



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:18 PM UTC

PDB ID : 4PPM / pdb_00004ppm
Title : Crystal structure of PigE: a transaminase involved in the biosynthesis of 2-methyl-3-n-amyI-pyrrole (MAP) from *Serratia* sp. FS14
Authors : Lou, X.D.; Ran, T.T.; Xu, D.Q.; Wang, W.W.
Deposited on : 2014-02-27
Resolution : 2.30 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

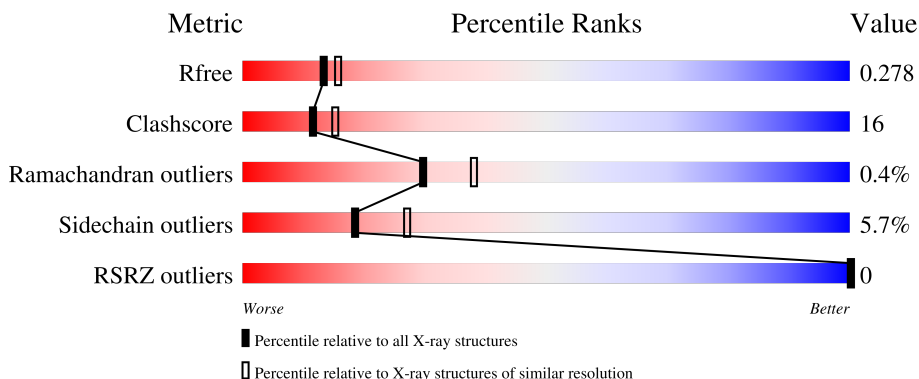
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	861	 33% 16% 5% 46%
1	B	861	 29% 21% • 46%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7493 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 Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3563	2265	617	657	24	0	0	0
1	B	462	3554	2263	615	652	24	0	0	0

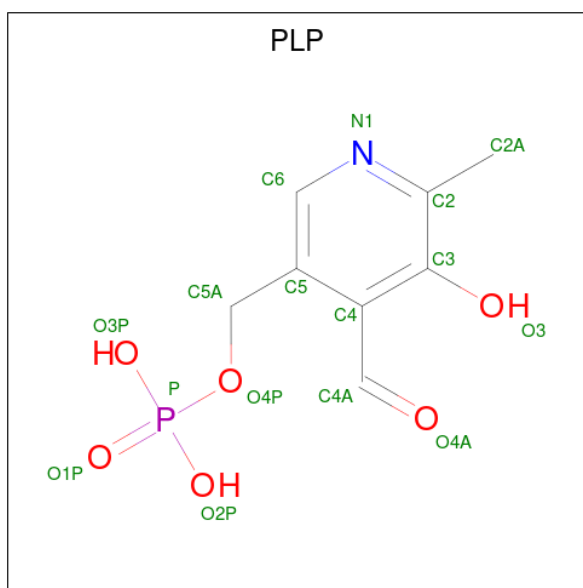
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	LEU	-	expression tag	UNP A0A059ZJX2
A	855	GLU	-	expression tag	UNP A0A059ZJX2
A	856	HIS	-	expression tag	UNP A0A059ZJX2
A	857	HIS	-	expression tag	UNP A0A059ZJX2
A	858	HIS	-	expression tag	UNP A0A059ZJX2
A	859	HIS	-	expression tag	UNP A0A059ZJX2
A	860	HIS	-	expression tag	UNP A0A059ZJX2
A	861	HIS	-	expression tag	UNP A0A059ZJX2
B	854	LEU	-	expression tag	UNP A0A059ZJX2
B	855	GLU	-	expression tag	UNP A0A059ZJX2
B	856	HIS	-	expression tag	UNP A0A059ZJX2
B	857	HIS	-	expression tag	UNP A0A059ZJX2
B	858	HIS	-	expression tag	UNP A0A059ZJX2
B	859	HIS	-	expression tag	UNP A0A059ZJX2
B	860	HIS	-	expression tag	UNP A0A059ZJX2
B	861	HIS	-	expression tag	UNP A0A059ZJX2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

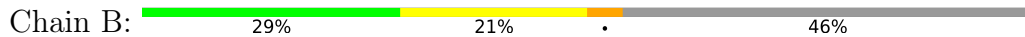
- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	160	160	160	0	0
4	B	184	184	184	0	0



