



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:09 AM UTC

PDB ID : 4R70 / pdb_00004r70
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

<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

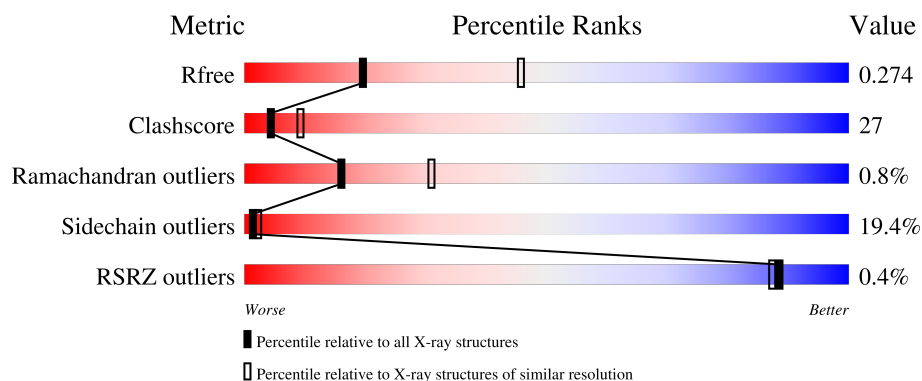
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	529	
1	B	529	

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.

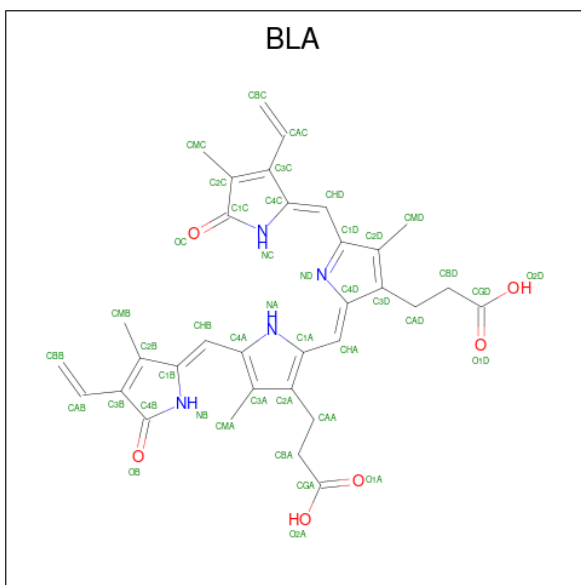
- Molecule 1 is a protein called Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB2.

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 (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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

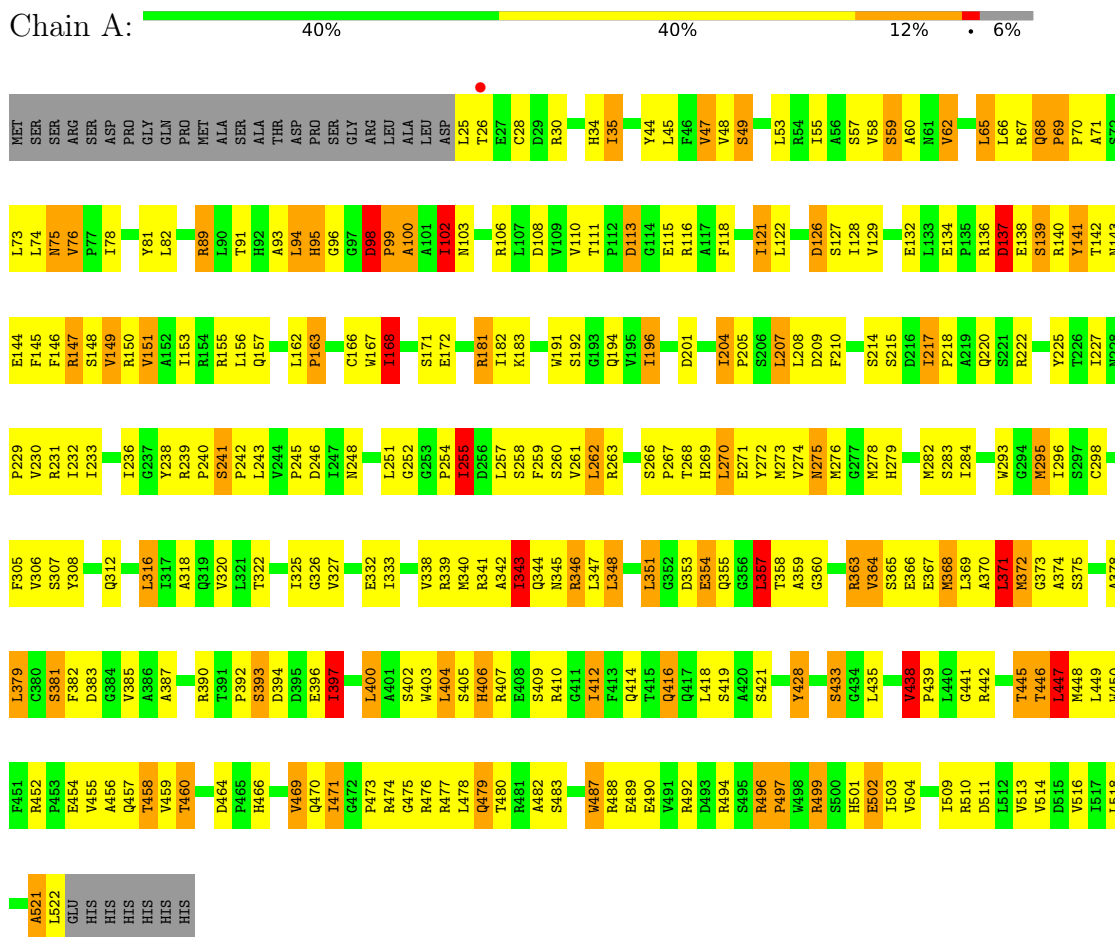
- Molecule 3 is water.

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, 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), PhyB2



- Molecule 1: Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB2



R477	L478	Q479	T480	R481	A482	S483	F484	E485	R488	V491	R492	D493	R494	P497	V498	R499	E502	I503	V504	I509	R510	D511	L512	V513	V514	D515	V516	I517	L518	A521	LEU	GLU	HIS	HIS	HIS	HIS	HIS																					
F413	Q414	T415	Q416	Q417	L418	S419	A420	F422	E426	V427	Y428	S429	D430	T431	A432	S433	G434	L435	L436	A437	V438	P439	L440	G441	R442	A443	S444	T445	T446	L447	M448	L449	W450	F451	R452	A456	Q457	T458	V459	T460	W461	G462	G463	D464	P465	H466	K467	P468	V469	GLN	ILE	GLY	PRO	ARG	GLY	ARG		
G352	D353	E354	Q355	G356	L357	T358	L361	R362	R363	Y364	S365	E366	E367	M368	L369	A370	L371	M372	G373	A374	S375	G376	F377	A378	L379	C380	S381	F382	D383	G384	V385	A386	A387	F388	G389	R390	T391	P392	S393	D394	D395	E396	I397	Q398	A399	L400	A401	S402	W403	L404	S405	H406	R407	E408	S409	R410	G411	I412
V274	M275	M276	G277	M278	H279	A280	A281	M282	S283	I284	S285	R291	L292	W293	G294	R295	I296	S297	C298	H299	N300	L301	T302	P303	V306	S307	E309	V310	A318	Q319	V320	L321	Q324	V327	L328	E329	E332	I333	V334	R335	H336	S337	R338	R339	M340	R341	Q344	L347	L348	L351								
P205	S206	L207	L208	D209	F210	H211	F212	P213	S214	S215	D216	I217	P218	A219	Q220	S221	R222	I227	M228	P229	V230	R231	I232	I236	G237	W238	R239	A240	S241	P242	L243	V244	P245	D246	I247	N248	P249	R250	L251	Q252	I255	F259	L262	R263	S264	V265	S266	P267	T268	H269	L270	E271	Y272	M273				
D64	L65	L66	R67	Q68	P69	P70	L73	L74	N75	V76	P77	I78	A79	H80	Y81	L82	S86	R89	H92	A93	L94	H95	G96	G97	I98	D98	P99	A100	A101	I102	N103	P104	I105	V110	T111	P112	D113	G114	E115	R116	A117	F118	N119	G120	I121	L122	H123	R124	H125	D126	S127	I128	L131	E132				
L133	E134	P135	R136	ASP	GLU	SER	Y141	T142	N143	E144	F145	F146	R147	S148	V149	R150	V151	R155	A160	T164	A165	C166	W167	I168	G97	A169	A170	S171	E172	V173	R174	R175	I176	T177	D180	R181	I182	K183	W184	Y185	Q186	F187	S192	G193	I196	A197	E198	D199	R200	D201	S202	G203	I204					

