (84%)	398 (90%)	34 (8%)	11 (2%)	4	22
All	All	906/1050 (86%)	816 (90%)	72 (8%)	18 (2%)	6	26

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	430	PRO

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Mol	Chain	Res	Type
1	B	66	ASP
1	A	164	GLY
1	A	379	PRO
1	B	65	ALA
1	B	379	PRO
1	A	341	HIS
1	A	383	ILE
1	B	111	ASP
1	B	501	VAL
1	B	220	PRO
1	B	240	PRO
1	A	220	PRO
1	B	452	PRO
1	B	499	ILE
1	B	450	GLY
1	B	451	ASN

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	382/424 (90%)	287 (75%)	95 (25%)	0	2
1	B	373/424 (88%)	295 (79%)	78 (21%)	1	5
All	All	755/848 (89%)	582 (77%)	173 (23%)	1	4

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	CYS
1	A	20	ILE
1	A	22	ILE
1	A	31	LEU
1	A	35	LEU
1	A	38	ASP
1	A	39	MET

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Mol	Chain	Res	Type
1	A	40	THR
1	A	41	ILE
1	A	51	LEU
1	A	56	ILE
1	A	59	LEU
1	A	62	ARG
1	A	63	SER
1	A	66	ASP
1	A	72	THR
1	A	76	LEU
1	A	78	ILE
1	A	80	LEU
1	A	91	ILE
1	A	95	PHE
1	A	106	SER
1	A	112	GLN
1	A	116	LEU
1	A	136	ASN
1	A	147	THR
1	A	150	SER
1	A	167	ARG
1	A	170	ILE
1	A	186	ARG
1	A	191	GLU
1	A	193	TYR
1	A	196	LEU
1	A	206	GLN
1	A	209	ARG
1	A	210	LEU
1	A	213	ILE
1	A	219	ILE
1	A	232	ASP
1	A	233	LEU
1	A	234	ASN
1	A	237	THR
1	A	239	ARG
1	A	241	ILE
1	A	247	ILE
1	A	259	MET
1	A	267	THR
1	A	269	SER
1	A	273	LEU

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Mol	Chain	Res	Type
1	A	278	LEU
1	A	297	ARG
1	A	298	GLN
1	A	302	LEU
1	A	303	VAL
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	333	LEU
1	A	341	HIS
1	A	344	ARG
1	A	347	LEU
1	A	363	LEU
1	A	364	CYS
1	A	371	VAL
1	A	377	THR
1	A	382	ILE
1	A	389	LEU
1	A	396	SER
1	A	398	LEU
1	A	400	GLN
1	A	403	ARG
1	A	404	LEU
1	A	410	GLU
1	A	419	SER
1	A	421	VAL
1	A	426	LEU
1	A	429	THR
1	A	433	ARG
1	A	436	LEU
1	A	439	ARG
1	A	442	VAL
1	A	444	GLN
1	A	445	THR
1	A	447	TYR
1	A	448	TRP
1	A	463	LEU
1	A	468	SER
1	A	472	TRP

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Mol	Chain	Res	Type
1	A	474	GLU
1	A	479	ARG
1	A	481	ILE
1	A	484	GLN
1	B	22	ILE
1	B	31	LEU
1	B	32	LEU
1	B	35	LEU
1	B	38	ASP
1	B	39	MET
1	B	40	THR
1	B	52	THR
1	B	60	ILE
1	B	63	SER
1	B	67	VAL
1	B	80	LEU
1	B	91	ILE
1	B	98	ARG
1	B	100	ASP
1	B	116	LEU
1	B	118	LEU
1	B	119	GLU
1	B	134	ARG
1	B	142	LEU
1	B	146	GLU
1	B	176	ASP
1	B	190	VAL
1	B	193	TYR
1	B	196	LEU
1	B	203	ILE
1	B	206	GLN
1	B	227	VAL
1	B	232	ASP
1	B	234	ASN
1	B	239	ARG
1	B	247	ILE
1	B	248	LEU
1	B	252	SER
1	B	260	ARG
1	B	267	THR
1	B	269	SER
1	B	278	LEU

