



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:02 am BST

PDB ID : 1YGP  
Title : PHOSPHORYLATED FORM OF YEAST GLYCOGEN PHOSPHORYLASE  
WITH PHOSPHATE BOUND IN THE ACTIVE SITE.  
Authors : Lin, K.; Rath, V.L.; Dai, S.C.; Fletterick, R.J.; Hwang, P.K.  
Deposited on : 1996-05-30  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

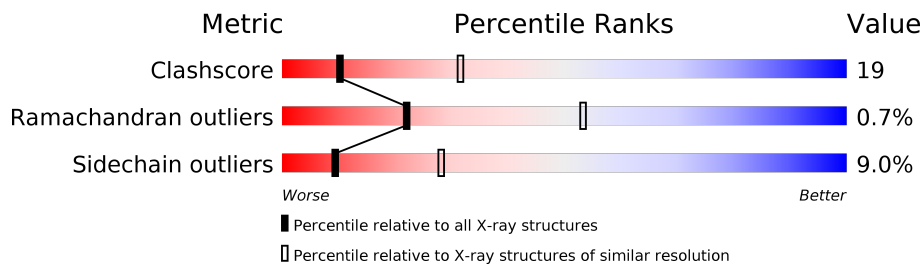
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	879	
1	B	879	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	1900	-	X	-	-
2	PO4	B	859	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13538 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.

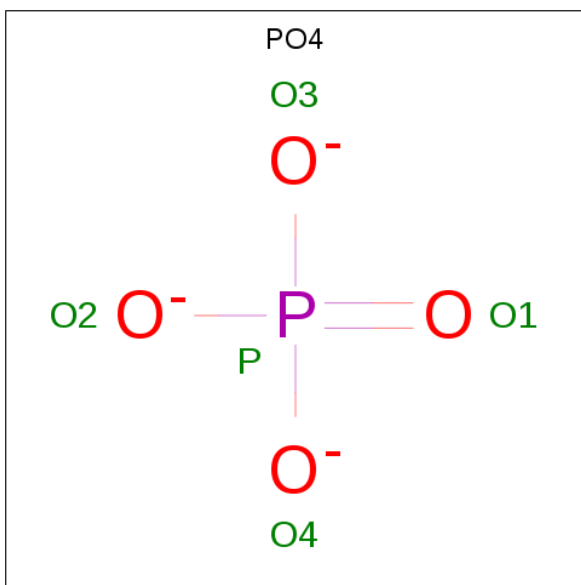
- Molecule 1 is a protein called YEAST GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	858	6744	4331	1140	1253	20	0	0	0
1	B	858	6744	4331	1140	1253	20	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

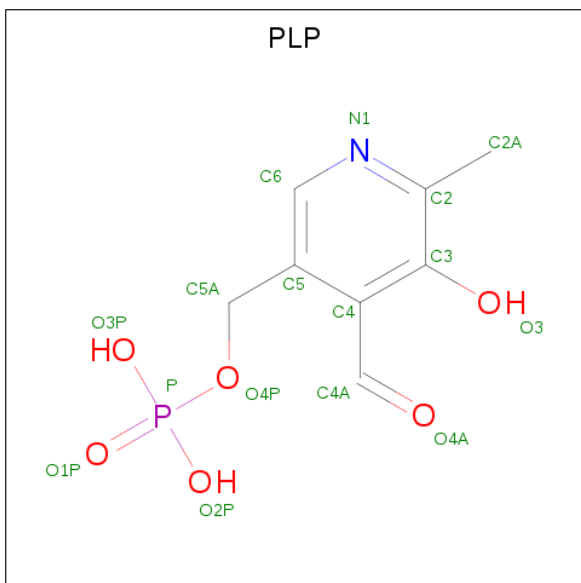
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	LEU	LYS	CONFLICT	UNP P06738
A	50	VAL	ALA	CONFLICT	UNP P06738
A	115	LEU	GLY	CONFLICT	UNP P06738
A	254	LEU	PHE	CONFLICT	UNP P06738
A	255	ASN	ALA	CONFLICT	UNP P06738
A	267	ALA	PRO	CONFLICT	UNP P06738
A	412	GLU	GLN	CONFLICT	UNP P06738
A	596	ARG	LYS	CONFLICT	UNP P06738
B	8	LEU	LYS	CONFLICT	UNP P06738
B	50	VAL	ALA	CONFLICT	UNP P06738
B	115	LEU	GLY	CONFLICT	UNP P06738
B	254	LEU	PHE	CONFLICT	UNP P06738
B	255	ASN	ALA	CONFLICT	UNP P06738
B	267	ALA	PRO	CONFLICT	UNP P06738
B	412	GLU	GLN	CONFLICT	UNP P06738
B	596	ARG	LYS	CONFLICT	UNP P06738

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



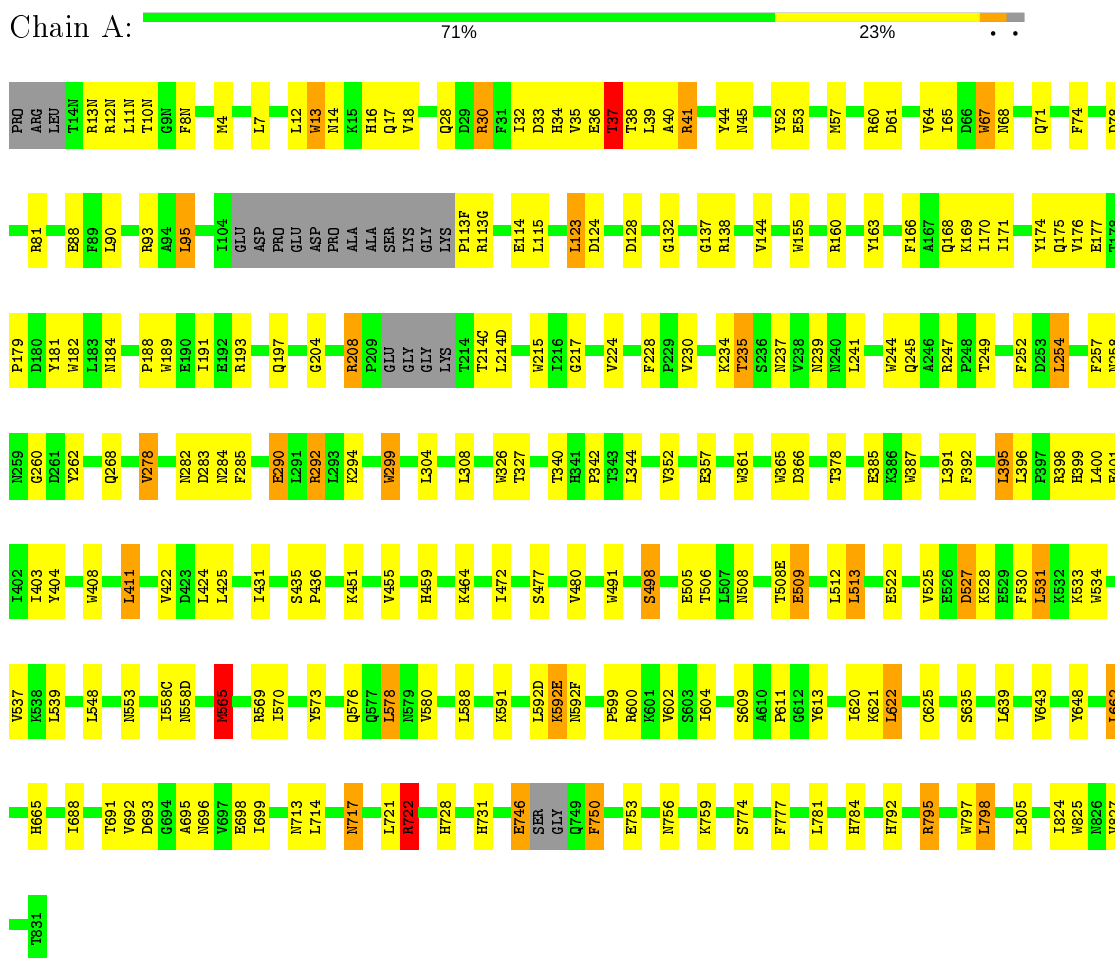
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0
3	B	1	15	8	1	5	1	0	0

### 3 Residue-property plots [i](#)

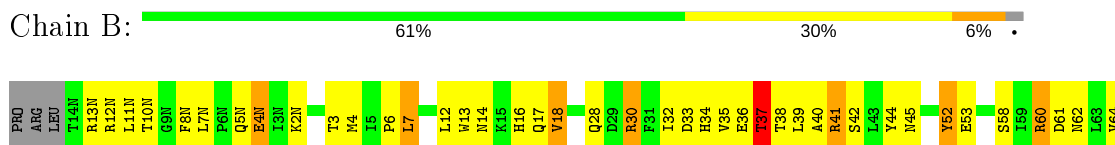
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