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 20.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.85) 98.1 (20.00-2.85)	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 0.203 , 0.274	Depositor DCC
R_{free} test set	1704 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	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, 0.333 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	1.46	26/4011 (0.6%)	1.65	64/5461 (1.2%)
1	B	1.46	31/3893 (0.8%)	1.59	55/5301 (1.0%)
All	All	1.46	57/7904 (0.7%)	1.62	119/10762 (1.1%)

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 (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	ALA	CA-CB	-10.52	1.36	1.53
1	B	165	ALA	CA-CB	-8.80	1.39	1.53
1	B	509	ILE	CA-CB	-8.45	1.44	1.54
1	A	412	ILE	CA-CB	-7.97	1.46	1.54
1	A	456	ALA	CA-CB	-7.91	1.41	1.53
1	B	296	ILE	CA-CB	-7.89	1.44	1.53
1	A	196	ILE	CA-CB	-7.76	1.45	1.54
1	B	170	ALA	CA-CB	-7.63	1.41	1.53
1	A	284	ILE	CA-CB	-7.21	1.45	1.54
1	A	378	ALA	CA-C	-7.02	1.44	1.52
1	A	496	ARG	CA-C	-6.87	1.45	1.53
1	A	342	ALA	CA-C	-6.81	1.44	1.52
1	B	456	ALA	CA-CB	-6.69	1.42	1.53
1	B	182	ILE	C-O	-6.68	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	THR	C-O	-6.65	1.16	1.24
1	B	111	THR	CA-C	6.64	1.58	1.52
1	B	320	VAL	CA-CB	-6.56	1.46	1.54
1	A	458	THR	CA-C	-6.53	1.44	1.52
1	B	338	VAL	CA-CB	-6.42	1.46	1.54
1	B	105	ILE	CA-CB	-6.42	1.46	1.54
1	A	514	VAL	CA-CB	-6.41	1.47	1.54
1	A	108	ASP	CA-C	-6.39	1.45	1.52
1	A	121	ILE	CA-CB	-6.31	1.45	1.53
1	A	320	VAL	CA-CB	-6.25	1.47	1.54
1	A	293	TRP	CA-C	-6.16	1.44	1.52
1	A	342	ALA	CA-CB	-6.10	1.43	1.53
1	B	364	VAL	CA-CB	-6.06	1.47	1.54
1	B	452	ARG	CA-C	-6.05	1.46	1.52
1	B	321	LEU	C-O	-5.92	1.17	1.24
1	B	467	LYS	C-N	5.90	1.38	1.33
1	A	153	ILE	CA-CB	-5.85	1.46	1.54
1	B	432	ALA	CA-CB	-5.75	1.45	1.52
1	A	325	ILE	CA-CB	-5.67	1.48	1.54
1	B	209	ASP	CA-C	-5.64	1.45	1.52
1	B	512	LEU	CA-C	-5.63	1.45	1.52
1	A	217	ILE	CA-CB	-5.60	1.47	1.54
1	A	128	ILE	CA-C	-5.53	1.48	1.52
1	B	320	VAL	N-CA	-5.51	1.40	1.46
1	A	233	ILE	CA-CB	-5.48	1.47	1.54
1	B	45	LEU	CA-C	5.38	1.59	1.52
1	A	487	TRP	CA-C	-5.36	1.46	1.52
1	B	284	ILE	CA-CB	-5.32	1.48	1.54
1	A	447	LEU	CA-C	-5.31	1.46	1.52
1	B	160	ALA	CA-CB	-5.23	1.45	1.53
1	B	284	ILE	CA-C	-5.21	1.46	1.52
1	A	387	ALA	CA-CB	-5.20	1.44	1.53
1	B	483	SER	CA-C	-5.17	1.46	1.52
1	A	168	ILE	CA-CB	-5.16	1.48	1.54
1	B	340	MET	N-CA	-5.14	1.40	1.46
1	A	499	ARG	CA-C	5.11	1.59	1.52
1	B	166	CYS	CA-C	-5.11	1.46	1.52
1	B	295	MET	CA-C	-5.10	1.46	1.52
1	A	521	ALA	CA-CB	-5.10	1.44	1.53
1	B	177	THR	CA-CB	-5.10	1.46	1.54
1	B	282	MET	CA-C	-5.08	1.46	1.52
1	B	166	CYS	C-O	-5.03	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	LEU	CA-C	-5.03	1.46	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	SER	N-CA-C	-12.51	98.11	113.50
1	A	217	ILE	CA-C-N	12.13	131.86	120.21
1	A	217	ILE	C-N-CA	12.13	131.86	120.21
1	B	452	ARG	CA-C-N	9.57	131.19	120.85
1	B	452	ARG	C-N-CA	9.57	131.19	120.85
1	A	357	LEU	N-CA-C	-9.56	100.19	112.23
1	A	464	ASP	CA-C-N	-9.48	109.92	120.45
1	A	464	ASP	C-N-CA	-9.48	109.92	120.45
1	A	496	ARG	CA-C-N	9.44	129.53	119.90
1	A	496	ARG	C-N-CA	9.44	129.53	119.90
1	A	438	VAL	CA-C-N	9.31	129.07	119.76
1	A	438	VAL	C-N-CA	9.31	129.07	119.76
1	A	241	SER	CA-C-N	-8.77	108.88	119.84
1	A	241	SER	C-N-CA	-8.77	108.88	119.84
1	B	208	LEU	N-CA-C	8.56	123.15	112.87
1	B	446	THR	N-CA-C	-8.47	93.70	108.69
1	B	42	HIS	N-CA-C	-7.83	103.71	113.18
1	B	117	ALA	N-CA-C	7.68	121.56	109.81
1	A	98	ASP	N-CA-C	-7.65	98.61	109.24
1	A	35	ILE	CA-C-N	-7.58	110.36	119.84
1	A	35	ILE	C-N-CA	-7.58	110.36	119.84
1	B	291	ARG	N-CA-C	-7.50	96.39	108.55
1	B	241	SER	CA-C-N	-7.40	110.59	119.84
1	B	241	SER	C-N-CA	-7.40	110.59	119.84
1	B	134	GLU	CA-C-N	7.31	127.07	119.76
1	B	134	GLU	C-N-CA	7.31	127.07	119.76
1	A	100	ALA	N-CA-C	-7.30	101.68	110.44
