



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:23 PM GMT

PDB ID : 1ORD  
Title : CRYSTALLOGRAPHIC STRUCTURE OF A PLP-DEPENDENT ORNITHINE DECARBOXYLASE FROM LACTOBACILLUS 30A TO 3.1 ANGSTROMS RESOLUTION  
Authors : Hackert, M.L.; Momany, C.; Ernst, S.; Ghosh, R.  
Deposited on : 1995-02-08  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

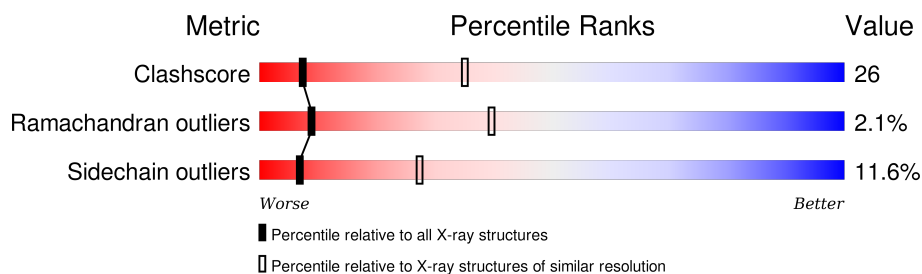
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	730	
1	B	730	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14561 atoms, of which 2752 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 ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	730	Total	C	H	N	O	S	0	0	0
			7105	3726	1269	982	1109	19			
1	B	730	Total	C	H	N	O	S	0	0	0
			7105	3726	1269	982	1109	19			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

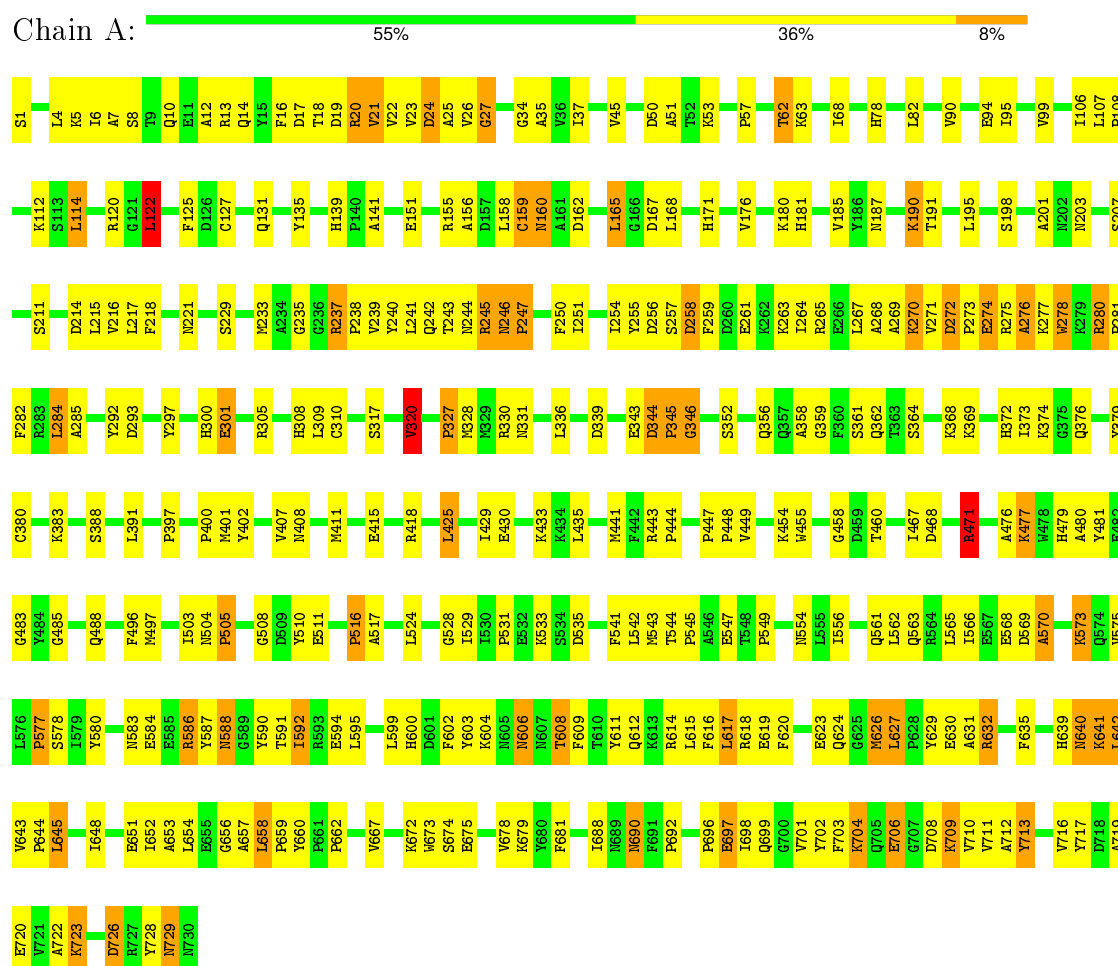
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	47	Total 141	H 94	O 47	0	0
3	B	60	Total 180	H 120	O 60	0	0

### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: ORNITHINE DECARBOXYLASE



K723	L642	Q574	Y481	H372	T279	T206	E103
V643	V643	V575	E482	I373	R280	S211	P108
P644	P644	L576	G483	K374	P281		
L645	L645	P577	Y484	G375	F282		
		S578	G485	Q376	S283	D214	K112
		L579	G488	Y379	L284	L215	H113
		Y580	Q488		A285	V216	L114
			Y489			L217	
			Y490	S388	Y292	F218	Y117
			P493	T395	A299	D219	R120
			F496	S396	E300	R220	G121
				P397	E301	N221	L122
				F398	V302		
			I503	Y399	V303	N228	C127
			N504	P400	K304	S229	P128
			P505	M401	R305	A230	G129
			E506		I306		H130
				Y407	G307	N233	Q131
			G508	M408	H308	A234	
			D509		L309	G235	Y135
			Y510	E415	C310	G236	Y136
			E511			R237	R137
				R418	S317	P238	K138
				L425		V239	H139
						Y240	P140
						L241	A141
						Q242	
			G528	T428	I326	T243	E151
			I529	A429	P327	N244	
			P531	E430	R328	R245	R155
			E532	A431	M329	N246	
			P533	R432	R330	P247	C159
			S534	K433	R331		N160
			D535	L435	S332	F250	
			F541	M441	L336	Y255	L165
			L542		I337	D256	G166
			N543	P447	D338	S257	D167
			T544	P448	D339	D258	L168
				V449		F259	H171
			E547	V450	E343	D260	
					D344	E261	
			K551	W455	G346	K262	A175
					I347	L264	V176
			L556	G458		R265	H181
				M459			
			Q561	T460	S352	D266	V185
			L562			L267	
			Q563	N465	K355	A268	K190
			R564		C356	A269	T191
			L565	D468	C357	K270	
			L566		A358	V271	L195
			E567	K471		D272	
			E568			P273	S198
			D569	A476		E274	
			A570	K477		R275	A201
			P571	W478		A276	
			L572	H479		K277	T204
			R573	A490		L278	V205

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.60 Å 195.60 Å 97.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.219 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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	0.75	0/5985	0.88	7/8118 (0.1%)
1	B	0.78	0/5985	0.89	9/8118 (0.1%)
All	All	0.77	0/11970	0.88	16/16236 (0.1%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	N-CA-C	-7.66	93.96	113.10
1	B	27	GLY	N-CA-C	-7.24	95.01	113.10
1	B	239	VAL	N-CA-C	-6.45	93.60	111.00
1	A	122	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	471	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	122	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	284	LEU	CA-CB-CG	5.84	128.72	115.30
1	A	284	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	471	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	239	VAL	N-CA-C	-5.23	96.89	111.00
1	A	391	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	218	PHE	N-CA-C	5.12	124.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	GLY	N-CA-C	-5.12	100.30	113.10
1	B	471	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	476	ALA	N-CA-C	5.02	124.56	111.00
1	A	346	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	TYR	Sidechain
1	A	713	TYR	Sidechain
1	B	713	TYR	Sidechain

