



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1K8Y  
Title : CRYSTAL STRUCTURE OF THE TRYPTOPHAN SYNTHASE BETA-SER178PRO MUTANT COMPLEXED WITH D,L-ALPHA-GLYCEROL-3-PHOSPHATE  
Authors : Weyand, M.; Schlichting, I.; Marabotti, A.; Mozzarelli, A.  
Deposited on : 2001-10-26  
Resolution : 1.50 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

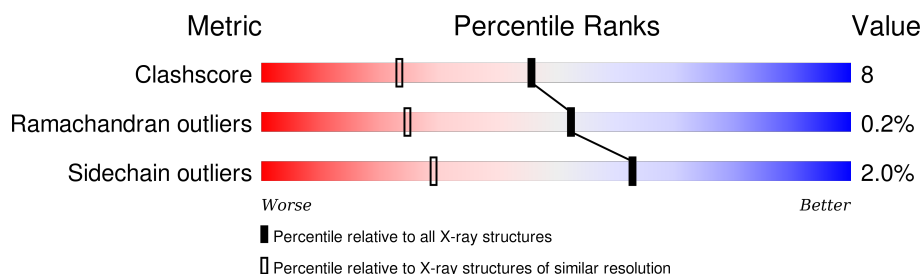
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

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	268	
2	B	396	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5617 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	6	0
			1947	1237	335	367	8			

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total	C	N	O	S	0	9	0
			2986	1873	527	566	20			

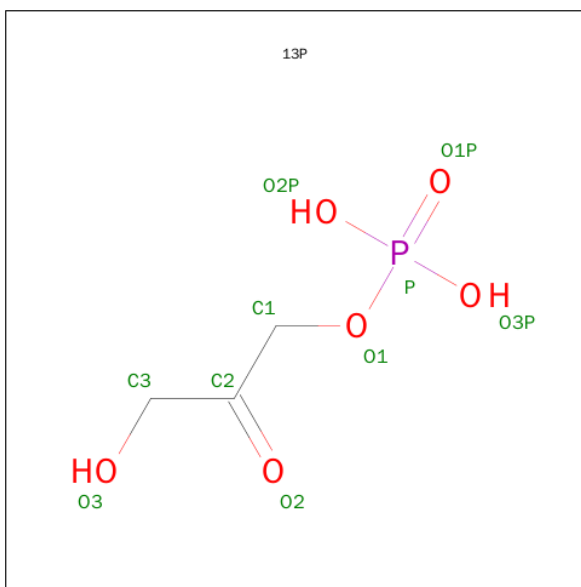
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	CLONING ARTIFACT	UNP P0A2K1
B	178	PRO	SER	ENGINEERED	UNP P0A2K1

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

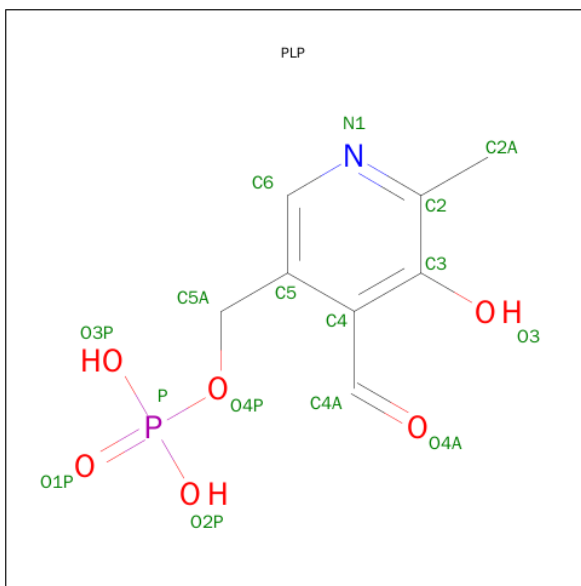
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		

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



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

- Molecule 6 is water.

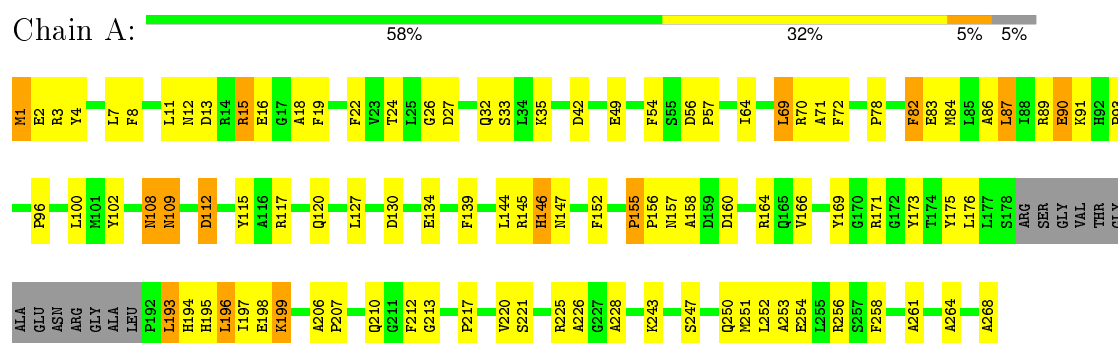
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	214	Total 214	O 214	0	0
6	B	444	Total 444	O 444	0	0