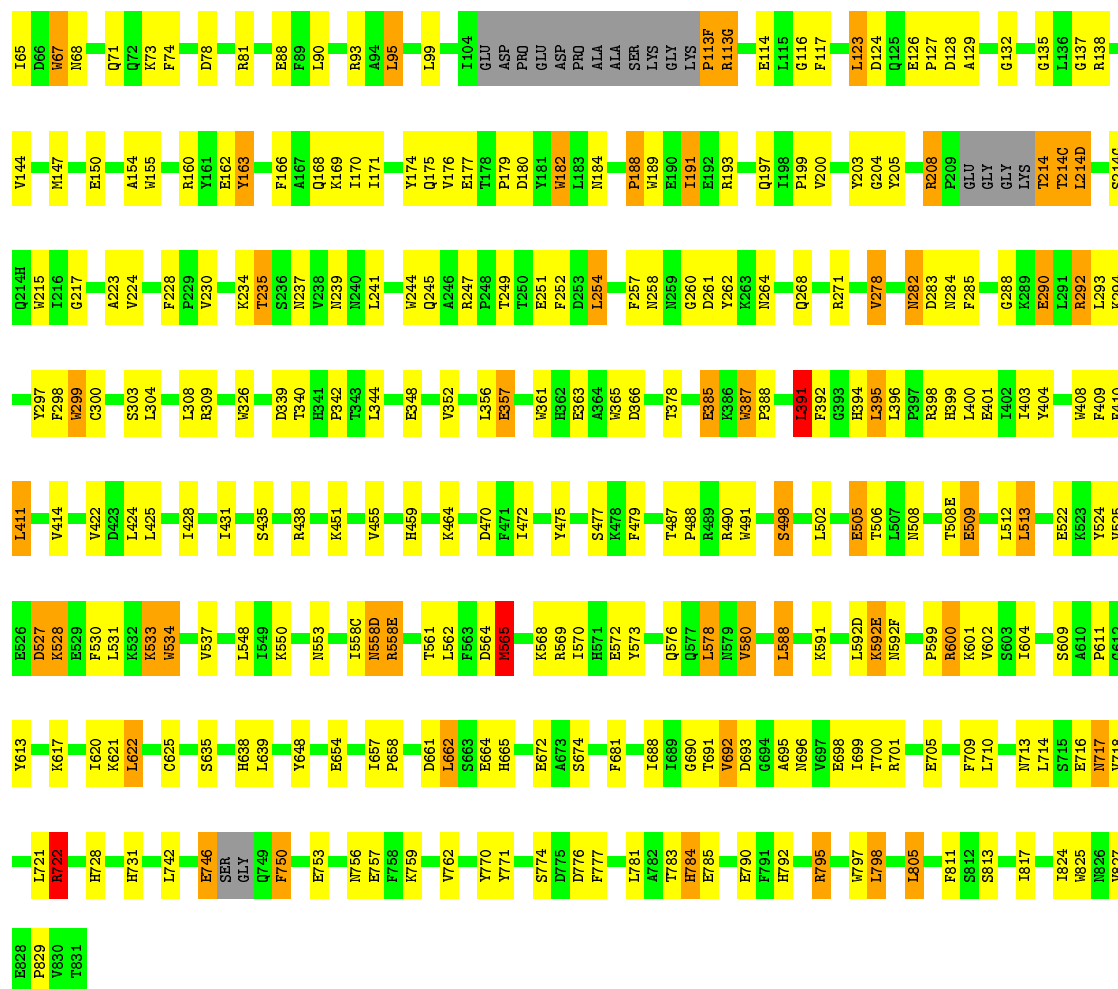
Note EDS was not executed.

- Molecule 1: YEAST GLYCOGEN PHOSPHORYLASE



- Molecule 1: YEAST GLYCOGEN PHOSPHORYLASE





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.91Å 143.93Å 169.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.179 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.74	0/6901	1.44	86/9378 (0.9%)
1	B	1.60	45/6901 (0.7%)	1.61	115/9378 (1.2%)
All	All	1.25	45/13802 (0.3%)	1.53	201/18756 (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	2
1	B	0	2
All	All	0	4

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	TRP	NE1-CE2	-6.96	1.28	1.37
1	B	361	TRP	CG-CD2	-6.92	1.31	1.43
1	B	357	GLU	CD-OE2	-6.83	1.18	1.25
1	B	150	GLU	CD-OE2	-6.79	1.18	1.25
1	B	790	GLU	CD-OE1	-6.69	1.18	1.25
1	B	365	TRP	CD1-NE1	-6.62	1.26	1.38
1	B	244	TRP	CG-CD2	-6.23	1.33	1.43
1	B	303	SER	CA-CB	-6.11	1.43	1.52
1	B	361	TRP	CD1-NE1	-6.11	1.27	1.38
1	B	299	TRP	CG-CD2	-6.09	1.33	1.43
1	B	155	TRP	CD1-NE1	-6.05	1.27	1.38
1	B	155	TRP	CG-CD2	-6.04	1.33	1.43
1	B	672	GLU	CD-OE1	-5.95	1.19	1.25
1	B	385	GLU	CD-OE2	-5.89	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	505	GLU	CD-OE2	-5.85	1.19	1.25
1	B	67	TRP	CG-CD2	-5.83	1.33	1.43
1	B	215	TRP	CG-CD2	-5.82	1.33	1.43
1	B	299	TRP	CD1-NE1	-5.71	1.28	1.38
1	B	365	TRP	CD2-CE2	-5.71	1.34	1.41
1	B	654	GLU	CD-OE2	-5.70	1.19	1.25
1	B	753	GLU	CD-OE2	-5.63	1.19	1.25
1	B	4(N)	GLU	CD-OE1	-5.60	1.19	1.25
1	B	300	CYS	CB-SG	-5.60	1.72	1.81
1	B	215	TRP	CD1-NE1	-5.58	1.28	1.38
1	B	572	GLU	CD-OE2	-5.57	1.19	1.25
1	B	785	GLU	CD-OE2	-5.51	1.19	1.25
1	B	829	PRO	N-CD	-5.47	1.40	1.47
1	B	182	TRP	CD1-NE1	-5.39	1.28	1.38
1	B	127	PRO	N-CD	-5.38	1.40	1.47
1	B	13	TRP	NE1-CE2	-5.38	1.30	1.37
1	B	757	GLU	CD-OE2	-5.36	1.19	1.25
1	B	188	PRO	N-CD	-5.35	1.40	1.47
1	B	326	TRP	NE1-CE2	-5.34	1.30	1.37
1	B	244	TRP	NE1-CE2	-5.28	1.30	1.37
1	B	534	TRP	CD1-NE1	-5.26	1.29	1.38
1	B	716	GLU	CD-OE2	-5.25	1.19	1.25
1	B	797	TRP	CD1-NE1	-5.24	1.29	1.38
1	B	784	HIS	CD2-NE2	-5.21	1.26	1.38
1	B	572	GLU	CD-OE1	-5.20	1.20	1.25
1	B	534	TRP	CG-CD2	-5.19	1.34	1.43
1	B	189	TRP	CD1-NE1	-5.18	1.29	1.38
1	B	790	GLU	CD-OE2	-5.14	1.20	1.25
1	B	664	GLU	CD-OE2	-5.11	1.20	1.25
1	B	658	PRO	N-CD	-5.09	1.40	1.47
1	B	199	PRO	N-CD	-5.09	1.40	1.47

