Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 10:38 pm BST

PDB ID	:	6S54
Title	:	Transaminase from Pseudomonas fluorescens
Authors	:	Smith, P.; Roura Padrosa, D.; Lopez-Gallego, F.; Paradisi, F.; Dreveny, I.
Deposited on	:	2019-06-30
Resolution	:	2.21 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 (i) symbol.

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

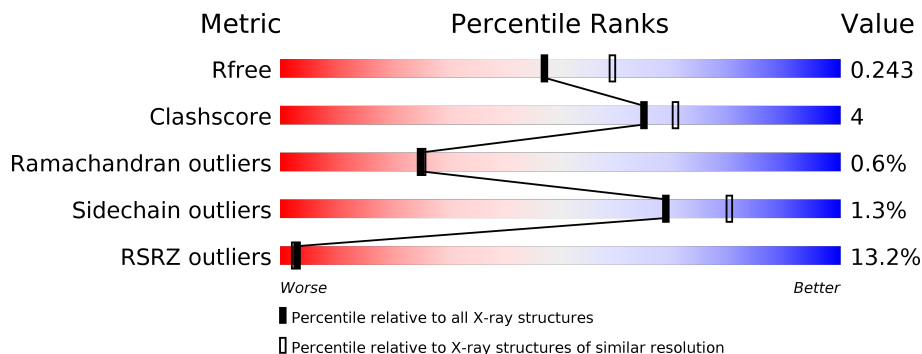|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.21 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		4
Ramachandran outliers		0.6%
Sidechain outliers		1.3%
RSRZ outliers		13.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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 <=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	479	89% 6% 5%
1	B	479	85% 9% 6%
1	C	479	27% 81% 12% 7%
1	D	479	23% 84% 9% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	C	1001	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14248 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 Aspartate aminotransferase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total 3489	C 2221	N 603	O 645	S 20	0	0	0
1	B	450	Total 3467	C 2210	N 598	O 639	S 20	0	0	0
1	C	447	Total 3432	C 2186	N 591	O 635	S 20	0	0	0
1	D	449	Total 3450	C 2198	N 595	O 637	S 20	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A2S8XV37
A	-18	GLY	-	expression tag	UNP A0A2S8XV37
A	-17	SER	-	expression tag	UNP A0A2S8XV37
A	-16	SER	-	expression tag	UNP A0A2S8XV37
A	-15	HIS	-	expression tag	UNP A0A2S8XV37
A	-14	HIS	-	expression tag	UNP A0A2S8XV37
A	-13	HIS	-	expression tag	UNP A0A2S8XV37
A	-12	HIS	-	expression tag	UNP A0A2S8XV37
A	-11	HIS	-	expression tag	UNP A0A2S8XV37
A	-10	HIS	-	expression tag	UNP A0A2S8XV37
A	-9	SER	-	expression tag	UNP A0A2S8XV37
A	-8	SER	-	expression tag	UNP A0A2S8XV37
A	-7	GLY	-	expression tag	UNP A0A2S8XV37
A	-6	LEU	-	expression tag	UNP A0A2S8XV37
A	-5	VAL	-	expression tag	UNP A0A2S8XV37
A	-4	PRO	-	expression tag	UNP A0A2S8XV37
A	-3	ARG	-	expression tag	UNP A0A2S8XV37
A	-2	GLY	-	expression tag	UNP A0A2S8XV37
A	-1	SER	-	expression tag	UNP A0A2S8XV37
A	0	HIS	-	expression tag	UNP A0A2S8XV37
A	1	MET	-	expression tag	UNP A0A2S8XV37