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

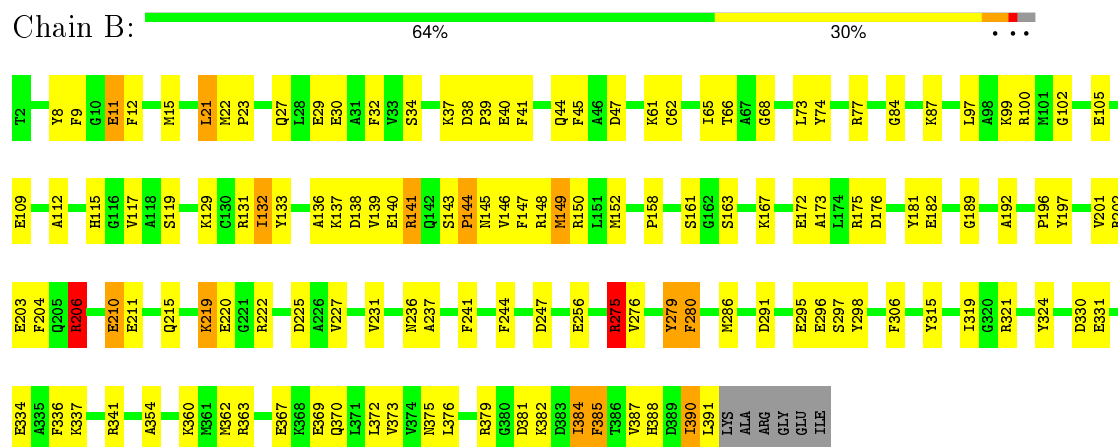
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: TRYPTOPHAN SYNTHASE ALPHA CHAIN



#### • Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.14Å 60.47Å 67.44Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50	Depositor
% Data completeness (in resolution range)	95.1 (20.00-1.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.171 , 0.209	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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: NA, 13P, 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	2.18	72/2014 (3.6%)	2.08	68/2733 (2.5%)
2	B	2.20	95/3100 (3.1%)	2.04	102/4185 (2.4%)
All	All	2.19	167/5114 (3.3%)	2.06	170/6918 (2.5%)

