



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 1YGP / pdb_00001ygp
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

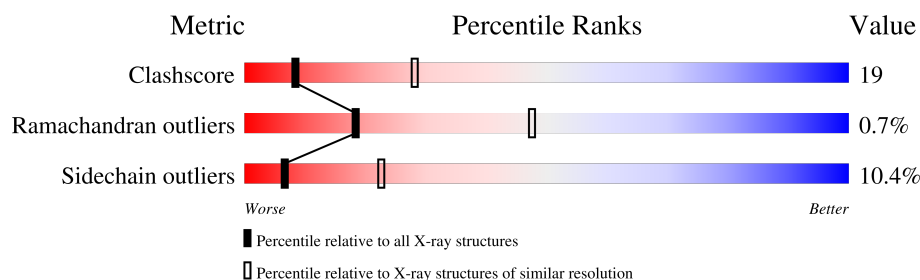
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	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.

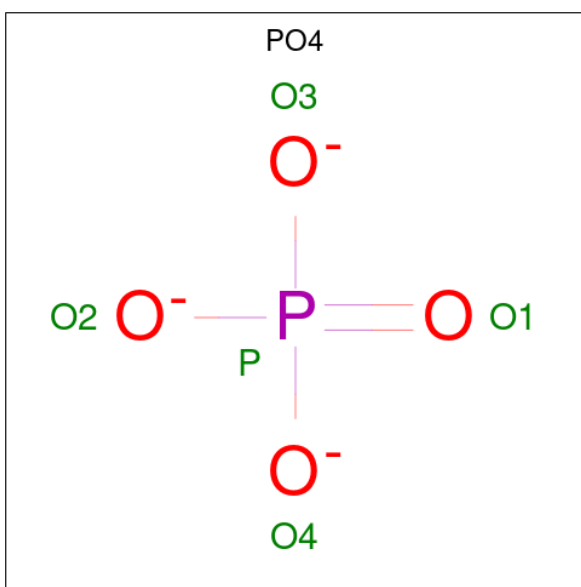
- Molecule 1 is a protein called YEAST GLYCOGEN PHOSPHORYLASE.

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

There are 16 discrepancies between the modelled and reference sequences:

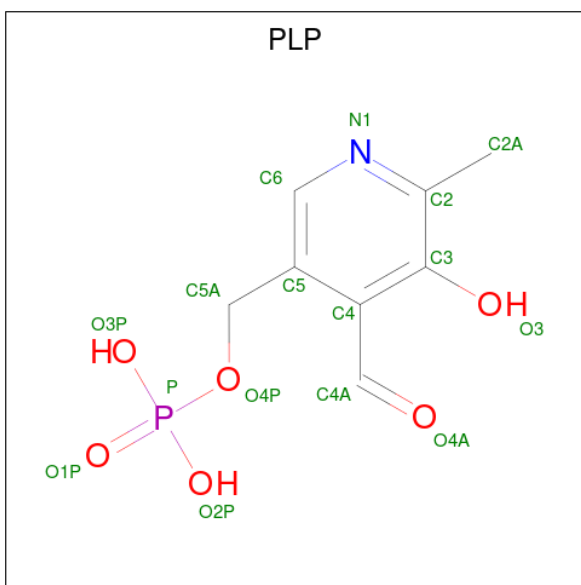
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	LEU	LYS	conflict	UNP P06738
A	50	VAL	ALA	conflict	UNP P06738
A	115	LEU	GLY	conflict	UNP P06738
A	254	LEU	PHE	conflict	UNP P06738
A	255	ASN	ALA	conflict	UNP P06738
A	267	ALA	PRO	conflict	UNP P06738
A	412	GLU	GLN	conflict	UNP P06738
A	596	ARG	LYS	conflict	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 (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



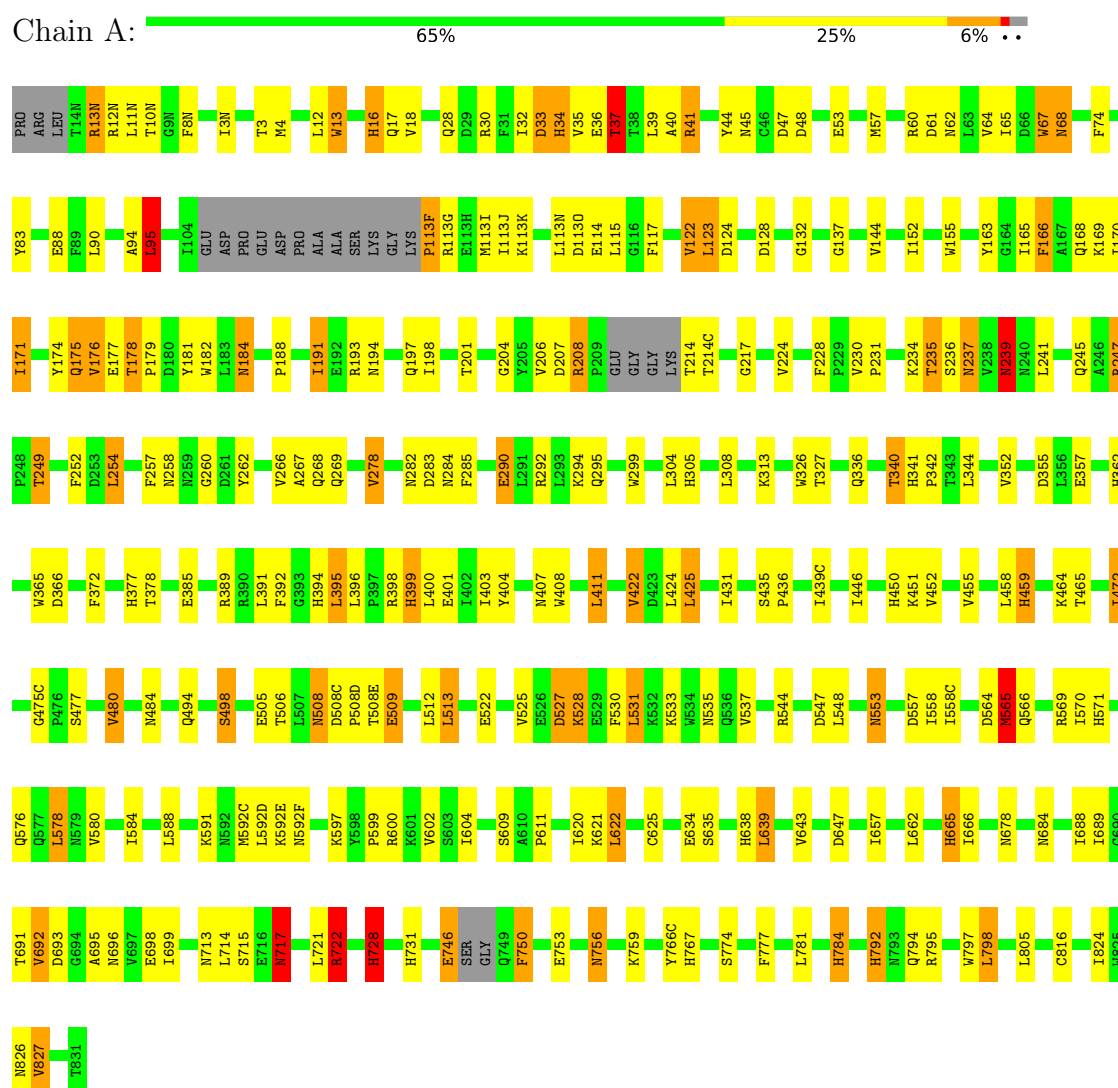
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

