Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:42 PM GMT

PDB ID	:	4PPM
Title	:	Crystal structure of PigE: a transaminase involved in the biosynthesis of 2-methyl-3-n-amyl-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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

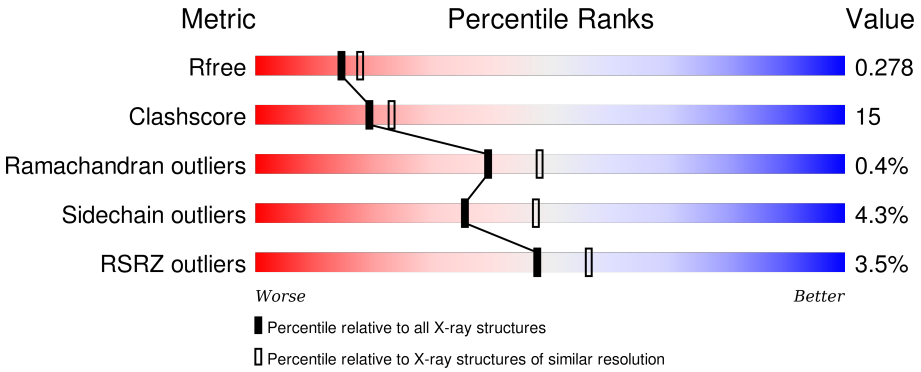
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 38% 15% • 46%
1	B	861	2% 35% 17% • 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
1	A	464	Total	C	N	O	S	0	0	0
			3563	2265	617	657	24			
1	B	462	Total	C	N	O	S	0	0	0
			3554	2263	615	652	24			

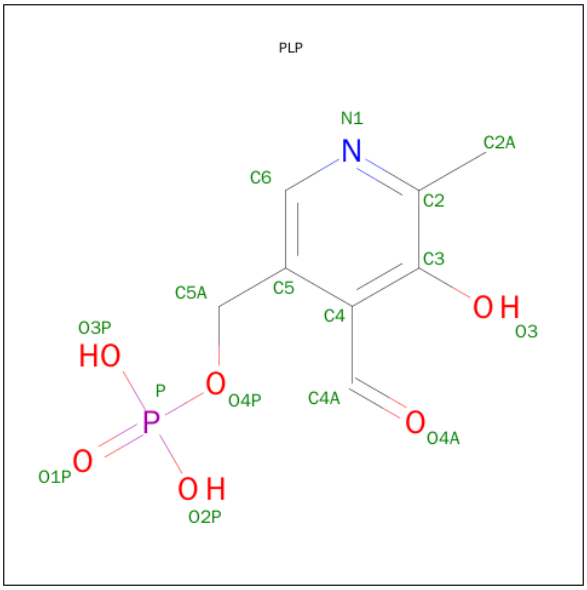
There are 16 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

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

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



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		

- Molecule 4 is water.

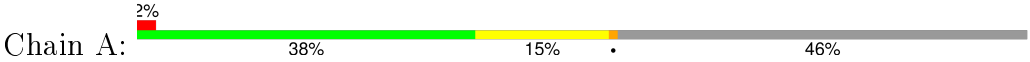
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total	O	0	0
			160	160		
4	B	184	Total	O	0	0
			184	184		