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	PHE	CD1-CE1	19.52	1.78	1.39
2	B	45	PHE	CG-CD1	16.51	1.63	1.38
1	A	169	TYR	CD1-CE1	15.63	1.62	1.39
2	B	319	ILE	C-O	15.55	1.52	1.23
2	B	149	MET	CG-SD	13.30	2.15	1.81
2	B	367[A]	GLU	CG-CD	-12.75	1.32	1.51
2	B	367[B]	GLU	CG-CD	-12.75	1.32	1.51
2	B	11	GLU	CD-OE2	12.35	1.39	1.25
2	B	385	PHE	CB-CG	-11.53	1.31	1.51
1	A	82	PHE	CE2-CZ	11.17	1.58	1.37
2	B	331	GLU	CD-OE2	10.99	1.37	1.25
2	B	385	PHE	CA-CB	-9.31	1.33	1.53
2	B	100	ARG	CZ-NH1	-8.86	1.21	1.33
2	B	360	LYS	CB-CG	-8.67	1.29	1.52
1	A	225	ARG	NE-CZ	8.52	1.44	1.33
1	A	89	ARG	CZ-NH2	8.35	1.43	1.33
2	B	210	GLU	CD-OE2	8.28	1.34	1.25
1	A	169	TYR	CG-CD1	-8.26	1.28	1.39
2	B	45	PHE	CE1-CZ	8.02	1.52	1.37
2	B	341	ARG	CZ-NH1	8.02	1.43	1.33
1	A	169	TYR	CE1-CZ	-7.97	1.28	1.38
2	B	41	PHE	CD1-CE1	7.87	1.54	1.39
2	B	29	GLU	CD-OE1	7.63	1.34	1.25
1	A	2	GLU	CD-OE1	7.44	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	388	HIS	CA-C	-7.29	1.33	1.52
1	A	83	GLU	CG-CD	7.29	1.62	1.51
2	B	173	ALA	CA-CB	7.25	1.67	1.52
2	B	41	PHE	CB-CG	7.25	1.63	1.51
1	A	8	PHE	CE1-CZ	7.24	1.51	1.37
2	B	39	PRO	C-O	7.21	1.37	1.23
2	B	152	MET	SD-CE	-7.16	1.37	1.77
2	B	139	VAL	CB-CG2	7.00	1.67	1.52
2	B	62	CYS	CB-SG	7.00	1.94	1.82
1	A	108	ASN	CG-ND2	-6.84	1.15	1.32
2	B	140	GLU	CD-OE1	6.84	1.33	1.25
1	A	109	ASN	CG-OD1	6.76	1.38	1.24
2	B	45	PHE	CD1-CE1	-6.76	1.25	1.39
1	A	173	TYR	CG-CD2	-6.76	1.30	1.39
2	B	141	ARG	C-O	6.73	1.36	1.23
2	B	167	LYS	CE-NZ	6.62	1.65	1.49
2	B	219[A]	LYS	CE-NZ	6.61	1.65	1.49
2	B	219[B]	LYS	CE-NZ	6.61	1.65	1.49
2	B	219[C]	LYS	CE-NZ	6.61	1.65	1.49
1	A	145	ARG	CZ-NH2	6.58	1.41	1.33
1	A	16	GLU	CB-CG	-6.56	1.39	1.52
2	B	41	PHE	C-O	6.55	1.35	1.23
1	A	220	VAL	CB-CG1	-6.54	1.39	1.52
2	B	237	ALA	CA-CB	6.50	1.66	1.52
2	B	143	SER	CA-CB	6.48	1.62	1.52
2	B	11	GLU	CG-CD	6.44	1.61	1.51
2	B	21	LEU	C-O	6.43	1.35	1.23
1	A	120	GLN	CG-CD	6.42	1.65	1.51
2	B	370	GLN	CG-CD	6.42	1.65	1.51
2	B	102	GLY	CA-C	-6.39	1.41	1.51
2	B	360	LYS	CE-NZ	6.36	1.65	1.49
1	A	173	TYR	CE2-CZ	-6.31	1.30	1.38
1	A	87	LEU	CG-CD1	6.26	1.75	1.51
1	A	120	GLN	CD-OE1	6.19	1.37	1.24
2	B	298	TYR	CE1-CZ	6.17	1.46	1.38
2	B	375	ASN	CG-OD1	6.17	1.37	1.24
2	B	306	PHE	CD1-CE1	6.14	1.51	1.39
2	B	105	GLU	CD-OE2	6.13	1.32	1.25
2	B	145	ASN	C-O	6.11	1.34	1.23
2	B	141	ARG	CZ-NH1	6.10	1.41	1.33
1	A	117	ARG	CG-CD	6.09	1.67	1.51
2	B	172	GLU	CD-OE2	6.09	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ALA	CA-CB	6.06	1.65	1.52
1	A	82	PHE	CE1-CZ	-6.03	1.25	1.37
2	B	341	ARG	CZ-NH2	6.02	1.40	1.33
1	A	134	GLU	CD-OE2	6.02	1.32	1.25
2	B	27	GLN	CB-CG	6.01	1.68	1.52
2	B	158	PRO	C-O	5.98	1.35	1.23
2	B	138	ASP	C-O	5.96	1.34	1.23
1	A	251	MET	C-O	5.87	1.34	1.23
2	B	8	TYR	CG-CD1	5.86	1.46	1.39
2	B	334	GLU	CD-OE2	5.86	1.32	1.25
2	B	181	TYR	CD1-CE1	5.85	1.48	1.39
1	A	84	MET	SD-CE	-5.83	1.45	1.77
1	A	115	TYR	CE2-CZ	-5.82	1.30	1.38
2	B	136	ALA	CA-CB	5.82	1.64	1.52
1	A	139	PHE	CE2-CZ	5.81	1.48	1.37
2	B	379[A]	ARG	CG-CD	5.74	1.66	1.51