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	TRP	CD1-CG-CD2	11.48	115.48	106.30
1	B	365	TRP	CE2-CD2-CG	-9.98	99.32	107.30
1	B	797	TRP	CD1-CG-CD2	9.78	114.12	106.30
1	B	299	TRP	CD1-CG-CD2	9.62	114.00	106.30
1	B	189	TRP	CD1-CG-CD2	9.23	113.69	106.30
1	A	408	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	B	182	TRP	CD1-CG-CD2	8.97	113.48	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	B	438	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	B	722	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	B	299	TRP	CE2-CD2-CG	-8.81	100.25	107.30
1	B	408	TRP	CD1-CG-CD2	8.77	113.32	106.30
1	B	182	TRP	CE2-CD2-CG	-8.76	100.29	107.30
1	A	365	TRP	CD1-CG-CD2	8.76	113.30	106.30
1	A	797	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	B	155	TRP	CE2-CD2-CG	-8.56	100.45	107.30
1	B	361	TRP	CE2-CD2-CG	-8.55	100.46	107.30
1	A	244	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	B	387	TRP	CD1-CG-CD2	8.43	113.05	106.30
1	A	138	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	326	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	B	189	TRP	CE2-CD2-CG	-8.28	100.67	107.30
1	A	387	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	B	113(F)	PRO	CA-N-CD	-8.23	99.97	111.50
1	A	155	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	B	60	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	A	408	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	B	534	TRP	CE2-CD2-CG	-8.05	100.86	107.30
1	A	365	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	B	155	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	A	182	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	A	189	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	A	13	TRP	CD1-CG-CD2	7.89	112.62	106.30
1	B	215	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	361	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	A	326	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	A	67	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	A	113(F)	PRO	CA-N-CD	-7.76	100.64	111.50
1	A	797	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	534	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	B	534	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	B	81	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	825	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	B	365	TRP	CG-CD1-NE1	-7.62	102.48	110.10
1	A	138	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	387	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	13	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	B	491	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	B	797	TRP	CE2-CD2-CG	-7.57	101.24	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	825	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	825	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	A	361	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	387	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	189	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B	490	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	155	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	182	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	B	408	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	795	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	244	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	113(F)	PRO	N-CA-CB	7.24	111.99	103.30
1	A	825	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	B	326	TRP	CD1-CG-CD2	7.20	112.06	106.30
1	B	365	TRP	CG-CD2-CE3	7.20	140.38	133.90
1	B	797	TRP	CG-CD1-NE1	-7.15	102.95	110.10
1	B	361	TRP	CD1-CG-CD2	7.14	112.02	106.30
1	B	215	TRP	CD1-CG-CD2	7.08	111.97	106.30
1	A	491	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	B	797	TRP	CG-CD2-CE3	7.06	140.25	133.90
1	B	113(F)	PRO	N-CA-CB	7.04	111.75	103.30
1	A	534	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	491	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	A	67	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	A	299	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	309	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	648	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	B	205	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	B	81	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	292	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	13	TRP	CD1-CG-CD2	6.73	111.69	106.30
1	B	578	LEU	CA-CB-CG	6.67	130.63	115.30
1	B	37	THR	N-CA-CB	-6.66	97.65	110.30
1	B	214(D)	LEU	CA-CB-CG	6.62	130.52	115.30
1	B	475	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	A	67	TRP	CG-CD2-CE3	6.59	139.83	133.90
1	B	292	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	215	TRP	CD1-CG-CD2	6.56	111.55	106.30
1	B	795	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	408	TRP	CG-CD2-CE3	6.53	139.78	133.90
1	A	408	TRP	CG-CD2-CE3	6.51	139.76	133.90
1	B	565	MET	CA-CB-CG	6.50	124.34	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	797	TRP	CB-CG-CD1	-6.49	118.56	127.00
1	B	558(E)	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	491	TRP	CE2-CD2-CG	-6.44	102.15	107.30
1	B	160	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	215	TRP	CE2-CD2-CG	-6.38	102.19	107.30
1	B	182	TRP	CG-CD2-CE3	6.37	139.64	133.90
1	B	750	PHE	N-CA-C	6.37	128.19	111.00
1	B	524	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	B	52	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	B	244	TRP	CD1-CG-CD2	6.20	111.26	106.30
1	B	408	TRP	CB-CG-CD1	-6.17	118.98	127.00
1	A	37	THR	N-CA-CB	-6.16	98.60	110.30
1	A	214(D)	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	52	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	B	648	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	A	67	TRP	CB-CG-CD1	-6.07	119.11	127.00
1	A	565	MET	CA-CB-CG	6.06	123.60	113.30
1	B	365	TRP	CB-CG-CD1	-6.05	119.14	127.00
1	B	189	TRP	CG-CD1-NE1	-6.04	104.06	110.10
1	A	182	TRP	CG-CD2-CE3	6.04	139.34	133.90
1	B	13	TRP	CG-CD2-CE3	6.04	139.33	133.90
1	B	771	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	A	662	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	93	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	578	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	600	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	B	491	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	A	750	PHE	N-CA-C	5.95	127.05	111.00
1	B	326	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	A	408	TRP	CB-CG-CD1	-5.93	119.30	127.00
1	B	41	ARG	N-CA-CB	-5.93	99.93	110.60
1	A	13	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	B	30	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	155	TRP	CG-CD2-CE3	5.83	139.15	133.90
1	B	408	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	A	797	TRP	CG-CD2-CE3	5.83	139.14	133.90
1	B	527	ASP	N-CA-C	5.83	126.73	111.00
1	A	41	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	299	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	A	160	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	326	TRP	CG-CD2-CE3	5.77	139.09	133.90
1	B	771	TYR	CG-CD1-CE1	-5.75	116.70	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	TRP	CB-CG-CD1	-5.73	119.55	127.00
1	A	408	TRP	CG-CD1-NE1	-5.72	104.38	110.10
1	B	509	GLU	CA-CB-CG	5.71	125.97	113.40
1	B	662	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	326	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	B	67	TRP	CE2-CD2-CG	-5.67	102.76	107.30
1	B	244	TRP	CE2-CD2-CG	-5.66	102.77	107.30
1	B	326	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	B	491	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	B	701	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	776	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	138	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	189	TRP	CG-CD2-CE3	5.59	138.94	133.90
1	A	480	VAL	N-CA-CB	-5.58	99.23	111.50
1	B	138	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	527	ASP	N-CA-C	5.52	125.91	111.00
1	B	93	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	189	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	B	528	LYS	N-CA-C	5.48	125.79	111.00
1	A	292	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	30	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	365	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	A	365	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	509	GLU	CA-CB-CG	5.41	125.30	113.40
1	A	722	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	81	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	299	TRP	CB-CG-CD2	-5.35	119.65	126.60
1	B	438	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	30	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	698	GLU	CA-CB-CG	-5.33	101.66	113.40
1	B	214	THR	CA-CB-CG2	5.33	119.86	112.40
1	B	193	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	113(F)	PRO	N-CD-CG	5.29	111.14	103.20
1	A	797	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	B	18	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	A	361	TRP	CB-CG-CD1	-5.24	120.19	127.00
1	B	297	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	B	326	TRP	CE2-CD2-CG	-5.23	103.11	107.30
1	A	244	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	B	811	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	B	692	VAL	CA-C-N	-5.20	105.77	117.20
1	B	160	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	299	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	326	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	A	527	ASP	CA-C-N	-5.13	105.91	117.20
1	B	491	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	B	580	VAL	CG1-CB-CG2	-5.13	102.70	110.90
1	A	93	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	81	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	491	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	A	797	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	A	155	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	B	155	TRP	CG-CD2-CE3	5.09	138.48	133.90
1	A	698	GLU	CA-CB-CG	-5.08	102.22	113.40
1	B	191	ILE	N-CA-C	-5.08	97.28	111.00
1	B	795	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	326	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	B	182	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	B	309	ARG	CD-NE-CZ	-5.06	116.51	123.60
1	A	534	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	B	13	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	B	13	TRP	CE2-CD2-CG	-5.04	103.26	107.30
1	B	162	GLU	CB-CA-C	-5.04	100.32	110.40
1	A	539	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	160	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	391	LEU	CA-CB-CG	5.01	126.82	115.30
1	B	163	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ARG	Peptide
1	A	435	SER	Peptide
1	B	208	ARG	Peptide
1	B	435	SER	Peptide

## 5.2 Too-close contacts [i](#)

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	6744	0	6429	372	1
1	B	6744	0	6434	425	32
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	2	0
All	All	13538	0	12877	496	32

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 19.