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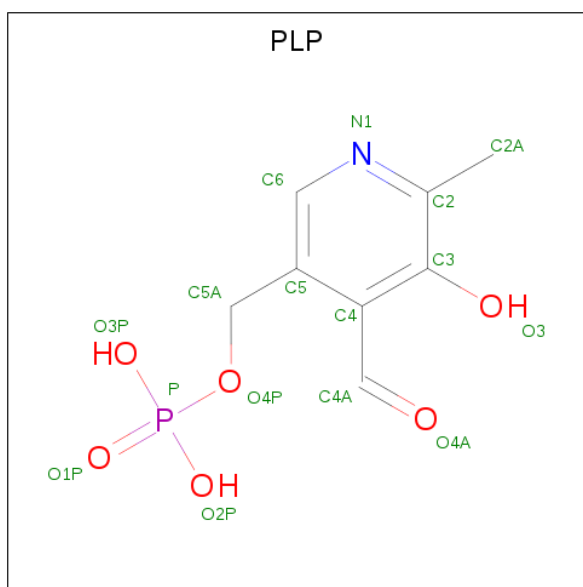
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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	-	expression tag	UNP A0A2S8XV37
A	3	PHE	-	expression tag	UNP A0A2S8XV37
A	4	LYS	-	expression tag	UNP A0A2S8XV37
A	5	ARG	-	expression tag	UNP A0A2S8XV37
A	6	SER	-	expression tag	UNP A0A2S8XV37
B	-19	MET	-	initiating methionine	UNP A0A2S8XV37
B	-18	GLY	-	expression tag	UNP A0A2S8XV37
B	-17	SER	-	expression tag	UNP A0A2S8XV37
B	-16	SER	-	expression tag	UNP A0A2S8XV37
B	-15	HIS	-	expression tag	UNP A0A2S8XV37
B	-14	HIS	-	expression tag	UNP A0A2S8XV37
B	-13	HIS	-	expression tag	UNP A0A2S8XV37
B	-12	HIS	-	expression tag	UNP A0A2S8XV37
B	-11	HIS	-	expression tag	UNP A0A2S8XV37
B	-10	HIS	-	expression tag	UNP A0A2S8XV37
B	-9	SER	-	expression tag	UNP A0A2S8XV37
B	-8	SER	-	expression tag	UNP A0A2S8XV37
B	-7	GLY	-	expression tag	UNP A0A2S8XV37
B	-6	LEU	-	expression tag	UNP A0A2S8XV37
B	-5	VAL	-	expression tag	UNP A0A2S8XV37
B	-4	PRO	-	expression tag	UNP A0A2S8XV37
B	-3	ARG	-	expression tag	UNP A0A2S8XV37
B	-2	GLY	-	expression tag	UNP A0A2S8XV37
B	-1	SER	-	expression tag	UNP A0A2S8XV37
B	0	HIS	-	expression tag	UNP A0A2S8XV37
B	1	MET	-	expression tag	UNP A0A2S8XV37
B	2	GLU	-	expression tag	UNP A0A2S8XV37
B	3	PHE	-	expression tag	UNP A0A2S8XV37
B	4	LYS	-	expression tag	UNP A0A2S8XV37
B	5	ARG	-	expression tag	UNP A0A2S8XV37
B	6	SER	-	expression tag	UNP A0A2S8XV37
C	-19	MET	-	initiating methionine	UNP A0A2S8XV37
C	-18	GLY	-	expression tag	UNP A0A2S8XV37
C	-17	SER	-	expression tag	UNP A0A2S8XV37
C	-16	SER	-	expression tag	UNP A0A2S8XV37
C	-15	HIS	-	expression tag	UNP A0A2S8XV37
C	-14	HIS	-	expression tag	UNP A0A2S8XV37
C	-13	HIS	-	expression tag	UNP A0A2S8XV37
C	-12	HIS	-	expression tag	UNP A0A2S8XV37
C	-11	HIS	-	expression tag	UNP A0A2S8XV37
C	-10	HIS	-	expression tag	UNP A0A2S8XV37
C	-9	SER	-	expression tag	UNP A0A2S8XV37