## 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	5836	1269	5623	295	0
1	B	5836	1269	5623	307	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
3	A	47	94	0	5	0
3	B	60	120	0	3	0
All	All	11809	2752	11260	589	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 (589) 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:269:ALA:HA	1:B:275:ARG:NH2	1.83	0.92
1:B:612:GLN:HA	1:B:615:LEU:HD12	1.57	0.86
1:B:273:PRO:O	1:B:277:LYS:HB2	1.74	0.86
1:B:20:ARG:HA	1:B:20:ARG:HE	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:HA	1:B:275:ARG:CZ	2.06	0.84
1:A:269:ALA:HA	1:A:275:ARG:NH2	1.92	0.84
1:A:273:PRO:O	1:A:277:LYS:HB2	1.77	0.83
1:A:26:VAL:HG11	1:A:45:VAL:HG13	1.60	0.83
1:B:719:ALA:O	1:B:723:LYS:HB2	1.77	0.82
1:A:20:ARG:HA	1:A:20:ARG:HE	1.44	0.81
1:A:477:LYS:HD2	1:A:477:LYS:H	1.46	0.80
1:B:623:GLU:O	1:B:672:LYS:HG2	1.82	0.79
1:A:612:GLN:HA	1:A:615:LEU:HD12	1.66	0.78
1:A:269:ALA:HA	1:A:275:ARG:CZ	2.13	0.78
1:A:623:GLU:O	1:A:672:LYS:HG2	1.84	0.78
1:A:719:ALA:O	1:A:723:LYS:HB2	1.83	0.78
1:A:645:LEU:O	1:A:648:ILE:HG22	1.84	0.78
1:A:271:VAL:HG12	1:A:274:GLU:HB2	1.65	0.77
1:A:723:LYS:HB3	1:A:723:LYS:NZ	1.98	0.77
1:B:271:VAL:HG12	1:B:274:GLU:HB2	1.66	0.77
1:B:565:LEU:HD13	1:B:575:VAL:HG22	1.68	0.76
1:B:120:ARG:HB2	1:B:122:LEU:HD22	1.68	0.76
1:B:704:LYS:HB2	1:B:713:TYR:CE1	2.22	0.75
1:B:726:ASP:HA	1:B:729:ASN:ND2	2.03	0.74
1:B:703:PHE:HB3	1:B:710:VAL:HG22	1.71	0.73
1:A:703:PHE:HB3	1:A:710:VAL:HG22	1.71	0.73
1:A:604:LYS:HD2	3:A:763:HOH:O	1.87	0.73
1:A:704:LYS:HB2	1:A:713:TYR:CE1	2.23	0.73
1:B:697:GLU:CD	1:B:697:GLU:H	1.92	0.72
1:B:301:GLU:O	1:B:305:ARG:HG3	1.89	0.72
1:A:122:LEU:HD12	1:B:528:GLY:HA2	1.71	0.72
1:A:569:ASP:OD1	1:A:591:THR:HB	1.90	0.72
1:A:1:SER:HB2	1:A:21:VAL:HG11	1.70	0.72
1:B:1:SER:HB2	1:B:21:VAL:HG11	1.69	0.72
1:B:26:VAL:HG11	1:B:45:VAL:HG13	1.71	0.71
1:B:263:LYS:HD2	1:B:267:LEU:HD22	1.72	0.71
1:B:657:ALA:HB1	1:B:681:PHE:CZ	2.25	0.71
1:B:477:LYS:HD2	1:B:477:LYS:H	1.55	0.71
1:B:76:ILE:HG21	3:B:742:HOH:O	1.91	0.71
1:A:565:LEU:HD13	1:A:575:VAL:HG22	1.71	0.71
1:B:504:ASN:OD1	1:B:505:PRO:HD2	1.92	0.70
1:A:479:HIS:CD2	1:A:481:TYR:HB2	2.27	0.70
1:A:51:ALA:O	1:A:53:LYS:HG2	1.90	0.70
1:A:697:GLU:H	1:A:697:GLU:CD	1.96	0.69
1:A:703:PHE:HB3	1:A:710:VAL:CG2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ASP:HA	1:A:729:ASN:ND2	2.08	0.68
1:A:237:ARG:HG2	1:A:270:LYS:HE2	1.76	0.68
1:A:374:LYS:HE3	3:A:773:HOH:O	1.93	0.68
1:A:660:TYR:HD1	1:A:697:GLU:O	1.76	0.68
1:B:275:ARG:HG3	1:B:276:ALA:H	1.59	0.68
1:A:471:ARG:NH1	1:A:471:ARG:HB3	2.08	0.68
1:A:271:VAL:CG1	1:A:274:GLU:HB2	2.24	0.68
1:B:471:ARG:NH1	1:B:471:ARG:HB3	2.09	0.67
1:B:723:LYS:NZ	1:B:723:LYS:HB3	2.09	0.67
1:A:20:ARG:HA	1:A:20:ARG:NE	2.09	0.67
1:A:602:PHE:O	1:A:606:ASN:HB2	1.93	0.67
1:A:528:GLY:HA2	1:B:122:LEU:HD12	1.76	0.67
1:A:344:ASP:HB2	1:A:345:PRO:HD2	1.77	0.67
1:B:660:TYR:HD1	1:B:697:GLU:O	1.77	0.67
1:B:476:ALA:HB2	1:B:479:HIS:CE1	2.30	0.66
1:B:20:ARG:HA	1:B:20:ARG:NE	2.08	0.66
1:B:476:ALA:CB	1:B:479:HIS:CE1	2.79	0.66
1:A:468:ASP:HA	1:A:471:ARG:NH2	2.11	0.66
1:B:344:ASP:HB2	1:B:345:PRO:HD2	1.78	0.66
1:A:301:GLU:O	1:A:305:ARG:HG3	1.95	0.66
1:B:271:VAL:CG1	1:B:274:GLU:HB2	2.26	0.65
1:B:479:HIS:CD2	1:B:481:TYR:HB2	2.31	0.65
1:B:703:PHE:HB3	1:B:710:VAL:CG2	2.26	0.65
1:B:640:ASN:HB3	1:B:654:LEU:CD1	2.26	0.65
1:B:51:ALA:O	1:B:53:LYS:HG2	1.95	0.65
1:A:516:PRO:HG2	1:A:599:LEU:HB3	1.79	0.64
1:B:235:GLY:HA2	1:B:629:TYR:HB2	1.77	0.64
1:B:90:VAL:O	1:B:94:GLU:HG3	1.97	0.64
1:A:278:TRP:CD1	1:A:278:TRP:N	2.61	0.64
1:A:8:SER:HG	1:A:16:PHE:HE1	1.44	0.64
1:A:235:GLY:HA2	1:A:629:TYR:HB2	1.79	0.63
1:B:645:LEU:O	1:B:648:ILE:HG22	1.98	0.63
1:B:602:PHE:O	1:B:606:ASN:HB2	1.98	0.63
1:A:723:LYS:HZ2	1:A:723:LYS:HB3	1.61	0.63
1:B:697:GLU:O	1:B:698:ILE:HD13	1.98	0.63
1:B:278:TRP:CD1	1:B:278:TRP:N	2.62	0.63
1:A:62:THR:HG21	1:A:68:ILE:HD11	1.81	0.62
1:A:476:ALA:CB	1:A:479:HIS:CE1	2.82	0.62
1:B:569:ASP:OD1	1:B:591:THR:HB	1.98	0.62
1:B:697:GLU:C	1:B:698:ILE:HD13	2.19	0.62
1:A:479:HIS:HD2	1:A:481:TYR:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:PRO:HG2	1:B:599:LEU:HB3	1.80	0.62
1:B:595:LEU:O	1:B:595:LEU:HD12	1.99	0.62
1:B:517:ALA:HB3	1:B:535:ASP:O	1.99	0.62
1:A:263:LYS:HD2	1:A:267:LEU:HD22	1.81	0.62
1:B:648:ILE:HD11	1:B:716:VAL:HG23	1.81	0.62
1:A:640:ASN:HB3	1:A:654:LEU:CD1	2.29	0.62
1:B:217:LEU:HD11	1:B:241:LEU:HD21	1.82	0.62
1:B:639:HIS:HB3	1:B:722:ALA:HB2	1.82	0.61
1:B:529:ILE:O	1:B:531:PRO:HD3	2.00	0.61
1:A:361:SER:O	1:A:362:GLN:HB2	2.01	0.61
1:A:247:PRO:HD2	1:A:480:ALA:HB1	1.82	0.61
1:B:247:PRO:HD2	1:B:480:ALA:HB1	1.81	0.61
1:A:63:LYS:HG3	1:A:82:LEU:HD11	1.82	0.61
1:A:517:ALA:HB3	1:A:535:ASP:O	2.01	0.61
1:B:479:HIS:HD2	1:B:481:TYR:HB2	1.65	0.61
1:B:76:ILE:HD13	3:B:742:HOH:O	2.00	0.61
1:A:504:ASN:OD1	1:A:505:PRO:HD2	2.01	0.61
1:B:1:SER:HB3	1:B:99:VAL:HG11	1.83	0.60
1:B:358:ALA:O	1:B:408:ASN:HB2	2.01	0.60
1:A:468:ASP:HA	1:A:471:ARG:HH22	1.67	0.60
1:A:1:SER:HB2	1:A:4:LEU:O	2.02	0.60
1:B:701:VAL:CG1	1:B:712:ALA:HB1	2.32	0.60
1:A:476:ALA:HB2	1:A:479:HIS:CE1	2.37	0.60
1:A:587:TYR:HA	1:A:590:TYR:CD1	2.37	0.60
1:B:151:GLU:O	1:B:155:ARG:HG2	2.01	0.60
1:A:706:GLU:HB2	1:A:711:VAL:HG23	1.84	0.60