2	B	379[B]	ARG	CG-CD	5.74	1.66	1.51
1	A	144	LEU	C-O	5.74	1.34	1.23
2	B	140	GLU	C-O	5.72	1.34	1.23
1	A	32	GLN	CG-CD	5.71	1.64	1.51
2	B	22	MET	SD-CE	-5.69	1.46	1.77
2	B	161	SER	CB-OG	5.67	1.49	1.42
2	B	295	GLU	CG-CD	5.66	1.60	1.51
2	B	37	LYS	C-O	5.63	1.34	1.23
2	B	375	ASN	CG-ND2	-5.61	1.18	1.32
1	A	12	ASN	CB-CG	5.61	1.64	1.51
1	A	258	PHE	CB-CG	-5.60	1.41	1.51
2	B	354	ALA	CA-CB	5.59	1.64	1.52
2	B	32	PHE	CG-CD1	5.59	1.47	1.38
2	B	68	GLY	C-O	5.59	1.32	1.23
1	A	4	TYR	CB-CG	-5.55	1.43	1.51
1	A	54	PHE	CD1-CE1	5.55	1.50	1.39
1	A	96	PRO	C-O	5.55	1.34	1.23
1	A	15	ARG	CA-CB	5.54	1.66	1.53
1	A	247	SER	CB-OG	5.53	1.49	1.42
2	B	336	PHE	CD1-CE1	5.48	1.50	1.39
2	B	387	VAL	CB-CG2	5.48	1.64	1.52
2	B	296	GLU	CD-OE2	-5.46	1.19	1.25
1	A	72	PHE	CD1-CE1	5.46	1.50	1.39
1	A	261	ALA	C-O	5.45	1.33	1.23
1	A	93	PRO	CG-CD	5.45	1.68	1.50
1	A	146	HIS	C-O	5.43	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	ASP	CB-CG	5.43	1.63	1.51
1	A	1	MET	CA-CB	5.41	1.65	1.53
2	B	220	GLU	CD-OE1	5.40	1.31	1.25
1	A	24	THR	C-O	5.40	1.33	1.23
1	A	16	GLU	CD-OE1	5.38	1.31	1.25
2	B	286	MET	CA-CB	5.38	1.65	1.53
2	B	369	GLU	CG-CD	5.36	1.59	1.51
1	A	117	ARG	CD-NE	5.35	1.55	1.46
2	B	286	MET	CB-CG	5.35	1.68	1.51
1	A	83	GLU	CD-OE1	5.33	1.31	1.25
2	B	315	TYR	CD1-CE1	5.33	1.47	1.39
2	B	133	TYR	CE2-CZ	5.33	1.45	1.38
1	A	4	TYR	CD1-CE1	5.32	1.47	1.39
2	B	211	GLU	CD-OE2	5.31	1.31	1.25
2	B	30	GLU	C-O	5.30	1.33	1.23
2	B	192	ALA	CA-CB	5.28	1.63	1.52
2	B	275	ARG	N-CA	5.26	1.56	1.46
1	A	175	TYR	CD2-CE2	-5.26	1.31	1.39
1	A	199	LYS	C-O	5.24	1.33	1.23
1	A	228	ALA	C-O	5.24	1.33	1.23
2	B	29	GLU	CG-CD	-5.24	1.44	1.51
1	A	225	ARG	CG-CD	5.23	1.65	1.51
1	A	243	LYS	CD-CE	5.23	1.64	1.51
1	A	207	PRO	CA-CB	5.22	1.64	1.53
2	B	219[A]	LYS	CD-CE	5.21	1.64	1.51
2	B	219[B]	LYS	CD-CE	5.21	1.64	1.51
2	B	219[C]	LYS	CD-CE	5.21	1.64	1.51
2	B	109	GLU	CA-CB	5.20	1.65	1.53
1	A	78	PRO	C-O	5.20	1.33	1.23
2	B	362	MET	SD-CE	-5.20	1.48	1.77
1	A	15	ARG	CG-CD	5.20	1.65	1.51
2	B	147	PHE	CD2-CE2	5.19	1.49	1.39
1	A	217	PRO	C-O	5.18	1.33	1.23
1	A	173	TYR	CD2-CE2	-5.18	1.31	1.39
1	A	26	GLY	CA-C	-5.18	1.43	1.51
1	A	18	ALA	CA-CB	5.16	1.63	1.52
1	A	115	TYR	CE1-CZ	5.16	1.45	1.38
2	B	32	PHE	CE2-CZ	5.15	1.47	1.37
1	A	120	GLN	N-CA	5.15	1.56	1.46
2	B	231	VAL	CB-CG2	-5.14	1.42	1.52
1	A	16	GLU	CG-CD	5.13	1.59	1.51
1	A	71	ALA	CA-CB	5.13	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	99	LYS	C-O	5.12	1.33	1.23
2	B	379[A]	ARG	CZ-NH1	-5.12	1.26	1.33
2	B	379[B]	ARG	CZ-NH1	-5.12	1.26	1.33
1	A	210	GLN	CG-CD	-5.11	1.39	1.51
1	A	226	ALA	CA-CB	-5.11	1.41	1.52
1	A	206	ALA	CA-CB	5.08	1.63	1.52
2	B	37	LYS	CG-CD	5.08	1.69	1.52
2	B	119	SER	CA-CB	5.06	1.60	1.52
1	A	109	ASN	N-CA	-5.06	1.36	1.46
1	A	70	ARG	CZ-NH1	5.05	1.39	1.33
1	A	93	PRO	N-CD	5.05	1.54	1.47
2	B	382	LYS	CD-CE	5.04	1.63	1.51
1	A	213	GLY	CA-C	5.02	1.59	1.51
2	B	244	PHE	CG-CD1	5.02	1.46	1.38
1	A	91	LYS	CE-NZ	5.02	1.61	1.49
2	B	373	VAL	CB-CG2	-5.02	1.42	1.52
2	B	256	GLU	CG-CD	5.01	1.59	1.51