MET	LYS	PHE	GLY	PHE	ILE	ILE	ALA	HIS	PRO	THR	SER	LEU	GLY	LEU	LYS	ARG	GLN	ARG	ASN	SER	GLY	GLY	TYR	THR	THR	GLN	HIS	SER	GLY	LEU	ASN	VAL	PRO	PHE	MET	ASN	PHE	ALA	ARG	ILE	THR	SER	ALA	THR	GLY	ALA														
THR	CYS	GLU	GLY	VAL	ILE	VAL	ILE	LYS	TYR	MET	PRO	LEU	VAL	ASP	GLU	GLY	ARG	ALA	VAL	VAL	VAL	GLN	GLY	ILE	ILE	GLU	GLU	GLY	GLY	GLY	GLY	GLY	PHE	THR	THR	ILE	VAL	VAL	GLY	GLY	GLY	ARG	ARG	ARG	GLY	ALA	THR	ALA												
LYS	SER	PRO	VAL	PRO	VAL	VAL	THR	SER	GLY	ASN	ASN	SER	LEU	VAL	THR	THR	THR	GLN	SER	TRP	VAL	TRP	LEU	GLU	GLY	ILE	ARG	PRO	GLU	GLU	GLY	ILE	ILE	CYS	VAL	VAL	PRO	THR	LEU	LEU	LEU	LEU	LEU	ALA	HIS	GLY	THR	SER												
LEU	HIS	LEU	LEU	HIS	ARG	VAL	ALA	GLY	ASN	HIS	ASP	ARG	LEU	THR	LEU	THR	GLY	ARG	PRO	GLU	VAL	THR	THR	LEU	ILE	THR	SER	ASP	PRO	ALA	PRO	ALA	ARG	CYS	VAL	VAL	THR	THR	ALA	VAL	VAL	VAL	LEU	LEU	ALA	ALA	PRO													
GLY	SER	ILE	PHE	ILE	ASP	VAL	ALA	ALA	ALA	PRO	ARG	ARG	ASP	ASP	ILE	ALA	SER	THR	THR	THR	ASP	ASP	GLY	GLY	GLY	CYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR													
ILE	VAL	ALA	ALA	GLU	GLY	ASN	ARG	ARG	ARG	GLU	ASN	PHE	ASP	SER	LEU	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR												
HIS	ASP	ILE	TYR	ALA	ALA	GLY	GLU	SER	ALA	ALA	ALA	A372	L373	P374	F380	I381	D382	A383	V384	Q387	T388	R391	E392	R397	Y398	M403	P404	P405	M406	V407	D408	F409	L410	K411	L412	Q413	R414	C415	V418	F419	R420	S421	A422	L427	Y428	D429	D430	M438	C444	L445	M446									
H449	N450	P451	Q452	P453	V454	V455	N456	L458	L458	K459	M460	Y461	G466	I473	S474	I475	P476	E477	E484	V485	L486	C487	R488	L489	A490	P491	R496	V497	S502	G503	T504	E505	A506	V507	E508	I513	A514	K520	P521	G522	L526	R527	N528	S529	Y530	H531	G532	K533	T534											
T541	G542	R543	D544	R547	R548	T551	P552	D555	A556	M557	V558	E559	V560	P561	F562	L568	A571	L572	N573	R574	A579	L580	M581	I585	E588	G589	V590	G591	H592	I593	P594	P595	A596	Q603	Q604	L605	L695	R696	E697	I698	Q701	D702	L703	H706	R709	M710	M711	G623												
R624	W633	I721	E637	A723	R724	D639	V640	L641	M642	L643	S644	K645	S646	L647	G733	S648	G734	M737	L738	G739	I740	Q741	F742	D743	GLN	ALA	PHE	THR	GLY	ALA	VAL	ASN	ALA	SER	ALA	ARG	GLU	PHE	N685	L686	E687	Y681	G684	N685	L686	A687	A691	L692	L695	R696	E697	I698	Q701	D702	L703	H706	R709	M710	M711	G623
Q716	E720	I721	A722	R724	R724	F725	P726	F727	V728	S729	E730	F731	R732	G733	R734	M737	L738	G739	I740	Q741	F742	D743	GLN	ALA	PHE	THR	GLY	ALA	VAL	ASN	ALA	SER	ALA	ARG	GLU	PHE	N685	L686	E687	Y681	G684	N685	L686	A687	A691	L692	L695	R696	E697	I698	Q701	D702	L703	H706	R709	M710	M711	G623		
E788	Q789	A790	L791	E792	M794	F795	C796	M797	K798	F799	V800	T801	I809	L810	I813	N816	S817	S818	T819	V820	I821	R822	I823	Q824	P825	I829	A832	E833	I834	F837	V838	F841	T843	V844	C845	E846	E847	L848	S849	T850	F851	L852	D853	L854	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS								

4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.10Å 228.10Å 67.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.30 19.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.89-2.30) 100.0 (19.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.30Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.238 , 0.272 0.251 , 0.278	Depositor DCC
R_{free} test set	4443 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.340 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.97	80/3633 (2.2%)	1.31	38/4920 (0.8%)
1	B	1.92	83/3626 (2.3%)	1.31	47/4912 (1.0%)
All	All	1.94	163/7259 (2.2%)	1.31	85/9832 (0.9%)