1	B	271	GLU	N-CA-C	-7.23	103.12	112.23
1	B	111	THR	CA-C-N	7.21	126.84	119.19
1	B	111	THR	C-N-CA	7.21	126.84	119.19
1	A	48	VAL	N-CA-C	7.16	118.43	108.12
1	B	347	LEU	N-CA-C	-7.14	102.54	111.11
1	A	483	SER	N-CA-C	7.11	120.15	108.99
1	B	208	LEU	CA-C-N	-7.08	110.82	122.08
1	B	208	LEU	C-N-CA	-7.08	110.82	122.08
1	A	134	GLU	CA-C-N	7.07	128.18	119.98
1	A	134	GLU	C-N-CA	7.07	128.18	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	ASN	CA-C-N	-7.02	112.55	121.04
1	B	228	ASN	C-N-CA	-7.02	112.55	121.04
1	A	255	ILE	CB-CA-C	-6.98	102.07	111.15
1	B	79	ALA	N-CA-C	6.96	120.66	111.75
1	A	275[A]	ASN	N-CA-C	-6.95	104.78	113.20
1	A	275[B]	ASN	N-CA-C	-6.95	104.78	113.20
1	A	433	SER	N-CA-C	-6.92	104.98	113.50
1	A	397	ILE	CG1-CB-CG2	-6.81	90.26	110.70
1	A	333	ILE	N-CA-C	6.80	117.56	110.62
1	A	445	THR	N-CA-C	-6.74	103.08	112.45
1	A	516	VAL	N-CA-C	-6.71	103.97	110.42
1	A	416	GLN	N-CA-C	-6.70	105.14	113.38
1	B	118	PHE	N-CA-C	6.68	119.33	109.24
1	B	36	PRO	CB-CA-C	-6.66	101.90	111.62
1	B	173	VAL	N-CA-CB	6.50	117.44	110.62
1	B	40	GLN	CA-C-N	6.35	127.78	119.84
1	B	40	GLN	C-N-CA	6.35	127.78	119.84
1	B	39	ILE	CB-CA-C	-6.34	100.90	111.29
1	B	101	ALA	N-CA-C	-6.31	102.86	110.44
1	B	148	SER	N-CA-C	-6.27	104.53	111.36
1	B	411	GLY	N-CA-C	-6.17	103.77	112.60
1	B	31	GLU	N-CA-C	6.15	117.65	109.83
1	B	374	ALA	N-CA-C	6.11	118.70	109.23
1	B	416	GLN	N-CA-C	-6.08	106.03	113.50
1	A	305	PHE	CA-C-N	-6.06	113.05	122.69
1	A	305	PHE	C-N-CA	-6.06	113.05	122.69
1	A	418	LEU	N-CA-C	-6.04	104.78	111.36
1	A	466	HIS	N-CA-C	5.97	120.56	113.16
1	A	229	PRO	CA-C-N	-5.95	114.14	122.71
1	A	229	PRO	C-N-CA	-5.95	114.14	122.71
1	A	457	GLN	CA-C-N	-5.94	114.62	122.99
1	A	457	GLN	C-N-CA	-5.94	114.62	122.99
1	A	348	LEU	N-CA-C	-5.85	103.88	111.02
1	B	111	THR	N-CA-CB	-5.83	103.95	111.35
1	B	48	VAL	N-CA-C	5.77	116.60	108.17
1	B	379	LEU	CA-C-N	-5.74	115.02	123.05
1	B	379	LEU	C-N-CA	-5.74	115.02	123.05
1	A	89	ARG	N-CA-C	-5.70	105.07	111.28
1	B	418	LEU	N-CA-C	-5.66	104.49	111.40
1	A	458	THR	N-CA-C	-5.60	99.77	108.90
1	B	396	GLU	N-CA-C	5.59	120.16	113.23
1	A	166	CYS	CA-CB-SG	-5.56	101.60	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	ALA	N-CA-C	5.55	119.15	112.38
1	A	102	ILE	N-CA-C	-5.54	104.90	113.16
1	B	447	LEU	N-CA-C	5.54	118.61	109.85
1	B	168	ILE	N-CA-C	-5.46	105.05	110.62
1	A	346	ARG	N-CA-C	-5.44	104.75	111.33
1	A	372	MET	N-CA-C	5.43	119.00	112.38
1	A	371	LEU	N-CA-C	-5.42	105.28	111.14
1	B	509	ILE	N-CA-C	5.41	115.62	110.53
1	A	128	ILE	CA-C-N	-5.37	116.53	123.19
1	A	128	ILE	C-N-CA	-5.37	116.53	123.19
1	A	140	ARG	CA-C-N	-5.37	114.62	122.19
1	A	140	ARG	C-N-CA	-5.37	114.62	122.19
1	B	111	THR	N-CA-C	5.35	114.30	108.14
1	B	33	ILE	N-CA-C	-5.30	105.80	113.07
1	B	187	PHE	N-CA-C	5.29	118.10	110.28
1	B	358	THR	N-CA-C	-5.28	105.42	111.07
1	A	181	ARG	N-CA-C	5.20	117.90	108.69
1	A	439	PRO	CB-CA-C	-5.19	104.31	111.21
1	B	110	VAL	N-CA-CB	5.16	116.16	110.53
1	B	68	GLN	CA-C-N	5.15	125.69	120.38
1	B	68	GLN	C-N-CA	5.15	125.69	120.38
1	A	255	ILE	N-CA-C	5.15	115.69	108.89
1	B	332	GLU	N-CA-C	-5.14	105.75	111.36
1	A	326	GLY	N-CA-C	5.14	118.90	112.73
1	A	318	ALA	CA-C-O	5.12	125.86	119.97
1	A	332	GLU	N-CA-C	-5.12	105.78	111.36
1	A	454	GLU	N-CA-C	-5.11	103.40	110.35
1	A	181	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	A	49	SER	N-CA-C	-5.09	102.33	109.96
1	A	497	PRO	CA-C-O	-5.08	115.62	121.36
1	B	113	ASP	N-CA-C	5.07	116.62	111.14
1	B	329	GLU	CA-C-O	-5.06	115.69	121.00
1	A	115	GLU	N-CA-C	5.05	117.37	110.24
1	B	372	MET	N-CA-C	-5.05	103.81	110.43
1	A	266	SER	CA-C-N	-5.05	113.84	119.19
1	A	266	SER	C-N-CA	-5.05	113.84	119.19
1	A	343	ILE	CB-CA-C	-5.03	105.36	112.14
1	A	239	ARG	CA-C-N	5.02	126.12	119.84
1	A	239	ARG	C-N-CA	5.02	126.12	119.84
1	B	206	SER	N-CA-C	5.01	117.56	109.40