1:A:639:HIS:HB3	1:A:722:ALA:HB2	1.84	0.60
1:B:569:ASP:HA	1:B:592:ILE:CD1	2.32	0.59
1:A:1:SER:OG	1:A:21:VAL:HG21	2.02	0.59
1:B:243:THR:HG21	1:B:245:ARG:NH2	2.18	0.59
1:B:243:THR:HG21	1:B:245:ARG:HH21	1.67	0.59
1:A:528:GLY:HA2	1:B:122:LEU:CD1	2.33	0.59
1:A:272:ASP:HA	1:A:275:ARG:NE	2.18	0.58
1:B:640:ASN:HB3	1:B:654:LEU:HD12	1.85	0.58
1:A:614:ARG:HA	1:A:617:LEU:HB2	1.83	0.58
1:A:703:PHE:HA	1:A:711:VAL:O	2.03	0.58
1:A:627:LEU:HB2	1:A:630:GLU:OE2	2.04	0.58
1:B:274:GLU:HG3	1:B:278:TRP:CZ3	2.38	0.58
1:B:569:ASP:HA	1:B:592:ILE:HD11	1.85	0.58
1:A:433:LYS:HZ1	1:A:460:THR:HG22	1.68	0.58
1:B:648:ILE:HD11	1:B:716:VAL:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:SER:HB3	1:A:99:VAL:HG11	1.86	0.58
1:B:274:GLU:HG3	1:B:278:TRP:CH2	2.38	0.57
1:A:471:ARG:HH11	1:A:471:ARG:CG	2.16	0.57
1:A:653:ALA:HB2	1:A:673:TRP:NE1	2.18	0.57
1:B:619:GLU:HG3	1:B:620:PHE:CD1	2.38	0.57
1:B:562:LEU:O	1:B:566:ILE:HG13	2.04	0.57
1:B:34:GLY:HA3	1:B:99:VAL:HG13	1.86	0.57
1:A:216:VAL:O	1:A:238:PRO:HA	2.05	0.57
1:B:361:SER:O	1:B:362:GLN:HB2	2.04	0.57
1:A:471:ARG:HH11	1:A:471:ARG:HG2	1.69	0.57
1:B:6:ILE:O	1:B:23:VAL:HA	2.05	0.57
1:A:7:ALA:HA	1:A:24:ASP:O	2.04	0.57
1:B:706:GLU:HB2	1:B:711:VAL:HG23	1.85	0.57
1:A:120:ARG:HB2	1:A:122:LEU:HD22	1.86	0.57
1:B:7:ALA:HA	1:B:24:ASP:O	2.04	0.57
1:A:328:MET:HE3	1:A:467:ILE:HD12	1.85	0.57
1:A:122:LEU:CD1	1:B:528:GLY:HA2	2.35	0.57
1:A:660:TYR:CD1	1:A:697:GLU:O	2.57	0.57
1:B:590:TYR:HA	1:B:594:GLU:OE1	2.04	0.57
1:A:247:PRO:HD2	1:A:480:ALA:CB	2.35	0.56
1:A:441:MET:CE	1:A:563:GLN:HG3	2.35	0.56
1:B:441:MET:CE	1:B:563:GLN:HG3	2.35	0.56
1:B:726:ASP:HA	1:B:729:ASN:HD21	1.69	0.56
1:A:181:HIS:O	1:A:185:VAL:HG23	2.06	0.56
1:A:657:ALA:HB1	1:A:681:PHE:CZ	2.40	0.56
1:A:590:TYR:HA	1:A:594:GLU:OE1	2.06	0.56
1:A:704:LYS:HB2	1:A:713:TYR:HE1	1.68	0.56
1:A:12:ALA:HB1	1:A:37:ILE:HG22	1.87	0.56
1:B:255:TYR:CD1	1:B:483:GLY:HA3	2.39	0.56
1:B:37:ILE:HD11	1:B:95:ILE:HD13	1.88	0.56
1:A:272:ASP:HA	1:A:275:ARG:HE	1.69	0.56
1:A:569:ASP:HA	1:A:592:ILE:CD1	2.36	0.56
1:B:211:SER:HB3	1:B:214:ASP:OD2	2.05	0.56
1:A:271:VAL:HG12	1:A:274:GLU:H	1.71	0.55
1:A:6:ILE:O	1:A:23:VAL:HA	2.06	0.55
1:B:195:LEU:HB3	1:B:401:MET:CE	2.36	0.55
1:A:640:ASN:HB3	1:A:654:LEU:HD11	1.87	0.55
1:B:240:TYR:O	1:B:618:ARG:NH1	2.39	0.55
1:A:374:LYS:HG3	1:A:379:TYR:CZ	2.42	0.55
1:A:264:ILE:HG21	1:A:309:LEU:HD13	1.88	0.55
1:B:624:GLN:OE1	1:B:627:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ARG:HG2	1:B:270:LYS:HE2	1.87	0.55
1:B:471:ARG:HH11	1:B:471:ARG:CG	2.18	0.55
1:A:330:ARG:HD2	1:A:336:LEU:HD12	1.89	0.55
1:A:645:LEU:HG	1:A:712:ALA:HB3	1.87	0.55
1:B:12:ALA:HB1	1:B:37:ILE:HG22	1.88	0.55
1:B:643:VAL:HG11	1:B:648:ILE:HA	1.87	0.55
1:A:195:LEU:HB3	1:A:401:MET:CE	2.36	0.55
1:A:477:LYS:CD	1:A:477:LYS:H	2.19	0.55
1:A:643:VAL:HB	1:A:648:ILE:HG13	1.89	0.55
1:A:697:GLU:C	1:A:698:ILE:HD13	2.27	0.55
1:B:62:THR:HG21	1:B:68:ILE:HD11	1.89	0.55
1:B:504:ASN:O	1:B:508:GLY:N	2.39	0.55
1:A:34:GLY:HA3	1:A:99:VAL:HG13	1.89	0.54
1:B:471:ARG:HH11	1:B:471:ARG:HG2	1.73	0.54
1:A:237:ARG:HG2	1:A:270:LYS:CE	2.37	0.54
1:A:282:PHE:O	1:A:310:CYS:HA	2.07	0.54
1:A:358:ALA:O	1:A:408:ASN:HB2	2.06	0.54
1:A:256:ASP:HA	1:A:488:GLN:HE22	1.73	0.54
1:A:611:TYR:CZ	1:A:679:LYS:HD2	2.43	0.54
1:B:1:SER:HB2	1:B:4:LEU:O	2.08	0.54
1:B:471:ARG:HH11	1:B:471:ARG:HB3	1.71	0.54
1:B:468:ASP:HA	1:B:471:ARG:NH2	2.23	0.54
1:B:275:ARG:HA	1:B:281:PRO:HB3	1.88	0.54
1:A:726:ASP:HA	1:A:729:ASN:HD21	1.72	0.54
1:B:645:LEU:HG	1:B:712:ALA:HB3	1.90	0.54
1:A:383:LYS:HB2	3:A:746:HOH:O	2.06	0.54
1:B:338:ASP:O	1:B:339:ASP:HB3	2.08	0.54
1:A:277:LYS:HB3	1:A:278:TRP:HD1	1.73	0.53
1:A:151:GLU:O	1:A:155:ARG:HG2	2.08	0.53
1:B:344:ASP:CB	1:B:345:PRO:HD2	2.38	0.53
1:B:243:THR:HG22	1:B:244:ASN:N	2.23	0.53
1:A:229:SER:HA	1:A:233:MET:HB2	1.90	0.53
1:B:255:TYR:CE1	1:B:483:GLY:HA3	2.43	0.53
1:B:374:LYS:HG3	1:B:379:TYR:CE2	2.44	0.53
1:B:271:VAL:HG12	1:B:274:GLU:H	1.73	0.53
1:B:587:TYR:HA	1:B:590:TYR:CD1	2.43	0.53
1:A:717:TYR:CZ	1:A:719:ALA:HA	2.44	0.53
1:B:704:LYS:HB2	1:B:713:TYR:HE1	1.73	0.53
1:A:640:ASN:O	1:A:641:LYS:HE3	2.09	0.53
1:A:372:HIS:CD2	1:A:373:ILE:HG23	2.43	0.53
1:A:90:VAL:O	1:A:94:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:HG3	1:B:379:TYR:CZ	2.44	0.53
1:A:586:ARG:NH1	1:A:690:ASN:O	2.41	0.53
1:A:708:ASP:C	1:A:709:LYS:HZ3	2.12	0.52
1:A:702:TYR:O	1:A:712:ALA:HA	2.09	0.52
1:B:607:ASN:ND2	1:B:610:THR:OG1	2.43	0.52
1:B:614:ARG:HA	1:B:617:LEU:HB2	1.90	0.52
1:A:246:ASN:HD22	1:A:246:ASN:N	2.07	0.52
1:A:648:ILE:HD11	1:A:716:VAL:HG23	1.91	0.52
1:B:1:SER:OG	1:B:21:VAL:HG21	2.09	0.52
1:B:221:ASN:OD1	1:B:245:ARG:NH2	2.43	0.52
1:B:653:ALA:HB2	1:B:673:TRP:NE1	2.24	0.52
1:B:433:LYS:NZ	1:B:458:GLY:O	2.43	0.52
1:A:697:GLU:O	1:A:698:ILE:HD13	2.09	0.52
1:A:468:ASP:OD1	1:A:471:ARG:NH2	2.43	0.52
1:A:587:TYR:HA	1:A:590:TYR:CE1	2.44	0.52
1:A:246:ASN:HD21	1:A:250:PHE:HB2	1.75	0.52
1:B:660:TYR:CD1	1:B:697:GLU:O	2.61	0.52
1:A:429:ILE:O	1:A:433:LYS:HG3	2.10	0.52
1:A:242:GLN:HB3	1:A:618:ARG:H	1.75	0.52
1:B:247:PRO:HD2	1:B:480:ALA:CB	2.40	0.52
1:B:580:TYR:HE1	1:B:587:TYR:O	1.92	0.52
1:B:330:ARG:HD2	1:B:336:LEU:HD12	1.92	0.52
1:A:255:TYR:CD1	1:A:483:GLY:HA3	2.45	0.51
1:B:717:TYR:CZ	1:B:719:ALA:HA	2.46	0.51