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	475	ILE	C-N	8.07	1.41	1.33
1	A	450	ASN	C-N	7.79	1.40	1.33
1	A	475	ILE	C-N	7.54	1.40	1.33
1	B	450	ASN	C-O	-7.39	1.20	1.23
1	B	452	GLN	C-O	-6.99	1.18	1.24
1	A	479	THR	C-O	-6.84	1.16	1.24
1	A	600	GLN	C-N	-6.77	1.25	1.33
1	B	733	GLY	C-O	-6.73	1.17	1.23
1	B	652	ILE	C-O	-6.63	1.17	1.23
1	A	452	GLN	C-O	-6.54	1.18	1.24
1	B	520	LYS	C-N	6.46	1.40	1.34
1	A	520	LYS	C-N	6.46	1.40	1.34
1	B	461	TYR	C-O	-6.44	1.16	1.24
1	B	450	ASN	C-N	6.33	1.41	1.33
1	A	824	GLN	C-N	6.32	1.40	1.33
1	A	400	GLN	C-O	-6.30	1.16	1.24
1	B	614	MET	C-O	-6.30	1.16	1.24
1	B	560	VAL	C-N	6.24	1.41	1.33
1	B	824	GLN	C-N	6.24	1.40	1.33
1	B	640	VAL	C-O	-6.20	1.17	1.24
1	A	408	ASP	C-O	-6.19	1.16	1.24
1	A	449	HIS	C-O	-6.14	1.16	1.23
1	B	508	GLU	N-CA	-6.11	1.39	1.46
1	A	593	ILE	C-N	6.06	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	VAL	C-O	-6.05	1.18	1.24
1	A	691	ALA	C-O	-5.94	1.17	1.24
1	B	397	ARG	C-O	-5.93	1.17	1.24
1	B	558	VAL	C-O	-5.92	1.17	1.24
1	A	640	VAL	C-O	-5.92	1.18	1.24
1	A	474	SER	C-O	-5.92	1.18	1.24
1	B	825	PRO	C-O	-5.91	1.17	1.24
1	A	429	ASP	C-O	-5.90	1.17	1.23
1	B	403	ASN	C-O	-5.88	1.17	1.24
1	A	594	PRO	C-N	5.84	1.40	1.33
1	A	637	GLU	C-N	5.84	1.40	1.33
1	A	441	GLY	C-O	-5.80	1.17	1.24
1	A	513	ILE	C-O	-5.80	1.17	1.24
1	B	684	GLY	C-O	-5.79	1.17	1.23
1	B	687	ALA	C-O	-5.77	1.17	1.24
1	B	581	MET	C-O	-5.73	1.17	1.23
1	A	667	ALA	C-O	-5.71	1.17	1.24
1	A	502	SER	C-O	-5.71	1.17	1.23
1	B	373	LEU	C-N	5.70	1.40	1.33
1	A	373	LEU	C-N	5.70	1.41	1.33
1	A	627	LYS	C-O	-5.69	1.16	1.23
1	A	808	LYS	C-O	-5.69	1.16	1.23
1	B	513	ILE	C-O	-5.69	1.17	1.24
1	A	715	LYS	C-O	-5.68	1.17	1.24
1	B	384	VAL	C-O	-5.67	1.17	1.24
1	B	454	VAL	C-O	-5.67	1.17	1.24
1	A	421	SER	C-O	-5.65	1.17	1.23
1	A	673	ARG	C-O	-5.64	1.16	1.24
1	A	490	ALA	C-N	5.64	1.40	1.33
1	B	473	ILE	C-O	-5.63	1.17	1.24
1	B	530	TYR	C-O	-5.62	1.17	1.23
1	A	713	TYR	C-O	-5.60	1.17	1.24
1	B	404	PRO	N-CD	5.59	1.55	1.47
1	A	497	VAL	C-O	-5.57	1.18	1.24
1	B	466	GLY	C-N	5.57	1.40	1.33
1	A	507	VAL	C-O	-5.55	1.17	1.24
1	A	828	ILE	C-O	-5.55	1.17	1.24
1	A	825	PRO	C-N	5.55	1.40	1.33
1	A	652	ILE	C-N	5.55	1.40	1.33
1	B	391	ARG	C-O	-5.54	1.17	1.24
1	A	467	PRO	C-O	-5.54	1.17	1.23
1	A	618	VAL	C-O	-5.52	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	502	SER	C-O	-5.52	1.18	1.24
1	B	456	ASN	C-O	-5.52	1.17	1.24
1	B	644	SER	C-O	-5.50	1.17	1.24
1	B	491	PRO	N-CD	5.49	1.55	1.47
1	B	476	PRO	C-O	-5.49	1.18	1.23
1	A	553	LEU	C-O	-5.48	1.18	1.23
1	B	637	GLU	C-N	5.47	1.40	1.33
1	A	655	GLY	C-O	-5.47	1.17	1.23
1	B	450	ASN	CA-C	-5.46	1.49	1.53
1	A	617	GLU	C-O	-5.45	1.16	1.23
1	B	701	GLN	C-O	-5.44	1.17	1.24
1	B	552	PRO	N-CD	5.44	1.55	1.47
1	A	693	SER	C-O	-5.43	1.17	1.24
1	B	476	PRO	N-CD	5.43	1.55	1.47
1	B	654	ILE	C-O	-5.43	1.17	1.23
1	B	652	ILE	C-N	5.42	1.40	1.33
1	A	832	ALA	C-O	-5.41	1.17	1.24
1	B	691	ALA	C-O	-5.41	1.17	1.24
1	A	614	MET	C-O	-5.40	1.17	1.24
1	B	477	GLU	C-O	-5.40	1.17	1.24
1	A	636	ILE	C-O	-5.38	1.18	1.24
1	A	433	GLU	C-O	-5.37	1.17	1.23
1	B	772	LEU	C-N	5.35	1.40	1.33
1	A	466	GLY	C-N	5.33	1.40	1.33
1	A	585	ILE	C-O	-5.33	1.18	1.24
1	A	825	PRO	C-O	-5.33	1.18	1.24
1	A	840	ALA	C-O	-5.33	1.17	1.24
1	B	643	LEU	C-O	-5.33	1.17	1.23
1	A	434	ALA	C-O	-5.31	1.17	1.23
1	B	403	ASN	C-N	5.31	1.40	1.34
1	A	833	GLU	C-O	-5.30	1.17	1.24
1	A	725	TYR	C-N	5.29	1.40	1.34
1	B	486	LEU	C-O	-5.28	1.18	1.24
1	B	695	LEU	C-O	-5.28	1.18	1.24
1	A	453	PRO	C-O	-5.27	1.17	1.24
1	B	638	PRO	N-CD	5.27	1.55	1.47
1	A	688	SER	C-O	-5.27	1.17	1.24
1	B	809	ILE	C-O	-5.26	1.18	1.24
1	B	593	ILE	C-O	-5.25	1.18	1.25
1	B	459	LYS	C-O	-5.25	1.18	1.24
1	B	594	PRO	C-N	5.24	1.40	1.33
1	B	460	ASN	C-O	-5.23	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	LEU	C-O	-5.23	1.17	1.23
1	B	686	LEU	C-O	-5.23	1.18	1.24
1	A	726	PRO	N-CD	5.22	1.55	1.47
1	B	692	LEU	C-O	-5.22	1.18	1.24
1	A	403	ASN	C-N	5.21	1.40	1.34
1	A	644	SER	C-O	-5.20	1.17	1.24
1	A	677	HIS	C-O	-5.20	1.17	1.24
1	B	677	HIS	C-O	-5.20	1.17	1.24
1	A	653	PRO	C-O	-5.20	1.17	1.23
1	B	490	ALA	C-N	5.20	1.39	1.33
1	B	595	PRO	N-CD	5.19	1.55	1.47
1	A	834	ILE	C-O	-5.18	1.18	1.24
1	A	404	PRO	N-CD	5.18	1.55	1.47
1	B	420	ARG	C-O	-5.17	1.17	1.24
1	B	444	CYS	C-O	-5.17	1.17	1.24
1	A	380	PHE	C-O	-5.16	1.18	1.24
1	A	783	ALA	C-O	-5.16	1.18	1.24
1	B	382	ASP	C-O	-5.16	1.18	1.24
1	A	476	PRO	N-CD	5.15	1.54	1.47
1	A	521	PRO	N-CD	5.15	1.54	1.47
1	A	803	LEU	C-O	-5.15	1.18	1.24
1	B	681	TYR	C-O	-5.14	1.17	1.24
1	B	488	ARG	C-O	-5.13	1.17	1.24
1	B	800	VAL	C-O	-5.13	1.18	1.24
1	A	385	ILE	C-O	-5.13	1.18	1.24
1	B	825	PRO	C-N	5.12	1.40	1.33
1	A	707	ALA	C-O	-5.12	1.18	1.24
1	A	623	GLY	C-O	-5.11	1.17	1.24
1	B	418	VAL	C-O	-5.11	1.18	1.24
1	B	698	ILE	C-O	-5.11	1.18	1.24
1	B	458	LEU	C-O	-5.10	1.18	1.24
1	B	585	ILE	C-O	-5.10	1.19	1.24
1	A	506	ALA	C-O	-5.08	1.17	1.24
1	A	599	LEU	C-N	-5.08	1.26	1.33
1	B	451	PRO	N-CD	5.07	1.54	1.47
1	A	397	ARG	C-O	-5.06	1.18	1.24
1	B	579	ALA	C-O	-5.06	1.17	1.23
1	A	374	PRO	N-CD	5.06	1.54	1.47
1	B	455	VAL	C-O	-5.05	1.18	1.24
1	A	526	LEU	C-O	-5.05	1.17	1.23
1	A	436	LEU	C-O	-5.05	1.17	1.24
1	B	380	PHE	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	GLY	C-O	-5.04	1.17	1.23
1	B	773	PRO	N-CD	5.04	1.54	1.47
1	B	457	ALA	C-O	-5.03	1.18	1.24
1	B	453	PRO	N-CD	5.03	1.54	1.47
1	B	579	ALA	CA-C	-5.03	1.46	1.52
1	B	505	GLU	C-O	-5.03	1.17	1.24
1	A	456	ASN	C-O	-5.03	1.18	1.24
1	B	709	ARG	C-O	-5.03	1.18	1.24
1	A	829	ILE	C-O	-5.02	1.18	1.24
1	B	653	PRO	N-CD	5.02	1.54	1.47
1	B	619	GLN	C-O	-5.01	1.17	1.24
1	A	642	MET	C-O	-5.01	1.18	1.24
1	A	773	PRO	N-CD	5.01	1.54	1.47