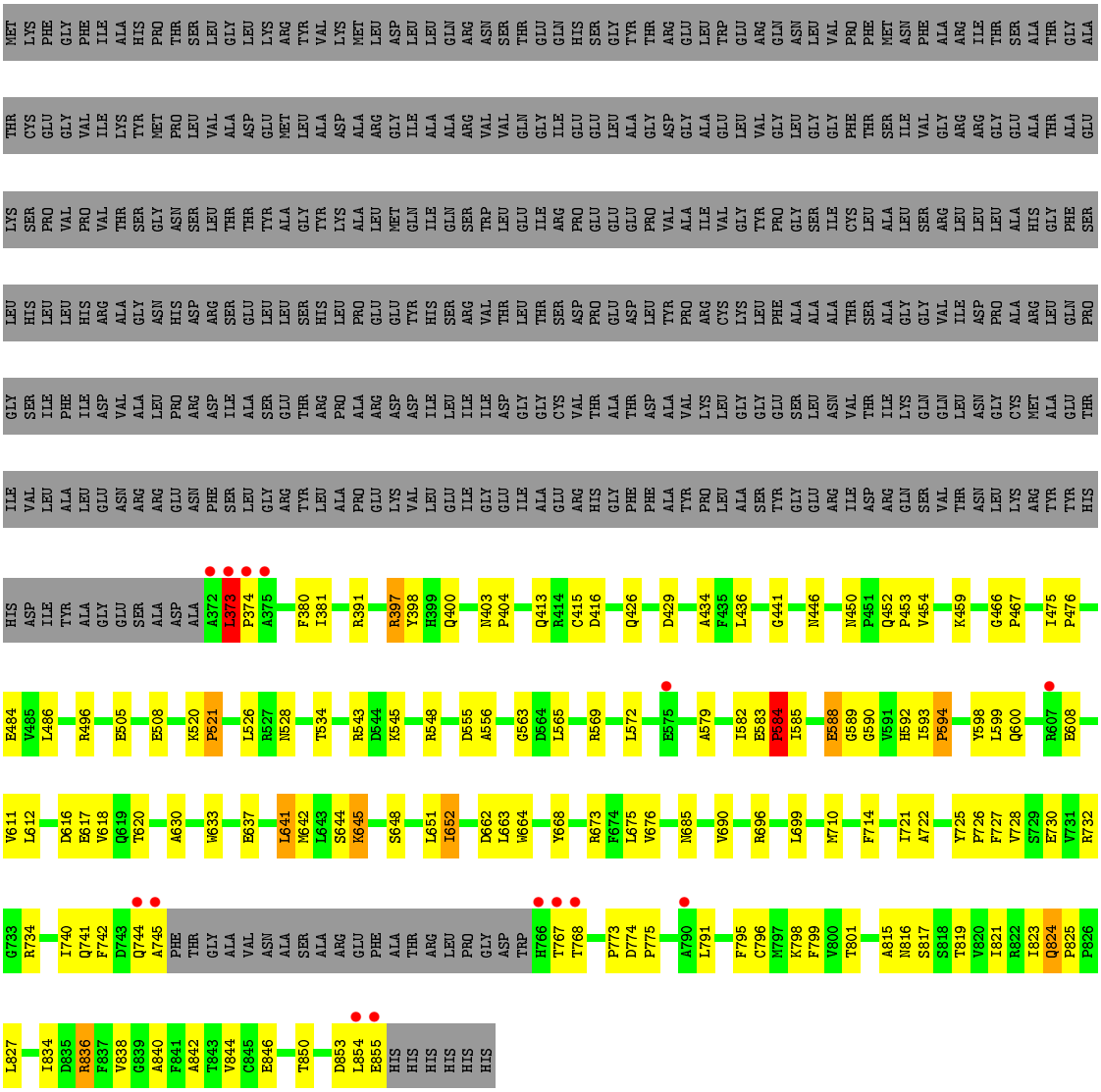
3 Residue-property plots (i)

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

- Molecule 1: Aminotransferase

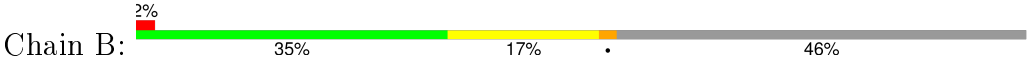
Chain A:

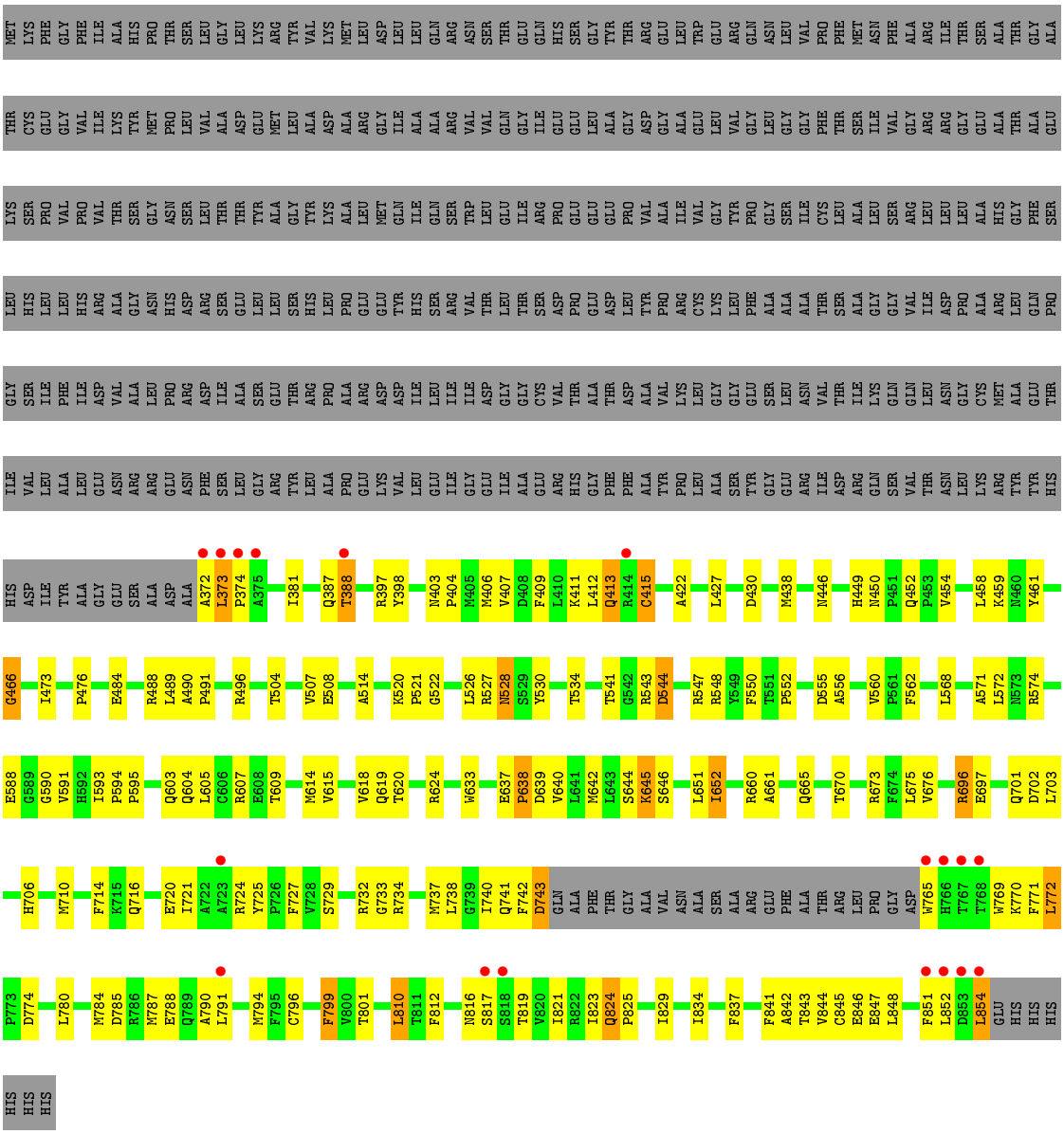




- Molecule 1: Aminotransferase

Chain B:




MET LYS PHE GLY PHE ILE ALA HIS PRO THR SER LEU GLY LEU LYS ARG TYR VAL LYS MET LEU ASP LEU LEU GLN ARG ASN SER THR GLU GLN HIS SER GLY TYR THR ARG GLU LEU GLN ARG GLN ASN LEU VAL PRO PHE MET ASN PHE ALA ARG ILE THR SER ALA THR GLY ALA
THR CYS GLU GLY VAL ILE LYS TYR MET PRO LEU VAL ALA ASP GLU MET LEU ALA ASP ALA ARG GLY ILE ALA ALA ARG VAL VAL GLN GLY ILE GLU GLU LEU ALA GLY ASP GLY ALA GLU LEU VAL GLY LEU GLY GLY PHE THR SER ILE VAL GLY ARG ARG GLY GLU ALA THR ALA GLU
LYS SER PRO VAL PRO VAL THR SER GLY ASN SER LEU THR THR TYR ALA GLY TYR LYS ALA LEU MET GLN ILE GLN SER TRP LEU GLU ILE ARG PRO GLU GLU GLU ILE ARG GLU PRO VAL ALA ILE VAL GLY TYR PRO GLY SER ILE CYS LEU ALA LEU LEU SER ARG LEU LEU LEU ALA HIS GLY PHE SER
LEU HIS LEU LEU HIS ARG ALA GLY ASN HIS ASP ARG SER GLU LEU LEU SER HIS LEU PRO ALA GLU GLU GLU ASP PRO ARG CYS LYS LEU PHE ALA ALA ALA THR SER ALA GLY GLY VAL ILE ASP PRO ALA ARG LEU GLN PRO
GLY SER ILE PHE ILE ASP VAL ALA LEU PRO ARG ASP ILE ALA SER GLU THR ARG PRO ALA ARG ASP ASP ILE LEU ILE ILE ASP GLY GLY CYS VAL THR ALA THR ASP ALA VAL LYS LEU GLY GLY GLU SER LEU ASN VAL THR ILE LYS GLN GLN LEU LEU ASN GLY CYS MET ALA GLU THR
ILE VAL LEU ALA LEU GLU ASN ARG ARG GLU ASN PHE SER LEU GLY ARG TYR LEU ALA PRO GLU LYS VAL LEU GLU ILE GLY GLU ILE ALA GLU ARG HIS GLY PHE PHE ALA TYR PRO LEU ALA SER TYR GLY GLU ARG ILE ASP ARG GLN SER VAL THR ASN LEU LYS ARG TYR HIS
HIS ASP ILE TYR ALA LEU GLU SER ALA ASP ALA A372 L373 P374 A375 I381 Q387 T388 R397 Y398 N403 P404 M405 M406 V407 D408 F409 L410 K411 L412 Q413 R414 C415 A422 L427 D430 M438 N446 H449 N450 P451 Q452 P453 V454 L458 K459 N460 Y461
G466 I473 P476 E484 R488 L489 A490 P491 R496 T504 V507 E508 A514 K520 P521 G522 L526 R527 N528 S529 Y530 T534 T541 G542 R543 D544 R547 R548 Y549 F550 T551 P552 D555 A556 V560 P561 F562 L568 A571 L572 N573 R574
E588 G589 G590 V591 H592 I593 P594 P595 Q603 Q604 L605 C606 R607 E608 T609 M614 V615 V618 Q619 T620 R624 w633 E637 P638 D639 V640 L641 M642 L643 S644 K645 S646 L651 I652 R660 A661 Q665 T670 R673 F674 L675 V676 R696 E697 Q701 D702 L703
H706 W710 F714 K715 Q716 E720 I721 A722 A723 R724 Y725 P726 F727 V728 S729 R732 G733 R734 M737 L738 G739 I740 Q741 F742 D743 GLN ALA PHE THR GLY ALA VAL ASN ALA SER ALA ARG GLU PHE ALA THR ARG LEU PRO GLY ASP W765 H766 T767 T768 W769 K770 F771 L772
P773 D774 L780 M784 D785 R786 M787 E788 Q789 A790 L791 M794 F795 C796 F799 V800 T801 L810 T811 F812 N816 S817 S818 T819 V820 I821 R822 I823 Q824 P825 I829 I834 F837 F841 A842 T843 V844 C845 E846 E847 L848 F851 L852 D853 L854 GLU 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
$< I/\sigma(I) >$ [1]	1.77 (at 2.30Å)	Xtriage
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 (5.28%)	DCC