All (496) 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:A:191:ILE:CD1	1:B:40:ALA:HB3	1.29	1.57
1:A:257:PHE:CZ	1:B:278:VAL:HG11	1.44	1.52
1:A:36:GLU:CD	1:B:18:VAL:HB	1.21	1.51
1:A:32:ILE:HG22	1:B:18:VAL:CG2	1.00	1.47
1:A:60:ARG:HH22	1:B:39:LEU:CA	1.23	1.46
1:A:285:PHE:CZ	1:B:262:TYR:CZ	2.04	1.46
1:A:32:ILE:CG2	1:B:18:VAL:HG23	1.00	1.44
1:A:64:VAL:HG13	1:B:41:ARG:N	1.30	1.44
1:A:64:VAL:CB	1:B:36:GLU:O	1.64	1.43
1:A:16:HIS:O	1:B:32:ILE:CD1	1.64	1.42
1:A:191:ILE:HD11	1:B:40:ALA:CB	1.50	1.40
1:A:32:ILE:HG22	1:B:18:VAL:CB	1.51	1.39
1:A:12:LEU:CD1	1:B:114:GLU:HG2	1.51	1.39
1:A:285:PHE:HZ	1:B:262:TYR:CZ	1.34	1.38
1:A:64:VAL:CG1	1:B:41:ARG:N	1.86	1.38
1:A:36:GLU:OE1	1:B:18:VAL:CB	1.70	1.37
1:A:32:ILE:HG21	1:B:18:VAL:N	1.38	1.34
1:A:32:ILE:CG2	1:B:18:VAL:N	1.88	1.33
1:A:191:ILE:CD1	1:B:40:ALA:CB	2.04	1.29
1:A:285:PHE:CZ	1:B:262:TYR:OH	1.85	1.29
1:A:36:GLU:HB3	1:B:65:ILE:CG1	1.60	1.29
1:A:36:GLU:HB3	1:B:65:ILE:CD1	1.64	1.27
1:A:611:PRO:HB2	1:B:258:ASN:CG	1.54	1.27
1:A:12:LEU:HD13	1:B:114:GLU:CG	1.63	1.27
1:A:18:VAL:HB	1:B:36:GLU:OE1	1.35	1.23
1:A:254:LEU:N	1:B:177:GLU:O	1.58	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:HD21	1:B:68:ASN:ND2	1.38	1.22
1:A:13:TRP:HH2	1:B:117:PHE:CE2	1.56	1.21
1:A:611:PRO:HB2	1:B:258:ASN:OD1	1.04	1.21
1:A:611:PRO:CB	1:B:258:ASN:CG	2.09	1.20
1:A:36:GLU:OE1	1:B:18:VAL:HB	1.27	1.20
1:A:285:PHE:CE1	1:B:262:TYR:CE2	2.31	1.19
1:A:114:GLU:O	1:B:12:LEU:HB2	1.38	1.18
1:A:28:GLN:OE1	1:B:16:HIS:CE1	1.95	1.18
1:A:64:VAL:HG13	1:B:40:ALA:C	1.58	1.18
1:A:36:GLU:HB3	1:B:65:ILE:HD11	1.26	1.17
1:A:64:VAL:HG11	1:B:41:ARG:H	1.06	1.16
1:A:60:ARG:NH2	1:B:39:LEU:HA	1.29	1.14
1:A:16:HIS:O	1:B:32:ILE:HD13	1.39	1.14
1:A:32:ILE:HG23	1:B:18:VAL:HG23	1.29	1.14
1:A:64:VAL:CG1	1:B:41:ARG:H	1.54	1.13
1:A:254:LEU:C	1:B:177:GLU:HB2	1.36	1.09
1:A:611:PRO:CB	1:B:258:ASN:OD1	1.99	1.09
1:A:32:ILE:HG22	1:B:18:VAL:CA	1.81	1.09
1:A:36:GLU:CD	1:B:18:VAL:CB	2.14	1.09
1:A:257:PHE:CZ	1:B:278:VAL:CG1	2.36	1.08
1:A:61:ASP:OD1	1:B:38:THR:N	1.86	1.08
1:A:65:ILE:HG13	1:B:36:GLU:HB3	1.35	1.06
1:A:41:ARG:HA	1:B:68:ASN:OD1	1.56	1.06
1:A:18:VAL:CB	1:B:36:GLU:OE1	2.04	1.06
1:A:13:TRP:CH2	1:B:117:PHE:CE2	2.44	1.05
1:A:68:ASN:OD1	1:B:41:ARG:C	1.94	1.04
1:A:18:VAL:HG21	1:B:32:ILE:C	1.71	1.03
1:A:285:PHE:HE1	1:B:262:TYR:CE2	1.73	1.03
1:A:191:ILE:HD12	1:B:40:ALA:HB3	1.05	1.03
1:A:37:THR:OG1	1:B:62:ASN:N	1.82	1.03
1:A:16:HIS:O	1:B:32:ILE:HD12	1.59	1.03
1:A:36:GLU:OE1	1:B:18:VAL:CG1	2.07	1.03
1:A:36:GLU:CB	1:B:65:ILE:HD11	1.89	1.02
1:A:32:ILE:CG2	1:B:18:VAL:CA	2.36	1.01
1:A:32:ILE:CG2	1:B:18:VAL:CG2	1.76	1.01
1:A:18:VAL:HB	1:B:36:GLU:CD	1.81	1.01
1:A:60:ARG:HG2	1:B:37:THR:O	1.59	1.01
1:A:285:PHE:CZ	1:B:262:TYR:CE2	2.45	1.00
1:A:193:ARG:HH21	1:B:41:ARG:NH1	1.59	1.00
1:A:32:ILE:HG22	1:B:18:VAL:HG22	1.40	1.00
1:A:64:VAL:HB	1:B:36:GLU:O	0.82	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:HB2	1:B:18:VAL:HG11	1.43	0.99
1:A:191:ILE:HD11	1:B:40:ALA:HB2	1.43	0.99
1:A:44:TYR:O	1:B:8(N):PHE:CE2	2.15	0.99
1:A:30:ARG:HD3	1:B:33:ASP:OD2	1.64	0.97
1:A:11(N):LEU:O	1:B:45:ASN:ND2	1.99	0.96
1:A:39:LEU:HA	1:B:60:ARG:HH22	1.29	0.96
1:A:64:VAL:CG1	1:B:36:GLU:O	2.14	0.95
1:A:32:ILE:HG21	1:B:17:GLN:C	1.88	0.94
1:A:36:GLU:CB	1:B:65:ILE:CG1	2.46	0.94
1:A:114:GLU:O	1:B:12:LEU:CB	2.16	0.93
1:A:257:PHE:HZ	1:B:278:VAL:CG1	1.75	0.93
1:A:41:ARG:CA	1:B:68:ASN:OD1	2.15	0.93
1:A:285:PHE:HE1	1:B:262:TYR:HE2	1.14	0.91
1:A:36:GLU:HB3	1:B:65:ILE:HG13	1.48	0.91
1:A:36:GLU:CG	1:B:18:VAL:HB	2.01	0.91
1:A:32:ILE:HD11	1:B:16:HIS:CB	2.02	0.90
1:A:32:ILE:CG2	1:B:18:VAL:H	1.60	0.90
1:A:191:ILE:HD12	1:B:40:ALA:CB	1.87	0.90
1:A:36:GLU:OE1	1:B:18:VAL:C	2.09	0.90
1:A:36:GLU:OE1	1:B:18:VAL:CA	2.20	0.89
1:A:11(N):LEU:HD22	1:B:41:ARG:HH11	1.37	0.89
1:A:41:ARG:NH1	1:B:11(N):LEU:HD22	1.88	0.89
1:B:197:GLN:HG2	1:B:224:VAL:HG22	1.54	0.89
1:A:45:ASN:ND2	1:B:68:ASN:ND2	2.21	0.88
1:A:611:PRO:HB3	1:B:258:ASN:CG	1.93	0.88
1:A:18:VAL:CG1	1:B:36:GLU:OE1	2.22	0.88
1:A:45:ASN:HD21	1:B:68:ASN:HD21	1.14	0.88
1:A:57:MET:O	1:B:37:THR:HG23	1.72	0.88
1:A:41:ARG:C	1:B:68:ASN:OD1	2.12	0.88
1:A:30:ARG:CD	1:B:33:ASP:OD2	2.13	0.87
1:A:32:ILE:CD1	1:B:16:HIS:HB3	2.03	0.86
1:A:37:THR:O	1:B:60:ARG:C	1.92	0.85
1:A:12:LEU:HD13	1:B:114:GLU:HG2	0.87	0.85
1:A:65:ILE:CG1	1:B:36:GLU:HB3	2.05	0.85
1:A:11(N):LEU:HD22	1:B:41:ARG:NH1	1.91	0.84
1:A:18:VAL:N	1:B:32:ILE:HG21	1.78	0.84
1:A:257:PHE:HZ	1:B:278:VAL:HG11	1.02	0.84
1:A:39:LEU:HA	1:B:60:ARG:NH2	1.93	0.83
1:A:32:ILE:HD12	1:B:16:HIS:HB3	1.59	0.83
1:A:611:PRO:C	1:B:258:ASN:HD21	1.81	0.83
1:A:32:ILE:HG23	1:B:18:VAL:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:H	1:B:32:ILE:HG21	1.41	0.83
1:A:258:ASN:ND2	1:B:617:LYS:NZ	2.27	0.83
1:A:36:GLU:OE1	1:B:18:VAL:HG12	1.77	0.82
1:A:33:ASP:OD2	1:B:30:ARG:HG2	1.77	0.82
1:A:60:ARG:NH2	1:B:39:LEU:CA	1.98	0.82
1:A:12:LEU:HD13	1:B:114:GLU:CB	2.08	0.82
1:A:61:ASP:OD2	1:B:33:ASP:OD1	1.99	0.81
1:A:262:TYR:OH	1:B:282:ASN:O	1.89	0.80
1:A:44:TYR:O	1:B:8(N):PHE:HE2	1.58	0.80
1:A:285:PHE:HZ	1:B:262:TYR:CE1	1.98	0.80
1:A:36:GLU:O	1:B:64:VAL:HB	1.82	0.80
1:A:260:GLY:CA	1:B:282:ASN:HD22	1.95	0.80
1:A:34:HIS:CE1	1:B:34:HIS:CE1	2.71	0.79
1:A:32:ILE:CD1	1:B:16:HIS:CB	2.50	0.78
1:A:60:ARG:CG	1:B:37:THR:O	2.32	0.78
1:B:171:ILE:HD12	1:B:176:VAL:HG21	1.65	0.78
1:A:191:ILE:HD11	1:B:40:ALA:HB3	1.16	0.78
1:A:171:ILE:HD12	1:A:176:VAL:HG21	1.66	0.78
1:A:64:VAL:HB	1:B:36:GLU:C	1.96	0.77
1:A:64:VAL:HG12	1:B:36:GLU:HA	1.64	0.77
1:A:193:ARG:NH2	1:B:41:ARG:CZ	2.48	0.77
1:A:285:PHE:CE1	1:B:262:TYR:CZ	2.59	0.77
1:A:64:VAL:CG1	1:B:36:GLU:HA	2.14	0.77
1:A:193:ARG:HH21	1:B:41:ARG:CZ	1.98	0.77
1:A:68:ASN:OD1	1:B:42:SER:N	2.18	0.77
1:A:197:GLN:HG2	1:A:224:VAL:HG22	1.66	0.77
1:A:8(N):PHE:HE2	1:B:44:TYR:HB3	1.50	0.77
1:A:114:GLU:CD	1:B:12:LEU:HD21	2.06	0.76
1:A:28:GLN:OE1	1:B:16:HIS:NE2	2.19	0.76
1:A:260:GLY:HA2	1:B:282:ASN:HD22	1.48	0.76
1:A:44:TYR:O	1:B:8(N):PHE:CZ	2.38	0.76
1:A:16:HIS:O	1:B:32:ILE:HD11	1.85	0.76
1:A:611:PRO:C	1:B:258:ASN:ND2	2.40	0.74
1:A:254:LEU:O	1:B:177:GLU:HB2	1.86	0.74
1:A:60:ARG:NH1	1:B:37:THR:O	2.21	0.74
1:A:33:ASP:C	1:B:30:ARG:NH1	2.38	0.73
1:A:611:PRO:O	1:B:258:ASN:ND2	2.21	0.73
1:A:12:LEU:HD22	1:B:114:GLU:CD	2.07	0.73
1:A:12:LEU:HB3	1:B:114:GLU:HB3	1.68	0.73
1:A:60:ARG:HD3	1:B:38:THR:HA	1.70	0.72
1:A:285:PHE:CE1	1:B:262:TYR:OH	2.42	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:HB2	1:B:18:VAL:CG1	2.18	0.71
1:A:11(N):LEU:HA	1:B:45:ASN:HB2	1.72	0.71
1:A:258:ASN:ND2	1:B:617:LYS:HZ2	1.88	0.71
1:A:36:GLU:HB3	1:B:65:ILE:HG12	1.71	0.71
1:B:665:HIS:HD2	1:B:688:ILE:HG23	1.56	0.71
1:A:41:ARG:HH12	1:B:11(N):LEU:HD22	1.56	0.70
1:B:214(C):THR:HG23	1:B:401:GLU:HB3	1.73	0.70
1:A:8(N):PHE:CE2	1:B:44:TYR:O	2.45	0.70
1:A:252:PHE:HE2	1:B:166:PHE:HB2	1.57	0.70
1:A:262:TYR:CE2	1:B:285:PHE:HZ	2.10	0.69
1:A:33:ASP:OD2	1:B:30:ARG:CG	2.32	0.69
1:B:404:TYR:HE1	1:B:431:ILE:HG12	1.57	0.69
1:A:8(N):PHE:CE2	1:B:44:TYR:HB3	2.27	0.69
1:A:285:PHE:CE2	1:B:260:GLY:HA3	2.28	0.69
1:A:13:TRP:CH2	1:B:117:PHE:HE2	2.07	0.69
1:A:254:LEU:CD2	1:B:177:GLU:N	2.49	0.68
1:A:68:ASN:CB	1:B:42:SER:HB3	2.23	0.68
1:A:193:ARG:NH2	1:B:41:ARG:NH1	2.37	0.68