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Mol	Chain	Res	Type
1	B	281	LEU
1	B	309	TRP
1	B	317	GLN
1	B	319	ILE
1	B	321	ARG
1	B	322	GLN
1	B	323	THR
1	B	329	ILE
1	B	330	GLN
1	B	340	LEU
1	B	341	HIS
1	B	344	ARG
1	B	347	LEU
1	B	354	LEU
1	B	358	MET
1	B	361	SER
1	B	364	CYS
1	B	367	SER
1	B	376	GLN
1	B	382	ILE
1	B	398	LEU
1	B	400	GLN
1	B	402	ASP
1	B	403	ARG
1	B	404	LEU
1	B	407	ILE
1	B	419	SER
1	B	421	VAL
1	B	436	LEU
1	B	438	PHE
1	B	441	GLU
1	B	442	VAL
1	B	476	THR
1	B	477	HIS
1	B	481	ILE
1	B	483	TRP
1	B	495	ARG
1	B	497	LEU
1	B	499	ILE
1	B	500	ASP

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

Mol	Chain	Res	Type
1	A	27	GLN
1	A	285	HIS
1	A	330	GLN
1	B	27	GLN
1	B	29	HIS
1	B	73	HIS
1	B	157	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	2.72	18 (39%)	66,67,67	1.91	17 (25%)
2	BLA	B	900	1	46,46,46	2.63	14 (30%)	66,67,67	1.99	20 (30%)

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	-	6/26/74/74	0/4/4/4
2	BLA	B	900	1	-	10/26/74/74	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	CHD-C4C	6.89	1.54	1.37
2	B	900	BLA	CHB-C1B	6.54	1.53	1.37
2	A	900	BLA	CHD-C1D	6.46	1.55	1.40
2	A	900	BLA	CHB-C4A	6.42	1.54	1.40
2	B	900	BLA	CHB-C4A	6.26	1.54	1.40
2	B	900	BLA	CHD-C4C	6.25	1.52	1.37
2	A	900	BLA	CHB-C1B	5.84	1.51	1.37
2	B	900	BLA	CHD-C1D	5.33	1.53	1.40
2	B	900	BLA	CBC-CAC	4.96	1.54	1.30
2	A	900	BLA	CBC-CAC	4.82	1.53	1.30
2	A	900	BLA	C4D-C3D	-4.34	1.38	1.45
2	B	900	BLA	C1D-C2D	-4.10	1.36	1.45
2	A	900	BLA	C1C-C2C	-4.04	1.38	1.48
2	B	900	BLA	C1C-C2C	-3.81	1.39	1.48
2	B	900	BLA	C1B-C2B	-3.46	1.38	1.45
2	B	900	BLA	C3C-C4C	-3.28	1.39	1.45
2	A	900	BLA	C1D-C2D	-3.18	1.38	1.45
2	B	900	BLA	C4D-C3D	-3.14	1.40	1.45
2	B	900	BLA	CAC-C3C	3.06	1.55	1.47
2	B	900	BLA	CAB-C3B	-2.97	1.39	1.47
2	A	900	BLA	CAB-C3B	-2.87	1.39	1.47
2	A	900	BLA	CAC-C3C	2.84	1.55	1.47
2	B	900	BLA	C1A-NA	-2.74	1.33	1.37
2	A	900	BLA	C3C-C4C	-2.72	1.40	1.45
2	A	900	BLA	CBA-CGA	2.68	1.56	1.50
2	B	900	BLA	C4A-NA	-2.67	1.33	1.37
2	A	900	BLA	C4A-NA	-2.64	1.33	1.37
2	A	900	BLA	C1B-C2B	-2.63	1.40	1.45
2	A	900	BLA	C1B-NB	-2.44	1.33	1.37
2	A	900	BLA	C1A-NA	-2.18	1.34	1.37
2	A	900	BLA	C4B-NB	-2.17	1.33	1.38
2	A	900	BLA	C4C-NC	-2.13	1.34	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	CHA-C4D-ND	5.86	136.91	124.60
2	B	900	BLA	C4A-CHB-C1B	-5.27	115.65	130.82
2	B	900	BLA	CAD-C3D-C4D	4.88	133.59	125.02
2	A	900	BLA	C4A-CHB-C1B	-4.88	116.78	130.82
2	A	900	BLA	CHA-C4D-C3D	-4.80	114.32	125.40
2	B	900	BLA	CHD-C1D-ND	4.33	134.31	124.95
2	B	900	BLA	C1A-CHA-C4D	-4.19	119.06	128.22
2	A	900	BLA	C4C-CHD-C1D	-4.13	117.91	128.06
2	B	900	BLA	CAD-C3D-C2D	-3.37	121.55	127.87
2	B	900	BLA	C1D-C2D-C3D	3.35	110.28	106.48
2	A	900	BLA	C3B-C4B-NB	3.26	110.23	106.13
2	B	900	BLA	CHD-C4C-C3C	-3.26	118.64	127.94
2	A	900	BLA	CMB-C2B-C1B	3.25	128.11	124.16
2	B	900	BLA	CHA-C4D-ND	2.94	130.76	124.60
2	B	900	BLA	CHA-C1A-C2A	-2.85	121.10	127.22
2	A	900	BLA	CHD-C1D-ND	2.77	130.93	124.95
2	B	900	BLA	C4C-CHD-C1D	-2.76	121.29	128.06
2	B	900	BLA	C4C-NC-C1C	-2.68	107.38	110.66
2	A	900	BLA	C1A-C2A-C3A	-2.61	104.58	107.62
2	B	900	BLA	CMA-C3A-C4A	2.56	129.34	125.62
2	A	900	BLA	C4D-ND-C1D	2.54	111.19	106.52
2	B	900	BLA	CHD-C1D-C2D	-2.46	118.55	124.87
2	A	900	BLA	CAA-C2A-C1A	2.46	129.67	125.77
2	A	900	BLA	CBC-CAC-C3C	-2.40	115.52	127.53
2	A	900	BLA	C1D-C2D-C3D	2.39	109.19	106.48
2	B	900	BLA	C3B-C4B-NB	2.37	109.11	106.13
2	B	900	BLA	CHA-C1A-NA	2.35	130.59	125.29
2	A	900	BLA	C1A-CHA-C4D	-2.32	123.16	128.22
2	B	900	BLA	C3C-C4C-NC	2.31	110.40	106.64
2	B	900	BLA	CHD-C4C-NC	2.29	130.95	126.06
2	A	900	BLA	CAA-CBA-CGA	2.24	119.61	113.67
2	A	900	BLA	C2D-C1D-ND	-2.23	105.72	110.58
2	B	900	BLA	CHB-C4A-C3A	2.17	132.84	127.53
2	A	900	BLA	CAD-CBD-CGD	-2.10	108.09	113.67
2	A	900	BLA	CHB-C4A-C3A	2.08	132.63	127.53
2	B	900	BLA	CBC-CAC-C3C	-2.02	117.44	127.53
2	B	900	BLA	CHB-C4A-NA	-2.01	120.75	125.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	BLA	C2B-C1B-CHB-C4A