1:A:698:ILE:HG22	1:A:699:GLN:N	2.26	0.51
1:A:471:ARG:HH11	1:A:471:ARG:HB3	1.74	0.51
1:B:448:PRO:HG2	1:B:449:VAL:H	1.74	0.51
1:A:237:ARG:HH22	1:A:271:VAL:HG21	1.75	0.51
1:A:275:ARG:HA	1:A:281:PRO:HB3	1.91	0.51
1:A:1:SER:CB	1:A:21:VAL:HG11	2.38	0.51
1:A:619:GLU:HG3	1:A:620:PHE:CD2	2.45	0.51
1:B:590:TYR:CD2	1:B:594:GLU:HB3	2.45	0.51
1:B:237:ARG:HH22	1:B:271:VAL:HG21	1.74	0.51
1:B:702:TYR:O	1:B:712:ALA:HA	2.10	0.51
1:B:708:ASP:C	1:B:709:LYS:HZ3	2.14	0.51
1:B:447:PRO:O	1:B:455:TRP:HB2	2.11	0.51
1:B:216:VAL:O	1:B:238:PRO:HA	2.11	0.51
1:A:397:PRO:HA	1:B:362:GLN:OE1	2.11	0.51
1:A:511:GLU:O	1:A:600:HIS:HE1	1.94	0.51
1:B:1:SER:CB	1:B:21:VAL:HG11	2.37	0.50
1:B:7:ALA:HB1	1:B:26:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:O	1:A:566:ILE:HG13	2.12	0.50
1:A:660:TYR:HB2	1:A:697:GLU:HG2	1.93	0.50
1:A:5:LYS:HG2	1:A:22:VAL:HB	1.93	0.50
1:B:372:HIS:CD2	1:B:373:ILE:HG23	2.46	0.50
1:B:583:ASN:ND2	1:B:692:PRO:HB2	2.26	0.50
1:B:221:ASN:OD1	1:B:243:THR:HG21	2.10	0.50
1:A:476:ALA:HB3	1:A:479:HIS:CE1	2.46	0.50
1:B:246:ASN:HD22	1:B:246:ASN:N	2.09	0.50
1:A:211:SER:HB3	1:A:214:ASP:OD2	2.11	0.50
1:A:274:GLU:HG3	1:A:278:TRP:CZ3	2.46	0.50
1:A:243:THR:HG21	1:A:245:ARG:NH2	2.27	0.50
1:A:644:PRO:HG3	1:A:713:TYR:CE2	2.47	0.50
1:B:274:GLU:HA	1:B:278:TRP:CZ2	2.47	0.50
1:A:327:PRO:O	1:A:330:ARG:HG2	2.12	0.50
1:A:274:GLU:HA	1:A:278:TRP:CE2	2.47	0.49
1:B:511:GLU:O	1:B:600:HIS:HE1	1.95	0.49
1:A:656:GLY:HA2	1:A:667:VAL:O	2.11	0.49
1:B:181:HIS:O	1:B:185:VAL:HG23	2.12	0.49
1:A:254:ILE:HG13	1:A:297:TYR:OH	2.12	0.49
1:B:246:ASN:HD21	1:B:250:PHE:HB2	1.77	0.49
1:A:62:THR:CG2	1:A:68:ILE:HD11	2.42	0.49
1:B:619:GLU:HG3	1:B:620:PHE:HD1	1.77	0.49
1:B:468:ASP:OD1	1:B:471:ARG:NH2	2.46	0.49
1:A:245:ARG:NH2	1:A:251:ILE:HG23	2.27	0.49
1:B:701:VAL:HG11	1:B:712:ALA:HB1	1.95	0.49
1:A:648:ILE:HD11	1:A:716:VAL:CG2	2.43	0.49
1:A:344:ASP:CB	1:A:345:PRO:HD2	2.40	0.49
1:B:590:TYR:HA	1:B:594:GLU:CD	2.33	0.49
1:A:257:SER:O	1:A:259:PHE:N	2.46	0.49
1:A:448:PRO:HG2	1:A:449:VAL:H	1.78	0.49
1:A:374:LYS:HG3	1:A:379:TYR:CE2	2.48	0.49
1:B:257:SER:O	1:B:259:PHE:N	2.46	0.49
1:B:5:LYS:HG2	1:B:22:VAL:HB	1.95	0.49
1:B:510:TYR:CE1	1:B:609:PHE:CD2	3.01	0.48
1:B:243:THR:CG2	1:B:245:ARG:HH21	2.26	0.48
1:B:229:SER:HA	1:B:233:MET:HB2	1.95	0.48
1:A:626:MET:HE3	1:A:652:ILE:HG21	1.94	0.48
1:A:1:SER:OG	1:A:21:VAL:CG2	2.60	0.48
1:A:243:THR:HG22	1:A:244:ASN:N	2.28	0.48
1:B:167:ASP:O	1:B:171:HIS:HA	2.12	0.48
1:B:274:GLU:HA	1:B:278:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ILE:O	1:A:99:VAL:HG23	2.13	0.48
1:A:660:TYR:CG	1:A:697:GLU:HG2	2.48	0.48
1:A:267:LEU:HD11	1:A:618:ARG:CZ	2.43	0.48
1:A:632:ARG:O	1:A:635:PHE:HB3	2.13	0.48
1:B:723:LYS:HB3	1:B:723:LYS:HZ2	1.77	0.48
1:B:242:GLN:HB3	1:B:618:ARG:H	1.79	0.48
1:B:264:ILE:HG21	1:B:309:LEU:HD13	1.96	0.48
1:B:640:ASN:HB3	1:B:654:LEU:HD11	1.95	0.48
1:A:529:ILE:O	1:A:531:PRO:HD3	2.13	0.48
1:A:644:PRO:O	1:A:648:ILE:HB	2.14	0.48
1:A:383:LYS:NZ	1:B:642:LEU:HD21	2.29	0.48
1:A:37:ILE:HD11	1:A:95:ILE:HD13	1.95	0.48
1:B:247:PRO:O	1:B:503:ILE:HD13	2.14	0.48
1:A:267:LEU:HD11	1:A:618:ARG:NE	2.28	0.48
1:A:653:ALA:HB2	1:A:673:TRP:HE1	1.76	0.48
1:A:243:THR:HG21	1:A:245:ARG:HH21	1.77	0.48
1:A:122:LEU:HG	1:B:530:ILE:HD11	1.96	0.48
1:A:569:ASP:HA	1:A:592:ILE:HD11	1.95	0.48
1:A:243:THR:HB	1:A:616:PHE:HB3	1.95	0.48
1:B:471:ARG:HA	1:B:490:TYR:HA	1.96	0.48
1:B:580:TYR:CE1	1:B:587:TYR:O	2.67	0.48
1:A:168:LEU:N	1:A:168:LEU:HD12	2.29	0.48
1:A:603:TYR:HB3	1:A:608:THR:OG1	2.14	0.48
1:B:698:ILE:HG22	1:B:699:GLN:N	2.29	0.47
1:A:471:ARG:NH1	1:A:471:ARG:CB	2.77	0.47
1:A:504:ASN:O	1:A:508:GLY:N	2.47	0.47
1:B:128:PRO:O	1:B:131:GLN:HG3	2.14	0.47
1:A:720:GLU:HA	1:A:723:LYS:HB2	1.96	0.47
1:B:429:ILE:O	1:B:433:LYS:HG3	2.14	0.47
1:B:611:TYR:CZ	1:B:679:LYS:HD2	2.49	0.47
1:B:688:ILE:HG23	1:B:695:ALA:CB	2.44	0.47
1:B:477:LYS:CD	1:B:477:LYS:H	2.22	0.47
1:A:510:TYR:CE1	1:A:609:PHE:CD2	3.02	0.47
1:B:317:SER:HB2	1:B:320:VAL:HG23	1.96	0.47
1:B:706:GLU:HB2	1:B:711:VAL:CG2	2.44	0.47
1:B:326:ILE:HD12	1:B:329:MET:SD	2.55	0.47
1:B:603:TYR:HB3	1:B:608:THR:OG1	2.14	0.47
1:B:435:LEU:HD23	1:B:556:ILE:HG23	1.96	0.47
1:A:221:ASN:OD1	1:A:243:THR:HG21	2.14	0.47
1:A:626:MET:CE	1:A:652:ILE:HG21	2.45	0.47
1:A:701:VAL:CG1	1:A:712:ALA:HB1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASN:OD1	1:B:505:PRO:CD	2.61	0.47
1:A:346:GLY:HA2	1:A:372:HIS:CE1	2.50	0.47
1:B:272:ASP:O	1:B:276:ALA:HB3	2.15	0.47
1:A:623:GLU:OE1	1:A:672:LYS:HD2	2.15	0.47
1:A:583:ASN:ND2	1:A:692:PRO:HB2	2.29	0.47
1:B:272:ASP:HA	1:B:275:ARG:NE	2.30	0.47
1:B:623:GLU:OE1	1:B:672:LYS:HD2	2.15	0.47
1:B:580:TYR:OH	1:B:588:ASN:HA	2.15	0.47
1:A:635:PHE:HA	1:A:654:LEU:HD13	1.97	0.47
1:B:256:ASP:HA	1:B:488:GLN:HE22	1.79	0.47
1:A:542:LEU:HD12	1:B:127:CYS:HB3	1.95	0.46
1:B:626:MET:CE	1:B:652:ILE:HG21	2.45	0.46
1:B:29:ASP:O	1:B:31:THR:HG23	2.14	0.46
1:A:255:TYR:CE1	1:A:483:GLY:HA3	2.49	0.46
1:B:117:TYR:HB2	1:B:165:LEU:HD11	1.98	0.46
1:A:281:PRO:HG2	1:A:282:PHE:CD2	2.50	0.46
1:B:476:ALA:CB	1:B:479:HIS:ND1	2.79	0.46
1:B:195:LEU:HB3	1:B:401:MET:HE2	1.96	0.46
1:A:706:GLU:HB2	1:A:711:VAL:CG2	2.44	0.46
1:B:614:ARG:HB3	1:B:620:PHE:CG	2.50	0.46