3 Residue-property plots [i](#)

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



S801	S715	C625	L558H	M484	Y404	E328	T250	W189	G113L	A54	PRO
V802	E716	D628	T561	T487	N407	F329	E251	E190	A113M	A55	ARG
L803	N717	D628	L562	T487	N407	P330	F252	I191	D113N	S56	LEU
L805	V718	F563	F563	P488	F409	D331	D253	L254	L1130	N57	T14N
F810	L721	N632	D564	R489	F410	Q332	L254	N194	E114	S58	R13N
S813	N722	D633	K565	R490	L411	Q336	F257	V196	L115	T59	R12N
D814	H728	S634	Q566	W491	E412	L337	M288	Q197	G116	R60	L11N
R815	V567	S635	Q568	N496	D413	N338	N259	I198	F117	D61	T10N
C816	K568	S636	K568	N496	V414	D339	G260	V200	D121	G62	G9N
I817	R569	L639	I570	S498	V422	T340	D261	V200	V122	L63	F8N
I824	H571	V642	H571	S498	D423	H341	Y262	T201	L123	P65	P6N
W825	R575	V642	R575	L502	L424	T343	M284	Y203	D124	D66	Q5N
N826	Q576	S651	Q576	E505	L425	L344	S265	G204	Q125	N67	E4N
V827	Q577	K652	Q577	E506	L426	L344	S266	Y205	E126	N68	I3N
E828	L578	K652	L578	T506	R427	E348	V266	Y205	P127	K73	K2N
P829	N579	V656	N579	L507	I428	L349	Q267	V206	D128	F74	S1N
V830	V580	P657	V580	N508	I431	V352	Q269	D207	A129	T75	T3
T831	D580C	P658	D580C	D508C	I431	V352	Q270	F209	G132	P79	M4
	P508D	D661	P508D	P508D	S435	L353	Q271	GLU	G135	K80	I5
	T583	L662	T583	E509	S435	D355	A277	GLY	L136	R81	P6
	E585	L662	E585	E509	R438	L356	V278	LYS	G137	V82	L7
	V586	H665	V586	L512	Q439	E357	L279	T214	R138	V83	R10
	R587	I666	R587	L513	I439C	W361	Y280	T214C	L139	V84	A11
	A589	S674	A589	D514	R440	H362	P281	S214E	V144	E88	L12
	K591	S674	K591	E522	I446	E363	N282	A214F	F89	F89	H16
	N592	N678	N592	V525	H450	A364	N284	S214G	M147	L90	Q17
	M592C	F681	M592C	E526	K450	V365	F285	Q214H	A154	R93	V18
	L592D	N684	L592D	E527	K451	D366	G288	W215	W155	A94	F21
	N592E	N684	N592E	K528	V452	T369	K289	T216	Y161	D96	N22
	N592F	N684	N592F	E529	V455	A373	E290	G217	E162	N97	N22
	V594	I688	V594	F530	V455	A373	L291	L222	Y163	A98	Q28
	K597	T689	K597	L531	L458	T375	R292	A223	G163	L99	D29
	Y598	T691	Y598	K533	H489	N376	L293	V224	I165	I100	R30
	P599	V692	P599	W534	S460	H377	K294	F228	F166	M101	F31
	R600	D693	R600	N535	E461	T378	Q295	V230	A167	I104	I32
	K601	S774	K601	Q536	L462	T378	Q296	V230	Q168	GLU	D33
	V602	F777	V602	V537	K463	E385	Y297	P231	K169	ASP	H34
	S603	L781	S603	I543	T465	K386	Q299	G232	I170	PRO	V35
	I604	T783	I604	D547	T466	P388	C300	F233	I171	T37	E36
	F605	H784	F605	L548	K469	L391	A301	K234	Y174	GLU	T38
	G606	S701	G606	I549	D470	F392	A302	T235	Q175	ASP	L39
	S609	E702	S609	K550	F471	G393	S303	S236	V176	ALA	A40
	A610	E705	A610	K551	I472	H394	L304	N237	E177	ALA	R41
	P611	D706	P611	N552	K473	L395	H305	V238	T178	SER	S42
	Y613	F709	Y613	N553	F474	L396	L308	R240	P179	LYS	L43
	K617	L710	K617	D557	P476	P397	R310	L241	D180	GLY	Y44
	I620	N713	I620	I558	S477	H399	F311	V244	Y181	LYS	N45
	N558C	L714	N558C	I558	K478	L400	K312	Q245	W182	P113F	C46
	R558E	L714	R558E	I558C	K478	E401	K313	K246	L183	E113H	D47
	L622	L714	L622	N558D	V490	I402	W326	R247	N184	S185	D48
				R558E	V490	I402	F248	T249	P188	M113I	Y52
							T327			I113J	E53

4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	Xtriage
Total number of atoms	13538	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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, PO4

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	0.90	23/6901 (0.3%)	1.73	141/9378 (1.5%)
1	B	2.14	208/6901 (3.0%)	1.92	201/9378 (2.1%)
All	All	1.64	231/13802 (1.7%)	1.83	342/18756 (1.8%)