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.5	EDS
Estimated twinning fraction	0.340 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 88591 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.41	7/3633 (0.2%)	0.94	19/4920 (0.4%)
1	B	1.36	6/3626 (0.2%)	0.95	20/4912 (0.4%)
All	All	1.39	13/7259 (0.2%)	0.95	39/9832 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	GLU	CD-OE2	-5.65	1.19	1.25
1	A	508	GLU	CD-OE1	-5.60	1.19	1.25
1	A	508	GLU	CD-OE2	-5.57	1.19	1.25
1	B	404	PRO	N-CD	5.52	1.55	1.47
1	B	552	PRO	N-CD	5.44	1.55	1.47
1	B	491	PRO	N-CD	5.42	1.55	1.47
1	B	476	PRO	N-CD	5.36	1.55	1.47
1	B	638	PRO	N-CD	5.20	1.55	1.47
1	A	726	PRO	N-CD	5.15	1.55	1.47
1	B	595	PRO	N-CD	5.12	1.55	1.47
1	A	404	PRO	N-CD	5.11	1.55	1.47
1	A	476	PRO	N-CD	5.08	1.54	1.47
1	A	521	PRO	N-CD	5.08	1.54	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	702	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	590	GLY	N-CA-C	6.99	130.58	113.10
1	A	593	ILE	C-N-CD	6.29	141.61	128.40
1	B	725	TYR	C-N-CD	6.16	141.34	128.40
1	A	594	PRO	C-N-CD	6.02	141.04	128.40
1	B	388	THR	C-N-CD	5.99	140.97	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	774	ASP	C-N-CD	5.93	140.85	128.40
1	B	373	LEU	C-N-CD	5.89	140.77	128.40
1	A	824	GLN	C-N-CD	5.85	140.68	128.40
1	A	583	GLU	C-N-CD	5.84	140.66	128.40
1	A	397	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	B	520	LYS	C-N-CD	5.81	140.60	128.40
1	A	637	GLU	C-N-CD	5.80	140.58	128.40
1	B	824	GLN	C-N-CD	5.76	140.49	128.40
1	A	466	GLY	C-N-CD	5.71	140.40	128.40
1	A	825	PRO	C-N-CD	5.64	140.25	128.40
1	B	560	VAL	C-N-CD	5.62	140.20	128.40
1	A	774	ASP	C-N-CD	5.59	140.13	128.40
1	A	652	ILE	C-N-CD	5.58	140.11	128.40
1	A	373	LEU	C-N-CD	5.54	140.04	128.40
1	A	520	LYS	C-N-CD	5.54	140.02	128.40
1	B	825	PRO	C-N-CD	5.53	140.02	128.40
1	B	772	LEU	C-N-CD	5.51	139.97	128.40
1	A	475	ILE	C-N-CD	5.50	139.95	128.40
1	B	652	ILE	C-N-CD	5.48	139.92	128.40
1	A	429	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	452	GLN	C-N-CD	5.41	139.77	128.40
1	B	594	PRO	C-N-CD	5.38	139.69	128.40
1	A	725	TYR	C-N-CD	5.34	139.61	128.40
1	A	450	ASN	C-N-CD	5.33	139.59	128.40
1	A	403	ASN	C-N-CD	5.32	139.57	128.40
1	B	696	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	B	450	ASN	C-N-CD	5.26	139.45	128.40
1	B	466	GLY	C-N-CD	5.22	139.36	128.40
1	B	490	ALA	C-N-CD	5.22	139.36	128.40
1	B	403	ASN	C-N-CD	5.13	139.18	128.40
1	B	637	GLU	C-N-CD	5.11	139.13	128.40
1	B	593	ILE	C-N-CD	5.09	139.09	128.40
1	A	584	PRO	CA-N-CD	-5.03	104.47	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3563	0	3567	100	0
1	B	3554	0	3558	132	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	216	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 15.