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	GLY	N-CA-C	10.92	130.58	114.10
1	B	551	THR	C-N-CD	7.73	137.61	120.60
1	B	490	ALA	CA-C-N	-7.28	113.31	120.52
1	B	490	ALA	C-N-CA	-7.28	113.31	120.52
1	B	475	ILE	N-CA-C	7.25	114.72	107.55
1	B	723	ALA	N-CA-C	-7.17	104.54	113.28
1	A	637	GLU	CA-C-N	-7.14	113.35	120.21
1	A	637	GLU	C-N-CA	-7.14	113.35	120.21
1	A	824	GLN	CA-C-N	-7.06	113.11	120.38
1	A	824	GLN	C-N-CA	-7.06	113.11	120.38
1	A	593	ILE	CA-C-N	-6.96	113.21	120.38
1	A	593	ILE	C-N-CA	-6.96	113.21	120.38
1	A	490	ALA	CA-C-N	-6.85	113.45	120.85
1	A	490	ALA	C-N-CA	-6.85	113.45	120.85
1	A	594	PRO	CA-C-N	-6.82	113.28	120.03
1	A	594	PRO	C-N-CA	-6.82	113.28	120.03
1	A	723	ALA	N-CA-C	-6.75	104.95	112.57
1	B	824	GLN	CA-C-N	-6.67	113.51	120.38
1	B	824	GLN	C-N-CA	-6.67	113.51	120.38
1	B	466	GLY	CA-C-N	-6.66	113.12	119.85
1	B	466	GLY	C-N-CA	-6.66	113.12	119.85
1	B	477	GLU	N-CA-C	6.65	118.53	111.28
1	A	520	LYS	CA-C-N	-6.59	113.42	120.47
1	A	520	LYS	C-N-CA	-6.59	113.42	120.47
1	A	558	VAL	N-CA-C	6.51	118.18	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	LYS	CA-C-N	-6.43	113.58	120.47
1	B	520	LYS	C-N-CA	-6.43	113.58	120.47
1	B	450	ASN	CA-C-N	-6.40	113.18	119.90
1	B	450	ASN	C-N-CA	-6.40	113.18	119.90
1	A	744	GLN	N-CA-C	6.34	118.77	107.80
1	B	373	LEU	CA-C-N	-6.33	113.44	120.14
1	B	373	LEU	C-N-CA	-6.33	113.44	120.14
1	B	560	VAL	CA-C-N	-6.21	113.88	120.03
1	B	560	VAL	C-N-CA	-6.21	113.88	120.03
1	B	532	GLY	N-CA-C	6.17	118.33	112.04
1	A	725	TYR	CA-C-N	-6.14	113.36	119.56
1	A	725	TYR	C-N-CA	-6.14	113.36	119.56
1	B	388	THR	CA-C-N	-6.11	113.39	119.99
1	B	388	THR	C-N-CA	-6.11	113.39	119.99
1	A	373	LEU	CA-C-N	-6.02	113.77	119.85
1	A	373	LEU	C-N-CA	-6.02	113.77	119.85
1	B	772	LEU	CA-C-N	-5.88	113.89	119.89
1	B	772	LEU	C-N-CA	-5.88	113.89	119.89
1	A	466	GLY	CA-C-N	-5.72	114.07	119.85
1	A	466	GLY	C-N-CA	-5.72	114.07	119.85
1	B	793	GLU	N-CA-C	-5.72	105.12	111.36
1	A	825	PRO	CA-C-N	-5.72	114.06	119.90
1	A	825	PRO	C-N-CA	-5.72	114.06	119.90
1	B	637	GLU	CA-C-N	-5.69	113.84	119.92
1	B	637	GLU	C-N-CA	-5.69	113.84	119.92
1	B	594	PRO	CA-C-N	-5.57	114.04	119.78
1	B	594	PRO	C-N-CA	-5.57	114.04	119.78
1	A	652	ILE	CA-C-N	-5.51	113.88	119.83
1	A	652	ILE	C-N-CA	-5.51	113.88	119.83
1	B	825	PRO	N-CA-C	5.50	117.41	110.70
1	B	838	VAL	N-CA-C	-5.43	105.42	110.53
1	A	812	PHE	N-CA-C	5.42	115.28	108.45
1	A	584	PRO	CA-N-CD	-5.38	104.47	112.00
1	B	825	PRO	CA-C-N	-5.37	114.22	119.76
1	B	825	PRO	C-N-CA	-5.37	114.22	119.76
1	A	543	ARG	N-CA-C	5.33	116.89	107.61
1	B	596	ALA	N-CA-C	5.33	122.14	110.80
1	B	558	VAL	N-CA-C	5.32	115.43	107.51
1	B	686	LEU	N-CA-C	5.28	116.73	110.97
1	A	767	THR	CB-CA-C	-5.25	101.10	110.70
1	B	774	ASP	CA-C-N	-5.23	113.36	119.32
1	B	774	ASP	C-N-CA	-5.23	113.36	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	622	LEU	N-CA-C	5.21	118.91	112.24
1	B	726	PRO	CA-N-CD	-5.19	104.73	112.00
1	A	774	ASP	CA-C-N	-5.15	113.88	119.24
1	A	774	ASP	C-N-CA	-5.15	113.88	119.24
1	A	426	GLN	N-CA-C	5.14	117.87	109.59
1	A	544	ASP	N-CA-C	5.14	117.62	111.71
1	B	428	TYR	N-CA-C	5.12	117.75	109.40
1	A	815	ALA	N-CA-C	5.12	117.75	111.82
1	B	849	SER	N-CA-C	-5.07	104.81	111.96
1	B	558	VAL	CB-CA-C	-5.07	104.22	111.31
1	A	403	ASN	CA-C-N	-5.06	113.82	119.19
1	A	403	ASN	C-N-CA	-5.06	113.82	119.19
1	B	832	ALA	N-CA-C	5.06	116.80	111.28
1	B	593	ILE	CA-C-N	-5.04	115.19	120.38
1	B	593	ILE	C-N-CA	-5.04	115.19	120.38
1	B	652	ILE	CA-C-N	-5.04	114.39	119.83
1	B	652	ILE	C-N-CA	-5.04	114.39	119.83
1	A	384	VAL	N-CA-C	5.01	115.24	110.53