1:A:13:TRP:NE1	1:B:116:GLY:CA	2.47	0.68
1:A:214(C):THR:HG23	1:A:401:GLU:HB3	1.74	0.68
1:A:282:ASN:HB3	1:B:262:TYR:CE1	2.29	0.68
1:A:282:ASN:HB3	1:B:262:TYR:HE1	1.59	0.67
1:A:64:VAL:HG11	1:B:41:ARG:N	1.75	0.67
1:A:252:PHE:CD1	1:B:179:PRO:HG3	1.75	0.67
1:B:245:GLN:HE21	1:B:247:ARG:HE	1.42	0.66
1:A:30:ARG:CD	1:B:33:ASP:OD1	2.36	0.66
1:A:166:PHE:CB	1:B:254:LEU:CD1	2.73	0.66
1:A:16:HIS:CE1	1:B:28:GLN:OE1	2.48	0.65
1:A:285:PHE:CE2	1:B:260:GLY:CA	2.79	0.65
1:B:464:LYS:HA	1:B:472:ILE:HD11	1.78	0.65
1:B:204:GLY:HA3	1:B:217:GLY:HA2	1.78	0.65
1:A:32:ILE:HD11	1:B:16:HIS:HB2	1.78	0.65
1:A:506:THR:HG21	1:A:530:PHE:HE1	1.62	0.64
1:B:506:THR:HG21	1:B:530:PHE:HE1	1.60	0.64
1:A:13:TRP:HE1	1:B:116:GLY:CA	2.08	0.64
1:A:40:ALA:HB3	1:B:191:ILE:HD11	1.77	0.64
1:B:411:LEU:HG	1:B:425:LEU:HG	1.78	0.64
1:A:36:GLU:CB	1:B:65:ILE:HG13	2.21	0.64
1:A:204:GLY:HA3	1:A:217:GLY:HA2	1.78	0.63
1:A:262:TYR:CE2	1:B:285:PHE:CZ	2.87	0.63
1:A:18:VAL:HG21	1:B:32:ILE:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:CD1	1:B:40:ALA:HB2	2.11	0.63
1:A:33:ASP:C	1:B:30:ARG:HH12	2.02	0.63
1:A:40:ALA:HB3	1:B:191:ILE:CD1	2.29	0.62
1:A:36:GLU:CB	1:B:65:ILE:CD1	2.53	0.62
1:A:12:LEU:HD13	1:B:114:GLU:HA	1.82	0.62
1:A:12:LEU:HD11	1:B:114:GLU:HG2	1.69	0.62
1:A:18:VAL:H	1:B:32:ILE:CG2	2.11	0.62
1:A:114:GLU:CD	1:B:12:LEU:CD2	2.68	0.62
1:A:179:PRO:HD3	1:B:252:PHE:O	2.00	0.62
1:B:235:THR:HB	1:B:237:ASN:H	1.65	0.62
1:A:611:PRO:CB	1:B:258:ASN:ND2	2.63	0.62
1:A:34:HIS:HE1	1:B:34:HIS:CE1	2.16	0.61
1:B:95:LEU:HD13	1:B:123:LEU:HD12	1.82	0.61
1:B:245:GLN:NE2	1:B:247:ARG:HE	1.99	0.61
1:A:88:GLU:HB2	1:A:132:GLY:HA2	1.83	0.61
1:A:611:PRO:HB3	1:B:258:ASN:CB	2.29	0.61
1:B:713:ASN:ND2	1:B:721:LEU:HD11	2.15	0.60
1:A:64:VAL:CG1	1:B:36:GLU:C	2.69	0.60
1:A:665:HIS:HD2	1:A:688:ILE:HG23	1.65	0.60
1:A:451:LYS:HG2	1:A:824:ILE:HG12	1.84	0.60
1:B:621:LYS:HE2	1:B:625:CYS:SG	2.42	0.60
1:A:166:PHE:HB2	1:B:254:LEU:HD13	1.83	0.60
1:B:451:LYS:HG2	1:B:824:ILE:HG12	1.84	0.60
1:A:34:HIS:N	1:B:30:ARG:HH12	1.99	0.60
1:A:36:GLU:CB	1:B:65:ILE:HG12	2.30	0.59
1:A:36:GLU:CG	1:B:65:ILE:HG12	2.33	0.59
1:A:411:LEU:HG	1:A:425:LEU:HG	1.84	0.59
1:A:11(N):LEU:HA	1:B:45:ASN:CB	2.32	0.59
1:A:166:PHE:CB	1:B:254:LEU:HD13	2.32	0.59
1:B:746:GLU:OE1	1:B:759:LYS:HG3	2.03	0.59
1:A:12:LEU:HD13	1:B:114:GLU:CA	2.31	0.59
1:A:713:ASN:ND2	1:A:721:LEU:HD11	2.17	0.59
1:A:32:ILE:HD11	1:B:16:HIS:HB3	1.75	0.58
1:A:60:ARG:HH22	1:B:39:LEU:HA	0.45	0.58
1:A:115:LEU:CD2	1:B:16:HIS:HB2	2.34	0.58
1:A:340:THR:HG21	1:A:385:GLU:HB3	1.84	0.58
1:B:234:LYS:HD2	1:B:513:LEU:HD21	1.85	0.58
1:B:283:ASP:HB3	1:B:292:ARG:HG3	1.86	0.58
1:A:61:ASP:OD1	1:B:37:THR:C	2.21	0.58
1:A:163:TYR:HE1	1:B:251:GLU:OE2	1.86	0.58
1:B:506:THR:HG21	1:B:530:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:CG	1:B:12:LEU:CD2	2.79	0.58
1:B:10(N):THR:HG22	1:B:67:TRP:HH2	1.68	0.58
1:A:234:LYS:HD2	1:A:513:LEU:HD21	1.86	0.58
1:A:64:VAL:HG11	1:B:35:VAL:O	2.03	0.58
1:A:191:ILE:HD12	1:B:39:LEU:O	2.04	0.58
1:A:41:ARG:NH1	1:B:11(N):LEU:CD2	2.64	0.58
1:B:692:VAL:HG11	1:B:714:LEU:HD23	1.86	0.57
1:A:8(N):PHE:HE2	1:B:44:TYR:O	1.87	0.57
1:A:245:GLN:HE21	1:A:247:ARG:HE	1.53	0.57
1:A:18:VAL:CG2	1:B:32:ILE:C	2.55	0.57
1:B:88:GLU:HB2	1:B:132:GLY:HA2	1.84	0.57
1:A:285:PHE:CE1	1:B:262:TYR:HE2	1.93	0.57
1:A:12:LEU:HD22	1:B:114:GLU:CG	2.34	0.57
1:B:340:THR:HG21	1:B:385:GLU:HB3	1.85	0.57
1:B:399:HIS:O	1:B:403:ILE:HG13	2.05	0.57
1:A:8(N):PHE:CZ	1:B:44:TYR:O	2.58	0.57
1:A:13:TRP:CD1	1:B:114:GLU:O	2.58	0.57
1:A:285:PHE:CZ	1:B:260:GLY:HA2	2.39	0.56
1:A:13:TRP:HE1	1:B:116:GLY:HA2	1.70	0.56
1:A:65:ILE:HD11	1:B:36:GLU:OE1	2.05	0.56
1:B:591:LYS:HA	1:B:592(D):LEU:HD12	1.88	0.56
1:A:68:ASN:CG	1:B:42:SER:HB3	2.25	0.56
1:A:68:ASN:HD21	1:B:45:ASN:HD21	1.53	0.56
1:B:592(E):LYS:HB3	1:B:592(E):LYS:HZ2	1.70	0.56
1:A:37:THR:HG21	1:B:30:ARG:HD2	1.88	0.56
1:A:591:LYS:HA	1:A:592(D):LEU:HD12	1.88	0.56
1:A:30:ARG:HD3	1:B:33:ASP:OD1	2.06	0.55
1:B:498:SER:HB2	1:B:537:VAL:HG13	1.88	0.55
1:A:36:GLU:HB2	1:B:65:ILE:HD11	1.86	0.55
1:B:693:ASP:O	1:B:696:ASN:HB2	2.07	0.55
1:A:64:VAL:CG1	1:B:41:ARG:O	2.55	0.55
1:A:285:PHE:CE2	1:B:260:GLY:HA2	2.41	0.55
1:B:580:VAL:HG11	1:B:622:LEU:HD13	1.89	0.55
1:A:163:TYR:CE1	1:B:251:GLU:OE2	2.60	0.54
1:A:60:ARG:NH2	1:B:39:LEU:C	2.60	0.54
1:A:166:PHE:CG	1:B:254:LEU:CD1	2.90	0.54
1:B:175:GLN:NE2	1:B:609:SER:H	2.06	0.54
1:A:64:VAL:HG13	1:B:41:ARG:CA	2.27	0.54
1:A:64:VAL:HG12	1:B:41:ARG:O	2.07	0.54
1:A:404:TYR:HE1	1:A:431:ILE:HG12	1.71	0.54
1:B:795:ARG:HG3	1:B:798:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASP:HA	1:B:18:VAL:CG1	2.37	0.53
1:A:115:LEU:HD21	1:B:16:HIS:HB2	1.90	0.53
1:B:565:MET:HB3	1:B:604:ILE:HB	1.90	0.53
1:B:88:GLU:O	1:B:137:GLY:HA2	2.07	0.53
1:A:565:MET:HB3	1:A:604:ILE:HB	1.90	0.53
1:A:464:LYS:HA	1:A:472:ILE:HD11	1.91	0.53
1:A:36:GLU:OE1	1:B:18:VAL:O	2.26	0.53
1:A:308:LEU:HD11	1:A:352:VAL:HG21	1.91	0.53
1:B:74:PHE:HE2	1:B:239:ASN:HD21	1.56	0.53
1:A:214(C):THR:CG2	1:A:401:GLU:HB3	2.39	0.53
1:B:455:VAL:H	1:B:459:HIS:HD2	1.56	0.53
1:A:175:GLN:NE2	1:A:609:SER:H	2.07	0.52
1:A:580:VAL:HG11	1:A:622:LEU:HD13	1.91	0.52
1:B:665:HIS:CD2	1:B:688:ILE:HG23	2.42	0.52
1:A:455:VAL:H	1:A:459:HIS:HD2	1.58	0.52
1:A:611:PRO:CB	1:B:258:ASN:CB	2.87	0.52
1:A:12:LEU:CD2	1:B:114:GLU:CD	2.78	0.52
1:A:114:GLU:C	1:B:12:LEU:CB	2.78	0.52
1:B:214(C):THR:CG2	1:B:401:GLU:HB3	2.39	0.52
1:B:599:PRO:HB2	1:B:792:HIS:NE2	2.24	0.52
1:A:68:ASN:ND2	1:B:45:ASN:HD21	2.08	0.52
1:A:570:ILE:HG13	1:A:620:ILE:HD11	1.92	0.51
1:A:592(E):LYS:HZ2	1:A:592(E):LYS:HB3	1.75	0.51
1:A:65:ILE:HG12	1:B:36:GLU:CD	2.31	0.51
1:B:522:GLU:HA	1:B:525:VAL:HG23	1.91	0.51
1:B:570:ILE:HG13	1:B:620:ILE:HD11	1.91	0.51
1:B:700:THR:HG23	1:B:705:GLU:HA	1.92	0.51
1:A:506:THR:HG21	1:A:530:PHE:CE1	2.43	0.51
1:A:254:LEU:HD22	1:B:177:GLU:N	2.21	0.51
1:A:68:ASN:OD1	1:B:42:SER:HB3	2.09	0.51
1:B:308:LEU:HD11	1:B:352:VAL:HG21	1.92	0.51
1:A:32:ILE:CG2	1:B:18:VAL:CB	2.38	0.51
1:A:746:GLU:OE1	1:A:759:LYS:HG3	2.10	0.51
1:A:12:LEU:CG	1:B:114:GLU:HG2	2.36	0.51
1:A:283:ASP:HB3	1:A:292:ARG:HG3	1.93	0.51
1:A:692:VAL:HG11	1:A:714:LEU:HD23	1.92	0.51
1:B:283:ASP:HA	1:B:288:GLY:HA3	1.93	0.51
1:A:795:ARG:HG3	1:A:798:LEU:HD22	1.93	0.51
1:B:147:MET:SD	1:B:154:ALA:CB	2.98	0.51
1:A:32:ILE:CG2	1:B:18:VAL:HG22	2.10	0.51
1:A:68:ASN:OD1	1:B:41:ARG:O	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HD13	1:B:17:GLN:CA	2.27	0.50
1:A:61:ASP:O	1:B:36:GLU:C	2.50	0.50
1:A:64:VAL:CG1	1:B:36:GLU:CA	2.86	0.50
1:B:60:ARG:HD2	1:B:188:PRO:O	2.11	0.50
1:A:191:ILE:HD12	1:B:39:LEU:C	2.32	0.50
1:A:695:ALA:O	1:A:699:ILE:HG12	2.12	0.50
1:A:64:VAL:HG11	1:B:36:GLU:HA	1.91	0.50
1:A:13:TRP:HH2	1:B:117:PHE:CZ	2.18	0.50
1:A:166:PHE:HB3	1:B:254:LEU:CD1	2.42	0.50
1:B:228:PHE:HB3	1:B:241:LEU:HB3	1.94	0.50
1:B:695:ALA:O	1:B:699:ILE:HG12	2.11	0.50
1:B:777:PHE:CE2	1:B:781:LEU:HD11	2.47	0.50
1:A:258:ASN:ND2	1:B:617:LYS:HZ1	2.05	0.50
1:B:214(D):LEU:HD11	1:B:409:PHE:CE2	2.47	0.50
1:B:404:TYR:CE1	1:B:431:ILE:HG12	2.43	0.50
1:B:717:ASN:O	1:B:721:LEU:HG	2.12	0.50
1:A:252:PHE:CE2	1:B:166:PHE:HB2	2.41	0.49
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.95	0.49