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

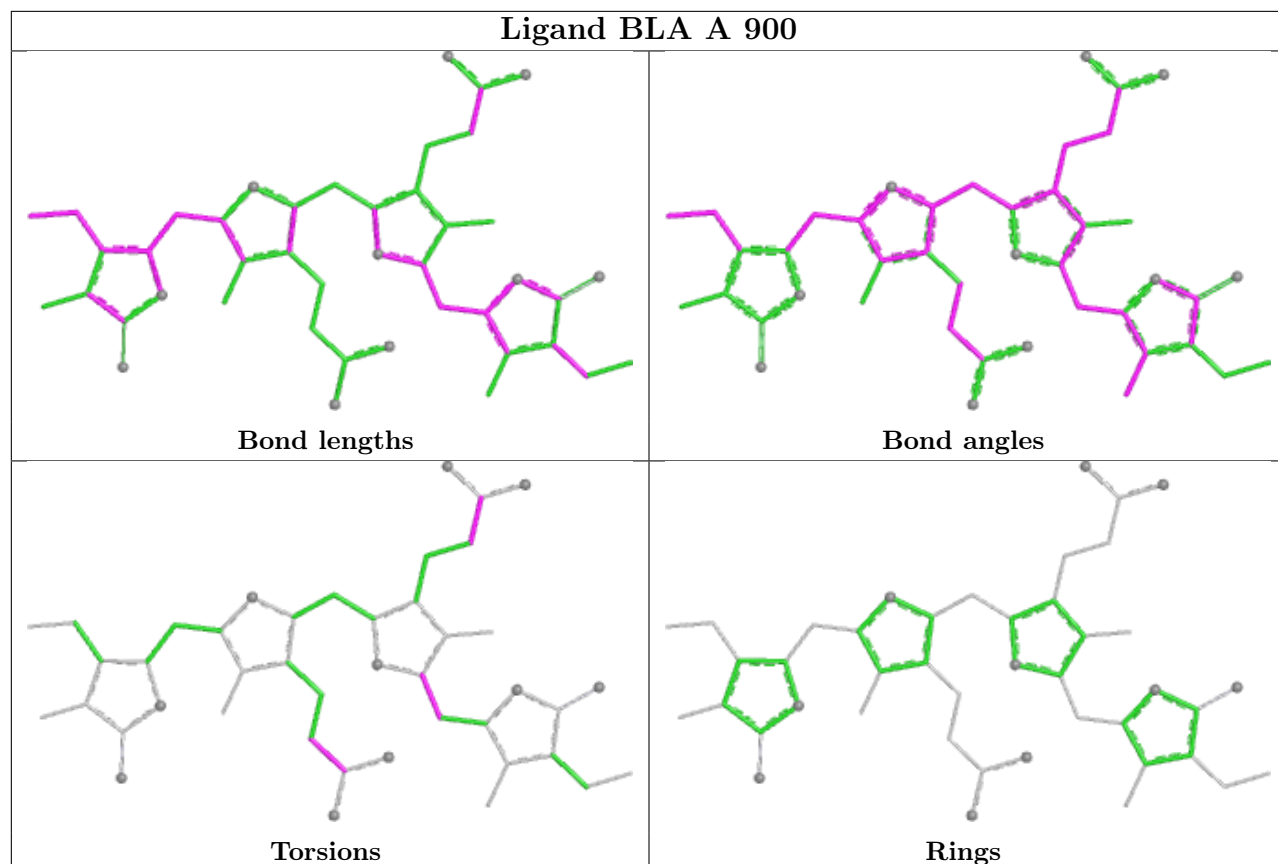
There are no ring outliers.