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	206	2
1	B	3806	0	3775	218	2
2	A	43	0	31	10	0
2	B	43	0	31	3	0
3	A	16	0	0	2	0
3	B	7	0	0	0	0
All	All	7830	0	7730	416	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 27.

All (416) 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:A:448:MET:HE1	1:A:513:VAL:HG21	1.51	0.91
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:B:448:MET:HE1	1:B:513:VAL:HG11	1.57	0.86
1:A:181:ARG:HE	1:A:183:LYS:HZ2	1.25	0.83
1:A:98:ASP:OD2	1:A:98:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLN:N	1:A:220:GLN:OE1	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:368:MET:HE2	1:B:509:ILE:HD13	1.68	0.75
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
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
1:B:365:SER:OG	1:B:366:GLU:N	2.23	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:92:HIS:O	1:B:96:GLY:N	2.26	0.69
1:B:460:THR:HG21	1:B:488:ARG:HH21	1.57	0.69
1:A:71:ALA:HA	1:A:74:LEU:HG	1.75	0.68
1:A:60:ALA:HB2	1:A:242:PRO:HD2	1.74	0.68
1:A:144:GLU:HA	1:A:147:ARG:NH1	2.09	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:155:ARG:HH12	1:B:175:ARG:HH12	1.44	0.66
1:B:381:SER:HB3	1:B:383:ASP:H	1.61	0.66
1:A:26:THR:O	1:A:30:ARG:HG3	1.96	0.66
1:B:398:GLN:O	1:B:402:SER:OG	2.14	0.66
1:B:232:ILE:HD12	1:B:282:MET:HE2	1.77	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:136:ARG:NH1	1:A:139:SER:OG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:208:LEU:HG	1:B:208:LEU:O	1.96	0.63
1:B:462:GLY:HA3	1:B:481:ARG:HH21	1.63	0.63
1:B:448:MET:HE1	1:B:513:VAL:CG1	2.28	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:145:PHE:O	1:B:148:SER:OG	2.17	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:A:207:LEU:HD21	1:A:276:MET:HE1	1.80	0.62
1:B:217:ILE:CG2	1:B:222:ARG:HG2	2.27	0.62
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:65:LEU:HD13	1:B:66:LEU:HG	1.82	0.62
1:B:462:GLY:HA3	1:B:481:ARG:NH2	2.14	0.62
1:A:347:LEU:CD2	1:A:351:LEU:HD23	2.29	0.62
1:A:351:LEU:HD12	1:A:351:LEU:O	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:198:GLU:OE2	1:B:206:SER:OG	2.12	0.61
1:B:354:GLU:OE1	1:B:356:GLY:N	2.30	0.61
1:A:412:ILE:CD1	1:A:438:VAL:HB	2.31	0.61
1:B:65:LEU:CD1	1:B:66:LEU:HG	2.30	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:A:347:LEU:HD11	1:A:368:MET:HE3	1.83	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:231:ARG:HH22	1:A:295:MET:HE1	1.66	0.59
1:B:132:GLU:HB3	1:B:262:LEU:HD12	1.84	0.59
1:A:345:ASN:O	1:A:346:ARG:C	2.46	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:338:VAL:HG21	1:B:149:VAL:HG21	1.86	0.58
1:A:445:THR:HB	1:A:446:THR:HG22	1.85	0.58
1:B:52:ASP:OD1	1:B:52:ASP:N	2.33	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:B:347:LEU:HD23	1:B:364:VAL:HG21	1.86	0.57
1:A:55:ILE:O	1:A:75:ASN:N	2.34	0.57
1:A:476:ARG:HE	1:A:478:LEU:CG	2.18	0.57
1:A:487:TRP:CZ3	1:A:489:GLU:HB2	2.40	0.57
1:B:58:VAL:HG22	1:B:62:VAL:HG21	1.87	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:A:358:THR:OG1	1:A:359:ALA:N	2.38	0.56
1:B:59:SER:O	1:B:62:VAL:HG23	2.05	0.56
1:A:283:SER:HB2	1:A:295:MET:CE	2.36	0.56
1:A:487:TRP:HZ3	1:A:489:GLU:HB2	1.71	0.56
1:A:155:ARG:NH1	1:A:172:GLU:OE2	2.38	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: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:A:231:ARG:NH2	1:A:295:MET:HE1	2.21	0.56
1:B:248:ASN:OD1	1:B:251:LEU:N	2.28	0.56
1:A:181:ARG:HH12	1:A:276:MET:HE2	1.71	0.55
1:A:269:HIS:O	1:A:272:TYR:HB3	2.06	0.55
1:A:273:MET:HE2	1:A:273:MET:HA	1.86	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:268:THR:HG23	1:A:478:LEU:O	2.07	0.54
1:A:341:ARG:CZ	1:B:101:ALA:HB1	2.36	0.54
1:A:94:LEU:HG	1:A:95:HIS:ND1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:81:TYR:C	1:B:110:VAL:HG12	2.33	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:431:ILE:C	1:B:431:ILE:HD12	2.33	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:A:147:ARG:HB2	1:A:147:ARG:HH11	1.73	0.52
1:A:354:GLU:OE1	1:A:363:ARG:HD3	2.09	0.52
1:B:50:GLU:O	1:B:53:LEU:N	2.42	0.52
1:B:415:THR:OG1	1:B:417:GLN:N	2.38	0.52
1:B:414:GLN:HG2	1:B:415:THR:N	2.19	0.52
1:A:347:LEU:O	1:A:351:LEU:HB3	2.10	0.52
1:A:402:SER:O	1:A:403:TRP:C	2.53	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:231:ARG:HH12	1:B:285:SER:HG	1.55	0.51
1:A:448:MET:CE	1:A:513:VAL:HG21	2.34	0.51
1:B:400:LEU:HD11	1:B:435:LEU:HD22	1.93	0.51
1:A:490:GLU:HG2	1:A:492:ARG:CZ	2.40	0.51
1:B:200:ARG:HD2	1:B:204:ILE:O	2.10	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:294:GLY:C	1:B:295:MET:HG2	2.34	0.51
1:A:89:ARG:HA	1:B:353:ASP:OD2	2.11	0.50
1:B:267:PRO:O	1:B:270:LEU:HB2	2.11	0.50
1:A:217:ILE:O	1:A:222:ARG:NH1	2.42	0.50
1:B:243:LEU:HD13	1:B:255:ILE:HD12	1.93	0.50
1:A:25:LEU:N	1:A:477:ARG:NH1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASP:HB3	1:B:204:ILE:HD13	1.91	0.50
1:A:316:LEU:HD22	1:B:338:VAL:HG13	1.94	0.50
1:B:99:PRO:HD2	1:B:101:ALA:HB3	1.93	0.50
1:B:283:SER:HB2	1:B:295:MET:HE2	1.93	0.50
1:A:137:ASP:CB	1:A:307:SER:HB3	2.42	0.50
1:A:471:ILE:HD11	1:A:475:GLY:HA2	1.93	0.50
1:B:369:LEU:HD22	1:B:374:ALA:O	2.12	0.50
1:A:73:LEU:O	1:A:73:LEU:HD12	2.12	0.50
1:A:341:ARG:O	1:A:344:GLN:HB3	2.11	0.50
1:A:69:PRO:CB	1:A:70:PRO:HD2	2.42	0.50
1:A:490:GLU:HG2	1:A:492:ARG:NH1	2.26	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:36:PRO:HG2	1:B:38:ALA:H	1.77	0.49
1:A:111:THR:HG23	1:A:113:ASP:O	2.11	0.49
1:A:232:ILE:HD12	1:A:282:MET:HE2	1.94	0.49
1:B:58:VAL:HG13	1:B:59:SER:N	2.28	0.49
1:A:66:LEU:C	1:A:68:GLN:H	2.20	0.49
1:B:499:ARG:N	1:B:502:GLU:OE1	2.32	0.49
1:B:412:ILE:HD13	1:B:412:ILE:H	1.77	0.49
1:A:416:GLN:OE1	1:A:497:PRO:HA	2.12	0.49
1:B:50:GLU:O	1:B:51:THR:C	2.56	0.49
1:B:379:LEU:HD12	1:B:447:LEU:O	2.12	0.49
1:B:468:PRO:HA	1:B:481:ARG:HD2	1.95	0.49
1:A:55:ILE:HD11	1:A:78:ILE:HG13	1.93	0.49
1:A:116:ARG:HB3	1:A:118:PHE:HE2	1.76	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: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:385:VAL:HG23	1:B:398:GLN:HE21	1.76	0.48
1:B:56:ALA:HB1	1:B:249:PRO:HG3	1.95	0.48
1:B:125:HIS:O	1:B:128:ILE:HG13	2.13	0.48
1:A:406:HIS:O	1:A:407:ARG:C	2.56	0.48
1:A:106:ARG:HH22	1:A:136:ARG:CZ	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TYR:CD1	1:A:273:MET:HE3	2.49	0.48
1:B:379:LEU:HA	1:B:447:LEU:O	2.14	0.48
1:B:397:ILE:HG12	1:B:398:GLN:N	2.29	0.48
1:A:95:HIS:ND1	1:A:95:HIS:N	2.59	0.47
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.72	0.47
1:A:271:GLU:O	1:A:275[A]:ASN:ND2	2.38	0.47
1:B:406:HIS:O	1:B:407:ARG:C	2.56	0.47
1:B:481:ARG:NH1	1:B:484:PHE:HE1	2.12	0.47
1:B:375:SER:O	1:B:390:ARG:N	2.43	0.47
1:A:521:ALA:C	1:A:522:LEU:HG	2.39	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
1:A:397:ILE:HG13	1:A:397:ILE:H	1.47	0.47