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	3563	0	3567	104	0
1	B	3554	0	3558	139	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
4	A	160	0	0	5	0
4	B	184	0	0	6	0
All	All	7493	0	7137	229	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 16.

All (229) 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:727:PHE:HB3	1:A:744:GLN:NE2	1.44	1.32
1:A:588:GLU:O	1:A:816:ASN:HB2	1.43	1.14
1:B:388:THR:HG22	4:B:1037:HOH:O	1.55	1.06
1:A:727:PHE:CB	1:A:744:GLN:HE21	1.69	1.05
1:A:727:PHE:HB3	1:A:744:GLN:HE21	0.89	1.04
1:A:588:GLU:HG3	1:A:815:ALA:HB3	1.47	0.96
1:A:675:LEU:HD21	1:B:406:MET:HE2	1.50	0.93
1:A:727:PHE:CB	1:A:744:GLN:NE2	2.30	0.93
1:A:397:ARG:HD3	1:B:484:GLU:OE2	1.70	0.91
1:A:589:GLY:O	1:A:592:HIS:CD2	2.26	0.89
1:B:438:MET:HB2	1:B:810:LEU:O	1.73	0.88
1:A:413:GLN:O	1:A:801:THR:HG23	1.75	0.86
1:A:545:LYS:CE	1:A:815:ALA:O	2.25	0.84
1:B:660:ARG:HD2	4:B:1182:HOH:O	1.79	0.81
1:B:614:MET:HE2	1:B:640:VAL:HG21	1.62	0.81
1:A:850:THR:O	1:A:854:LEU:HD13	1.81	0.80
1:B:543:ARG:HD3	1:B:816:ASN:HB3	1.64	0.80
1:B:843:THR:O	1:B:846:GLU:HG2	1.81	0.80
1:B:854:LEU:HD13	1:B:854:LEU:H	1.46	0.78
1:A:842:ALA:O	1:A:846:GLU:HG3	1.82	0.78
1:B:372:ALA:HB3	1:B:373:LEU:HA	1.65	0.77
1:A:588:GLU:O	1:A:816:ASN:CB	2.29	0.75
1:A:699:LEU:HD12	1:B:381:ILE:CD1	2.17	0.75
1:B:422:ALA:HB2	1:B:427:LEU:HD23	1.68	0.74
1:A:588:GLU:CG	1:A:815:ALA:HB3	2.18	0.74
1:B:785:ASP:O	1:B:788:GLU:N	2.21	0.74
1:B:741:GLN:HG3	1:B:742:PHE:N	2.03	0.73
1:B:588:GLU:O	1:B:816:ASN:HB2	1.89	0.73
1:B:620:THR:HG22	1:B:737:MET:HE1	1.70	0.73
1:B:661:ALA:O	1:B:665:GLN:HG2	1.89	0.72
1:B:581:MET:SD	1:B:642:MET:HE1	2.31	0.71
1:B:409:PHE:O	1:B:412:LEU:HB3	1.90	0.71
1:B:740:ILE:HD12	1:B:823:ILE:HD11	1.72	0.70
1:A:563:GLY:HA2	1:A:598:TYR:CE1	2.27	0.70
1:B:514:ALA:HB2	1:B:614:MET:HE1	1.73	0.70
1:B:603:GLN:HE21	1:B:607:ARG:NH2	1.90	0.69
1:B:817:SER:HB3	4:B:1062:HOH:O	1.93	0.69
1:A:484:GLU:OE2	1:B:397:ARG:NE	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:SER:OG	1:A:819:THR:HG22	1.94	0.68
1:A:545:LYS:HE2	1:A:815:ALA:O	1.94	0.67
1:A:740:ILE:HG13	1:A:823:ILE:HD13	1.76	0.67
1:B:526:LEU:HD13	1:B:562:PHE:HD1	1.60	0.67
1:A:633:TRP:CE2	1:A:734:ARG:HD3	2.30	0.67
1:B:372:ALA:HB3	1:B:373:LEU:CA	2.26	0.66
1:B:484:GLU:O	1:B:488:ARG:HG2	1.96	0.66
1:B:799:PHE:CE1	1:B:844:VAL:HG12	2.31	0.66
1:A:721:ILE:HD11	1:A:838:VAL:HG13	1.78	0.65
1:A:675:LEU:HD21	1:B:406:MET:CE	2.25	0.65
1:B:799:PHE:HE2	1:B:841:PHE:CD1	2.13	0.65
1:B:568:LEU:HD23	1:B:605:LEU:HD23	1.79	0.65
1:B:721:ILE:O	1:B:724:ARG:HB2	1.97	0.65
1:B:590:GLY:O	1:B:732:ARG:NH2	2.23	0.64
1:B:526:LEU:HD13	1:B:562:PHE:CD1	2.33	0.64
1:B:843:THR:O	1:B:847:GLU:HG3	1.99	0.63
1:A:569:ARG:NH1	1:A:608:GLU:OE1	2.28	0.63
1:A:721:ILE:CD1	1:A:838:VAL:HG13	2.29	0.62
1:A:741:GLN:HE22	1:A:819:THR:HG23	1.63	0.62
1:B:785:ASP:O	1:B:788:GLU:HB3	1.99	0.62
1:B:639:ASP:OD1	1:B:660:ARG:NH2	2.33	0.61
1:B:854:LEU:H	1:B:854:LEU:CD1	2.13	0.61
1:B:446:ASN:OD1	1:B:624:ARG:NH2	2.34	0.61
1:A:579:ALA:HA	1:A:611:VAL:HG13	1.83	0.60
1:B:619:GLN:OE1	1:B:824:GLN:NE2	2.34	0.60
1:B:799:PHE:CE2	1:B:841:PHE:CE1	2.89	0.60
1:B:591:VAL:O	1:B:591:VAL:HG13	2.01	0.60
1:A:373:LEU:HD23	1:A:374:PRO:CD	2.32	0.60
1:B:514:ALA:HB2	1:B:614:MET:CE	2.30	0.60
1:B:670:THR:OG1	1:B:673:ARG:HG3	2.02	0.60
1:B:770:LYS:HD3	1:B:771:PHE:CE2	2.37	0.60
1:B:496:ARG:NH1	1:B:665:GLN:HE22	2.01	0.59
1:A:652:ILE:HD12	1:A:690:VAL:HG21	1.85	0.59
1:B:398:TYR:HD1	1:B:407:VAL:CG2	2.15	0.59
1:B:727:PHE:O	1:B:743:ASP:N	2.32	0.59
1:A:699:LEU:CD1	1:B:381:ILE:CD1	2.82	0.58