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH2	-27.61	106.50	120.30
1	A	70	ARG	NE-CZ-NH1	19.32	129.96	120.30
1	A	3	ARG	NE-CZ-NH1	18.64	129.62	120.30
2	B	131	ARG	NE-CZ-NH1	18.55	129.57	120.30
2	B	321	ARG	NE-CZ-NH2	-16.97	111.82	120.30
2	B	47	ASP	CB-CG-OD2	12.81	129.82	118.30
2	B	330	ASP	CB-CG-OD1	12.57	129.61	118.30
1	A	82	PHE	CB-CG-CD1	-12.55	112.02	120.80
2	B	385	PHE	CB-CA-C	-12.05	86.30	110.40
2	B	141	ARG	NE-CZ-NH2	-11.53	114.53	120.30
2	B	41	PHE	CB-CG-CD1	-11.22	112.94	120.80
2	B	286	MET	CA-CB-CG	11.18	132.31	113.30
2	B	363	ARG	NE-CZ-NH1	11.12	125.86	120.30
2	B	321	ARG	NE-CZ-NH1	10.14	125.37	120.30
2	B	77	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	196	LEU	CB-CG-CD1	9.87	127.78	111.00
1	A	176	LEU	CB-CG-CD2	-9.53	94.79	111.00
2	B	315	TYR	CB-CG-CD1	-9.29	115.43	121.00
2	B	241	PHE	CB-CG-CD2	-9.24	114.33	120.80
2	B	148	ARG	NE-CZ-NH2	-9.24	115.68	120.30
2	B	381	ASP	CB-CG-OD1	9.10	126.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ARG	NE-CZ-NH2	-9.06	115.77	120.30
2	B	291[A]	ASP	CB-CG-OD1	-8.65	110.51	118.30
2	B	291[B]	ASP	CB-CG-OD1	-8.65	110.51	118.30
2	B	77	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	A	256	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	155	PRO	N-CD-CG	-8.56	90.36	103.20
1	A	164	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	225	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	93	PRO	N-CD-CG	-8.32	90.72	103.20
1	A	252	LEU	CB-CG-CD2	-8.31	96.88	111.00
2	B	133	TYR	CB-CG-CD1	-8.25	116.05	121.00
1	A	175	TYR	CB-CG-CD1	-8.22	116.06	121.00
2	B	286	MET	CG-SD-CE	-8.18	87.12	100.20
1	A	89	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	171	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	160	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	145	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	B	152	MET	CG-SD-CE	-7.72	87.85	100.20
2	B	133	TYR	CZ-CE2-CD2	-7.69	112.88	119.80
1	A	82	PHE	CD1-CE1-CZ	-7.67	110.89	120.10
2	B	298	TYR	CD1-CE1-CZ	-7.67	112.90	119.80
1	A	70	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	56	ASP	CB-CG-OD1	7.57	125.12	118.30
2	B	367[A]	GLU	OE1-CD-OE2	-7.38	114.45	123.30
2	B	367[B]	GLU	OE1-CD-OE2	-7.38	114.45	123.30
2	B	331	GLU	OE1-CD-OE2	-7.31	114.53	123.30
1	A	35	LYS	CD-CE-NZ	7.29	128.46	111.70
2	B	12	PHE	CG-CD1-CE1	-7.20	112.88	120.80
2	B	150	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	152	PHE	CB-CG-CD1	-7.14	115.80	120.80
1	A	164	ARG	NE-CZ-NH2	-7.13	116.73	120.30
2	B	203	GLU	OE1-CD-OE2	-7.12	114.75	123.30
2	B	158	PRO	N-CD-CG	-7.11	92.53	103.20
2	B	45	PHE	CD1-CE1-CZ	7.10	128.62	120.10
2	B	144	PRO	N-CD-CG	-7.10	92.56	103.20
2	B	298	TYR	CA-CB-CG	-7.09	99.92	113.40
2	B	279	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	A	109	ASN	N-CA-CB	-6.89	98.20	110.60
1	A	19	PHE	CB-CG-CD1	-6.88	115.98	120.80
2	B	146	VAL	CG1-CB-CG2	-6.88	99.90	110.90
2	B	131	ARG	NH1-CZ-NH2	-6.87	111.84	119.40
2	B	225	ASP	CB-CG-OD2	6.86	124.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	LEU	CB-CG-CD2	6.82	122.60	111.00
1	A	87	LEU	CB-CG-CD1	6.74	122.47	111.00
2	B	390	ILE	CG1-CB-CG2	6.59	125.90	111.40
2	B	222[A]	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	B	222[B]	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	69	LEU	CB-CG-CD1	-6.54	99.88	111.00
2	B	227	VAL	CA-CB-CG2	6.54	120.71	110.90
2	B	363	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	221	SER	O-C-N	6.40	132.94	122.70
2	B	197	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	A	42	ASP	CB-CG-OD2	-6.33	112.61	118.30
2	B	280	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	A	134	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	A	4	TYR	CZ-CE2-CD2	6.26	125.43	119.80
2	B	376	LEU	CB-CG-CD2	-6.20	100.46	111.00
2	B	206[A]	ARG	NE-CZ-NH1	-6.18	117.21	120.30
2	B	206[B]	ARG	NE-CZ-NH1	-6.18	117.21	120.30
2	B	175	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	145	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	B	385	PHE	CB-CG-CD1	-6.15	116.50	120.80
2	B	202	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	B	47	ASP	OD1-CG-OD2	-6.10	111.72	123.30