1:B:39:ILE:HD12	1:B:40:GLN:C	2.40	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:282:MET:HE1	1:B:306:VAL:HG12	1.96	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:75:ASN:O	1:A:75:ASN:ND2	2.47	0.47
1:A:396:GLU:HB2	1:A:428:TYR:CE1	2.50	0.47
1:B:297:SER:C	1:B:298:CYS:SG	2.98	0.47
1:A:126:ASP:OD2	1:A:251:LEU:HD12	2.14	0.46
1:A:204:ILE:HG23	1:A:205:PRO:HD2	1.97	0.46
1:A:58:VAL:HG21	1:A:62:VAL:HG21	1.97	0.46
1:A:93:ALA:C	1:A:96:GLY:H	2.22	0.46
1:B:229:PRO:C	1:B:231:ARG:HH11	2.23	0.46
1:A:267:PRO:HA	1:A:270:LEU:HB2	1.97	0.46
1:A:473:PRO:HD2	1:A:476:ARG:HH12	1.81	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:B:245:PRO:CG	1:B:247:ILE:HG12	2.44	0.46
1:B:272:TYR:O	1:B:275:ASN:HB2	2.16	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:A:157:GLN:OE1	1:B:335:ARG:NH1	2.48	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:302:THR:OG1	1:B:303:PRO:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ARG:O	1:A:502:GLU:N	2.39	0.46
1:B:33:ILE:HD13	1:B:220:GLN:HG2	1.97	0.46
1:B:448:MET:HE3	1:B:448:MET:HB2	1.84	0.46
1:A:366:GLU:O	1:A:370:ALA:N	2.41	0.46
1:A:400:LEU:HD11	1:A:435:LEU:CD2	2.45	0.46
1:B:123:HIS:CE1	1:B:259:PHE:HB2	2.51	0.46
1:B:213:PRO:HD2	1:B:216:ASP:OD1	2.16	0.46
1:A:132:GLU:OE2	1:A:260:SER:OG	2.20	0.46
1:B:81:TYR:O	1:B:110:VAL:HG12	2.15	0.46
1:B:99:PRO:O	1:B:100:ALA:C	2.59	0.46
1:A:58:VAL:HG22	1:A:59:SER:H	1.79	0.46
1:B:50:GLU:C	1:B:53:LEU:H	2.24	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:181:ARG:NE	1:A:183:LYS:HZ2	2.04	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: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:B:436:LEU:HD12	1:B:436:LEU:HA	1.51	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:B:381:SER:HB3	1:B:383:ASP:OD1	2.17	0.45
1:B:385:VAL:HG21	1:B:397:ILE:HD11	1.97	0.45
1:A:47:VAL:HA	1:A:129:VAL:O	2.16	0.45
1:A:100:ALA:HA	1:A:102:ILE:HD13	1.99	0.45
1:A:368:MET:HE2	1:A:509:ILE:CG2	2.47	0.45
1:B:396:GLU:O	1:B:399:ALA:HB3	2.17	0.45
1:A:347:LEU:O	1:A:348:LEU:C	2.60	0.45
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:B:407:ARG:C	1:B:409:SER:H	2.26	0.45
1:A:150:ARG:HG3	1:B:335:ARG:O	2.17	0.44
1:B:113:ASP:OD1	1:B:114:GLY:N	2.50	0.44
1:B:211:HIS:CD2	1:B:459:VAL:HG23	2.51	0.44
1:A:338:VAL:O	1:A:339:ARG:C	2.59	0.44
1:B:44:TYR:CD1	1:B:61:ASN:ND2	2.85	0.44
1:A:341:ARG:NH1	1:B:101:ALA:HB1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:236:ILE:HG23	1:B:279:HIS:C	2.42	0.44
1:A:81:TYR:N	1:A:81:TYR:CD2	2.84	0.44
1:A:369:LEU:HD22	1:A:374:ALA:O	2.16	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:B:377:PHE:C	1:B:377:PHE:CD1	2.95	0.44
1:A:393:SER:CB	1:A:396:GLU:HG2	2.47	0.44
1:A:232:ILE:HB	1:A:282:MET:HG3	1.99	0.44
1:B:403:TRP:CE3	1:B:404:LEU:HD13	2.53	0.44
1:B:464:ASP:OD1	1:B:464:ASP:N	2.51	0.44
1:B:491:VAL:O	1:B:491:VAL:HG13	2.18	0.44
1:A:55:ILE:HD12	1:A:73:LEU:HD11	2.00	0.44
1:A:98:ASP:O	1:A:99:PRO:C	2.61	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
1:B:416:GLN:HE21	1:B:497:PRO:HA	1.83	0.44
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:A:368:MET:HE2	1:A:509:ILE:HG23	1.99	0.43
1:B:120:GLY:C	1:B:121:ILE:HD12	2.42	0.43
1:B:383:ASP:OD1	1:B:383:ASP:N	2.52	0.43
1:A:390:ARG:HA	1:A:390:ARG:HD3	1.68	0.43
1:B:248:ASN:O	1:B:252:GLY:HA2	2.19	0.43
1:A:53:LEU:O	1:A:78:ILE:HG22	2.18	0.43
1:A:181:ARG:HG2	1:A:183:LYS:HZ2	1.83	0.43
1:A:402:SER:O	1:A:405:SER:N	2.51	0.43
1:B:267:PRO:O	1:B:268:THR:C	2.61	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: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: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:B:285:SER:HB3	1:B:292:LEU:HD11	2.01	0.43
1:B:181:ARG:HE	1:B:183:LYS:NZ	2.16	0.43
1:A:267:PRO:O	1:A:268:THR:C	2.62	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:246:ASP:OD2	1:A:254:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275[B]:ASN:HD21	1:A:482:ALA:HA	1.84	0.43
1:A:347:LEU:CD2	1:A:364:VAL:HG21	2.49	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:B:214:SER:C	1:B:216:ASP:N	2.76	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:309:GLU:H	1:B:309:GLU:CD	2.22	0.42
1:A:182:ILE:HD12	1:A:182:ILE:HG23	1.79	0.42
2:A:900:BLA:NB	2:A:900:BLA:CMA	2.83	0.42
1:B:272:TYR:CE2	1:B:484:PHE:HZ	2.37	0.42
1:B:281:ALA:HA	1:B:298:CYS:O	2.19	0.42
1:B:478:LEU:CG	1:B:479:GLN:H	2.31	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:79:ALA:C	1:B:81:TYR:H	2.27	0.42
1:B:180:ASP:HB3	1:B:204:ILE:HG12	2.02	0.42
1:B:481:ARG:NH1	1:B:484:PHE:CE1	2.88	0.42
2:A:900:BLA:HAD2	2:A:900:BLA:HHA	1.85	0.42
1:B:231:ARG:NH2	1:B:295:MET:HE1	2.34	0.42
1:B:390:ARG:HA	1:B:390:ARG:HD3	1.81	0.42
1:B:452:ARG:NH2	1:B:502:GLU:OE2	2.52	0.42
1:A:217:ILE:HA	1:A:218:PRO:HD2	1.81	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
1:B:56:ALA:CB	1:B:249:PRO:HG3	2.49	0.42
1:B:348:LEU:C	1:B:348:LEU:HD23	2.45	0.42
1:B:361:LEU:HD23	1:B:361:LEU:HA	1.80	0.42
1:B:515:ASP:O	1:B:518:LEU:HB2	2.20	0.42
1:A:147:ARG:O	1:A:151:VAL:HG13	2.20	0.42
1:A:295:MET:HE3	1:A:295:MET:HB3	1.57	0.42
1:A:365:SER:OG	1:A:366:GLU:N	2.53	0.42
2:A:900:BLA:CMA	2:A:900:BLA:HB	2.33	0.42
1:B:460:THR:HG21	1:B:488:ARG:NH2	2.29	0.42
1:A:66:LEU:C	1:A:68:GLN:N	2.76	0.41
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:A:368:MET:HE2	1:A:509:ILE:HD13	2.00	0.41
1:A:400:LEU:HD22	1:A:404:LEU:HD22	2.02	0.41
1:B:44:TYR:CD2	1:B:65:LEU:HD23	2.55	0.41
1:B:92:HIS:O	1:B:93:ALA:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:VAL:C	1:B:336:HIS:H	2.28	0.41
1:B:428:TYR:O	1:B:429:SER:C	2.63	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:94:LEU:HA	1:B:94:LEU:HD23	1.65	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:A:59:SER:HB2	1:A:241:SER:OG	2.20	0.41
1:A:409:SER:O	1:A:410:ARG:HD3	2.21	0.41
1:B:208:LEU:O	1:B:208:LEU:CG	2.66	0.41
1:B:344:GLN:O	1:B:348:LEU:HB2	2.20	0.41
1:A:210:PHE:N	1:A:210:PHE:CD2	2.88	0.41
1:A:255:ILE:HG22	1:A:257:LEU:HG	2.03	0.41
1:B:266:SER:HB3	2:B:900:BLA:HBD2	2.03	0.41
1:B:324:GLN:HA	1:B:327:VAL:HG13	2.01	0.41
1:A:283:SER:HB2	1:A:295:MET:HE1	2.02	0.41
1:A:94:LEU:HG	1:A:95:HIS:CE1	2.56	0.41
1:A:274:VAL:C	1:A:276:MET:H	2.29	0.41
1:B:391:THR:OG1	1:B:392:PRO:O	2.38	0.41
1:A:403:TRP:CE3	1:A:404:LEU:HD13	2.56	0.41
1:B:413:PHE:CG	1:B:414:GLN:N	2.88	0.41
1:A:272:TYR:HD1	1:A:273:MET:HE3	1.86	0.40
1:A:347:LEU:HG	1:A:364:VAL:HG21	2.03	0.40
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.72	0.40
1:B:387:ALA:C	1:B:388:PHE:CD2	2.99	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
1:A:496:ARG:HA	1:A:497:PRO:HD3	1.85	0.40
1:B:102:ILE:HG12	1:B:103:ASN:N	2.35	0.40
1:B:131:LEU:HG	1:B:132:GLU:N	2.34	0.40
1:A:257:LEU:O	1:A:258:SER:C	2.65	0.40
1:A:412:ILE:HA	1:A:412:ILE:HD13	1.84	0.40
1:B:132:GLU:HB3	1:B:262:LEU:CD1	2.51	0.40
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