1:B:799:PHE:CE2	1:B:841:PHE:CD1	2.91	0.58
1:A:620:THR:HG22	1:A:737:MET:HE1	1.84	0.58
1:B:615:VAL:HG21	1:B:638:PRO:HG3	1.84	0.57
1:B:496:ARG:NH1	1:B:665:GLN:NE2	2.53	0.57
1:B:398:TYR:CD1	1:B:407:VAL:CG2	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:PHE:CE2	1:A:799:PHE:CE1	2.92	0.57
1:B:571:ALA:O	1:B:574:ARG:HG3	2.04	0.57
1:A:426:GLN:HE21	1:A:434:ALA:HB1	1.70	0.55
1:A:373:LEU:HD23	1:A:374:PRO:HD3	1.87	0.55
1:B:710:MET:HE3	1:B:834:ILE:HD12	1.89	0.55
1:B:530:TYR:HA	1:B:541:THR:HG23	1.88	0.55
1:A:612:LEU:HD21	1:A:663:LEU:HD21	1.89	0.55
1:B:372:ALA:CB	1:B:373:LEU:CA	2.85	0.54
1:A:668:TYR:HA	1:A:673:ARG:HB3	1.89	0.54
1:B:720:GLU:HB2	4:B:1151:HOH:O	2.08	0.54
1:A:545:LYS:NZ	1:A:815:ALA:O	2.41	0.53
1:B:541:THR:O	1:B:547:ARG:HD2	2.08	0.53
1:A:589:GLY:O	1:A:592:HIS:HD2	1.85	0.53
1:A:668:TYR:CE1	1:A:676:VAL:CG1	2.91	0.53
1:B:790:ALA:O	1:B:794:MET:HG3	2.08	0.53
1:A:441:GLY:N	4:A:1067:HOH:O	2.33	0.53
1:A:853:ASP:C	1:A:854:LEU:HD12	2.34	0.53
1:A:548:ARG:NH2	4:A:1147:HOH:O	2.41	0.53
1:A:742:PHE:HE2	1:A:799:PHE:CE1	2.27	0.52
1:B:591:VAL:HG13	1:B:732:ARG:HB2	1.90	0.52
1:A:589:GLY:O	1:A:592:HIS:NE2	2.42	0.52
1:A:710:MET:HE2	1:A:834:ILE:HD12	1.91	0.52
1:A:744:GLN:O	1:A:745:ALA:HB3	2.09	0.52
1:B:799:PHE:CD1	1:B:848:LEU:HD12	2.45	0.52
1:B:507:VAL:HG22	1:B:642:MET:SD	2.50	0.51
1:B:854:LEU:CD1	1:B:854:LEU:N	2.73	0.51
1:B:633:TRP:CB	1:B:734:ARG:NH1	2.74	0.51
1:A:641:LEU:HG	1:A:642:MET:N	2.26	0.51
1:B:727:PHE:O	1:B:742:PHE:HA	2.11	0.51
1:B:555:ASP:O	1:B:556:ALA:HB3	2.10	0.51
1:B:620:THR:CG2	1:B:737:MET:HE1	2.38	0.51
1:A:840:ALA:O	1:A:844:VAL:HG23	2.11	0.51
1:A:397:ARG:CD	1:B:484:GLU:OE2	2.53	0.50
1:A:594:PRO:HG2	1:A:599:LEU:HD11	1.93	0.50
1:A:727:PHE:CA	1:A:744:GLN:NE2	2.74	0.50
1:B:673:ARG:HA	1:B:676:VAL:HG23	1.93	0.50
1:B:696:ARG:HD3	1:B:696:ARG:C	2.36	0.50
1:A:588:GLU:HG3	1:A:815:ALA:CB	2.31	0.50
1:B:837:PHE:CD1	1:B:837:PHE:C	2.89	0.50
1:A:617:GLU:HG3	1:A:641:LEU:HD11	1.94	0.50
1:B:430:ASP:HB2	4:B:1122:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:NH1	4:A:1101:HOH:O	2.45	0.49
1:A:767:THR:OG1	1:A:768:THR:N	2.43	0.49
1:A:699:LEU:CD1	1:B:381:ILE:HD11	2.42	0.49
1:B:854:LEU:HD13	1:B:854:LEU:N	2.22	0.49
1:A:616:ASP:HA	1:A:642:MET:HB2	1.95	0.49
1:B:461:TYR:CE2	1:B:466:GLY:HA3	2.48	0.49
1:B:824:GLN:O	1:B:824:GLN:HG2	2.12	0.49
1:B:588:GLU:HB2	1:B:816:ASN:CG	2.38	0.49
1:B:458:LEU:HD11	1:B:652:ILE:HD11	1.94	0.48
1:B:543:ARG:CD	1:B:816:ASN:HB3	2.40	0.48
1:B:780:LEU:O	1:B:784:MET:HB2	2.13	0.48
1:A:796:CYS:O	1:A:799:PHE:HB2	2.13	0.48
1:B:846:GLU:CG	1:B:847:GLU:N	2.77	0.48
1:A:742:PHE:HE1	1:A:821:ILE:HG13	1.79	0.48
1:B:796:CYS:SG	1:B:819:THR:HA	2.54	0.48
1:A:467:PRO:O	1:A:685:ASN:HB2	2.14	0.48
1:A:579:ALA:CA	1:A:611:VAL:HG13	2.43	0.48
1:A:618:VAL:HG12	1:A:645:LYS:HD2	1.96	0.47
1:B:588:GLU:HB3	1:B:816:ASN:H	1.79	0.47
1:B:697:GLU:OE2	1:B:701:GLN:NE2	2.41	0.47
1:B:741:GLN:HG3	1:B:742:PHE:H	1.76	0.47
1:A:391:ARG:NH2	1:A:416:ASP:O	2.44	0.47
1:A:496:ARG:NH1	1:A:664:TRP:CE3	2.83	0.47
1:B:799:PHE:CZ	1:B:844:VAL:HG12	2.50	0.47
1:A:850:THR:O	1:A:850:THR:HG22	2.15	0.47
1:A:836:ARG:NH1	4:A:1083:HOH:O	2.39	0.46
1:B:604:GLN:HE21	1:B:604:GLN:N	2.13	0.46
1:B:706:HIS:O	1:B:710:MET:HB2	2.15	0.46
1:A:740:ILE:HG13	1:A:823:ILE:CD1	2.45	0.46
1:A:400:GLN:O	1:B:496:ARG:NH2	2.49	0.46
1:A:648:SER:HB2	1:A:652:ILE:O	2.15	0.46
1:B:413:GLN:O	1:B:801:THR:HG23	2.15	0.46
1:A:572:LEU:HG	1:A:611:VAL:HG21	1.97	0.46
1:B:742:PHE:HE1	1:B:821:ILE:HG13	1.81	0.46
1:A:534:THR:HG22	1:B:508:GLU:HG2	1.98	0.45