2 monomers are involved in 13 short contacts:

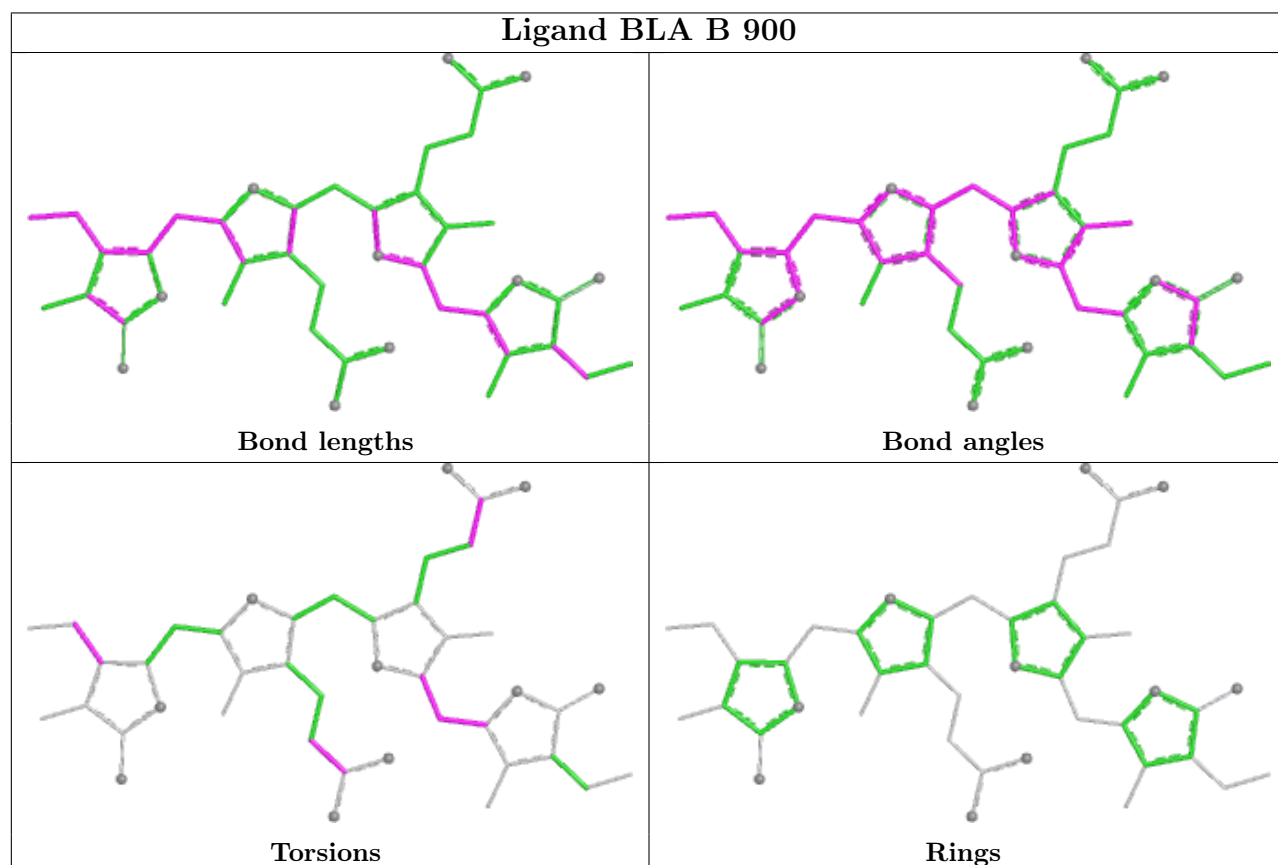
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	7	0
2	B	900	BLA	6	0