2	B	9	PHE	CB-CG-CD1	-6.09	116.54	120.80
2	B	241	PHE	CG-CD2-CE2	-6.07	114.12	120.80
2	B	8	TYR	CZ-CE2-CD2	6.07	125.26	119.80
2	B	275	ARG	NE-CZ-NH2	6.06	123.33	120.30
2	B	379[A]	ARG	CG-CD-NE	-6.05	99.08	111.80
2	B	379[B]	ARG	CG-CD-NE	-6.05	99.08	111.80
1	A	196	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	93	PRO	O-C-N	-6.04	113.03	122.70
2	B	372	LEU	CB-CG-CD1	-6.01	100.78	111.00
2	B	379[A]	ARG	NE-CZ-NH1	-5.99	117.31	120.30
2	B	379[B]	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	A	127	LEU	CB-CG-CD1	-5.98	100.83	111.00
1	A	112	ASP	CB-CG-OD1	5.95	123.66	118.30
2	B	34	SER	N-CA-CB	-5.94	101.59	110.50
2	B	84	GLY	CA-C-O	-5.84	110.09	120.60
1	A	213	GLY	CA-C-O	-5.84	110.09	120.60
2	B	315	TYR	CG-CD1-CE1	-5.83	116.64	121.30
1	A	160	ASP	OD1-CG-OD2	-5.81	112.27	123.30
2	B	133	TYR	CG-CD1-CE1	-5.80	116.66	121.30
1	A	1	MET	N-CA-C	-5.79	95.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	CYS	CA-CB-SG	-5.78	103.59	114.00
1	A	166	VAL	CA-CB-CG1	5.77	119.55	110.90
2	B	176	ASP	N-CA-CB	-5.76	100.22	110.60
2	B	74	TYR	CB-CG-CD1	5.73	124.44	121.00
2	B	279	TYR	CB-CG-CD1	5.72	124.43	121.00
1	A	82	PHE	CD1-CG-CD2	5.72	125.74	118.30
1	A	82	PHE	CE1-CZ-CE2	5.72	130.30	120.00
1	A	82	PHE	CZ-CE2-CD2	-5.71	113.25	120.10
2	B	204	PHE	CB-CG-CD2	-5.71	116.81	120.80
1	A	64	ILE	CA-CB-CG1	-5.69	100.18	111.00
2	B	73	LEU	CB-CG-CD2	-5.66	101.38	111.00
2	B	247	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	173	TYR	CG-CD2-CE2	5.65	125.82	121.30
1	A	16	GLU	OE1-CD-OE2	-5.64	116.53	123.30
2	B	315	TYR	CZ-CE2-CD2	-5.64	114.72	119.80
2	B	331	GLU	CG-CD-OE1	5.64	129.58	118.30
2	B	74	TYR	CB-CG-CD2	-5.60	117.64	121.00
2	B	15	MET	CA-CB-CG	-5.60	103.79	113.30
1	A	70	ARG	NH1-CZ-NH2	-5.55	113.29	119.40
2	B	87	LYS	CB-CG-CD	-5.55	97.17	111.60
2	B	141	ARG	N-CA-CB	5.53	120.55	110.60
2	B	39	PRO	N-CD-CG	-5.50	94.95	103.20
2	B	129	LYS	N-CA-CB	-5.43	100.82	110.60
2	B	275	ARG	NE-CZ-NH1	-5.43	117.58	120.30
2	B	100	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	B	45	PHE	CG-CD1-CE1	-5.42	114.84	120.80
1	A	91	LYS	CD-CE-NZ	-5.41	99.25	111.70
2	B	390	ILE	CB-CA-C	-5.41	100.77	111.60
2	B	143	SER	CB-CA-C	5.38	120.33	110.10
1	A	8	PHE	CZ-CE2-CD2	5.37	126.55	120.10
2	B	201	VAL	O-C-N	-5.36	114.12	122.70
2	B	330	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	253	ALA	N-CA-CB	-5.36	102.59	110.10
2	B	298	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	A	33	SER	O-C-N	5.32	131.20	122.70
2	B	384	ILE	C-N-CA	-5.31	108.42	121.70
1	A	247	SER	N-CA-CB	5.27	118.41	110.50
2	B	315	TYR	CD1-CG-CD2	5.27	123.70	117.90
2	B	12	PHE	CB-CG-CD1	-5.26	117.12	120.80
2	B	132	ILE	O-C-N	5.25	131.10	122.70
2	B	40	GLU	N-CA-CB	5.23	120.01	110.60
1	A	193	LEU	CB-CA-C	5.22	120.11	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LEU	CB-CG-CD1	5.21	119.87	111.00
2	B	66	THR	O-C-N	-5.21	114.36	122.70
1	A	130	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	18	ALA	N-CA-CB	-5.15	102.89	110.10
2	B	324	TYR	CB-CG-CD1	-5.14	117.91	121.00
2	B	203	GLU	CG-CD-OE1	5.13	128.56	118.30
1	A	127	LEU	CB-CG-CD2	5.12	119.71	111.00
1	A	27	ASP	CB-CG-OD1	-5.12	113.69	118.30
2	B	117	VAL	O-C-N	-5.12	114.52	122.70
1	A	251	MET	CG-SD-CE	5.11	108.38	100.20
1	A	83	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	A	147	ASN	CB-CG-OD1	-5.08	111.44	121.60
2	B	41	PHE	CG-CD1-CE1	-5.07	115.22	120.80
2	B	37	LYS	CB-CG-CD	-5.07	98.41	111.60
2	B	381	ASP	OD1-CG-OD2	-5.05	113.69	123.30
1	A	93	PRO	CA-C-N	5.05	128.30	117.20
2	B	8	TYR	CB-CG-CD2	5.04	124.03	121.00
1	A	175	TYR	CD1-CE1-CZ	-5.03	115.27	119.80
1	A	8	PHE	CG-CD1-CE1	5.03	126.33	120.80
2	B	276	VAL	CG1-CB-CG2	-5.02	102.87	110.90
1	A	90[A]	GLU	CA-C-N	5.01	128.23	117.20
1	A	90[B]	GLU	CA-C-N	5.01	128.23	117.20
1	A	11	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	1947	0	1955	41	0
2	B	2986	0	2959	38	0
3	B	1	0	0	0	0
4	A	10	0	5	0	0
5	B	15	0	7	0	0
6	A	214	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	444	0	0	5	0
All	All	5617	0	4926	76	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 8.