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%)	16	31
1	B	480/529 (91%)	440 (92%)	36 (8%)	4 (1%)	16	31
All	All	978/1058 (92%)	889 (91%)	81 (8%)	8 (1%)	16	31

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 [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	421/445 (95%)	336 (80%)	85 (20%)	1	2
1	B	409/445 (92%)	333 (81%)	76 (19%)	1	2
All	All	830/890 (93%)	669 (81%)	161 (19%)	1	2

All (161) 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	76	VAL
1	A	82	LEU
1	A	91	THR
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	149	VAL
1	A	151	VAL
1	A	156	LEU
1	A	163	PRO
1	A	168	ILE
1	A	171	SER
1	A	192	SER
1	A	194	GLN
1	A	196	ILE
1	A	204	ILE
1	A	207	LEU
1	A	215	SER
1	A	230	VAL

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Mol	Chain	Res	Type
1	A	255	ILE
1	A	261	VAL
1	A	262	LEU
1	A	270	LEU
1	A	295	MET
1	A	298	CYS
1	A	306	VAL
1	A	316	LEU
1	A	327	VAL
1	A	340	MET
1	A	343	ILE
1	A	351	LEU
1	A	354	GLU
1	A	355	GLN
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	455	VAL
1	A	458	THR
1	A	459	VAL
1	A	460	THR
1	A	469	VAL

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Mol	Chain	Res	Type
1	A	471	ILE
1	A	474	ARG
1	A	479	GLN
1	A	494	ARG
1	A	501	HIS
1	A	502	GLU
1	A	503	ILE
1	A	504	VAL
1	B	51	THR
1	B	52	ASP
1	B	58	VAL
1	B	68	GLN
1	B	75	ASN
1	B	78	ILE
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	128	ILE
1	B	149	VAL
1	B	151	VAL
1	B	164	THR
1	B	168	ILE
1	B	171	SER
1	B	176	ILE
1	B	192	SER
1	B	196	ILE
1	B	202	SER
1	B	204	ILE
1	B	214	SER
1	B	227	ILE
1	B	230	VAL
1	B	231	ARG
1	B	239	ARG
1	B	241	SER
1	B	247	ILE

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Mol	Chain	Res	Type
1	B	274	VAL
1	B	276	MET
1	B	295	MET
1	B	302	THR
1	B	319	GLN
1	B	327	VAL
1	B	328	LEU
1	B	338	VAL
1	B	341	ARG
1	B	351	LEU
1	B	357	LEU
1	B	358	THR
1	B	363	ARG
1	B	364	VAL
1	B	367	GLU
1	B	368	MET
1	B	371	LEU
1	B	381	SER
1	B	391	THR
1	B	394	ASP
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	440	LEU
1	B	446	THR
1	B	459	VAL
1	B	460	THR
1	B	464	ASP
1	B	469	VAL
1	B	479	GLN
1	B	493	ASP
1	B	494	ARG
1	B	503	ILE
1	B	504	VAL
1	B	510	ARG
1	B	513	VAL
1	B	514	VAL
1	B	516	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	A	501	HIS
1	B	40	GLN
1	B	42	HIS
1	B	75	ASN
1	B	80	HIS
1	B	211	HIS
1	B	269	HIS
1	B	319	GLN
1	B	344	GLN
1	B	416	GLN
1	B	501	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	900	1	46,46,46	2.68	17 (36%)	66,67,67	2.20	21 (31%)
2	BLA	A	900	1	46,46,46	2.67	19 (41%)	66,67,67	1.95	21 (31%)