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 (231) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	784	HIS	CD2-NE2	-10.32	1.26	1.37
1	B	305	HIS	CD2-NE2	-9.82	1.27	1.37
1	B	665	HIS	CD2-NE2	-8.90	1.28	1.37
1	B	459	HIS	CD2-NE2	-8.82	1.28	1.37
1	B	34	HIS	CD2-NE2	-8.82	1.28	1.37
1	B	341	HIS	CD2-NE2	-8.72	1.28	1.37
1	B	394	HIS	CD2-NE2	-8.68	1.28	1.37
1	B	394	HIS	CG-ND1	-8.65	1.28	1.38
1	B	792	HIS	CD2-NE2	-8.37	1.28	1.37
1	B	67	TRP	NE1-CE2	-8.13	1.28	1.37
1	B	665	HIS	CG-ND1	-7.92	1.29	1.38
1	B	34	HIS	CG-ND1	-7.82	1.29	1.38
1	B	377	HIS	CD2-NE2	-7.11	1.30	1.37
1	B	301	ALA	N-CA	-7.07	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	TYR	C-O	-7.05	1.20	1.23
1	B	760	PRO	CA-CB	-7.01	1.43	1.53
1	B	638	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	638	HIS	CD2-NE2	-6.95	1.30	1.37
1	B	606	GLY	N-CA	-6.89	1.39	1.45
1	B	281	PRO	CA-CB	-6.88	1.44	1.53
1	A	34	HIS	CD2-NE2	-6.87	1.30	1.37
1	B	784	HIS	CG-ND1	-6.86	1.30	1.38
1	A	377	HIS	CD2-NE2	-6.83	1.30	1.37
1	B	199	PRO	CA-CB	-6.82	1.45	1.53
1	B	508(C)	ASP	N-CA	-6.77	1.39	1.46
1	B	829	PRO	CA-CB	-6.77	1.44	1.53
1	A	459	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	29	ASP	N-CA	-6.69	1.38	1.46
1	B	533	LYS	N-CA	-6.69	1.38	1.46
1	B	450	HIS	CG-ND1	-6.67	1.30	1.38
1	B	361	TRP	CG-CD2	-6.59	1.31	1.43
1	A	665	HIS	CD2-NE2	-6.48	1.30	1.37
1	B	337	LEU	CA-C	-6.38	1.45	1.52
1	B	305	HIS	ND1-CE1	-6.36	1.26	1.32
1	B	222	LEU	CA-C	-6.35	1.44	1.52
1	B	16	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	459	HIS	ND1-CE1	-6.33	1.26	1.32
1	B	598	TYR	N-CA	-6.32	1.39	1.46
1	B	622	LEU	N-CA	-6.31	1.38	1.46
1	B	414	VAL	N-CA	-6.30	1.39	1.46
1	B	728	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	394	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	57	MET	N-CA	-6.27	1.38	1.46
1	B	13	TRP	NE1-CE2	-6.26	1.30	1.37
1	A	792	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	16	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	399	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	122	VAL	CA-CB	6.24	1.62	1.54
1	A	341	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	305	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	326	TRP	NE1-CE2	-6.22	1.30	1.37
1	B	82	VAL	CA-CB	-6.19	1.46	1.54
1	B	611	PRO	CA-CB	-6.16	1.45	1.53
1	B	244	TRP	NE1-CE2	-6.15	1.30	1.37
1	B	269	GLN	CA-C	-6.13	1.44	1.52
1	A	450	HIS	CD2-NE2	-6.12	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	SER	CA-CB	-6.10	1.43	1.53
1	B	450	HIS	CD2-NE2	-6.10	1.31	1.37
1	B	290	GLU	N-CA	-6.08	1.39	1.46
1	A	362	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	657	ILE	C-O	-6.06	1.19	1.24
1	A	571	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	728	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	476	PRO	CA-CB	-6.00	1.45	1.53
1	B	42	SER	CA-C	-6.00	1.45	1.52
1	B	628	ASP	CA-C	-6.00	1.44	1.52
1	B	354	VAL	C-O	-5.98	1.18	1.24
1	B	652	LYS	N-CA	-5.98	1.39	1.46
1	B	571	HIS	CD2-NE2	-5.96	1.31	1.37
1	B	96	ASP	CA-CB	-5.94	1.43	1.53
1	B	244	TRP	CG-CD2	-5.94	1.33	1.43
1	B	613	TYR	N-CA	-5.92	1.39	1.46
1	B	362	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	399	HIS	CD2-NE2	-5.89	1.31	1.37
1	B	425	LEU	N-CA	-5.88	1.39	1.46
1	B	233	PHE	CA-CB	-5.87	1.45	1.53
1	B	553	ASN	CA-CB	-5.87	1.45	1.53
1	B	490	ARG	CA-C	-5.87	1.45	1.53
1	B	363	GLU	CA-CB	-5.86	1.43	1.53
1	B	792	HIS	CG-ND1	-5.85	1.31	1.38
1	B	1(N)	SER	N-CA	-5.84	1.39	1.46
1	B	696	ASN	N-CA	-5.82	1.39	1.46
1	B	299	TRP	CG-CD2	-5.81	1.33	1.43
1	B	37	THR	N-CA	-5.80	1.39	1.46
1	B	8(N)	PHE	N-CA	-5.77	1.39	1.46
1	B	155	TRP	CG-CD2	-5.76	1.33	1.43
1	B	767	HIS	CD2-NE2	-5.76	1.31	1.37
1	B	63	LEU	CA-C	-5.75	1.45	1.52
1	B	571	HIS	CE1-NE2	-5.75	1.26	1.32
1	A	767	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	68	ASN	N-CA	-5.73	1.39	1.46
1	B	795	ARG	N-CA	-5.73	1.39	1.46
1	B	139	LEU	CA-C	-5.73	1.45	1.52
1	B	277	ALA	CA-C	-5.71	1.45	1.52
1	B	392	PHE	CA-C	-5.71	1.45	1.52
1	B	341	HIS	CG-ND1	-5.71	1.31	1.38
1	B	794	GLN	CA-C	-5.70	1.46	1.53
1	B	32	ILE	CA-C	-5.70	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	ALA	CA-CB	-5.70	1.44	1.53
1	B	693	ASP	N-CA	-5.69	1.39	1.46
1	B	5(N)	GLN	N-CA	-5.67	1.39	1.46
1	B	66	ASP	CA-CB	-5.66	1.44	1.53
1	B	474	PHE	N-CA	-5.66	1.39	1.46
1	B	161	TYR	CA-CB	-5.66	1.44	1.53
1	B	365	TRP	N-CA	-5.66	1.39	1.46
1	B	338	ASN	N-CA	-5.66	1.39	1.46
1	B	163	TYR	N-CA	-5.64	1.39	1.46