1:B:247:PRO:HG3	1:B:609:PHE:CE1	2.50	0.46
1:B:631:ALA:O	1:B:654:LEU:HD22	2.15	0.46
1:B:17:ASP:O	1:B:19:ASP:N	2.41	0.46
1:A:415:GLU:HA	1:A:418:ARG:CG	2.46	0.46
1:A:443:ARG:HG3	1:A:444:PRO:HD2	1.97	0.46
1:A:274:GLU:HG3	1:A:278:TRP:CH2	2.50	0.46
1:A:719:ALA:O	1:A:723:LYS:N	2.42	0.46
1:B:264:ILE:O	1:B:267:LEU:HB3	2.16	0.46
1:A:476:ALA:CB	1:A:479:HIS:ND1	2.79	0.46
1:B:346:GLY:HA2	1:B:372:HIS:CE1	2.51	0.46
1:A:544:THR:O	1:A:547:GLU:HG2	2.15	0.46
1:A:108:PRO:HG2	1:A:407:VAL:HA	1.96	0.46
1:A:407:VAL:O	1:A:411:MET:HG3	2.15	0.46
1:A:125:PHE:CZ	1:B:551:LYS:HG2	2.51	0.46
1:B:276:ALA:O	1:B:277:LYS:HG2	2.16	0.46
1:A:274:GLU:HA	1:A:278:TRP:CZ2	2.51	0.46
1:A:524:LEU:HD13	1:A:531:PRO:HG3	1.98	0.46
1:A:280:ARG:HB3	1:A:280:ARG:HE	1.53	0.46
1:B:63:LYS:HG3	1:B:82:LEU:HD11	1.98	0.46
1:B:660:TYR:HB2	1:B:697:GLU:HG2	1.98	0.46
1:B:282:PHE:O	1:B:310:CYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLY:N	1:B:488:GLN:OE1	2.49	0.46
1:B:703:PHE:HA	1:B:711:VAL:O	2.15	0.46
1:B:468:ASP:HA	1:B:471:ARG:HH22	1.79	0.46
1:A:5:LYS:HB3	1:A:22:VAL:O	2.16	0.46
1:A:187:ASN:O	1:A:369:LYS:HE3	2.16	0.46
1:B:479:HIS:O	1:B:480:ALA:HB3	2.15	0.45
1:A:619:GLU:HG3	1:A:620:PHE:HD2	1.80	0.45
1:A:631:ALA:O	1:A:654:LEU:HD22	2.15	0.45
1:A:195:LEU:HB3	1:A:401:MET:HE2	1.98	0.45
1:B:635:PHE:HA	1:B:654:LEU:HD13	1.98	0.45
1:B:586:ARG:NH1	1:B:690:ASN:O	2.47	0.45
1:B:159:CYS:SG	1:B:160:ASN:N	2.88	0.45
1:B:198:SER:HA	1:B:201:ALA:HB3	1.98	0.45
1:B:272:ASP:HA	1:B:275:ARG:HE	1.80	0.45
1:B:441:MET:HE3	1:B:563:GLN:HG3	1.98	0.45
1:A:277:LYS:HB3	1:A:278:TRP:CD1	2.51	0.45
1:B:644:PRO:O	1:B:648:ILE:HB	2.17	0.45
1:B:573:LYS:O	1:B:577:PRO:HA	2.17	0.45
1:A:271:VAL:HG11	1:A:274:GLU:OE1	2.15	0.45
1:B:267:LEU:HD11	1:B:618:ARG:CZ	2.47	0.45
1:B:627:LEU:HB2	1:B:630:GLU:OE2	2.16	0.45
1:B:327:PRO:HB2	1:B:465:ASN:HD21	1.81	0.45
1:B:643:VAL:HB	1:B:648:ILE:HG13	1.98	0.45
1:A:570:ALA:N	1:A:592:ILE:HD11	2.31	0.45
1:B:570:ALA:HB1	1:B:571:PRO:CD	2.47	0.45
1:A:221:ASN:OD1	1:A:245:ARG:NH2	2.49	0.45
1:A:198:SER:HA	1:A:201:ALA:HB3	1.99	0.45
1:A:158:LEU:HB3	1:A:162:ASP:OD2	2.16	0.45
1:A:7:ALA:HB1	1:A:26:VAL:HG22	1.98	0.45
1:B:595:LEU:C	1:B:595:LEU:HD12	2.37	0.45
1:B:701:VAL:HG13	1:B:712:ALA:HB1	1.98	0.45
1:B:4:LEU:CD1	1:B:103:GLU:HB2	2.47	0.45
1:B:471:ARG:HH11	1:B:471:ARG:CB	2.29	0.45
1:B:476:ALA:HB3	1:B:479:HIS:CE1	2.51	0.45
1:B:230:ALA:O	1:B:234:ALA:HB3	2.16	0.45
1:A:237:ARG:NH2	1:A:271:VAL:HG21	2.31	0.45
1:B:308:HIS:HE1	1:B:343:GLU:HB3	1.82	0.45
1:B:352:SER:HA	1:B:364:SER:HB3	1.99	0.45
1:B:430:GLU:OE2	1:B:460:THR:HG21	2.16	0.45
1:B:237:ARG:HG2	1:B:270:LYS:CE	2.47	0.45
1:A:293:ASP:OD1	1:A:533:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:O	1:A:171:HIS:HA	2.16	0.45
1:A:246:ASN:HD21	1:A:250:PHE:H	1.64	0.44
1:A:165:LEU:N	1:A:165:LEU:HD22	2.32	0.44
1:A:246:ASN:ND2	1:A:250:PHE:HB2	2.32	0.44
1:B:280:ARG:HB3	1:B:280:ARG:HE	1.57	0.44
1:A:139:HIS:CD2	1:A:141:ALA:H	2.35	0.44
1:B:271:VAL:O	1:B:275:ARG:HG2	2.18	0.44
1:B:269:ALA:CA	1:B:275:ARG:CZ	2.87	0.44
1:A:247:PRO:O	1:A:503:ILE:HD13	2.17	0.44
1:A:308:HIS:HE1	1:A:343:GLU:HB3	1.82	0.44
1:A:127:CYS:HB3	1:B:542:LEU:HD12	1.99	0.44
1:B:228:ASN:O	1:B:233:MET:HG3	2.17	0.44
1:A:17:ASP:O	1:A:19:ASP:N	2.45	0.44
1:B:303:VAL:HG11	1:B:347:ILE:HD11	1.98	0.44
1:B:730:ASN:HB3	3:B:791:HOH:O	2.16	0.44
1:B:139:HIS:CD2	1:B:141:ALA:H	2.36	0.44
1:A:496:PHE:HB3	1:A:541:PHE:HB2	1.99	0.44
1:A:672:LYS:HB3	1:A:672:LYS:HE2	1.72	0.44
1:B:285:ALA:HB2	1:B:310:CYS:SG	2.57	0.44
1:B:496:PHE:HB3	1:B:541:PHE:HB2	1.99	0.44
1:A:642:LEU:O	1:A:713:TYR:HD2	2.01	0.44
1:A:471:ARG:HH11	1:A:471:ARG:CB	2.31	0.44
1:B:577:PRO:HG2	1:B:578:SER:H	1.82	0.44
1:B:471:ARG:NH1	1:B:471:ARG:CB	2.79	0.44
1:B:533:LYS:HB3	1:B:533:LYS:HE2	1.75	0.44
1:A:590:TYR:CD2	1:A:594:GLU:HB3	2.53	0.43
1:A:433:LYS:NZ	1:A:460:THR:HG22	2.33	0.43
1:A:352:SER:HA	1:A:364:SER:HB3	1.99	0.43
1:B:108:PRO:HG2	1:B:407:VAL:HA	1.99	0.43
1:B:171:HIS:C	1:B:176:VAL:HB	2.38	0.43
3:A:732:HOH:O	1:B:140:PRO:HB3	2.18	0.43
1:A:265:ARG:O	1:A:268:ALA:HB3	2.18	0.43
1:B:206:THR:HG21	1:B:230:ALA:HB2	2.00	0.43
1:A:573:LYS:O	1:A:577:PRO:HA	2.18	0.43
1:B:425:LEU:HD11	1:B:493:PRO:HB2	2.00	0.43
1:A:635:PHE:HB2	1:A:654:LEU:HB3	2.01	0.43
1:A:203:ASN:O	1:A:207:SER:HB2	2.18	0.43
1:B:717:TYR:CE2	1:B:719:ALA:HB2	2.53	0.43
1:A:704:LYS:O	1:A:711:VAL:N	2.48	0.43
1:B:632:ARG:O	1:B:635:PHE:HB3	2.19	0.43
1:A:580:TYR:OH	1:A:588:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:PRO:O	1:A:455:TRP:HB2	2.18	0.43
1:B:246:ASN:HD22	1:B:246:ASN:H	1.67	0.43
1:B:246:ASN:HD21	1:B:250:PHE:H	1.65	0.43
1:B:327:PRO:O	1:B:330:ARG:HG2	2.18	0.43
1:B:356:GLN:NE2	1:B:543:MET:O	2.51	0.43
1:B:265:ARG:O	1:B:268:ALA:HB3	2.18	0.43
1:A:275:ARG:HG3	1:A:276:ALA:H	1.84	0.43
1:B:660:TYR:CG	1:B:697:GLU:HG2	2.54	0.43
1:B:587:TYR:HA	1:B:590:TYR:CE1	2.53	0.43
1:B:618:ARG:C	1:B:620:PHE:H	2.22	0.43
1:B:247:PRO:HA	1:B:609:PHE:CD1	2.54	0.43
1:A:211:SER:O	1:A:214:ASP:HB2	2.18	0.43
1:B:704:LYS:O	1:B:711:VAL:N	2.51	0.43
1:B:476:ALA:HB3	1:B:479:HIS:CD2	2.53	0.43
1:A:688:ILE:HG12	1:A:696:PRO:HD2	2.00	0.43
1:A:159:CYS:SG	1:A:160:ASN:N	2.92	0.43
1:B:215:LEU:HD23	1:B:237:ARG:HE	1.84	0.42
1:B:720:GLU:HA	1:B:723:LYS:HB2	2.00	0.42
1:B:643:VAL:HB	1:B:648:ILE:CG1	2.49	0.42