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	B	900	1	-	10/26/74/74	0/4/4/4
2	BLA	A	900	1	-	9/26/74/74	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	CHD-C4C	7.68	1.56	1.37
2	A	900	BLA	CHD-C4C	6.99	1.54	1.37
2	B	900	BLA	CHD-C1D	6.51	1.55	1.40
2	A	900	BLA	CHD-C1D	6.24	1.55	1.40
2	A	900	BLA	C1C-C2C	-5.47	1.35	1.48
2	B	900	BLA	CHB-C4A	4.99	1.51	1.40
2	B	900	BLA	CBC-CAC	4.78	1.53	1.30
2	A	900	BLA	CHB-C4A	4.76	1.51	1.40
2	A	900	BLA	CBC-CAC	4.66	1.52	1.30
2	B	900	BLA	C1C-C2C	-4.41	1.37	1.48
2	A	900	BLA	C4D-C3D	-4.34	1.38	1.45
2	A	900	BLA	CHB-C1B	4.18	1.47	1.37
2	B	900	BLA	C1D-C2D	-4.13	1.36	1.45
2	B	900	BLA	CHB-C1B	4.02	1.47	1.37
2	B	900	BLA	C4A-NA	-3.65	1.31	1.37
2	A	900	BLA	C4A-NA	-3.49	1.31	1.37
2	A	900	BLA	C1B-C2B	-3.47	1.38	1.45
2	B	900	BLA	C1A-NA	-3.47	1.31	1.37
2	B	900	BLA	CAB-C3B	-3.43	1.38	1.47
2	B	900	BLA	CMA-C3A	3.37	1.57	1.50
2	A	900	BLA	C1D-C2D	-3.18	1.38	1.45
2	A	900	BLA	CAB-C3B	-3.15	1.39	1.47
2	A	900	BLA	C1B-NB	-3.15	1.32	1.37
2	B	900	BLA	C4D-C3D	-3.12	1.40	1.45
2	B	900	BLA	C1B-C2B	-3.00	1.39	1.45
2	A	900	BLA	CBA-CGA	2.88	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	CAC-C3C	2.75	1.54	1.47
2	B	900	BLA	C1B-NB	-2.74	1.33	1.37
2	B	900	BLA	C3C-C4C	-2.48	1.41	1.45
2	A	900	BLA	C4C-NC	-2.48	1.33	1.37
2	A	900	BLA	CAC-C3C	2.44	1.53	1.47
2	A	900	BLA	C1A-NA	-2.35	1.33	1.37
2	A	900	BLA	C3C-C4C	-2.29	1.41	1.45
2	A	900	BLA	C3B-C4B	-2.13	1.38	1.47
2	A	900	BLA	C4B-NB	-2.02	1.33	1.38
2	B	900	BLA	C4D-ND	-2.00	1.34	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	CHA-C4D-ND	5.40	135.95	124.60
2	B	900	BLA	C4A-CHB-C1B	-5.27	115.66	130.82
2	B	900	BLA	CHD-C1D-ND	5.27	136.33	124.95
2	B	900	BLA	CHB-C4A-NA	-5.00	113.99	125.29
2	B	900	BLA	CHB-C4A-C3A	4.88	139.49	127.53
2	B	900	BLA	CHA-C4D-ND	4.16	133.34	124.60
2	B	900	BLA	CMB-C2B-C1B	4.08	129.12	124.16
2	A	900	BLA	CMB-C2B-C1B	3.86	128.85	124.16
2	A	900	BLA	O1D-CGD-CBD	-3.85	110.88	123.09
2	A	900	BLA	CBC-CAC-C3C	-3.72	108.92	127.53
2	A	900	BLA	CHA-C4D-C3D	-3.67	116.92	125.40
2	B	900	BLA	C3B-C4B-NB	3.67	110.74	106.13
2	B	900	BLA	C1B-NB-C4B	-3.66	106.17	110.66
2	A	900	BLA	C4A-CHB-C1B	-3.55	120.62	130.82
2	A	900	BLA	C4D-ND-C1D	3.38	112.72	106.52
2	B	900	BLA	CHA-C4D-C3D	-3.29	117.81	125.40
2	B	900	BLA	CMA-C3A-C4A	3.25	130.34	125.62
2	B	900	BLA	CHD-C1D-C2D	-3.12	116.87	124.87
2	A	900	BLA	CHD-C1D-ND	3.05	131.55	124.95
2	B	900	BLA	C1D-C2D-C3D	3.03	109.91	106.48
2	B	900	BLA	CAD-CBD-CGD	-2.89	106.00	113.67
2	A	900	BLA	CHB-C4A-C3A	2.78	134.35	127.53
2	B	900	BLA	C2B-C1B-NB	2.77	111.00	106.97
2	B	900	BLA	CBC-CAC-C3C	-2.76	113.73	127.53
2	A	900	BLA	C1A-CHA-C4D	-2.62	122.49	128.22
2	A	900	BLA	C4A-NA-C1A	2.56	114.28	109.78
2	A	900	BLA	C2D-C1D-ND	-2.56	104.99	110.58
2	A	900	BLA	O2D-CGD-O1D	2.54	129.86	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C3D-C4D-ND	-2.51	106.50	110.04
2	A	900	BLA	C1D-C2D-C3D	2.48	109.29	106.48
2	A	900	BLA	C1A-C2A-C3A	-2.37	104.87	107.62
2	A	900	BLA	C3A-C4A-NA	-2.35	104.23	107.43
2	B	900	BLA	O1A-CGA-CBA	-2.24	115.98	123.09
2	A	900	BLA	CAC-C3C-C4C	2.20	130.11	123.66
2	A	900	BLA	O1A-CGA-CBA	-2.20	116.12	123.09
2	B	900	BLA	C4C-CHD-C1D	-2.19	122.69	128.06
2	A	900	BLA	CMB-C2B-C3B	-2.14	123.24	128.43
2	B	900	BLA	CHD-C4C-C3C	-2.14	121.84	127.94
2	B	900	BLA	CAA-C2A-C1A	2.10	129.10	125.77
2	A	900	BLA	CAD-CBD-CGD	-2.09	108.13	113.67
2	B	900	BLA	C1A-CHA-C4D	-2.08	123.67	128.22
2	B	900	BLA	C1A-C2A-C3A	-2.07	105.21	107.62

There are no chirality outliers.

All (19) torsion outliers are listed below:

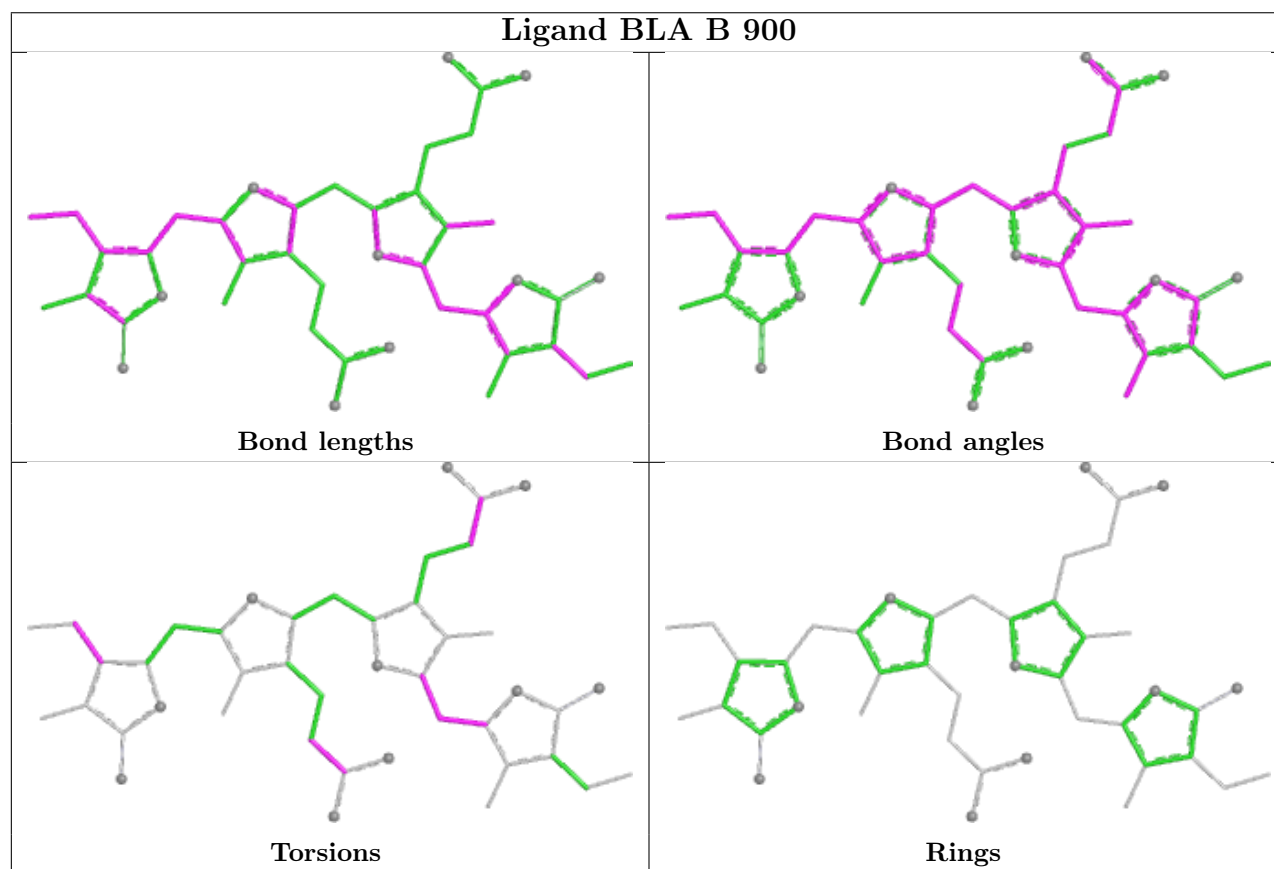
Mol	Chain	Res	Type	Atoms
2	A	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	C4C-C3C-CAC-CBC
2	B	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C2B-C1B-CHB-C4A
2	B	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	C4C-C3C-CAC-CBC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