1	B	305	HIS	N-CA	-5.63	1.39	1.46
1	B	191	ILE	N-CA	-5.63	1.38	1.46
1	B	571	HIS	CA-C	-5.63	1.45	1.52
1	B	738	LEU	N-CA	-5.60	1.39	1.46
1	B	375	THR	N-CA	-5.59	1.39	1.46
1	B	535	ASN	CA-CB	-5.59	1.44	1.53
1	B	195	GLU	C-N	-5.59	1.27	1.33
1	B	52	TYR	CA-C	-5.58	1.46	1.52
1	B	633	ASP	N-CA	-5.58	1.39	1.46
1	B	67	TRP	CG-CD2	-5.56	1.33	1.43
1	B	609	SER	CA-C	-5.56	1.45	1.52
1	B	373	ALA	N-CA	-5.56	1.39	1.45
1	B	632	ASN	CA-C	-5.56	1.45	1.52
1	B	361	TRP	NE1-CE2	-5.55	1.31	1.37
1	B	215	TRP	CG-CD2	-5.55	1.33	1.43
1	B	28	GLN	CA-C	-5.55	1.45	1.52
1	B	592(F)	ASN	N-CA	-5.54	1.39	1.46
1	B	543	ILE	CA-C	-5.54	1.45	1.52
1	A	341	HIS	CG-ND1	-5.54	1.32	1.38
1	B	3(N)	ILE	CA-CB	-5.54	1.47	1.54
1	B	289	LYS	CA-C	-5.54	1.45	1.52
1	B	330	PRO	N-CA	-5.53	1.40	1.47
1	B	79	PRO	N-CA	-5.52	1.40	1.47
1	B	342	PRO	N-CA	-5.52	1.40	1.47
1	B	461	GLU	CA-CB	-5.51	1.44	1.53
1	B	824	ILE	CA-C	-5.51	1.45	1.52
1	B	305	HIS	CG-ND1	-5.50	1.32	1.38
1	B	491	TRP	N-CA	-5.50	1.38	1.46
1	B	657	ILE	CA-CB	-5.49	1.51	1.54
1	B	774	SER	N-CA	-5.48	1.39	1.46
1	B	113(M)	ALA	N-CA	-5.48	1.39	1.46
1	B	827	VAL	C-O	-5.48	1.18	1.24
1	B	473	LYS	CA-C	-5.47	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	472	ILE	CA-CB	-5.47	1.47	1.54
1	B	101	ASN	CA-C	-5.46	1.47	1.53
1	B	304	LEU	CA-C	-5.45	1.45	1.52
1	B	298	PHE	C-N	-5.45	1.26	1.33
1	B	604	ILE	N-CA	-5.43	1.39	1.46
1	B	258	ASN	CA-CB	-5.42	1.44	1.53
1	B	466	THR	CA-C	-5.42	1.45	1.52
1	B	591	LYS	CA-C	-5.41	1.46	1.52
1	B	829	PRO	N-CD	-5.40	1.40	1.47
1	B	55	ALA	CA-CB	-5.40	1.44	1.53
1	B	745	ILE	N-CA	-5.38	1.39	1.46
1	B	235	THR	C-N	-5.36	1.26	1.33
1	B	297	TYR	N-CA	-5.35	1.40	1.46
1	B	684	ASN	CA-C	-5.35	1.46	1.52
1	B	84	TYR	N-CA	-5.34	1.39	1.46
1	A	450	HIS	CG-ND1	-5.32	1.32	1.38
1	B	563	PHE	N-CA	-5.32	1.39	1.46
1	B	270	GLN	N-CA	-5.32	1.40	1.46
1	B	462	LEU	CA-C	-5.31	1.45	1.52
1	B	127	PRO	N-CD	-5.31	1.40	1.47
1	B	365	TRP	CD1-NE1	-5.31	1.26	1.37
1	B	526	GLU	N-CA	-5.31	1.39	1.46
1	A	784	HIS	CD2-NE2	-5.30	1.32	1.37
1	B	362	HIS	CE1-NE2	-5.30	1.27	1.32
1	B	401	GLU	CA-CB	-5.29	1.45	1.53
1	B	147	MET	N-CA	-5.29	1.40	1.46
1	B	311	PHE	CA-C	-5.29	1.46	1.52
1	B	43	LEU	N-CA	-5.29	1.39	1.46
1	B	188	PRO	N-CD	-5.28	1.40	1.47
1	B	179	PRO	CA-CB	-5.28	1.46	1.53
1	B	355	ASP	C-O	-5.28	1.17	1.24
1	B	784	HIS	ND1-CE1	-5.27	1.27	1.32
1	B	369	THR	N-CA	-5.27	1.40	1.46
1	B	439(C)	ILE	CA-CB	-5.27	1.47	1.54
1	B	817	ILE	N-CA	-5.26	1.39	1.46
1	B	329	PHE	CA-C	-5.26	1.46	1.52
1	A	399	HIS	CG-ND1	-5.25	1.32	1.38
1	B	621	LYS	CA-C	-5.25	1.46	1.52
1	B	766(C)	TYR	CA-C	-5.25	1.46	1.52
1	B	63	LEU	CB-CG	-5.24	1.43	1.53
1	A	728	HIS	CG-ND1	-5.24	1.32	1.38
1	B	514	ASP	CA-C	-5.23	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	GLU	C-O	-5.22	1.17	1.24
1	B	589	ALA	N-CA	-5.22	1.40	1.46
1	B	584	ILE	CA-C	-5.22	1.46	1.52
1	B	341	HIS	ND1-CE1	-5.21	1.27	1.32
1	B	332	GLN	CA-CB	-5.21	1.46	1.54
1	B	692	VAL	CA-C	-5.21	1.48	1.52
1	B	728	HIS	CG-ND1	-5.19	1.32	1.38
1	B	162	GLU	CA-C	-5.19	1.46	1.52
1	B	403	ILE	N-CA	-5.19	1.40	1.46
1	B	732	PRO	CA-C	-5.19	1.46	1.52
1	B	558(D)	ASN	CA-CB	-5.18	1.46	1.53
1	B	257	PHE	C-N	-5.18	1.26	1.34
1	B	496	ASN	N-CA	-5.17	1.41	1.46
1	B	713	ASN	CA-C	-5.17	1.46	1.52
1	B	656	ILE	C-O	-5.16	1.18	1.24
1	B	53	GLU	N-CA	-5.16	1.40	1.46
1	B	586	ARG	C-O	-5.16	1.18	1.24
1	B	551	LYS	N-CA	-5.15	1.40	1.46
1	B	412	GLU	CA-CB	-5.15	1.45	1.53
1	B	681	PHE	N-CA	-5.15	1.40	1.46
1	B	399	HIS	CG-ND1	-5.15	1.32	1.38
1	B	651	SER	CA-C	-5.14	1.46	1.52
1	B	575	ARG	N-CA	-5.14	1.38	1.46
1	B	7	LEU	C-O	-5.13	1.18	1.24
1	B	825	TRP	N-CA	-5.12	1.39	1.46
1	B	310	ARG	CA-CB	-5.12	1.45	1.53
1	B	312	LYS	N-CA	-5.12	1.39	1.46
1	B	10	ARG	N-CA	-5.12	1.40	1.46
1	B	438	ARG	CD-NE	-5.12	1.39	1.46
1	B	605	PHE	CA-C	-5.11	1.46	1.52
1	B	801	SER	N-CA	-5.11	1.40	1.46
1	B	10	ARG	C-O	-5.11	1.18	1.24
1	B	33	ASP	N-CA	-5.11	1.40	1.46
1	B	567	VAL	N-CA	-5.10	1.39	1.46
1	B	16	HIS	CG-ND1	-5.09	1.32	1.38
1	B	176	VAL	N-CA	-5.07	1.40	1.46
1	B	364	ALA	CA-C	-5.07	1.46	1.52
1	B	59	ILE	CA-CB	-5.06	1.48	1.54
1	B	302	ALA	C-N	-5.06	1.27	1.33
1	B	64	VAL	N-CA	-5.05	1.40	1.46
1	A	638	HIS	CG-ND1	-5.04	1.32	1.38
1	B	12	LEU	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	THR	N-CA	-5.04	1.40	1.46
1	B	638	HIS	CG-ND1	-5.04	1.32	1.38
1	B	214(E)	SER	N-CA	-5.03	1.39	1.45
1	B	393	GLY	N-CA	-5.02	1.39	1.45
1	B	658	PRO	N-CD	-5.02	1.40	1.47
1	B	199	PRO	N-CD	-5.02	1.40	1.47
1	B	207	ASP	N-CA	-5.01	1.39	1.46