1:A:717:TYR:CE2	1:A:719:ALA:HB2	2.54	0.42
1:B:632:ARG:O	1:B:635:PHE:N	2.51	0.42
1:A:640:ASN:HB3	1:A:654:LEU:HD12	2.00	0.42
1:B:719:ALA:O	1:B:723:LYS:CB	2.59	0.42
1:B:246:ASN:HB2	1:B:480:ALA:HB3	2.01	0.42
1:B:544:THR:O	1:B:547:GLU:HG2	2.19	0.42
1:B:719:ALA:O	1:B:723:LYS:N	2.47	0.42
1:A:587:TYR:C	1:A:590:TYR:HD1	2.22	0.42
1:A:425:LEU:HD13	1:A:425:LEU:HA	1.68	0.42
1:A:702:TYR:N	1:A:702:TYR:CD1	2.88	0.42
1:B:570:ALA:N	1:B:592:ILE:HD11	2.34	0.42
1:A:433:LYS:NZ	1:A:458:GLY:O	2.52	0.42
1:B:195:LEU:HD12	1:B:397:PRO:HB3	2.00	0.42
1:B:62:THR:CG2	1:B:68:ILE:HD11	2.49	0.42
1:B:168:LEU:HD12	1:B:168:LEU:N	2.34	0.42
1:A:435:LEU:HD21	1:A:556:ILE:HG12	2.00	0.42
1:A:237:ARG:HG3	1:A:627:LEU:HD21	2.02	0.42
1:B:415:GLU:HA	1:B:418:ARG:CG	2.49	0.42
1:A:217:LEU:HB3	1:A:285:ALA:HA	2.01	0.42
1:B:618:ARG:HG3	1:B:618:ARG:O	2.18	0.42
1:B:617:LEU:HD23	1:B:619:GLU:HG2	2.01	0.42
1:B:635:PHE:HB2	1:B:654:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:HE2	1:A:191:THR:O	2.20	0.42
1:A:180:LYS:NZ	1:A:180:LYS:HB3	2.34	0.42
1:B:642:LEU:O	1:B:713:TYR:HD2	2.02	0.42
1:A:35:ALA:HA	1:A:57:PRO:HG2	2.02	0.42
1:B:660:TYR:HA	1:B:661:PRO:HA	1.92	0.42
1:A:618:ARG:C	1:A:620:PHE:H	2.23	0.42
1:A:359:GLY:O	1:B:130:HIS:HD2	2.03	0.42
1:A:485:GLY:N	1:A:488:GLN:OE1	2.51	0.42
1:A:246:ASN:HD22	1:A:246:ASN:H	1.67	0.42
1:B:299:ALA:HB2	1:B:332:SER:O	2.19	0.42
1:B:242:GLN:HB3	1:B:618:ARG:N	2.35	0.42
1:A:264:ILE:O	1:A:267:LEU:HB3	2.20	0.42
1:B:243:THR:HB	1:B:616:PHE:HB3	2.01	0.42
1:A:256:ASP:HA	1:A:488:GLN:NE2	2.34	0.42
1:B:190:LYS:HE2	1:B:191:THR:O	2.20	0.42
1:B:271:VAL:HG11	1:B:274:GLU:OE1	2.20	0.41
1:A:285:ALA:HB2	1:A:310:CYS:SG	2.60	0.41
1:A:703:PHE:HB3	1:A:710:VAL:HG21	2.00	0.41
1:B:371:SER:HA	1:B:374:LYS:NZ	2.34	0.41
1:A:139:HIS:HD2	1:A:141:ALA:H	1.68	0.41
1:A:645:LEU:HA	1:A:645:LEU:HD22	1.89	0.41
1:A:651:GLU:OE1	1:A:716:VAL:HG11	2.20	0.41
1:B:658:LEU:HB3	1:B:699:GLN:HB2	2.02	0.41
1:B:217:LEU:HB3	1:B:285:ALA:HA	2.01	0.41
1:A:361:SER:HB2	1:B:398:PHE:HA	2.02	0.41
1:A:588:ASN:ND2	3:A:762:HOH:O	2.52	0.41
1:A:454:LYS:HB3	1:A:454:LYS:HE2	1.90	0.41
1:B:237:ARG:NH2	1:B:271:VAL:HG21	2.34	0.41
1:A:242:GLN:HB3	1:A:618:ARG:N	2.35	0.41
1:B:255:TYR:O	1:B:256:ASP:C	2.59	0.41
1:A:504:ASN:HA	1:A:505:PRO:HD3	1.68	0.41
1:B:435:LEU:HD21	1:B:556:ILE:HG12	2.01	0.41
1:A:240:TYR:O	1:A:241:LEU:HD23	2.20	0.41
1:B:237:ARG:HB2	1:B:237:ARG:HE	1.76	0.41
1:B:643:VAL:HB	1:B:648:ILE:HD12	2.01	0.41
1:B:586:ARG:NH2	1:B:590:TYR:OH	2.53	0.41
1:B:168:LEU:HA	1:B:175:ALA:HB1	2.03	0.41
1:A:300:HIS:CD2	1:A:331:ASN:O	2.74	0.41
1:A:18:THR:HG22	1:A:18:THR:O	2.20	0.41
1:B:592:ILE:HD12	1:B:593:ARG:H	1.85	0.41
1:B:449:VAL:O	1:B:450:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HD13	1:B:140:PRO:HB2	2.01	0.41
1:B:20:ARG:NE	1:B:20:ARG:CA	2.79	0.41
1:B:591:THR:O	1:B:594:GLU:HB2	2.20	0.41
1:A:356:GLN:NE2	1:A:543:MET:O	2.53	0.41
1:A:626:MET:HG2	1:A:630:GLU:HB2	2.03	0.41
1:A:719:ALA:O	1:A:723:LYS:CB	2.63	0.41
1:A:648:ILE:HG12	1:A:648:ILE:O	2.20	0.41
1:B:246:ASN:ND2	1:B:250:PHE:HB2	2.36	0.41
1:A:504:ASN:OD1	1:A:505:PRO:CD	2.69	0.41
1:A:590:TYR:HA	1:A:594:GLU:CD	2.40	0.41
1:B:435:LEU:CD2	1:B:556:ILE:HG23	2.51	0.41
1:A:368:LYS:NZ	1:A:380:CYS:O	2.49	0.41
1:A:215:LEU:HD23	1:A:237:ARG:HE	1.86	0.41
1:B:1:SER:OG	1:B:21:VAL:CG2	2.69	0.41
1:B:16:PHE:CD1	1:B:37:ILE:HG21	2.56	0.41
1:A:708:ASP:OD1	1:A:709:LYS:HG2	2.21	0.41
1:B:688:ILE:HG12	1:B:696:PRO:HD2	2.02	0.41
1:B:320:VAL:HB	1:B:321:GLY:H	1.58	0.41
1:B:302:VAL:O	1:B:306:ILE:HG13	2.20	0.41
1:B:428:THR:CG2	1:B:432:ARG:HH21	2.34	0.41
1:A:476:ALA:HB3	1:A:479:HIS:CG	2.56	0.41
1:A:573:LYS:HG3	1:A:580:TYR:CE1	2.56	0.41
1:B:651:GLU:O	1:B:672:LYS:HA	2.20	0.40
1:A:471:ARG:NH1	1:A:471:ARG:CG	2.80	0.40
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.95	0.40
1:A:171:HIS:C	1:A:176:VAL:HB	2.42	0.40
1:A:573:LYS:HZ3	1:A:573:LYS:H	1.69	0.40
1:A:114:LEU:HD21	1:A:156:ALA:HB1	2.03	0.40
1:B:137:ARG:C	1:B:137:ARG:HD2	2.42	0.40
1:A:276:ALA:O	1:A:277:LYS:HG2	2.20	0.40
1:A:20:ARG:CA	1:A:20:ARG:NE	2.83	0.40
1:B:504:ASN:HA	1:B:505:PRO:HD3	1.62	0.40
1:A:247:PRO:HA	1:A:609:PHE:CD1	2.56	0.40
1:A:63:LYS:HE3	1:A:63:LYS:HB3	1.92	0.40
1:B:219:ASP:HB3	1:B:222:ASN:ND2	2.36	0.40
1:B:618:ARG:HD3	1:B:618:ARG:HH11	1.78	0.40
1:B:5:LYS:HB3	1:B:22:VAL:O	2.21	0.40
1:B:679:LYS:HE3	1:B:679:LYS:HB2	1.81	0.40
1:B:204:THR:HG23	1:B:388:SER:HB3	2.02	0.40
1:B:277:LYS:HB3	1:B:278:TRP:HD1	1.86	0.40
1:A:643:VAL:HB	1:A:648:ILE:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:LEU:HB3	1:A:699:GLN:HB2	2.03	0.40
1:A:660:TYR:CB	1:A:697:GLU:HG2	2.51	0.40
1:A:632:ARG:O	1:A:635:PHE:N	2.55	0.40
1:A:444:PRO:HA	1:A:497:MET:O	2.22	0.40
1:A:674:SER:O	1:A:678:VAL:HG23	2.22	0.40
1:A:317:SER:HB2	1:A:320:VAL:HG23	2.03	0.40
1:B:651:GLU:OE1	1:B:716:VAL:HG11	2.22	0.40
1:B:504:ASN:HB3	1:B:507:THR:OG1	2.21	0.40
1:A:618:ARG:O	1:A:618:ARG:HG3	2.22	0.40
1:A:430:GLU:OE2	1:A:460:THR:HG21	2.21	0.40
1:B:356:GLN:OE1	1:B:542:LEU:HD22	2.20	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	728/730 (100%)	642 (88%)	70 (10%)	16 (2%)	8	38
1	B	728/730 (100%)	643 (88%)	70 (10%)	15 (2%)	9	40
All	All	1456/1460 (100%)	1285 (88%)	140 (10%)	31 (2%)	9	40