All (216) 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:B:514:ALA:HB2	1:B:614:MET:HE1	1.39	1.02
1:A:588:GLU:HG3	1:A:815:ALA:HB3	1.47	0.96
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: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:H	1:B:854:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:661:ALA:O	1:B:665:GLN:HG2	1.89	0.72
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: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
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:A:675:LEU:HD21	1:B:406:MET:CE	2.25	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: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:A:675:LEU:HD21	1:B:406:MET:HE2	1.78	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:770:LYS:HD3	1:B:771:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:THR:OG1	1:B:673:ARG:HG3	2.02	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:727:PHE:O	1:B:743:ASP:N	2.32	0.59
1:B:398:TYR:HD1	1:B:407:VAL:CG2	2.15	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: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
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: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:A:744:GLN:O	1:A:745:ALA:HB3	2.09	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:548:ARG:NH2	4:A:1147:HOH:O	2.41	0.53
1:A:710:MET:HE2	1:A:834:ILE:HD12	1.90	0.53
1:B:591:VAL:HG13	1:B:732:ARG:HB2	1.90	0.52
1:A:742:PHE:HE2	1:A:799:PHE:CE1	2.27	0.52
1:A:589:GLY:O	1:A:592:HIS:NE2	2.42	0.52
1:B:555:ASP:O	1:B:556:ALA:HB3	2.10	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:A:710:MET:HE2	1:A:834:ILE:CD1	2.41	0.51
1:B:633:TRP:CB	1:B:734:ARG:NH1	2.74	0.51
1:B:727:PHE:O	1:B:742:PHE:HA	2.11	0.51
1:A:641:LEU:HG	1:A:642:MET:N	2.26	0.51
1:B:710:MET:HE3	1:B:834:ILE:HD12	1.93	0.51
1:A:840:ALA:O	1:A:844:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:CD	1:B:484:GLU:OE2	2.53	0.50
1:A:767:THR:OG1	1:A:768:THR:N	2.43	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:A:594:PRO:HG2	1:A:599:LEU:HD11	1.93	0.50
1:A:588:GLU:HG3	1:A:815:ALA:CB	2.31	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
1:A:548:ARG:NH1	4:A:1101:HOH:O	2.45	0.49
1:B:854:LEU:N	1:B:854:LEU:HD13	2.22	0.49
1:A:699:LEU:CD1	1:B:381:ILE:HD11	2.42	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: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:853:ASP:C	1:A:854:LEU:HD12	2.34	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:579:ALA:CA	1:A:611:VAL:HG13	2.43	0.48
1:A:467:PRO:O	1:A:685:ASN:HB2	2.14	0.48
1:B:588:GLU:HB3	1:B:816:ASN:H	1.79	0.47
1:A:618:VAL:HG12	1:A:645:LYS:HD2	1.96	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:B:620:THR:HG22	1:B:737:MET:HE1	1.97	0.47