1:A:581:MET:HE2	1:A:614:MET:HE3	1.98	0.45
1:B:848:LEU:O	1:B:852:LEU:HB2	2.15	0.45
1:B:373:LEU:HB3	1:B:374:PRO:CD	2.46	0.45
1:A:662:ASP:OD1	1:A:663:LEU:N	2.49	0.45
1:B:618:VAL:CG1	1:B:645:LYS:HD2	2.47	0.45
1:A:824:GLN:O	1:A:824:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:PRO:CB	1:A:775:PRO:HD2	2.47	0.45
1:B:675:LEU:HD23	1:B:675:LEU:HA	1.72	0.45
1:B:372:ALA:HB3	1:B:373:LEU:C	2.42	0.44
1:A:584:PRO:O	1:A:585:ILE:HG13	2.17	0.44
1:A:740:ILE:CG1	1:A:823:ILE:HD13	2.45	0.44
1:B:454:VAL:HG12	1:B:651:LEU:HD12	1.99	0.44
1:B:851:PHE:O	1:B:851:PHE:CG	2.70	0.44
1:A:528:ASN:OD1	1:A:543:ARG:HD3	2.17	0.44
1:A:398:TYR:OH	4:A:1004:HOH:O	2.20	0.44
1:A:380:PHE:CZ	1:B:488:ARG:HG3	2.53	0.44
1:A:555:ASP:O	1:A:556:ALA:HB3	2.17	0.44
1:A:699:LEU:HD12	1:B:381:ILE:HD13	1.98	0.44
1:A:620:THR:HB	1:A:630:ALA:HB2	1.99	0.44
1:B:388:THR:CG2	4:B:1037:HOH:O	2.34	0.43
1:A:452:GLN:HB3	1:A:453:PRO:HD3	1.99	0.43
1:B:473:ILE:HD12	1:B:473:ILE:HA	1.88	0.43
1:B:791:LEU:HD23	1:B:791:LEU:HA	1.73	0.43
1:A:696:ARG:HD3	1:A:696:ARG:C	2.43	0.43
1:B:411:LYS:HE3	1:B:411:LYS:HB3	1.83	0.43
1:B:527:ARG:O	1:B:528:ASN:HB2	2.16	0.43
1:B:730:GLU:CD	1:B:732:ARG:HD3	2.43	0.43
1:A:413:GLN:O	1:A:415:CYS:SG	2.74	0.43
1:A:459:LYS:HG2	1:B:459:LYS:HG2	2.00	0.43
1:A:620:THR:CG2	1:A:737:MET:HE1	2.49	0.43
1:B:413:GLN:OE1	1:B:801:THR:OG1	2.37	0.43
1:B:721:ILE:HD13	1:B:842:ALA:HB2	2.00	0.43
1:A:730:GLU:OE2	1:A:732:ARG:NH2	2.50	0.43
1:B:413:GLN:HB3	1:B:415:CYS:SG	2.59	0.43
1:B:633:TRP:CG	1:B:734:ARG:NH1	2.87	0.43
1:A:526:LEU:HD11	1:A:582:ILE:HG22	2.00	0.43
1:B:618:VAL:HG12	1:B:645:LYS:HD2	2.00	0.43
1:B:846:GLU:C	1:B:848:LEU:H	2.27	0.43
1:A:413:GLN:C	1:A:415:CYS:HG	2.24	0.42
1:A:436:LEU:HB2	1:A:836:ARG:NH1	2.34	0.42
1:A:741:GLN:NE2	1:A:819:THR:HG23	2.32	0.42
1:A:795:PHE:O	1:A:798:LYS:HB3	2.19	0.42
1:B:710:MET:CE	1:B:834:ILE:HD12	2.48	0.42
1:B:733:GLY:HA3	1:B:738:LEU:HD23	2.02	0.42
1:B:769:TRP:HA	1:B:772:LEU:HD12	2.02	0.42
1:B:504:THR:HG21	1:B:534:THR:HG23	2.01	0.42
1:B:615:VAL:O	1:B:642:MET:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:GLN:HG2	1:B:388:THR:N	2.34	0.41
1:B:648:SER:C	1:B:650:GLY:N	2.76	0.41
1:B:701:GLN:HB2	1:B:703:LEU:HG	2.02	0.41
1:B:422:ALA:CB	1:B:427:LEU:HD23	2.44	0.41
1:B:797:MET:HE1	1:B:813:ILE:HG12	2.01	0.41
1:A:543:ARG:HB2	1:A:816:ASN:ND2	2.35	0.41
1:B:829:ILE:HG12	1:B:834:ILE:HG13	2.03	0.41
1:B:422:ALA:HB1	1:B:449:HIS:CG	2.56	0.41
1:B:603:GLN:HG2	1:B:604:GLN:NE2	2.35	0.41
1:B:791:LEU:HD23	1:B:794:MET:HE3	2.02	0.41
1:A:446:ASN:HB3	1:A:827:LEU:HD12	2.03	0.41
1:B:673:ARG:HA	1:B:676:VAL:CG2	2.51	0.41
1:A:454:VAL:HG12	1:A:651:LEU:HD12	2.03	0.41
1:B:544:ASP:OD2	1:B:548:ARG:NH2	2.53	0.41
1:B:790:ALA:O	1:B:794:MET:CG	2.69	0.41
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.95	0.41
1:B:530:TYR:CG	1:B:588:GLU:HG3	2.56	0.41
1:B:696:ARG:HD3	1:B:696:ARG:O	2.21	0.41
1:B:522:GLY:HA2	1:B:556:ALA:O	2.21	0.40
1:B:851:PHE:O	1:B:851:PHE:CD2	2.74	0.40
1:B:496:ARG:HH11	1:B:665:GLN:HE22	1.69	0.40
1:B:852:LEU:HD23	1:B:852:LEU:HA	1.71	0.40
1:A:579:ALA:HA	1:A:611:VAL:CG1	2.50	0.40
1:A:587:GLY:C	1:A:589:GLY:H	2.29	0.40
1:A:722:ALA:HB1	1:A:728:VAL:HG12	2.02	0.40
1:A:381:ILE:HD11	1:B:489:LEU:HD11	2.04	0.40
1:A:522:GLY:C	1:A:523:ILE:HG13	2.46	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	460/861 (53%)	432 (94%)	26 (6%)	2 (0%)	30	38
1	B	458/861 (53%)	440 (96%)	16 (4%)	2 (0%)	30	38
All	All	918/1722 (53%)	872 (95%)	42 (5%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	645	LYS
1	B	645	LYS
1	A	644	SER
1	B	644	SER