All (342) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	VAL	N-CA-CB	-10.36	99.23	112.60
1	B	165	ILE	N-CA-C	-9.97	102.18	111.45
1	A	165	ILE	N-CA-C	-9.70	102.43	111.45
1	B	508	ASN	OD1-CG-ND2	-9.46	113.14	122.60
1	B	558	ILE	N-CA-C	-9.31	102.83	111.67
1	B	527	ASP	N-CA-C	9.11	126.73	107.70
1	B	237	ASN	CA-CB-CG	8.90	121.50	112.60
1	A	33	ASP	CA-CB-CG	8.81	121.41	112.60
1	A	527	ASP	N-CA-C	8.71	125.91	107.70
1	B	547	ASP	CA-CB-CG	8.65	121.25	112.60
1	B	480	VAL	N-CA-CB	-8.65	101.44	112.60
1	B	269	GLN	OE1-CD-NE2	-8.64	113.96	122.60
1	B	113(F)	PRO	CA-N-CD	-8.59	99.97	112.00
1	B	459	HIS	CB-CG-CD2	-8.36	120.33	131.20
1	B	553	ASN	CA-CB-CG	-8.32	104.28	112.60
1	A	113(F)	PRO	N-CA-CB	8.17	111.99	103.00
1	B	750	PHE	N-CA-C	8.16	128.19	110.80
1	A	113(F)	PRO	CA-N-CD	-8.12	100.64	112.00
1	A	340	THR	N-CA-C	8.01	121.11	111.82
1	B	446	ILE	CB-CA-C	-8.01	101.71	111.97
1	B	113(F)	PRO	N-CA-CB	7.96	111.75	103.00
1	A	553	ASN	CA-CB-CG	-7.88	104.72	112.60
1	A	484	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	B	571	HIS	CB-CG-CD2	-7.87	120.96	131.20
1	B	33	ASP	CA-CB-CG	7.83	120.43	112.60
1	B	266	VAL	N-CA-CB	-7.77	102.24	112.26
1	B	62	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	A	407	ASN	OD1-CG-ND2	-7.67	114.93	122.60
1	B	564	ASP	CA-CB-CG	7.67	120.27	112.60
1	A	750	PHE	N-CA-C	7.63	127.05	110.80
1	A	571	HIS	CB-CG-CD2	-7.63	121.28	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	558	ILE	N-CA-C	-7.54	104.51	111.67
1	B	47	ASP	CA-CB-CG	7.53	120.13	112.60
1	B	94	ALA	N-CA-C	7.52	120.94	111.69
1	B	657	ILE	O-C-N	-7.47	115.64	120.42
1	A	178	THR	O-C-N	-7.46	116.93	121.71
1	A	508	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	128	ASP	CA-CB-CG	7.43	120.03	112.60
1	B	305	HIS	CB-CG-CD2	-7.39	121.59	131.20
1	B	557	ASP	CA-CB-CG	7.39	119.99	112.60
1	A	152	ILE	N-CA-C	-7.39	102.28	108.63
1	B	178	THR	O-C-N	-7.38	116.99	121.71
1	B	484	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	B	249	THR	N-CA-C	-7.28	103.06	112.23
1	B	175	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	B	535	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	A	166	PHE	CA-CB-CG	7.19	120.99	113.80
1	B	678	ASN	OD1-CG-ND2	-7.17	115.43	122.60
1	B	41	ARG	N-CA-CB	-7.14	99.93	111.22
1	B	231	PRO	CA-C-N	7.14	127.11	122.18
1	B	231	PRO	C-N-CA	7.14	127.11	122.18
1	B	124	ASP	CA-CB-CG	-7.13	105.47	112.60
1	B	666	ILE	N-CA-C	7.07	124.05	109.34
1	B	37	THR	N-CA-CB	-7.05	97.65	110.27
1	B	528	LYS	N-CA-C	7.04	125.79	110.80
1	B	584	ILE	CA-C-O	-7.04	113.71	121.17
1	B	571	HIS	CB-CG-ND1	7.02	133.23	122.70
1	A	564	ASP	CA-CB-CG	7.00	119.60	112.60
1	B	236	SER	N-CA-C	-6.99	104.06	112.59
1	A	94	ALA	N-CA-C	6.97	120.27	111.69
1	A	237	ASN	CA-CB-CG	6.96	119.56	112.60
1	B	715	SER	N-CA-C	6.92	119.67	111.71
1	B	176	VAL	N-CA-C	-6.90	98.54	108.48
1	A	266	VAL	N-CA-CB	-6.90	103.36	112.26
1	A	657	ILE	O-C-N	-6.88	116.02	120.42
1	A	547	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	355	ASP	N-CA-C	6.88	118.86	111.36
1	B	377	HIS	CB-CG-CD2	-6.87	122.28	131.20
1	B	578	LEU	N-CA-C	-6.74	103.86	111.14
1	A	665	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	A	459	HIS	CB-CG-CD2	-6.73	122.45	131.20
1	B	206	VAL	N-CA-C	-6.72	98.70	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	B	201	THR	CA-CB-OG1	-6.69	99.56	109.60
1	A	535	ASN	OD1-CG-ND2	-6.67	115.94	122.60
1	A	175	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	B	657	ILE	CA-C-O	-6.62	114.25	118.69
1	B	48	ASP	N-CA-C	6.61	118.57	111.36
1	A	47	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	267	ALA	N-CA-C	6.58	119.30	111.33
1	B	214	THR	CA-CB-OG1	-6.57	99.74	109.60
1	B	362	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	B	365	TRP	CE2-CD2-CG	-6.57	99.32	107.20
1	B	340	THR	N-CA-C	6.55	119.42	111.82
1	B	97	ASN	OD1-CG-ND2	-6.53	116.08	122.60
1	B	284	ASN	CB-CG-ND2	6.53	126.19	116.40
1	A	37	THR	N-CA-CB	-6.52	98.60	110.27
1	A	62	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	A	214	THR	CA-CB-OG1	-6.51	99.84	109.60
1	B	184	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	A	267	ALA	N-CA-C	6.50	119.20	111.33
1	B	407	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	B	784	HIS	CA-CB-CG	-6.49	107.31	113.80
1	B	422	VAL	N-CA-C	6.48	122.83	109.34
1	A	231	PRO	CA-C-N	6.48	126.65	122.18
1	A	231	PRO	C-N-CA	6.48	126.65	122.18
1	B	365	TRP	CG-CD2-CE3	6.48	140.38	133.90
1	A	722	ARG	N-CA-C	-6.48	104.14	111.07
1	A	394	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	B	95	LEU	N-CA-C	6.45	118.89	111.02
1	B	185	SER	N-CA-C	-6.44	102.71	110.44
1	A	508	ASN	CB-CG-ND2	6.41	126.02	116.40
1	B	459	HIS	CB-CG-ND1	6.40	132.30	122.70
1	A	528	LYS	N-CA-C	6.38	124.38	110.80
1	B	166	PHE	CA-CB-CG	6.37	120.17	113.80
1	B	797	TRP	CG-CD2-CE3	6.35	140.25	133.90
1	A	446	ILE	CB-CA-C	-6.34	103.85	111.97
1	B	583	ILE	CB-CA-C	-6.34	103.72	112.02
1	B	508	ASN	CB-CG-ND2	6.32	125.88	116.40
1	A	237	ASN	N-CA-C	-6.31	98.93	108.96
1	A	678	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	284	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	191	ILE	N-CA-C	-6.29	97.28	107.28
1	A	362	HIS	CB-CG-CD2	-6.29	123.03	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	792	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	A	592(F)	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	B	642	VAL	N-CA-C	-6.22	99.41	108.11
1	B	698	GLU	CA-CB-CG	-6.22	101.66	114.10
1	B	329	PHE	CA-C-O	-6.21	112.92	118.63
1	B	162	GLU	CB-CA-C	-6.20	100.32	110.85
1	B	592(F)	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	B	784	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	A	422	VAL	N-CA-C	6.17	122.16	109.34
1	B	702	GLU	N-CA-C	6.14	117.64	111.07
1	B	750	PHE	CA-CB-CG	-6.13	107.67	113.80
1	A	657	ILE	N-CA-CB	-6.12	105.68	110.45
1	A	95	LEU	N-CA-C	6.11	118.48	111.02
1	B	16	HIS	CB-CG-CD2	-6.11	123.25	131.20
1	A	13(N)	ARG	N-CA-C	6.09	123.77	110.80
1	A	362	HIS	CA-CB-CG	-6.08	107.72	113.80
1	B	341	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	A	666	ILE	N-CA-C	6.04	121.89	109.34
1	A	206	VAL	N-CA-C	-6.03	99.72	108.71
1	B	717	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	B	377	HIS	CB-CG-ND1	6.02	131.73	122.70
1	A	191	ILE	N-CA-C	-6.02	98.97	107.75
1	A	578	LEU	N-CA-C	-6.00	104.82	111.36
1	B	207	ASP	N-CA-C	-6.00	98.62	108.76
1	A	689	ILE	N-CA-C	-6.00	99.10	107.80
1	A	377	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	B	579	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	717	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	B	459	HIS	N-CA-C	-5.97	104.68	111.07
1	A	305	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	A	792	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	A	295	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	A	698	GLU	CA-CB-CG	-5.94	102.22	114.10
1	B	365	TRP	CG-CD1-NE1	-5.94	102.48	110.20
1	A	784	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	67	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	A	465	THR	CA-CB-OG1	-5.93	100.70	109.60
1	B	509	GLU	CA-CB-CG	5.93	125.97	114.10
1	B	558(E)	ARG	N-CA-C	5.93	118.53	111.71
1	A	34	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	B	237	ASN	N-CA-C	-5.91	99.56	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	465	THR	CA-CB-OG1	-5.90	100.75	109.60
1	B	362	HIS	CA-CB-CG	-5.90	107.90	113.80
1	A	459	HIS	CB-CG-ND1	5.89	131.54	122.70
1	B	37	THR	CA-CB-OG1	-5.89	100.77	109.60
1	A	207	ASP	N-CA-C	-5.88	98.81	108.76
1	B	408	TRP	CG-CD2-CE3	5.88	139.78	133.90
1	B	198	ILE	CA-C-N	5.87	126.32	119.99
1	B	198	ILE	C-N-CA	5.87	126.32	119.99
1	A	484	ASN	CB-CG-ND2	5.86	125.20	116.40
1	A	408	TRP	CG-CD2-CE3	5.86	139.76	133.90
1	B	706	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	472	ILE	CB-CA-C	-5.86	104.14	112.22
1	B	693	ASP	CA-CB-CG	5.86	118.45	112.60
1	A	247	ARG	CA-C-N	5.85	125.83	120.03
1	A	247	ARG	C-N-CA	5.85	125.83	120.03
1	A	571	HIS	CB-CG-ND1	5.84	131.46	122.70
1	B	472	ILE	CB-CA-C	-5.83	104.17	112.22