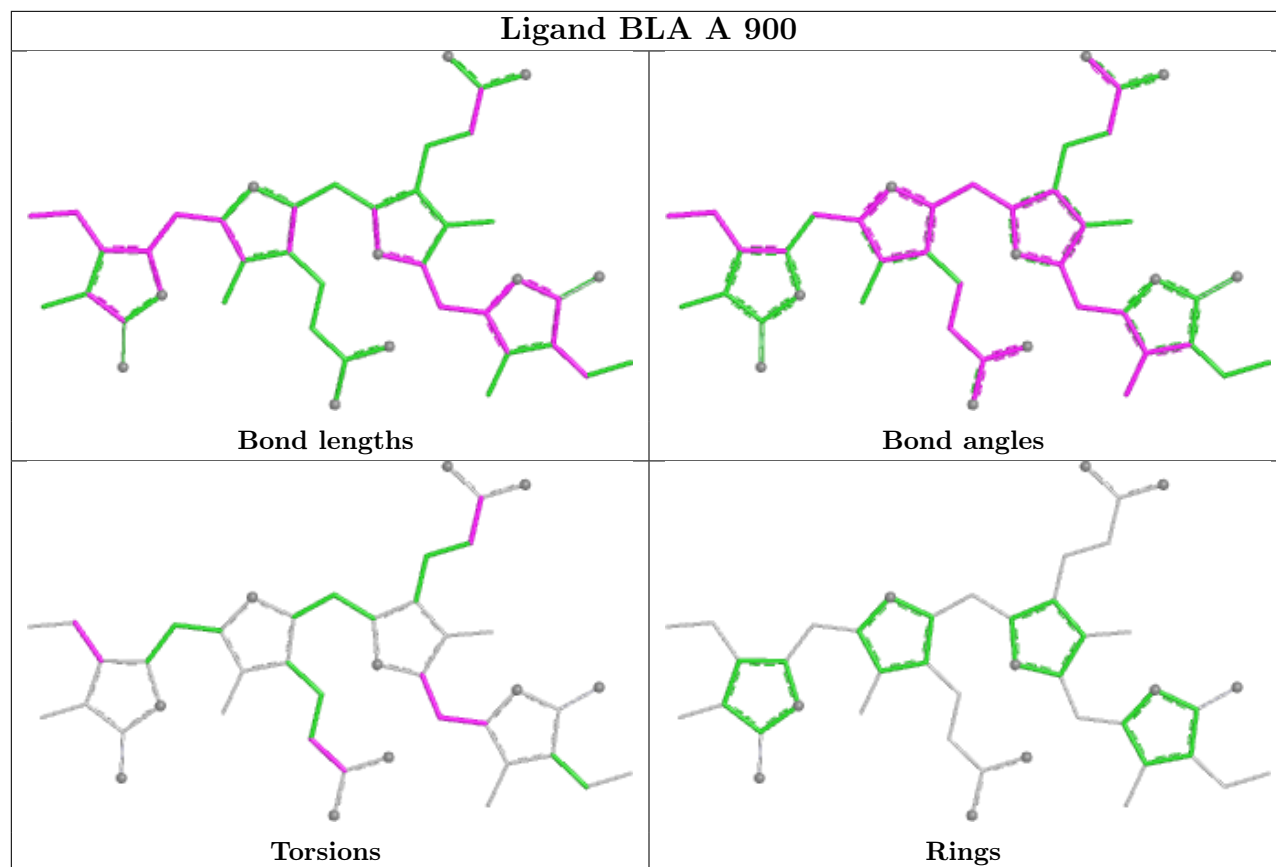
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	BLA	3	0
2	A	900	BLA	10	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	498/529 (94%)	-0.63	1 (0%) 91 91	41, 107, 181, 236	2 (0%)
1	B	486/529 (91%)	-0.44	3 (0%) 85 82	65, 132, 200, 232	0
All	All	984/1058 (93%)	-0.54	4 (0%) 88 87	41, 119, 194, 236	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	ALA	3.2
1	A	26	THR	2.4
1	B	33	ILE	2.1
1	B	478	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 [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	0.95	0.08	82,104,136,142	0

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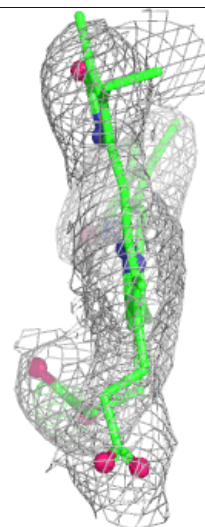
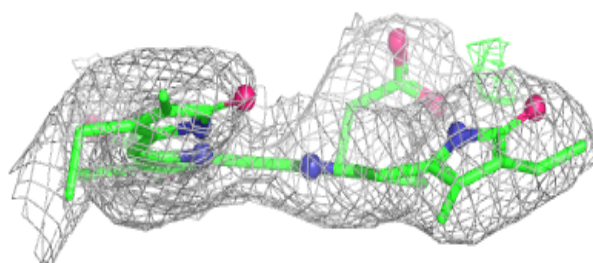
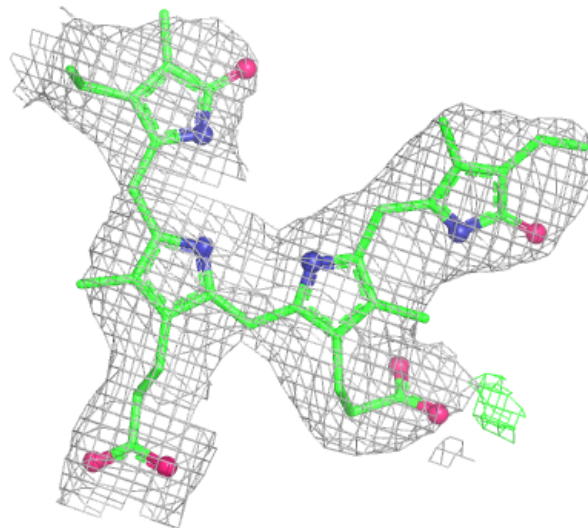
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BLA	B	900	43/43	0.95	0.10	108,145,171,175	0

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.

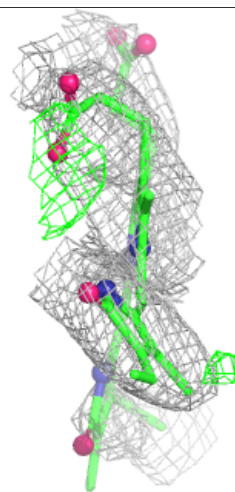
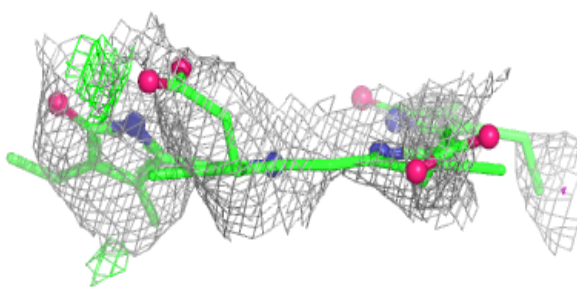
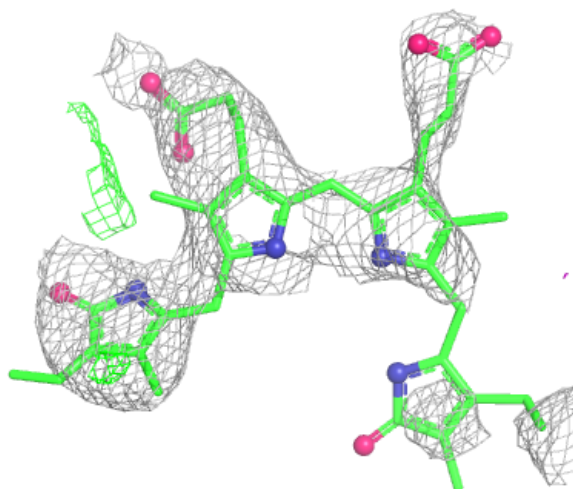
Electron density around BLA A 900:

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



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.