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	372/692 (54%)	352 (95%)	20 (5%)	20	29
1	B	371/692 (54%)	349 (94%)	22 (6%)	18	26
All	All	743/1384 (54%)	701 (94%)	42 (6%)	18	27

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LEU
1	A	415	CYS
1	A	497	VAL
1	A	521	PRO
1	A	572	LEU
1	A	584	PRO
1	A	588	GLU
1	A	600	GLN
1	A	604	GLN
1	A	607	ARG
1	A	641	LEU
1	A	642	MET

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Mol	Chain	Res	Type
1	A	645	LYS
1	A	708	GLU
1	A	770	LYS
1	A	791	LEU
1	A	808	LYS
1	A	823	ILE
1	A	836	ARG
1	A	855	GLU
1	B	392	GLU
1	B	413	GLN
1	B	415	CYS
1	B	497	VAL
1	B	508	GLU
1	B	521	PRO
1	B	543	ARG
1	B	544	ASP
1	B	572	LEU
1	B	604	GLN
1	B	609	THR
1	B	646	SER
1	B	716	GLN
1	B	721	ILE
1	B	729	SER
1	B	784	MET
1	B	810	LEU
1	B	813	ILE
1	B	821	ILE
1	B	838	VAL
1	B	845	CYS
1	B	854	LEU

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

Mol	Chain	Res	Type
1	A	387	GLN
1	A	426	GLN
1	A	546	HIS
1	A	586	GLN
1	A	741	GLN
1	A	744	GLN
1	A	777	GLN
1	B	399	HIS

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Mol	Chain	Res	Type
1	B	600	GLN
1	B	665	GLN
1	B	777	GLN
1	B	824	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are 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$
3	PLP	B	902	1	15,15,16	2.69	8 (53%)	21,22,23	1.65	5 (23%)
3	PLP	A	902	1	15,15,16	2.88	9 (60%)	21,22,23	1.91	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
3	PLP	B	902	1	-	1/6/6/8	0/1/1/1
3	PLP	A	902	1	-	2/6/6/8	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	PLP	C5-C4	5.92	1.47	1.40
3	B	902	PLP	C5-C4	5.44	1.46	1.40
3	A	902	PLP	C3-C2	4.12	1.45	1.41
3	B	902	PLP	C3-C2	4.06	1.45	1.41
3	A	902	PLP	P-O3P	-3.91	1.40	1.54
3	A	902	PLP	P-O2P	-3.78	1.40	1.54
3	B	902	PLP	P-O2P	-3.72	1.41	1.54
3	B	902	PLP	P-O3P	-3.49	1.41	1.54
3	A	902	PLP	P-O1P	-3.36	1.40	1.50
3	B	902	PLP	P-O1P	-3.13	1.40	1.50
3	A	902	PLP	C3-C4	3.00	1.45	1.40
3	B	902	PLP	C4A-C4	-2.99	1.45	1.51
3	B	902	PLP	O3-C3	-2.46	1.31	1.36
3	B	902	PLP	C3-C4	2.37	1.44	1.40
3	A	902	PLP	O3-C3	-2.33	1.31	1.36
3	A	902	PLP	P-O4P	-2.16	1.53	1.60
3	A	902	PLP	C4A-C4	-2.10	1.47	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	PLP	C4A-C4-C5	5.04	126.13	120.94
3	B	902	PLP	O3P-P-O2P	3.13	119.54	107.80
3	B	902	PLP	O4P-C5A-C5	2.77	114.54	109.36
3	A	902	PLP	O3P-P-O2P	2.66	117.79	107.80
3	B	902	PLP	C4A-C4-C5	2.62	123.64	120.94
3	B	902	PLP	C6-N1-C2	2.59	123.90	119.20
3	A	902	PLP	O4P-C5A-C5	2.43	113.92	109.36
3	A	902	PLP	C6-N1-C2	2.42	123.59	119.20
3	A	902	PLP	C3-C4-C5	-2.30	115.83	118.59
3	A	902	PLP	C2A-C2-N1	2.09	121.59	117.64
3	B	902	PLP	C2A-C2-N1	2.06	121.53	117.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	PLP	C6-C5-C5A-O4P
3	A	902	PLP	C4-C5-C5A-O4P
3	B	902	PLP	C5A-O4P-P-O1P

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	464/861 (53%)	-1.41	0 100 100	17, 33, 60, 93	0
1	B	462/861 (53%)	-1.38	0 100 100	17, 38, 68, 96	0
All	All	926/1722 (53%)	-1.40	0 100 100	17, 36, 65, 96	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	901	1/1	0.97	0.04	30,30,30,30	0
2	MG	B	901	1/1	0.99	0.04	30,30,30,30	0
3	PLP	A	902	15/16	1.00	0.02	21,26,33,35	0
3	PLP	B	902	15/16	1.00	0.03	24,29,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.