1	B	93	ARG	CA-C-O	5.82	126.72	120.38
1	A	249	THR	N-CA-C	-5.79	104.93	112.23
1	B	299	TRP	CE2-CD2-CG	-5.79	100.25	107.20
1	A	269	GLN	CG-CD-NE2	5.78	125.08	116.40
1	A	784	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	A	236	SER	N-CA-C	-5.77	105.55	112.59
1	B	269	GLN	CG-CD-NE2	5.77	125.06	116.40
1	B	290	GLU	CA-CB-CG	-5.77	102.56	114.10
1	B	362	HIS	CB-CG-ND1	5.77	131.36	122.70
1	B	182	TRP	CE2-CD2-CG	-5.76	100.29	107.20
1	B	13(N)	ARG	N-CA-C	5.75	123.05	110.80
1	B	481	ASN	CA-CB-CG	-5.74	106.86	112.60
1	B	365	TRP	CD1-CG-CD2	5.74	115.48	106.30
1	B	465	THR	N-CA-CB	-5.74	101.49	110.44
1	B	182	TRP	CG-CD2-CE3	5.74	139.64	133.90
1	B	245	GLN	CA-C-O	-5.73	114.63	120.71
1	B	427	ARG	N-CA-C	5.72	117.59	111.36
1	B	441	MET	N-CA-C	5.71	117.18	111.07
1	A	41	ARG	N-CA-CB	-5.71	102.20	111.22
1	B	232	GLY	O-C-N	-5.70	118.12	123.25
1	B	175	GLN	CG-CD-NE2	5.70	124.95	116.40
1	A	117	PHE	N-CA-C	5.67	118.14	108.90
1	A	794	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	B	178	THR	CA-CB-OG1	-5.64	101.14	109.60
1	B	309	ARG	CD-NE-CZ	-5.63	116.51	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	VAL	CA-C-O	5.63	127.53	122.63
1	B	155	TRP	CE2-CD2-CG	-5.62	100.45	107.20
1	B	361	TRP	CE2-CD2-CG	-5.62	100.46	107.20
1	B	828	GLU	CA-C-N	5.62	125.55	119.76
1	B	828	GLU	C-N-CA	5.62	125.55	119.76
1	A	284	ASN	CB-CG-ND2	5.61	124.81	116.40
1	A	565	MET	N-CA-C	5.60	118.86	109.95
1	B	7(N)	LEU	CA-C-N	5.60	125.71	119.32
1	B	7(N)	LEU	C-N-CA	5.60	125.71	119.32
1	A	509	GLU	CA-CB-CG	5.60	125.30	114.10
1	B	797	TRP	CG-CD1-NE1	-5.58	102.95	110.20
1	A	665	HIS	CB-CG-ND1	5.56	131.04	122.70
1	B	797	TRP	CB-CG-CD1	-5.56	118.56	126.90
1	A	239	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	16	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	341	HIS	CA-C-O	-5.53	112.58	120.16
1	B	692	VAL	O-C-N	5.52	126.59	121.96
1	B	295	GLN	OE1-CD-NE2	-5.51	117.08	122.60
1	B	469	LYS	N-CA-C	5.51	117.73	111.11
1	A	198	ILE	CA-C-N	5.51	125.27	119.76
1	A	198	ILE	C-N-CA	5.51	125.27	119.76
1	B	214	THR	CA-CB-CG2	5.50	119.86	110.50
1	A	313	LYS	CB-CG-CD	-5.50	98.64	111.30
1	B	728	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	B	284	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	767	HIS	CA-CB-CG	-5.49	108.31	113.80
1	B	722	ARG	N-CA-C	-5.48	105.22	111.14
1	A	647	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	558	ILE	CB-CA-C	-5.45	105.38	111.80
1	A	182	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	B	189	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	B	13	TRP	CG-CD2-CE3	5.43	139.33	133.90
1	B	349	LEU	N-CA-C	-5.42	105.37	111.28
1	B	713	ASN	O-C-N	5.42	129.26	122.86
1	A	37	THR	CA-CB-OG1	-5.42	101.47	109.60
1	B	583	ILE	N-CA-CB	5.42	117.51	110.57
1	B	22	ASN	N-CA-C	-5.41	106.59	114.12
1	B	313	LYS	CB-CG-CD	-5.39	98.91	111.30
1	B	491	TRP	CG-CD2-CE3	5.38	139.28	133.90
1	B	407	ASN	CB-CG-ND2	5.36	124.45	116.40
1	A	48	ASP	N-CA-C	5.36	117.20	111.36
1	A	816	CYS	CB-CA-C	-5.36	101.57	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	HIS	CB-CG-ND1	5.36	130.74	122.70
1	A	715	SER	N-CA-C	5.35	117.86	111.71
1	A	766(C)	TYR	O-C-N	-5.35	116.34	121.85
1	A	408	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	B	355	ASP	N-CA-C	5.34	117.19	111.36
1	A	284	ASN	CA-CB-CG	5.34	117.94	112.60
1	B	299	TRP	CD2-CE2-CZ2	-5.34	117.06	122.40
1	B	665	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	13	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	B	194	ASN	CA-C-N	5.32	127.84	120.29
1	B	194	ASN	C-N-CA	5.32	127.84	120.29
1	B	121	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	810	PHE	CA-CB-CG	5.31	119.11	113.80
1	B	113(F)	PRO	N-CD-CG	5.29	111.14	103.20
1	B	336	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	B	558(H)	LEU	N-CA-C	5.29	117.73	111.33
1	B	534	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	A	83	TYR	N-CA-C	-5.28	100.30	108.90
1	B	408	TRP	CB-CG-CD1	-5.28	118.98	126.90
1	A	557	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	565	MET	N-CA-C	5.27	118.32	109.95
1	A	377	HIS	CA-CB-CG	5.26	119.06	113.80
1	A	475(C)	GLY	CA-C-N	5.26	126.42	119.84
1	A	475(C)	GLY	C-N-CA	5.26	126.42	119.84
1	B	67	TRP	N-CA-C	-5.25	105.45	111.07
1	A	767	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	A	155	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	B	247	ARG	CA-C-N	5.25	125.22	120.03
1	B	247	ARG	C-N-CA	5.25	125.22	120.03
1	A	365	TRP	CE2-CD2-CG	-5.25	100.91	107.20
1	B	340	THR	CA-CB-OG1	-5.25	101.73	109.60
1	B	594	VAL	N-CA-C	-5.25	105.49	110.42
1	A	797	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	B	803	LEU	CA-C-O	-5.24	114.87	120.42
1	A	634	GLU	N-CA-C	5.24	117.67	111.33
1	A	372	PHE	N-CA-C	5.23	118.53	110.42
1	A	827	VAL	N-CA-CB	-5.23	102.29	111.39
1	A	756	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	176	VAL	N-CA-C	-5.21	100.98	108.48
1	A	67	TRP	CB-CG-CD1	-5.19	119.11	126.90
1	B	326	TRP	CG-CD2-CE3	5.19	139.09	133.90
1	B	266	VAL	CB-CA-C	5.19	117.63	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	767	HIS	CA-CB-CG	-5.19	108.61	113.80
1	B	128	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	399	HIS	N-CA-C	-5.18	105.81	111.82
1	B	735	LEU	CA-C-N	5.18	125.09	119.76
1	B	735	LEU	C-N-CA	5.18	125.09	119.76
1	B	365	TRP	CB-CG-CD1	-5.18	119.14	126.90
1	A	826	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	584	ILE	CA-C-O	-5.16	115.90	121.27
1	B	215	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	B	245	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	B	826	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	A	544	ARG	CB-CA-C	-5.15	102.80	110.88
1	B	756	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	B	566	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	B	767	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	A	201	THR	CA-CB-OG1	-5.14	101.89	109.60
1	A	326	TRP	CE2-CD2-CG	-5.14	101.04	107.20
1	B	117	PHE	N-CA-C	5.13	117.77	109.40
1	B	235	THR	N-CA-C	-5.13	103.15	110.59
1	A	728	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	565	MET	CA-CB-CG	5.12	124.34	114.10
1	A	389	ARG	N-CA-C	5.11	116.86	111.28
1	B	299	TRP	CB-CG-CD2	-5.11	119.65	126.80
1	B	126	GLU	O-C-N	-5.11	116.65	121.35
1	A	326	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	B	117	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	657	ILE	CA-C-N	5.10	124.82	119.82
1	B	657	ILE	C-N-CA	5.10	124.82	119.82
1	A	67	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	B	394	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	175	GLN	CG-CD-NE2	5.09	124.04	116.40
1	A	336	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	494	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	535	ASN	CB-CG-ND2	5.09	124.03	116.40
1	A	480	VAL	CB-CA-C	5.08	118.16	111.19
1	A	797	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	B	827	VAL	N-CA-CB	-5.08	102.55	111.39
1	A	340	THR	N-CA-CB	-5.08	102.41	110.28
1	A	408	TRP	CB-CG-CD1	-5.07	119.30	126.90
1	B	326	TRP	CB-CG-CD1	-5.07	119.29	126.90
1	A	684	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	194	ASN	CA-C-N	5.06	127.48	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ASN	C-N-CA	5.06	127.48	120.29
1	B	376	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	566	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	439(C)	ILE	N-CA-C	-5.05	100.47	107.80
1	A	68	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	B	610	ALA	CA-C-N	5.04	124.83	119.28
1	B	610	ALA	C-N-CA	5.04	124.83	119.28
1	A	178	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	184	ASN	CA-CB-CG	-5.04	107.56	112.60
1	B	189	TRP	CG-CD2-CE3	5.04	138.94	133.90
1	B	21	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	791	PHE	N-CA-C	5.03	116.45	111.07
1	B	825	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	B	665	HIS	CB-CG-ND1	5.02	130.23	122.70
1	B	751	SER	N-CA-C	5.01	120.89	109.81
1	B	794	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	B	231	PRO	O-C-N	5.00	129.11	123.00