All (76) 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:82:PHE:CE1	1:A:82:PHE:CD1	1.78	1.65
1:A:87:LEU:CD1	1:A:87:LEU:CG	1.75	1.63
2:B:149:MET:SD	2:B:149:MET:CG	2.15	1.34
1:A:49[B]:GLU:OE2	1:A:100[B]:LEU:CD2	1.89	1.17
2:B:337:LYS:HE2	2:B:391:LEU:HD11	1.31	1.12
1:A:49[B]:GLU:OE2	1:A:100[B]:LEU:HD21	0.94	1.08
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:HD11	1.79	1.02
2:B:337:LYS:CE	2:B:391:LEU:HD11	1.92	0.99
1:A:82:PHE:CD1	1:A:82:PHE:CZ	2.52	0.96
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:HD21	1.92	0.89
2:B:337:LYS:CE	2:B:391:LEU:CD1	2.51	0.88
1:A:108:ASN:HD21	2:B:275:ARG:HH22	1.18	0.87
2:B:337:LYS:HZ1	2:B:391:LEU:HD13	1.38	0.87
2:B:337:LYS:HE3	2:B:391:LEU:HD21	1.57	0.86
1:A:254[B]:GLU:HG3	6:A:909:HOH:O	1.74	0.86
2:B:337:LYS:NZ	2:B:391:LEU:HD13	1.91	0.86
2:B:337:LYS:HE2	2:B:391:LEU:CD1	2.05	0.85
1:A:100[A]:LEU:HG	6:A:914:HOH:O	1.77	0.84
2:B:206[A]:ARG:HD3	2:B:210:GLU:OE2	1.81	0.80
1:A:49[A]:GLU:OE2	6:A:913:HOH:O	2.01	0.77
1:A:49[B]:GLU:OE1	1:A:100[B]:LEU:HD11	1.82	0.77
1:A:194:HIS:O	1:A:198:GLU:HG2	1.85	0.77
2:B:141:ARG:HD2	6:B:1028:HOH:O	1.84	0.77
1:A:108:ASN:OD1	1:A:109:ASN:ND2	2.19	0.76
2:B:337:LYS:HZ1	2:B:391:LEU:HD22	1.48	0.75
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:CD1	2.56	0.74
1:A:87:LEU:CD1	1:A:87:LEU:CD2	2.65	0.73
1:A:87:LEU:CD1	1:A:87:LEU:HG	2.12	0.71
2:B:337:LYS:HZ1	2:B:391:LEU:CD1	2.04	0.70
2:B:337:LYS:NZ	2:B:391:LEU:HD22	2.08	0.69
2:B:337:LYS:NZ	2:B:391:LEU:CD1	2.56	0.68
1:A:108:ASN:HD21	2:B:275:ARG:NH2	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49[B]:GLU:HG2	1:A:100[B]:LEU:HG	1.80	0.64
2:B:337:LYS:HZ1	2:B:391:LEU:CD2	2.12	0.63
2:B:149:MET:CB	2:B:149:MET:SD	2.86	0.63
1:A:195:HIS:CE1	1:A:199:LYS:HE2	2.34	0.63
2:B:337:LYS:HE3	2:B:391:LEU:CD2	2.28	0.62
1:A:108:ASN:ND2	2:B:275:ARG:HH22	1.95	0.61
2:B:390:ILE:HG22	2:B:391:LEU:N	2.14	0.60
2:B:215:GLN:O	2:B:219[C]:LYS:HD2	2.02	0.59
2:B:44:GLN:HG3	6:B:969:HOH:O	2.05	0.56
2:B:132:ILE:HD13	2:B:149:MET:SD	2.46	0.56
1:A:22:PHE:CD2	1:A:100[B]:LEU:HD12	2.42	0.55
2:B:206[A]:ARG:CD	2:B:210:GLU:OE2	2.52	0.55
2:B:337:LYS:NZ	2:B:391:LEU:CD2	2.69	0.54
2:B:337:LYS:CE	2:B:391:LEU:CD2	2.88	0.51
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.94	0.51
1:A:49[B]:GLU:OE2	1:A:100[B]:LEU:HD11	2.09	0.50
1:A:195:HIS:HE1	1:A:199:LYS:HE2	1.77	0.50
1:A:157:ASN:O	1:A:158:ALA:C	2.49	0.50
2:B:137:LYS:HE3	2:B:163:SER:O	2.12	0.49
1:A:1:MET:N	6:A:880:HOH:O	2.46	0.48
2:B:279:TYR:CG	2:B:280:PHE:N	2.82	0.48
2:B:38:ASP:OD1	2:B:38:ASP:C	2.53	0.47
1:A:100[A]:LEU:HD21	6:A:846:HOH:O	2.15	0.46
1:A:250:GLN:NE2	1:A:254[A]:GLU:OE2	2.39	0.46
1:A:254[B]:GLU:CG	6:A:909:HOH:O	2.50	0.46
2:B:61:LYS:HE2	6:B:1006:HOH:O	2.16	0.46
1:A:49[B]:GLU:CD	1:A:100[B]:LEU:CG	2.84	0.46
1:A:195:HIS:CE1	1:A:199:LYS:CE	2.99	0.45
1:A:193:LEU:O	1:A:197:ILE:HG13	2.16	0.45
1:A:22:PHE:CE2	1:A:100[B]:LEU:HD12	2.52	0.45
1:A:250:GLN:O	1:A:254[A]:GLU:HG3	2.17	0.45
2:B:112:ALA:HB3	6:B:1077:HOH:O	2.17	0.45
1:A:86:ALA:O	1:A:90[B]:GLU:HG3	2.16	0.44
2:B:11:GLU:HG2	2:B:11:GLU:O	2.17	0.44
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.53	0.43
2:B:337:LYS:HE3	2:B:391:LEU:HD11	1.94	0.42
1:A:49[B]:GLU:CG	1:A:100[B]:LEU:HG	2.47	0.42
1:A:155:PRO:HA	1:A:156:PRO:HD3	1.86	0.42
1:A:15:ARG:O	1:A:268:ALA:HB2	2.19	0.41
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.55	0.41
2:B:21:LEU:HA	2:B:21:LEU:HD23	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49[B]:GLU:HG2	1:A:100[B]:LEU:CG	2.49	0.40
2:B:384:ILE:HG13	2:B:385:PHE:N	2.36	0.40
2:B:182:GLU:HB3	6:B:871:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	257/268 (96%)	251 (98%)	5 (2%)	1 (0%)	39 14
2	B	398/396 (100%)	389 (98%)	9 (2%)	0	100 100
All	All	655/664 (99%)	640 (98%)	14 (2%)	1 (0%)	52 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