1:B:10(N):THR:HG22	1:B:67:TRP:CH2	2.45	0.49
1:A:39:LEU:HA	1:B:60:ARG:CZ	2.31	0.49
1:A:228:PHE:HB3	1:A:241:LEU:HB3	1.95	0.49
1:B:129:ALA:HA	1:B:182:TRP:CE3	2.47	0.49
1:B:99:LEU:HB3	1:B:113(G):ARG:HG3	1.95	0.49
1:B:388:PRO:HG2	1:B:391:LEU:HB3	1.95	0.49
1:B:4:MET:N	1:B:4:MET:SD	2.86	0.49
1:B:722:ARG:O	1:B:728:HIS:HB2	2.13	0.49
1:A:254:LEU:HD12	1:B:177:GLU:HB3	1.65	0.49
1:A:693:ASP:O	1:A:696:ASN:HB2	2.12	0.48
1:A:166:PHE:CG	1:B:254:LEU:HD13	2.48	0.48
1:A:245:GLN:NE2	1:A:247:ARG:HE	2.11	0.48
1:B:169:LYS:HB2	1:B:176:VAL:CG2	2.43	0.48
1:B:214(D):LEU:HD11	1:B:409:PHE:CZ	2.48	0.48
1:B:290:GLU:O	1:B:294:LYS:HB2	2.13	0.48
1:A:18:VAL:HG12	1:B:36:GLU:OE1	2.09	0.48
1:B:135:GLY:CA	3:B:860:PLP:H5A2	2.43	0.48
1:A:68:ASN:CG	1:B:42:SER:CB	2.82	0.48
1:A:169:LYS:HB2	1:A:176:VAL:CG2	2.43	0.48
1:A:37:THR:O	1:B:60:ARG:O	2.31	0.48
1:B:410:PHE:O	1:B:414:VAL:HG23	2.14	0.48
1:A:621:LYS:HE2	1:A:625:CYS:SG	2.54	0.48
1:A:32:ILE:HG21	1:B:17:GLN:CA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:ILE:HG12	1:B:681:PHE:CE1	2.48	0.48
1:A:235:THR:HB	1:A:237:ASN:H	1.79	0.48
1:A:61:ASP:O	1:B:36:GLU:O	2.32	0.48
1:A:40:ALA:O	1:B:64:VAL:HG22	1.93	0.48
1:A:509:GLU:HB3	1:A:512:LEU:HD12	1.95	0.47
1:A:37:THR:HG21	1:B:30:ARG:CD	2.44	0.47
1:B:533:LYS:O	1:B:537:VAL:HG23	2.13	0.47
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.96	0.47
1:B:568:LYS:HE2	1:B:568:LYS:HB3	1.67	0.47
1:B:576:GLN:O	1:B:580:VAL:HG23	2.14	0.47
1:B:18:VAL:HG12	1:B:65:ILE:HD11	1.96	0.47
1:A:399:HIS:O	1:A:403:ILE:HG13	2.14	0.47
1:A:576:GLN:O	1:A:580:VAL:HG23	2.14	0.47
1:A:498:SER:HB2	1:A:537:VAL:HG13	1.95	0.47
1:A:10(N):THR:HG22	1:A:67:TRP:HH2	1.78	0.47
1:A:36:GLU:O	1:B:64:VAL:CB	2.60	0.47
1:B:33:ASP:O	1:B:37:THR:HB	2.15	0.47
1:B:58:SER:O	1:B:61:ASP:HB2	2.15	0.47
1:B:558(C):ILE:HD11	1:B:602:VAL:HG11	1.95	0.47
1:A:45:ASN:ND2	1:B:68:ASN:HD21	1.97	0.47
1:A:36:GLU:CB	1:B:18:VAL:CG1	2.93	0.47
1:A:395:LEU:HD13	1:A:396:LEU:HG	1.96	0.46
1:A:522:GLU:HA	1:A:525:VAL:HG23	1.97	0.46
1:B:395:LEU:HD13	1:B:396:LEU:HG	1.97	0.46
1:B:509:GLU:HB3	1:B:512:LEU:HD12	1.95	0.46
1:A:144:VAL:HG12	1:A:230:VAL:HG11	1.96	0.46
1:B:564:ASP:OD2	1:B:601:LYS:HE3	2.16	0.46
1:A:600:ARG:HA	1:A:639:LEU:O	2.15	0.46
1:A:611:PRO:HB3	1:B:258:ASN:HB2	1.94	0.46
1:A:38:THR:OG1	1:B:61:ASP:OD1	2.30	0.46
1:A:169:LYS:HB2	1:A:176:VAL:HG22	1.98	0.46
1:A:41:ARG:HH12	1:B:11(N):LEU:CD2	2.24	0.46
1:B:13(N):ARG:HE	1:B:12(N):ARG:HH21	1.63	0.46
1:A:254:LEU:HD12	1:B:166:PHE:HB2	1.36	0.46
1:B:170:ILE:HA	1:B:174:TYR:O	2.15	0.46
1:B:550:LYS:HD2	1:B:558(E):ARG:HH12	1.81	0.46
1:B:600:ARG:HA	1:B:639:LEU:O	2.15	0.46
1:A:278:VAL:HG11	1:B:257:PHE:CZ	2.51	0.46
1:B:464:LYS:HE3	1:B:479:PHE:HB2	1.98	0.46
1:B:144:VAL:HG12	1:B:230:VAL:HG11	1.97	0.45
1:A:28:GLN:HB3	1:B:16:HIS:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HD2	1:A:188:PRO:O	2.16	0.45
1:A:722:ARG:O	1:A:728:HIS:HB2	2.16	0.45
1:A:170:ILE:HA	1:A:174:TYR:O	2.17	0.45
1:A:252:PHE:CE2	1:B:166:PHE:CB	3.00	0.45
1:A:4:MET:SD	1:A:4:MET:N	2.90	0.45
1:A:74:PHE:HE2	1:A:239:ASN:HD21	1.63	0.45
1:A:777:PHE:CE2	1:A:781:LEU:HD11	2.52	0.45
1:A:11(N):LEU:HD23	1:B:45:ASN:HB2	1.98	0.45
1:B:428:ILE:HD12	1:B:470:ASP:HB3	1.98	0.45
1:B:169:LYS:HB2	1:B:176:VAL:HG22	1.99	0.45
1:A:16:HIS:ND1	1:B:28:GLN:OE1	2.50	0.45
1:A:18:VAL:HG12	1:A:65:ILE:HD11	1.98	0.45
1:A:177:GLU:HB2	1:B:254:LEU:HB3	0.97	0.44
1:A:344:LEU:HD21	1:A:392:PHE:CZ	2.52	0.44
1:B:200:VAL:HG11	1:B:298:PHE:HA	2.00	0.44
1:A:33:ASP:HA	1:B:18:VAL:HG11	1.98	0.44
1:B:170:ILE:HD13	1:B:175:GLN:HA	1.99	0.44
1:B:534:TRP:CH2	1:B:805:LEU:HG	2.53	0.44
1:A:65:ILE:CD1	1:B:36:GLU:OE1	2.64	0.44
1:B:813:SER:O	1:B:817:ILE:HG12	2.18	0.44
1:A:12:LEU:CD1	1:B:114:GLU:CG	2.44	0.44
1:A:32:ILE:HG21	1:B:18:VAL:CA	2.18	0.44
1:B:502:LEU:O	1:B:506:THR:HG23	2.18	0.44
1:A:599:PRO:HB2	1:A:792:HIS:NE2	2.33	0.44
1:A:254:LEU:HD13	1:B:177:GLU:HA	1.77	0.43
1:A:191:ILE:CG1	1:B:40:ALA:HB3	2.30	0.43
1:B:561:THR:HG23	1:B:600:ARG:HG2	2.00	0.43
1:A:12:LEU:CD2	1:B:114:GLU:CG	2.96	0.43
1:B:163:TYR:O	1:B:180:ASP:HB3	2.19	0.43
1:B:455:VAL:HG23	1:B:674:SER:HB2	2.00	0.43
1:A:254:LEU:C	1:B:177:GLU:CB	2.33	0.43
1:B:171:ILE:HB	1:B:176:VAL:CG1	2.49	0.43
1:A:32:ILE:HD13	1:B:17:GLN:HA	2.00	0.43
1:A:455:VAL:HG22	1:A:459:HIS:CD2	2.54	0.43
1:A:33:ASP:HA	1:B:18:VAL:HG13	2.00	0.43
1:B:588:LEU:HA	1:B:588:LEU:HD12	1.87	0.43
1:B:73:LYS:HB3	1:B:73:LYS:HE2	1.87	0.43
1:A:254:LEU:HD23	1:B:177:GLU:N	2.30	0.43
1:B:2(N):LYS:HD3	1:B:2(N):LYS:HA	1.80	0.43
1:A:36:GLU:CA	1:B:65:ILE:HG13	2.49	0.43
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558(C):ILE:HD11	1:A:602:VAL:HG11	2.00	0.43
1:A:95:LEU:HD13	1:A:123:LEU:HD12	2.00	0.42
1:A:68:ASN:CB	1:B:42:SER:CB	2.97	0.42
1:A:308:LEU:CD1	1:A:352:VAL:HG21	2.49	0.42
1:A:60:ARG:O	1:B:37:THR:HA	2.16	0.42
1:B:339:ASP:O	1:B:342:PRO:HD2	2.19	0.42
1:B:344:LEU:HD21	1:B:392:PHE:CZ	2.53	0.42
1:A:260:GLY:CA	1:B:282:ASN:ND2	2.74	0.42
1:A:278:VAL:HG11	1:B:257:PHE:CE2	2.55	0.42
1:B:308:LEU:CD1	1:B:352:VAL:HG21	2.49	0.42
1:A:179:PRO:N	1:B:252:PHE:HD2	2.16	0.42
1:B:352:VAL:HB	1:B:356:LEU:HD12	2.01	0.42
1:A:68:ASN:OD1	1:B:42:SER:CB	2.67	0.42
1:B:52:TYR:OH	1:B:126:GLU:HG3	2.20	0.42
1:B:299:TRP:CH2	1:B:342:PRO:HB3	2.55	0.42
1:A:378:THR:O	1:A:459:HIS:HE1	2.02	0.42
1:B:348:GLU:OE1	1:B:399:HIS:HE1	2.03	0.42
1:B:487:THR:HA	1:B:488:PRO:HD3	1.88	0.42
1:B:722:ARG:NH1	1:B:770:TYR:O	2.53	0.42
1:B:562:LEU:HD12	1:B:661:ASP:HB3	2.01	0.42
1:A:604:ILE:HD13	1:A:643:VAL:HB	2.02	0.41
1:B:455:VAL:HG22	1:B:459:HIS:CD2	2.55	0.41
1:B:214:THR:HG22	1:B:214(D):LEU:HD23	2.02	0.41
1:B:718:VAL:O	1:B:722:ARG:HB2	2.20	0.41
1:A:17:GLN:HA	1:B:32:ILE:HD13	2.01	0.41
1:A:717:ASN:O	1:A:721:LEU:HG	2.21	0.41
1:B:293:LEU:HD13	1:B:387:TRP:CE2	2.56	0.41
1:A:299:TRP:CH2	1:A:342:PRO:HB3	2.56	0.41
1:B:197:GLN:HA	1:B:223:ALA:O	2.21	0.41
1:A:262:TYR:CZ	1:B:282:ASN:N	2.86	0.41
1:B:558(D):ASN:OD1	1:B:638:HIS:ND1	2.54	0.41
1:A:344:LEU:HD21	1:A:392:PHE:HZ	1.85	0.41
1:A:166:PHE:CG	1:B:254:LEU:HD11	2.56	0.41
1:B:592(E):LYS:HB3	1:B:592(E):LYS:NZ	2.33	0.41
1:A:258:ASN:HA	1:B:611:PRO:HB2	1.35	0.41
1:A:191:ILE:HG23	1:B:39:LEU:O	2.21	0.41
1:A:60:ARG:HD3	1:B:38:THR:CA	2.44	0.41
1:A:181:TYR:OH	1:B:252:PHE:N	2.52	0.40
1:A:290:GLU:O	1:A:294:LYS:HB2	2.20	0.40
1:B:175:GLN:HE22	1:B:609:SER:H	1.67	0.40
1:B:378:THR:O	1:B:459:HIS:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:LEU:HB3	1:B:762:VAL:HG13	2.03	0.40
1:B:742:LEU:HD22	1:B:762:VAL:HG22	2.03	0.40
1:A:10(N):THR:HG22	1:A:67:TRP:CH2	2.54	0.40
1:A:88:GLU:O	1:A:137:GLY:HA2	2.22	0.40
1:A:12:LEU:CD2	1:B:114:GLU:HG2	2.51	0.40
1:B:690:GLY:O	1:B:710:LEU:HA	2.20	0.40
1:A:13(N):ARG:HE	1:A:12(N):ARG:HH21	1.70	0.40
1:A:40:ALA:HB1	1:B:64:VAL:HA	1.62	0.40
1:A:531:LEU:HG	1:A:798:LEU:HB3	2.03	0.40
1:B:135:GLY:HA2	3:B:860:PLP:H5A2	2.03	0.40
1:B:203:TYR:CE1	1:B:395:LEU:HD23	2.56	0.40
1:B:214(G):SER:HB2	1:B:398:ARG:NE	2.36	0.40
1:A:177:GLU:C	1:B:254:LEU:HB2	2.41	0.40
1:B:709:PHE:HB3	1:B:783:THR:CG2	2.51	0.40
1:B:7(N):LEU:HB2	1:B:4(N):GLU:HG3	2.04	0.40
1:B:245:GLN:HE21	1:B:247:ARG:NE	2.14	0.40
1:A:60:ARG:CD	1:B:37:THR:O	2.70	0.40
1:A:35:VAL:O	1:B:64:VAL:HG11	2.22	0.40
1:B:74:PHE:HE2	1:B:239:ASN:ND2	2.19	0.40