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 ⓘ

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	377	1
1	B	6744	0	6434	433	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13538	0	12877	505	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 (505) 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:36:GLU:CD	1:B:18:VAL:HB	1.21	1.55
1:A:257:PHE:CZ	1:B:278:VAL:HG11	1.44	1.52
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:64:VAL:CG1	1:B:41:ARG:N	1.86	1.38
1:A:285:PHE:HZ	1:B:262:TYR:CZ	1.34	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:611:PRO:HB2	1:B:258:ASN:CG	1.54	1.32
1:A:191:ILE:CD1	1:B:40:ALA:CB	2.04	1.29
1:A:36:GLU:HB3	1:B:65:ILE:CG1	1.60	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:CD1	1.64	1.27
1:A:12:LEU:HD13	1:B:114:GLU:CG	1.63	1.27
1:A:611:PRO:CB	1:B:258:ASN:CG	2.09	1.25
1:A:18:VAL:HB	1:B:36:GLU:OE1	1.35	1.23
1:A:64:VAL:HG13	1:B:40:ALA:C	1.58	1.22
1:A:254:LEU:N	1:B:177:GLU:O	1.58	1.22
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:254:LEU:C	1:B:177:GLU:HB2	1.36	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:36:GLU:CD	1:B:18:VAL:CB	2.14	1.13
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:68:ASN:OD1	1:B:41:ARG:C	1.94	1.09
1:A:18:VAL:HG21	1:B:32:ILE:C	1.71	1.08
1:A:61:ASP:OD1	1:B:38:THR:N	1.86	1.08
1:A:257:PHE:CZ	1:B:278:VAL:CG1	2.36	1.08
1:A:65:ILE:HG13	1:B:36:GLU:HB3	1.35	1.06
1:A:18:VAL:HB	1:B:36:GLU:CD	1.81	1.06
1:A:18:VAL:CB	1:B:36:GLU:OE1	2.04	1.06
1:A:41:ARG:HA	1:B:68:ASN:OD1	1.56	1.06
1:A:13:TRP:CH2	1:B:117:PHE:CE2	2.44	1.05
1:A:191:ILE:HD12	1:B:40:ALA:HB3	1.05	1.03
1:A:285:PHE:HE1	1:B:262:TYR:CE2	1.73	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: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
1:A:36:GLU:HB2	1:B:18:VAL:HG11	1.43	0.99
1:A:32:ILE:HG21	1:B:17:GLN:C	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:OE1	1:B:18:VAL:C	2.09	0.94
1:A:37:THR:O	1:B:60:ARG:C	1.92	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:611:PRO:HB3	1:B:258:ASN:CG	1.93	0.93
1:A:41:ARG:C	1:B:68:ASN:OD1	2.12	0.92
1:A:36:GLU:HB3	1:B:65:ILE:HG13	1.48	0.91
1:A:285:PHE:HE1	1:B:262:TYR:HE2	1.14	0.91
1:A:36:GLU:CG	1:B:18:VAL:HB	2.01	0.91
1:A:32:ILE:CG2	1:B:18:VAL:CG2	1.76	0.90
1:A:64:VAL:HB	1:B:36:GLU:C	1.96	0.90
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: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:C	1:B:258:ASN:HD21	1.81	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: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: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:18:VAL:H	1:B:32:ILE:HG21	1.41	0.83
1:A:32:ILE:HG23	1:B:18:VAL:H	1.42	0.83
1:A:258:ASN:ND2	1:B:617:LYS:NZ	2.27	0.83
1:A:33:ASP:OD2	1:B:30:ARG:HG2	1.77	0.82
1:A:36:GLU:OE1	1:B:18:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:CD	1:B:12:LEU:HD21	2.06	0.81
1:A:61:ASP:OD2	1:B:33:ASP:OD1	1.99	0.81
1:A:44:TYR:O	1:B:8(N):PHE:HE2	1.58	0.80
1:A:262:TYR:OH	1:B:282:ASN:O	1.89	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:611:PRO:C	1:B:258:ASN:ND2	2.40	0.79
1:A:34:HIS:CE1	1:B:34:HIS:CE1	2.71	0.79
1:A:12:LEU:HD22	1:B:114:GLU:CD	2.07	0.78
1:A:32:ILE:CD1	1:B:16:HIS:CB	2.50	0.78
1:A:33:ASP:C	1:B:30:ARG:NH1	2.38	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: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:8(N):PHE:HE2	1:B:44:TYR:HB3	1.50	0.77
1:A:197:GLN:HG2	1:A:224:VAL:HG22	1.66	0.77
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: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:611:PRO:O	1:B:258:ASN:ND2	2.21	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
1:A:11(N):LEU:HA	1:B:45:ASN:HB2	1.72	0.71
1:A:36:GLU:HB2	1:B:18:VAL:CG1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:ASP:OD2	1:B:30:ARG:CG	2.32	0.69
1:A:262:TYR:CE2	1:B:285:PHE:HZ	2.10	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:61:ASP:OD1	1:B:37:THR:C	2.21	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:33:ASP:C	1:B:30:ARG:HH12	2.02	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:A:114:GLU:CD	1:B:12:LEU:CD2	2.68	0.66
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:A:64:VAL:CG1	1:B:36:GLU:C	2.69	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
1:A:191:ILE:CD1	1:B:40:ALA:HB2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:68:ASN:CG	1:B:42:SER:HB3	2.25	0.61
1:A:88:GLU:HB2	1:A:132:GLY:HA2	1.83	0.61
1:A:18:VAL:CG2	1:B:32:ILE:C	2.55	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: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:11(N):LEU:HA	1:B:45:ASN:CB	2.32	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: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:60:ARG:NH2	1:B:39:LEU:C	2.60	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: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
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:592(E):LYS:HB3	1:A:592(E):LYS:HZ2	1.67	0.58
1:A:64:VAL:HG11	1:B:35:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NH1	1:B:11(N):LEU:CD2	2.64	0.58
1:A:191:ILE:HD12	1:B:39:LEU:O	2.04	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:611:PRO:CB	1:B:258:ASN:ND2	2.63	0.57
1:A:245:GLN:HE21	1:A:247:ARG:HE	1.53	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:12:LEU:CD2	1:B:114:GLU:CD	2.78	0.57
1:A:13:TRP:CD1	1:B:114:GLU:O	2.58	0.57
1:B:592(C):MET:HE1	1:B:597:LYS:HD3	1.87	0.57
1:A:114:GLU:C	1:B:12:LEU:CB	2.78	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:A:285:PHE:CZ	1:B:260:GLY:HA2	2.39	0.56
1:B:591:LYS:HA	1:B:592(D):LEU:HD12	1.88	0.56
1:A:65:ILE:HG12	1:B:36:GLU:CD	2.31	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:592(C):MET:HE1	1:A:597:LYS:HD3	1.88	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:36:GLU:HB2	1:B:65:ILE:HD11	1.86	0.55
1:B:498:SER:HB2	1:B:537:VAL:HG13	1.88	0.55
1:A:61:ASP:O	1:B:36:GLU:C	2.50	0.55
1:B:693:ASP:O	1:B:696:ASN:HB2	2.07	0.55
1:A:191:ILE:HD12	1:B:39:LEU:C	2.32	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: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:88:GLU:O	1:B:137:GLY:HA2	2.07	0.53
1:B:565:MET:HB3	1:B:604:ILE:HB	1.90	0.53
1:A:565:MET:HB3	1:A:604:ILE:HB	1.90	0.53
1:A:68:ASN:CG	1:B:42:SER:CB	2.82	0.53
1:A:464:LYS:HA	1:A:472:ILE:HD11	1.91	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: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: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:36:GLU:OE1	1:B:18:VAL:O	2.26	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:12:LEU:CG	1:B:114:GLU:HG2	2.36	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: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
1:A:32:ILE:HD13	1:B:17:GLN:CA	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:LEU:HA	1:B:60:ARG:CZ	2.31	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: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:4:MET:SD	1:B:4:MET:N	2.86	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: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:166:PHE:CG	1:B:254:LEU:HD13	2.48	0.48
1:A:693:ASP:O	1:A:696:ASN:HB2	2.12	0.48
1:A:18:VAL:HG12	1:B:36:GLU:OE1	2.09	0.48
1:A:245:GLN:NE2	1:A:247:ARG:HE	2.11	0.48
1:B:135:GLY:CA	3:B:860:PLP:H5A2	2.43	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:169:LYS:HB2	1:A:176:VAL:CG2	2.43	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
1:B:657:ILE:HG12	1:B:681:PHE:CE1	2.48	0.48
1:A:61:ASP:O	1:B:36:GLU:O	2.32	0.48
1:A:235:THR:HB	1:A:237:ASN:H	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:45:ASN:ND2	1:B:68:ASN:HD21	1.97	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: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:41:ARG:HH12	1:B:11(N):LEU:CD2	2.24	0.46
1:A:169:LYS:HB2	1:A:176:VAL:HG22	1.98	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:A:28:GLN:HB3	1:B:16:HIS:CG	2.51	0.45
1:B:144:VAL:HG12	1:B:230:VAL:HG11	1.97	0.45
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: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: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: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:A:177:GLU:C	1:B:254:LEU:HB2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ILE:HD12	1:B:470:ASP:HB3	1.98	0.45
1:A:16:HIS:ND1	1:B:28:GLN:OE1	2.50	0.45
1:B:169:LYS:HB2	1:B:176:VAL:HG22	1.99	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:30:ARG:HD3	1:B:33:ASP:OD1	2.06	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:64:VAL:HG11	1:B:36:GLU:C	2.42	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:B:815:ARG:HD2	1:B:815:ARG:C	2.43	0.44
1:A:599:PRO:HB2	1:A:792:HIS:NE2	2.33	0.44
1:A:191:ILE:CG1	1:B:40:ALA:HB3	2.30	0.43
1:A:254:LEU:HD13	1:B:177:GLU:HA	1.77	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:40:ALA:O	1:B:64:VAL:HG22	1.93	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:33:ASP:HA	1:B:18:VAL:HG13	2.00	0.43
1:A:455:VAL:HG22	1:A:459:HIS:CD2	2.54	0.43
1:B:73:LYS:HB3	1:B:73:LYS:HE2	1.87	0.43
1:B:588:LEU:HD12	1:B:588:LEU:HA	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
1:A:558(C):ILE:HD11	1:A:602:VAL:HG11	2.00	0.43
1:A:68:ASN:CB	1:B:42:SER:CB	2.97	0.42
1:A:95:LEU:HD13	1:A:123:LEU:HD12	2.00	0.42
1:A:60:ARG:O	1:B:37:THR:HA	2.16	0.42
1:A:308:LEU:CD1	1:A:352:VAL:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:53:GLU:C	2.62	0.42
1:B:52:TYR:OH	1:B:126:GLU:HG3	2.20	0.42
1:B:80:LYS:HG3	1:B:332:GLN:C	2.44	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:36:GLU:CD	1:B:18:VAL:CA	2.84	0.41
1:A:262:TYR:CZ	1:B:282:ASN:N	2.86	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:B:558(D):ASN:OD1	1:B:638:HIS:ND1	2.54	0.41
1:A:37:THR:O	1:B:60:ARG:O	2.31	0.41
1:A:166:PHE:CG	1:B:254:LEU:HD11	2.56	0.41
1:A:258:ASN:HA	1:B:611:PRO:HB2	1.35	0.41
1:A:344:LEU:HD21	1:A:392:PHE:HZ	1.85	0.41
1:B:592(E):LYS:HB3	1:B:592(E):LYS:NZ	2.33	0.41
1:A:64:VAL:CB	1:B:36:GLU:C	2.68	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:258:ASN:HB2	1:B:177:GLU:CD	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:THR:O	1:B:459:HIS:HE1	2.02	0.40
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:12:LEU:CD2	1:B:114:GLU:HG2	2.51	0.40
1:A:88:GLU:O	1:A:137:GLY:HA2	2.22	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:44:TYR:C	1:B:8(N):PHE:HE2	2.28	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:A:181:TYR:OH	1:B:251:GLU:C	2.26	0.40
1:B:7(N):LEU:HB2	1:B:4(N):GLU:HG3	2.04	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:B:709:PHE:HB3	1:B:783:THR:CG2	2.51	0.40
1:A:35:VAL:O	1:B:64:VAL:HG11	2.22	0.40
1:A:60:ARG:CD	1:B:37:THR:O	2.70	0.40
1:B:74:PHE:HE2	1:B:239:ASN:ND2	2.19	0.40
1:B:245:GLN:HE21	1:B:247:ARG:NE	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:5(N):GLN:CD	1:B:261:ASP:CG[4_535]	1.89	0.31
1:B:3:THR:OG1	1:B:271:ARG:NH1[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:5(N):GLN:CA	1:B:264:ASN:OD1[4_535]	2.14	0.06
1:B:6:PRO:CA	1:B:394:HIS:ND1[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 ⓘ