### 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	205/208 (99%)	203 (99%)	2 (1%)	82 62
2	B	316/310 (102%)	307 (97%)	9 (3%)	51 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	521/518 (101%)	510 (98%)	11 (2%)	63 27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	196	LEU
2	B	23	PRO
2	B	65	ILE
2	B	144	PRO
2	B	196	PRO
2	B	206[A]	ARG
2	B	206[B]	ARG
2	B	236	ASN
2	B	275	ARG
2	B	297	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	66	ASN
1	A	108	ASN
1	A	109	ASN
1	A	195	HIS
2	B	236	ASN
2	B	375	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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$
4	13P	A	701	-	9,9,9	4.59	6 (66%)	9,12,12	6.34	4 (44%)
5	PLP	B	702	2	15,15,16	3.81	5 (33%)	21,22,23	2.38	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	13P	A	701	-	-	1/7/8/8	0/0/0/0
5	PLP	B	702	2	-	0/6/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	PLP	C3-C2	-13.28	1.31	1.40
5	B	702	PLP	P-O4P	-2.85	1.50	1.60
5	B	702	PLP	C3-C4	-2.74	1.33	1.40
5	B	702	PLP	C5A-C5	2.16	1.57	1.50
4	A	701	13P	P-O2P	2.39	1.63	1.54
4	A	701	13P	O3-C3	2.96	1.51	1.41
5	B	702	PLP	C6-N1	3.00	1.40	1.34
4	A	701	13P	O1-C1	3.17	1.45	1.43
4	A	701	13P	C3-C2	3.73	1.60	1.50
4	A	701	13P	C1-C2	5.34	1.61	1.50
4	A	701	13P	O2-C2	10.83	1.41	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	13P	O2-C2-C3	-15.01	94.07	120.74
4	A	701	13P	O2-C2-C1	-10.89	100.97	120.45
5	B	702	PLP	C4A-C4-C5	-3.43	117.31	120.88
5	B	702	PLP	C2A-C2-N1	-2.94	111.43	117.95
4	A	701	13P	O3-C3-C2	-2.89	102.07	112.09
5	B	702	PLP	C6-C5-C4	-2.72	115.84	118.15
4	A	701	13P	O3P-P-O2P	2.39	116.46	107.38
5	B	702	PLP	C5A-C5-C4	3.64	126.47	121.65
5	B	702	PLP	O4P-C5A-C5	5.05	117.35	108.99
5	B	702	PLP	C2A-C2-C3	6.15	128.46	121.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	13P	O2-C2-C3-O3

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.