1:A:391:ARG:NH2	1:A:416:ASP:O	2.44	0.47
1:A:675:LEU:HD21	1:B:406:MET:HE1	1.95	0.47
1:B:799:PHE:CZ	1:B:844:VAL:HG12	2.50	0.47
1:A:496:ARG:NH1	1:A:664:TRP:CE3	2.83	0.47
1:A:850:THR:HG22	1:A:850:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:PHE:HE1	1:B:821:ILE:HG13	1.81	0.46
1:A:572:LEU:HG	1:A:611:VAL:HG21	1.97	0.46
1:A:534:THR:HG22	1:B:508:GLU:HG2	1.98	0.45
1:B:696:ARG:HD3	1:B:696:ARG:C	2.36	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:B:837:PHE:C	1:B:837:PHE:CD1	2.89	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
1:B:675:LEU:HD23	1:B:675:LEU:HA	1.72	0.45
1:A:773:PRO:CB	1:A:775:PRO:HD2	2.47	0.45
1:B:588:GLU:HB2	1:B:816:ASN:CG	2.38	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:A:584:PRO:O	1:A:585:ILE:HG13	2.17	0.44
1:B:851:PHE:CG	1:B:851:PHE:O	2.70	0.44
1:A:528:ASN:OD1	1:A:543:ARG:HD3	2.17	0.44
1:B:620:THR:HG22	1:B:737:MET:CE	2.47	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:699:LEU:HD12	1:B:381:ILE:HD13	1.98	0.44
1:A:555:ASP:O	1:A:556:ALA:HB3	2.17	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:B:791:LEU:HD23	1:B:791:LEU:HA	1.73	0.43
1:B:473:ILE:HD12	1:B:473:ILE:HA	1.88	0.43
1:A:452:GLN:HB3	1:A:453:PRO:HD3	1.99	0.43
1:B:411:LYS:HB3	1:B:411:LYS:HE3	1.83	0.43
1:B:527:ARG:O	1:B:528:ASN:HB2	2.16	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:B:721:ILE:HD13	1:B:842:ALA:HB2	2.00	0.43
1:B:413:GLN:OE1	1:B:801:THR:OG1	2.37	0.43
1:A:730:GLU:OE2	1:A:732:ARG:NH2	2.50	0.43
1:B:633:TRP:CG	1:B:734:ARG:NH1	2.87	0.43
1:B:413:GLN:HB3	1:B:415:CYS:SG	2.59	0.43
1:B:618:VAL:HG12	1:B:645:LYS:HD2	2.00	0.43
1:A:526:LEU:HD11	1:A:582:ILE:HG22	2.00	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:387:GLN:HG2	1:B:388:THR:N	2.34	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: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:614:MET:CE	1:B:640:VAL:HG21	2.50	0.41
1:B:673:ARG:HA	1:B:676:VAL:CG2	2.51	0.41
1:A:446:ASN:HB3	1:A:827:LEU:HD12	2.03	0.41
1:B:790:ALA:O	1:B:794:MET:CG	2.69	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:530:TYR:CG	1:B:588:GLU:HG3	2.56	0.41
1:B:696:ARG:O	1:B:696:ARG:HD3	2.21	0.41
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.95	0.41
1:B:522:GLY:HA2	1:B:556:ALA:O	2.21	0.40
1:B:851:PHE:CD2	1:B:851:PHE:O	2.74	0.40
1:B:496:ARG:HH11	1:B:665:GLN:HE22	1.69	0.40
1:B:852:LEU:HA	1:B:852:LEU:HD23	1.71	0.40
1:A:579:ALA:HA	1:A:611:VAL:CG1	2.50	0.40
1:A:722:ALA:HB1	1:A:728:VAL:HG12	2.02	0.40
1:A:675:LEU:HD11	1:B:406:MET:HE1	2.03	0.40
1:A:381:ILE:HD11	1:B:489:LEU:HD11	2.04	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%)	39 48
1	B	458/861 (53%)	440 (96%)	16 (4%)	2 (0%)	39 48
All	All	918/1722 (53%)	872 (95%)	42 (5%)	4 (0%)	39 48