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	850/879 (97%)	802 (94%)	43 (5%)	5 (1%)	21	51
1	B	850/879 (97%)	800 (94%)	43 (5%)	7 (1%)	16	44
All	All	1700/1758 (97%)	1602 (94%)	86 (5%)	12 (1%)	18	47

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	VAL
1	A	528	LYS

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Mol	Chain	Res	Type
1	A	750	PHE
1	B	422	VAL
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%)	624 (90%)	73 (10%)	6	22
1	B	697/781 (89%)	625 (90%)	72 (10%)	7	23
All	All	1394/1562 (89%)	1249 (90%)	145 (10%)	7	22

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3(N)	ILE
1	A	3	THR
1	A	37	THR
1	A	53	GLU
1	A	90	LEU
1	A	95	LEU
1	A	113(F)	PRO
1	A	113(G)	ARG
1	A	113(I)	MET
1	A	113(J)	ILE
1	A	113(K)	LYS
1	A	113(N)	LEU
1	A	113(O)	ASP

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Mol	Chain	Res	Type
1	A	122	VAL
1	A	123	LEU
1	A	124	ASP
1	A	171	ILE
1	A	178	THR
1	A	184	ASN
1	A	235	THR
1	A	239	ASN
1	A	249	THR
1	A	254	LEU
1	A	268	GLN
1	A	278	VAL
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	425	LEU
1	A	452	VAL
1	A	458	LEU
1	A	477	SER
1	A	480	VAL
1	A	498	SER
1	A	505	GLU
1	A	508	ASN
1	A	508(C)	ASP
1	A	508(D)	PRO
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	565	MET
1	A	569	ARG
1	A	578	LEU

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Mol	Chain	Res	Type
1	A	588	LEU
1	A	622	LEU
1	A	635	SER
1	A	639	LEU
1	A	662	LEU
1	A	691	THR
1	A	692	VAL
1	A	717	ASN
1	A	722	ARG
1	A	728	HIS
1	A	746	GLU
1	A	753	GLU
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	3(N)	ILE
1	B	3	THR
1	B	37	THR
1	B	53	GLU
1	B	90	LEU
1	B	95	LEU
1	B	113(F)	PRO
1	B	113(G)	ARG
1	B	113(I)	MET
1	B	113(J)	ILE
1	B	113(K)	LYS
1	B	113(N)	LEU
1	B	113(O)	ASP
1	B	122	VAL
1	B	123	LEU
1	B	124	ASP
1	B	171	ILE
1	B	178	THR
1	B	184	ASN
1	B	235	THR
1	B	249	THR
1	B	254	LEU
1	B	268	GLN
1	B	278	VAL

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Mol	Chain	Res	Type
1	B	290	GLU
1	B	304	LEU
1	B	327	THR
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	425	LEU
1	B	452	VAL
1	B	458	LEU
1	B	477	SER
1	B	480	VAL
1	B	498	SER
1	B	505	GLU
1	B	508	ASN
1	B	508(C)	ASP
1	B	508(D)	PRO
1	B	508(E)	THR
1	B	513	LEU
1	B	527	ASP
1	B	531	LEU
1	B	533	LYS
1	B	548	LEU
1	B	553	ASN
1	B	565	MET
1	B	569	ARG
1	B	578	LEU
1	B	588	LEU
1	B	622	LEU
1	B	635	SER
1	B	639	LEU
1	B	662	LEU
1	B	691	THR
1	B	692	VAL
1	B	717	ASN
1	B	722	ARG
1	B	737	SER
1	B	746	GLU
1	B	753	GLU

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Mol	Chain	Res	Type
1	B	756	ASN
1	B	774	SER
1	B	784	HIS
1	B	798	LEU
1	B	805	LEU
1	B	827	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	16	HIS
1	A	34	HIS
1	A	133	ASN
1	A	175	GLN
1	A	237	ASN
1	A	239	ASN
1	A	240	ASN
1	A	245	GLN
1	A	264	ASN
1	A	332	GLN
1	A	399	HIS
1	A	439	GLN
1	A	459	HIS
1	A	481	ASN
1	A	494	GLN
1	A	496	ASN
1	A	520	GLN
1	A	536	GLN
1	A	540	ASN
1	A	541	ASN
1	A	579	ASN
1	A	592(F)	ASN
1	A	684	ASN
1	A	713	ASN
1	A	784	HIS
1	B	14	ASN
1	B	34	HIS
1	B	68	ASN
1	B	133	ASN
1	B	184	ASN
1	B	237	ASN

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Mol	Chain	Res	Type
1	B	239	ASN
1	B	240	ASN
1	B	245	GLN
1	B	258	ASN
1	B	264	ASN
1	B	296	GLN
1	B	332	GLN
1	B	399	HIS
1	B	439	GLN
1	B	459	HIS
1	B	481	ASN
1	B	494	GLN
1	B	536	GLN
1	B	540	ASN
1	B	579	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 oligosaccharides 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$
3	PLP	A	860	1	15,15,16	1.85	1 (6%)	21,22,23	1.28	3 (14%)
2	PO4	A	859	-	4,4,4	1.93	2 (50%)	6,6,6	0.52	0
3	PLP	B	860	1	15,15,16	2.08	2 (13%)	21,22,23	1.34	3 (14%)
2	PO4	B	1900	-	4,4,4	2.44	3 (75%)	6,6,6	0.64	0
2	PO4	A	1900	-	4,4,4	1.70	1 (25%)	6,6,6	0.25	0
2	PO4	B	859	-	4,4,4	2.69	4 (100%)	6,6,6	0.50	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	B	860	1	-	4/6/6/8	0/1/1/1
3	PLP	A	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	-6.51	1.38	1.51
3	A	860	PLP	C4A-C4	-5.73	1.40	1.51
2	B	1900	PO4	P-O2	-3.12	1.45	1.54
2	B	859	PO4	P-O4	-2.97	1.46	1.54
2	B	859	PO4	P-O2	-2.95	1.46	1.54
2	B	859	PO4	P-O3	-2.46	1.47	1.54
2	B	1900	PO4	P-O3	-2.38	1.47	1.54
2	B	859	PO4	P-O1	-2.31	1.45	1.50
2	A	859	PO4	P-O2	-2.30	1.47	1.54
2	A	859	PO4	P-O4	-2.27	1.48	1.54
3	B	860	PLP	C3-C2	-2.22	1.38	1.41
2	B	1900	PO4	P-O4	-2.10	1.48	1.54
2	A	1900	PO4	P-O3	-2.03	1.48	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	860	PLP	O3P-P-O1P	3.34	123.84	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	860	PLP	O3P-P-O1P	3.25	123.51	110.83
3	A	860	PLP	C6-C5-C4	2.59	120.22	118.10
3	B	860	PLP	C6-C5-C4	2.54	120.18	118.10
3	B	860	PLP	O2P-P-O4P	-2.45	100.29	106.67
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.