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ALA
1	A	339	ASP
1	A	376	GLN
1	B	339	ASP
1	B	376	GLN
1	A	131	GLN
1	A	258	ASP

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Mol	Chain	Res	Type
1	A	270	LYS
1	A	690	ASN
1	A	729	ASN
1	B	25	ALA
1	B	131	GLN
1	B	270	LYS
1	B	276	ALA
1	B	690	ASN
1	B	729	ASN
1	A	276	ALA
1	A	505	PRO
1	B	258	ASP
1	A	726	ASP
1	B	505	PRO
1	A	570	ALA
1	A	608	THR
1	B	277	LYS
1	B	320	VAL
1	B	355	LYS
1	A	320	VAL
1	A	27	GLY
1	A	577	PRO
1	B	27	GLY
1	B	577	PRO

### 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	617/617 (100%)	544 (88%)	73 (12%)	6	26
1	B	617/617 (100%)	547 (89%)	70 (11%)	7	28
All	All	1234/1234 (100%)	1091 (88%)	143 (12%)	7	27

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	13	ARG
1	A	14	GLN
1	A	20	ARG
1	A	21	VAL
1	A	24	ASP
1	A	50	ASP
1	A	62	THR
1	A	78	HIS
1	A	112	LYS
1	A	114	LEU
1	A	122	LEU
1	A	135	TYR
1	A	159	CYS
1	A	160	ASN
1	A	165	LEU
1	A	190	LYS
1	A	218	PHE
1	A	237	ARG
1	A	245	ARG
1	A	246	ASN
1	A	247	PRO
1	A	258	ASP
1	A	261	GLU
1	A	272	ASP
1	A	274	GLU
1	A	278	TRP
1	A	280	ARG
1	A	284	LEU
1	A	292	TYR
1	A	301	GLU
1	A	320	VAL
1	A	327	PRO
1	A	344	ASP
1	A	345	PRO
1	A	388	SER
1	A	400	PRO
1	A	425	LEU
1	A	471	ARG
1	A	477	LYS
1	A	516	PRO
1	A	545	PRO
1	A	549	PRO