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.

Ligand BLA A 900



Ligand BLA B 900



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	473/525 (90%)	0.14	13 (2%) 56 38	79, 125, 206, 294	0
1	B	455/525 (86%)	0.45	23 (5%) 33 22	106, 174, 272, 340	0
All	All	928/1050 (88%)	0.29	36 (3%) 43 29	79, 149, 250, 340	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	SER	3.7
1	B	33	LEU	3.6
1	B	484	GLN	3.3
1	A	354	LEU	3.2
1	B	502	ILE	3.2
1	B	158	GLU	3.0
1	A	369	GLU	2.9
1	B	93	VAL	2.8
1	B	469	PHE	2.7
1	B	144	ALA	2.7
1	A	380	GLY	2.7
1	A	451	ASN	2.6
1	B	90	PRO	2.5
1	B	400	GLN	2.5
1	B	466	ARG	2.4
1	B	433	ARG	2.4
1	A	383	ILE	2.4
1	A	333	LEU	2.4
1	B	325	LYS	2.3
1	B	329	ILE	2.3
1	B	365	LEU	2.3
1	A	370	GLY	2.3
1	A	427	SER	2.3
1	B	398	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	444	GLN	2.3
1	A	101	ALA	2.2
1	B	97	MET	2.2
1	B	399	PHE	2.2
1	A	96	THR	2.2
1	A	361	SER	2.2
1	B	443	ALA	2.1
1	B	378	PRO	2.1
1	B	344	ARG	2.1
1	B	467	THR	2.0
1	A	382	ILE	2.0
1	B	379	PRO	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 [i](#)

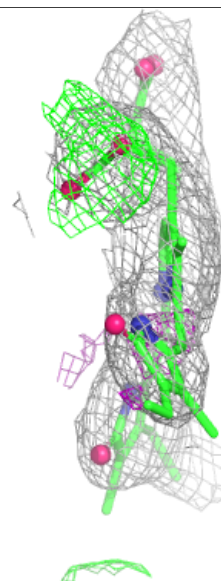
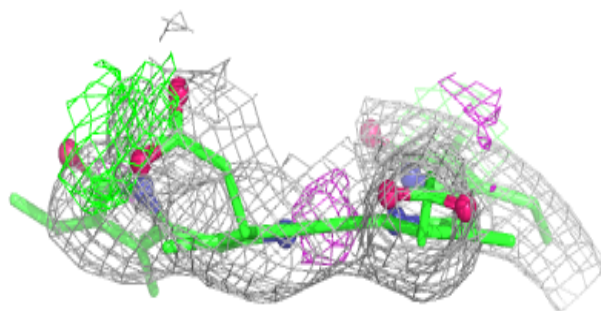
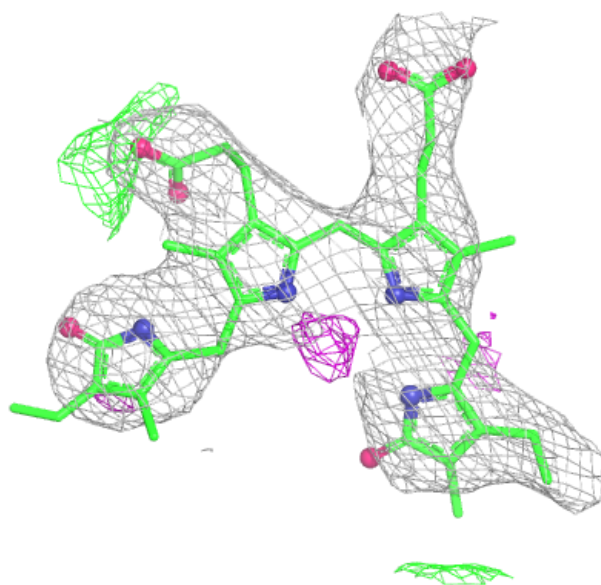
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