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%)	360 (97%)	12 (3%)	46 62
1	B	371/692 (54%)	351 (95%)	20 (5%)	27 36
All	All	743/1384 (54%)	711 (96%)	32 (4%)	35 47

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LEU
1	A	521	PRO
1	A	565	LEU
1	A	584	PRO
1	A	588	GLU
1	A	600	GLN
1	A	641	LEU
1	A	696	ARG
1	A	714	PHE
1	A	791	LEU
1	A	836	ARG
1	A	855	GLU

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Mol	Chain	Res	Type
1	B	413	GLN
1	B	415	CYS
1	B	521	PRO
1	B	528	ASN
1	B	544	ASP
1	B	550	PHE
1	B	572	LEU
1	B	609	THR
1	B	646	SER
1	B	714	PHE
1	B	716	GLN
1	B	729	SER
1	B	743	ASP
1	B	765	TRP
1	B	787	MET
1	B	799	PHE
1	B	810	LEU
1	B	812	PHE
1	B	845	CYS
1	B	854	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	GLN
1	A	452	GLN
1	A	741	GLN
1	A	744	GLN
1	A	777	GLN
1	A	805	GLN
1	B	665	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 carbohydrates 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	A	902	1	15,15,16	3.09	9 (60%)	21,22,23	2.02	7 (33%)
3	PLP	B	902	1	15,15,16	2.94	7 (46%)	21,22,23	1.70	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	902	1	-	0/6/6/8	0/1/1/1
3	PLP	B	902	1	-	0/6/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	PLP	P-O3P	-4.02	1.40	1.54
3	A	902	PLP	P-O2P	-3.88	1.40	1.54
3	B	902	PLP	P-O2P	-3.82	1.41	1.54
3	B	902	PLP	P-O3P	-3.59	1.41	1.54
3	A	902	PLP	P-O1P	-3.39	1.40	1.51
3	B	902	PLP	P-O1P	-3.17	1.40	1.51
3	B	902	PLP	C4A-C4	-2.96	1.45	1.51
3	B	902	PLP	O3-C3	-2.47	1.31	1.37
3	A	902	PLP	O3-C3	-2.34	1.31	1.37
3	A	902	PLP	C4A-C4	-2.08	1.47	1.51
3	A	902	PLP	P-O4P	-2.02	1.53	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	PLP	C3-C4	2.32	1.45	1.40
3	B	902	PLP	C5-C4	5.30	1.46	1.40
3	A	902	PLP	C5-C4	5.77	1.47	1.40
3	B	902	PLP	C3-C2	6.38	1.45	1.40
3	A	902	PLP	C3-C2	6.47	1.45	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	PLP	C3-C4-C5	-2.70	115.83	118.78
3	A	902	PLP	C6-N1-C2	2.11	123.59	119.28
3	B	902	PLP	C6-N1-C2	2.27	123.90	119.28
3	A	902	PLP	O3P-P-O1P	2.46	118.50	110.58
3	A	902	PLP	C5A-C5-C4	2.54	125.02	121.65
3	B	902	PLP	C4A-C4-C5	2.64	123.64	120.88
3	A	902	PLP	O3P-P-O2P	2.73	117.79	107.38
3	A	902	PLP	O4P-C5A-C5	2.98	113.92	108.99
3	B	902	PLP	O3P-P-O2P	3.19	119.54	107.38
3	B	902	PLP	O4P-C5A-C5	3.36	114.54	108.99
3	A	902	PLP	C4A-C4-C5	5.04	126.13	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.22	14 (3%)	54	63	17, 33, 60, 93	0
1	B	462/861 (53%)	-0.14	18 (3%)	43	52	17, 38, 68, 96	0
All	All	926/1722 (53%)	-0.18	32 (3%)	48	56	17, 36, 65, 96	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	765	TRP	7.3
1	B	372	ALA	6.0
1	B	374	PRO	5.2
1	B	766	HIS	5.0
1	A	372	ALA	4.9
1	B	373	LEU	4.6
1	B	791	LEU	4.4
1	A	766	HIS	4.4
1	A	374	PRO	4.4
1	B	375	ALA	4.2
1	B	767	THR	3.8
1	A	373	LEU	3.8
1	A	854	LEU	3.7
1	B	818	SER	3.3
1	A	767	THR	3.1
1	B	851	PHE	3.1
1	A	855	GLU	3.1
1	B	768	THR	3.0
1	B	854	LEU	2.9
1	B	817	SER	2.9
1	B	852	LEU	2.7
1	B	853	ASP	2.6
1	A	745	ALA	2.4
1	A	790	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	607	ARG	2.3
1	A	744	GLN	2.2
1	A	768	THR	2.2
1	B	414	ARG	2.1
1	B	723	ALA	2.1
1	B	388	THR	2.1
1	A	575	GLU	2.0
1	A	375	ALA	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MG	B	901	1/1	0.88	0.20	0.47	30,30,30,30	0
3	PLP	A	902	15/16	0.97	0.08	-0.72	21,26,33,35	0
3	PLP	B	902	15/16	0.98	0.09	-0.88	24,29,33,34	0
2	MG	A	901	1/1	0.87	0.06	-1.91	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.