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Mol	Chain	Res	Type
1	A	554	ASN
1	A	561	GLN
1	A	568	GLU
1	A	573	LYS
1	A	578	SER
1	A	584	GLU
1	A	586	ARG
1	A	588	ASN
1	A	592	ILE
1	A	595	LEU
1	A	606	ASN
1	A	617	LEU
1	A	624	GLN
1	A	626	MET
1	A	627	LEU
1	A	632	ARG
1	A	640	ASN
1	A	641	LYS
1	A	642	LEU
1	A	645	LEU
1	A	658	LEU
1	A	659	PRO
1	A	662	PRO
1	A	675	GLU
1	A	697	GLU
1	A	704	LYS
1	A	706	GLU
1	A	709	LYS
1	A	723	LYS
1	A	728	TYR
1	B	3	SER
1	B	10	GLN
1	B	13	ARG
1	B	14	GLN
1	B	20	ARG
1	B	21	VAL
1	B	24	ASP
1	B	50	ASP
1	B	62	THR
1	B	78	HIS
1	B	112	LYS
1	B	114	LEU

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Mol	Chain	Res	Type
1	B	135	TYR
1	B	159	CYS
1	B	160	ASN
1	B	165	LEU
1	B	190	LYS
1	B	218	PHE
1	B	237	ARG
1	B	242	GLN
1	B	245	ARG
1	B	246	ASN
1	B	247	PRO
1	B	258	ASP
1	B	261	GLU
1	B	272	ASP
1	B	274	GLU
1	B	278	TRP
1	B	280	ARG
1	B	284	LEU
1	B	292	TYR
1	B	301	GLU
1	B	320	VAL
1	B	327	PRO
1	B	344	ASP
1	B	388	SER
1	B	395	THR
1	B	400	PRO
1	B	425	LEU
1	B	471	ARG
1	B	477	LYS
1	B	516	PRO
1	B	561	GLN
1	B	564	ARG
1	B	568	GLU
1	B	573	LYS
1	B	578	SER
1	B	584	GLU
1	B	586	ARG
1	B	588	ASN
1	B	592	ILE
1	B	595	LEU
1	B	606	ASN
1	B	617	LEU

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Mol	Chain	Res	Type
1	B	624	GLN
1	B	626	MET
1	B	627	LEU
1	B	632	ARG
1	B	640	ASN
1	B	641	LYS
1	B	642	LEU
1	B	645	LEU
1	B	658	LEU
1	B	659	PRO
1	B	675	GLU
1	B	697	GLU
1	B	704	LYS
1	B	706	GLU
1	B	709	LYS
1	B	723	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	139	HIS
1	A	187	ASN
1	A	202	ASN
1	A	222	ASN
1	A	246	ASN
1	A	308	HIS
1	A	465	ASN
1	A	479	HIS
1	A	494	ASN
1	A	583	ASN
1	A	600	HIS
1	A	607	ASN
1	A	624	GLN
1	B	10	GLN
1	B	101	ASN
1	B	139	HIS
1	B	187	ASN
1	B	202	ASN
1	B	222	ASN
1	B	246	ASN
1	B	300	HIS

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Mol	Chain	Res	Type
1	B	308	HIS
1	B	351	GLN
1	B	465	ASN
1	B	479	HIS
1	B	583	ASN
1	B	600	HIS
1	B	607	ASN
1	B	624	GLN
1	B	640	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	PLP	A	731	1	15,15,16	1.83	3 (20%)	21,22,23	1.88	7 (33%)
2	PLP	B	731	1	15,15,16	2.11	6 (40%)	21,22,23	1.50	3 (14%)

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	PLP	A	731	1	-	0/6/6/8	0/1/1/1
2	PLP	B	731	1	-	0/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	731	PLP	P-O2P	-2.25	1.46	1.54
2	B	731	PLP	P-O3P	-2.11	1.47	1.54
2	B	731	PLP	O3-C3	2.43	1.42	1.37
2	B	731	PLP	P-O4P	2.78	1.69	1.60
2	A	731	PLP	C2-N1	3.08	1.40	1.34
2	B	731	PLP	C2-N1	3.29	1.41	1.34
2	B	731	PLP	C4A-C4	3.45	1.58	1.51
2	B	731	PLP	C6-N1	3.87	1.42	1.34
2	A	731	PLP	C2A-C2	3.96	1.58	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	731	PLP	C5A-C5-C4	-3.39	117.16	121.65
2	A	731	PLP	O4P-P-O1P	-2.96	99.60	107.14
2	B	731	PLP	C2A-C2-C3	-2.77	117.70	121.04
2	A	731	PLP	C2A-C2-C3	-2.77	117.70	121.04
2	B	731	PLP	C5A-C5-C4	-2.33	118.56	121.65
2	A	731	PLP	O2P-P-O1P	-2.17	103.59	110.58
2	A	731	PLP	C4A-C4-C5	-2.01	118.79	120.88
2	B	731	PLP	C2A-C2-N1	2.36	123.18	117.95
2	A	731	PLP	C6-C5-C4	2.81	120.53	118.15
2	A	731	PLP	O3P-P-O4P	3.15	115.64	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.