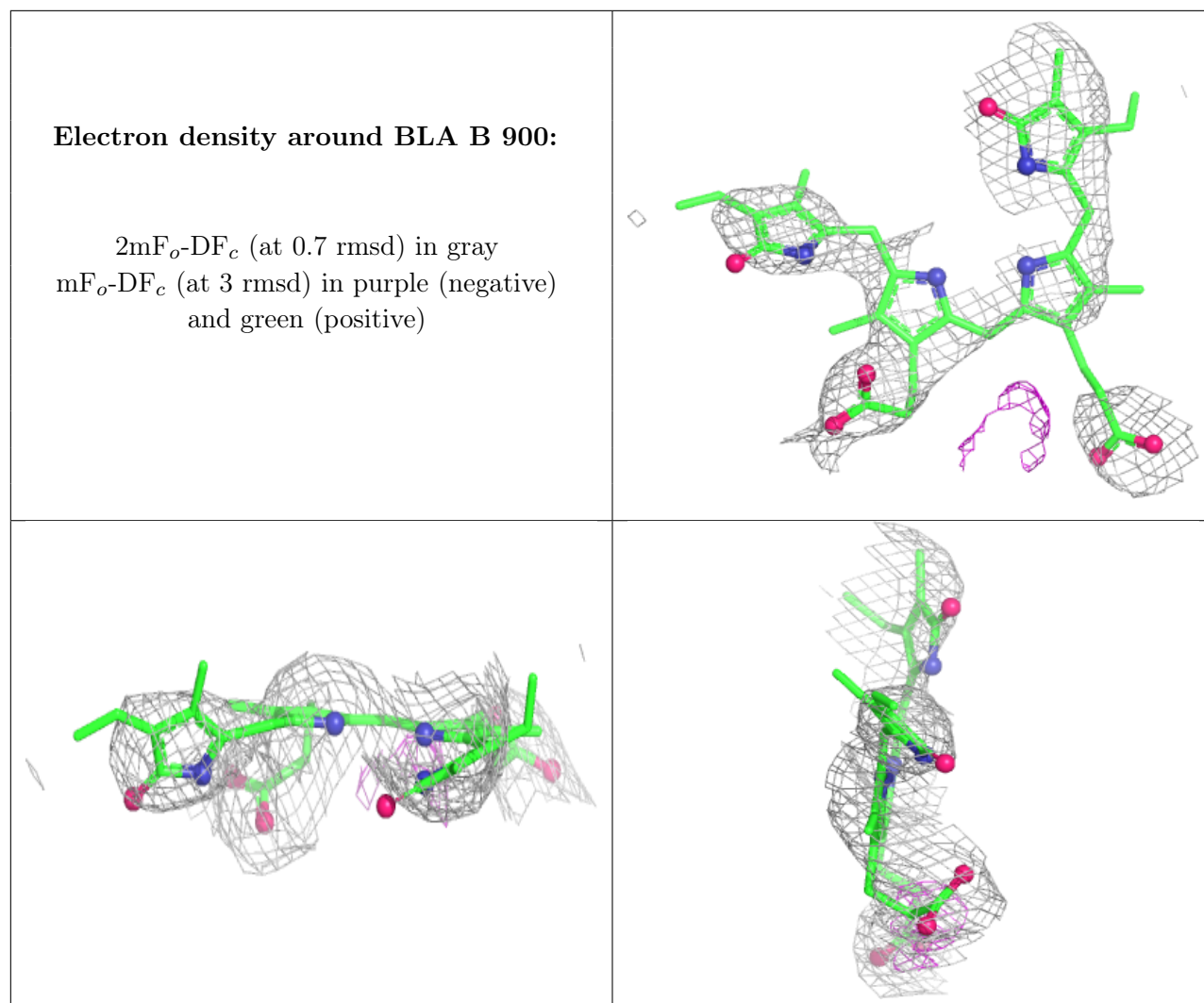
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BLA	A	900	43/43	0.89	0.16	80,115,135,145	0
2	BLA	B	900	43/43	0.92	0.16	134,144,172,183	0

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 A 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.