All (32) 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:B:7:LEU:CD2	1:B:203:TYR:CA[4_535]	0.92	1.28
1:B:6:PRO:CA	1:B:394:HIS:CE1[4_535]	0.93	1.27
1:B:5(N):GLN:CG	1:B:261:ASP:OD2[4_535]	1.22	0.98
1:B:7:LEU:CD2	1:B:203:TYR:CB[4_535]	1.29	0.91
1:B:6:PRO:CB	1:B:394:HIS:CE1[4_535]	1.33	0.87
1:B:7:LEU:CG	1:B:203:TYR:CB[4_535]	1.38	0.82
1:B:3:THR:CB	1:B:271:ARG:NH1[4_535]	1.39	0.81
1:B:7:LEU:CD2	1:B:203:TYR:C[4_535]	1.42	0.78
1:B:5(N):GLN:CD	1:B:261:ASP:OD2[4_535]	1.43	0.77
1:B:5(N):GLN:CG	1:B:261:ASP:CG[4_535]	1.59	0.61
1:B:6:PRO:CB	1:B:394:HIS:ND1[4_535]	1.61	0.59
1:B:6:PRO:C	1:B:394:HIS:CE1[4_535]	1.64	0.56
1:B:7:LEU:CG	1:B:204:GLY:N[4_535]	1.64	0.56
1:B:6:PRO:CA	1:B:394:HIS:NE2[4_535]	1.65	0.55
1:B:5(N):GLN:CG	1:B:261:ASP:OD1[4_535]	1.73	0.47
1:B:5(N):GLN:OE1	1:B:261:ASP:OD2[4_535]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5(N):GLN:CB	1:B:264:ASN:OD1[4_535]	1.73	0.47
1:B:7:LEU:CD2	1:B:203:TYR:N[4_535]	1.74	0.46
1:B:7:LEU:CD1	1:B:203:TYR:CB[4_535]	1.79	0.41
1:B:6:PRO:CB	1:B:394:HIS:NE2[4_535]	1.84	0.36
1:B:3:THR:OG1	1:B:271:ARG:NH1[4_535]	1.89	0.31
1:B:5(N):GLN:CD	1:B:261:ASP:CG[4_535]	1.89	0.31
1:B:7:LEU:CB	1:B:203:TYR:CB[4_535]	1.99	0.21
1:B:7:LEU:CG	1:B:203:TYR:CA[4_535]	1.99	0.21
1:B:7:LEU:CG	1:B:203:TYR:C[4_535]	2.04	0.16
1:B:7:LEU:CD2	1:B:204:GLY:N[4_535]	2.08	0.12
1:A:436:PRO:CG	1:B:363:GLU:OE1[4_435]	2.12	0.08
1:B:7:LEU:N	1:B:394:HIS:CE1[4_535]	2.13	0.07
1:B:6:PRO:CA	1:B:394:HIS:ND1[4_535]	2.14	0.06
1:B:5(N):GLN:CA	1:B:264:ASN:OD1[4_535]	2.14	0.06
1:B:6:PRO:CB	1:B:394:HIS:CG[4_535]	2.17	0.03
1:B:3:THR:CB	1:B:271:ARG:CZ[4_535]	2.19	0.01

## 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	850/879 (97%)	802 (94%)	43 (5%)	5 (1%)	25	56
1	B	850/879 (97%)	800 (94%)	43 (5%)	7 (1%)	19	49
All	All	1700/1758 (97%)	1602 (94%)	86 (5%)	12 (1%)	22	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	VAL
1	A	528	LYS
1	A	750	PHE
1	B	422	VAL

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Mol	Chain	Res	Type
1	B	528	LYS
1	B	750	PHE
1	A	208	ARG
1	A	731	HIS
1	B	208	ARG
1	B	731	HIS
1	B	282	ASN
1	B	214(C)	THR

### 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	697/781 (89%)	634 (91%)	63 (9%)	9	28
1	B	697/781 (89%)	635 (91%)	62 (9%)	9	28
All	All	1394/1562 (89%)	1269 (91%)	125 (9%)	9	28

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	14	ASN
1	A	37	THR
1	A	53	GLU
1	A	71	GLN
1	A	78	ASP
1	A	90	LEU
1	A	95	LEU
1	A	113(G)	ARG
1	A	123	LEU
1	A	124	ASP
1	A	128	ASP
1	A	184	ASN
1	A	235	THR
1	A	249	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	254	LEU
1	A	268	GLN
1	A	278	VAL
1	A	284	ASN
1	A	290	GLU
1	A	304	LEU
1	A	327	THR
1	A	357	GLU
1	A	366	ASP
1	A	391	LEU
1	A	395	LEU
1	A	400	LEU
1	A	411	LEU
1	A	424	LEU
1	A	477	SER
1	A	498	SER
1	A	505	GLU
1	A	508	ASN
1	A	508(E)	THR
1	A	513	LEU
1	A	527	ASP
1	A	531	LEU
1	A	533	LYS
1	A	548	LEU
1	A	553	ASN
1	A	558(D)	ASN
1	A	565	MET
1	A	569	ARG
1	A	573	TYR
1	A	578	LEU
1	A	588	LEU
1	A	592(E)	LYS
1	A	592(F)	ASN
1	A	613	TYR
1	A	622	LEU
1	A	635	SER
1	A	662	LEU
1	A	691	THR
1	A	717	ASN
1	A	722	ARG
1	A	746	GLU
1	A	753	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	756	ASN
1	A	774	SER
1	A	784	HIS
1	A	798	LEU
1	A	805	LEU
1	A	827	VAL
1	B	7	LEU
1	B	14	ASN
1	B	37	THR
1	B	53	GLU
1	B	71	GLN
1	B	78	ASP
1	B	90	LEU
1	B	95	LEU
1	B	113(F)	PRO
1	B	113(G)	ARG
1	B	123	LEU
1	B	124	ASP
1	B	128	ASP
1	B	184	ASN
1	B	235	THR
1	B	249	THR
1	B	254	LEU
1	B	268	GLN
1	B	278	VAL
1	B	284	ASN
1	B	290	GLU
1	B	304	LEU
1	B	357	GLU
1	B	366	ASP
1	B	391	LEU
1	B	395	LEU
1	B	400	LEU
1	B	411	LEU
1	B	424	LEU
1	B	477	SER
1	B	498	SER
1	B	505	GLU
1	B	508	ASN
1	B	508(E)	THR
1	B	513	LEU
1	B	527	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	531	LEU
1	B	533	LYS
1	B	548	LEU
1	B	553	ASN
1	B	558(D)	ASN
1	B	565	MET
1	B	569	ARG
1	B	573	TYR
1	B	578	LEU
1	B	588	LEU
1	B	592(E)	LYS
1	B	592(F)	ASN
1	B	613	TYR
1	B	622	LEU
1	B	635	SER
1	B	662	LEU
1	B	691	THR
1	B	717	ASN
1	B	722	ARG
1	B	746	GLU
1	B	756	ASN
1	B	774	SER
1	B	784	HIS
1	B	798	LEU
1	B	805	LEU
1	B	827	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	14	ASN
1	A	16	HIS
1	A	175	GLN
1	A	237	ASN
1	A	239	ASN
1	A	240	ASN
1	A	245	GLN
1	A	399	HIS
1	A	459	HIS
1	A	481	ASN
1	A	494	GLN
1	A	592(F)	ASN

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Mol	Chain	Res	Type
1	A	713	ASN
1	A	784	HIS
1	B	14	ASN
1	B	68	ASN
1	B	237	ASN
1	B	239	ASN
1	B	240	ASN
1	B	245	GLN
1	B	258	ASN
1	B	399	HIS
1	B	459	HIS
1	B	481	ASN
1	B	494	GLN
1	B	558(D)	ASN
1	B	592(F)	ASN
1	B	713	ASN
1	B	784	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

6 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	PO4	A	859	-	4,4,4	1.87	2 (50%)	6,6,6	0.49	0
3	PLP	A	860	1	15,15,16	1.79	1 (6%)	20,22,23	1.29	3 (15%)
3	PLP	B	860	1	15,15,16	2.01	2 (13%)	20,22,23	1.35	3 (15%)
2	PO4	B	859	-	4,4,4	2.61	4 (100%)	6,6,6	0.47	0
2	PO4	A	1900	-	4,4,4	1.64	0	6,6,6	0.24	0
2	PO4	B	1900	-	4,4,4	2.37	4 (100%)	6,6,6	0.62	0

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
3	PLP	A	860	1	-	4/6/6/8	0/1/1/1
3	PLP	B	860	1	-	4/6/6/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	860	PLP	C4A-C4	-6.26	1.38	1.51
3	A	860	PLP	C4A-C4	-5.51	1.40	1.51
2	B	1900	PO4	P-O2	-3.01	1.45	1.54
2	B	859	PO4	P-O4	-2.86	1.46	1.54
2	B	859	PO4	P-O2	-2.85	1.46	1.54
2	B	859	PO4	P-O3	-2.37	1.47	1.54
2	B	859	PO4	P-O1	-2.33	1.45	1.50
2	B	1900	PO4	P-O3	-2.30	1.47	1.54
3	B	860	PLP	C3-C2	-2.23	1.38	1.40
2	A	859	PO4	P-O2	-2.22	1.47	1.54
2	A	859	PO4	P-O4	-2.19	1.48	1.54
2	B	1900	PO4	P-O4	-2.03	1.48	1.54
2	B	1900	PO4	P-O1	-2.00	1.46	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	860	PLP	O3P-P-O1P	3.36	123.84	110.68
3	B	860	PLP	O3P-P-O1P	3.28	123.51	110.68
3	A	860	PLP	C6-C5-C4	2.62	120.22	118.16
3	B	860	PLP	C6-C5-C4	2.57	120.18	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	860	PLP	O2P-P-O4P	-2.42	100.29	106.73
3	A	860	PLP	C4A-C4-C5	-2.03	118.85	120.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C5A-O4P-P-O2P
3	A	860	PLP	C5A-O4P-P-O3P
3	B	860	PLP	C5A-O4P-P-O2P
3	B	860	PLP	C5A-O4P-P-O3P
3	B	860	PLP	C4-C5-C5A-O4P
3	A	860	PLP	C6-C5-C5A-O4P
3	B	860	PLP	C6-C5-C5A-O4P
3	A	860	PLP	C4-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	860	PLP	2	0

## 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.