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP A0A2S8XV37
C	-7	GLY	-	expression tag	UNP A0A2S8XV37
C	-6	LEU	-	expression tag	UNP A0A2S8XV37
C	-5	VAL	-	expression tag	UNP A0A2S8XV37
C	-4	PRO	-	expression tag	UNP A0A2S8XV37
C	-3	ARG	-	expression tag	UNP A0A2S8XV37
C	-2	GLY	-	expression tag	UNP A0A2S8XV37
C	-1	SER	-	expression tag	UNP A0A2S8XV37
C	0	HIS	-	expression tag	UNP A0A2S8XV37
C	1	MET	-	expression tag	UNP A0A2S8XV37
C	2	GLU	-	expression tag	UNP A0A2S8XV37
C	3	PHE	-	expression tag	UNP A0A2S8XV37
C	4	LYS	-	expression tag	UNP A0A2S8XV37
C	5	ARG	-	expression tag	UNP A0A2S8XV37
C	6	SER	-	expression tag	UNP A0A2S8XV37
D	-19	MET	-	initiating methionine	UNP A0A2S8XV37
D	-18	GLY	-	expression tag	UNP A0A2S8XV37
D	-17	SER	-	expression tag	UNP A0A2S8XV37
D	-16	SER	-	expression tag	UNP A0A2S8XV37
D	-15	HIS	-	expression tag	UNP A0A2S8XV37
D	-14	HIS	-	expression tag	UNP A0A2S8XV37
D	-13	HIS	-	expression tag	UNP A0A2S8XV37
D	-12	HIS	-	expression tag	UNP A0A2S8XV37
D	-11	HIS	-	expression tag	UNP A0A2S8XV37
D	-10	HIS	-	expression tag	UNP A0A2S8XV37
D	-9	SER	-	expression tag	UNP A0A2S8XV37
D	-8	SER	-	expression tag	UNP A0A2S8XV37
D	-7	GLY	-	expression tag	UNP A0A2S8XV37
D	-6	LEU	-	expression tag	UNP A0A2S8XV37
D	-5	VAL	-	expression tag	UNP A0A2S8XV37
D	-4	PRO	-	expression tag	UNP A0A2S8XV37
D	-3	ARG	-	expression tag	UNP A0A2S8XV37
D	-2	GLY	-	expression tag	UNP A0A2S8XV37
D	-1	SER	-	expression tag	UNP A0A2S8XV37
D	0	HIS	-	expression tag	UNP A0A2S8XV37
D	1	MET	-	expression tag	UNP A0A2S8XV37
D	2	GLU	-	expression tag	UNP A0A2S8XV37
D	3	PHE	-	expression tag	UNP A0A2S8XV37
D	4	LYS	-	expression tag	UNP A0A2S8XV37
D	5	ARG	-	expression tag	UNP A0A2S8XV37
D	6	SER	-	expression tag	UNP A0A2S8XV37

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).

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

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
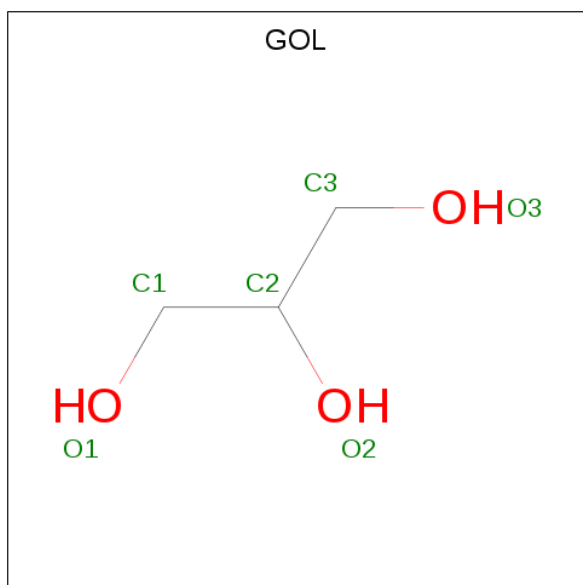
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
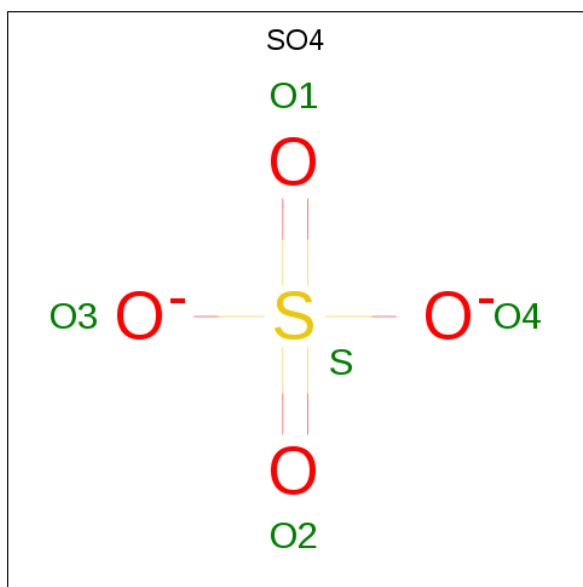
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total 158	O 158	0	0
5	B	126	Total 126	O 126	0	0
5	C	26	Total 26	O 26	0	0
5	D	18	Total 18	O 18	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.
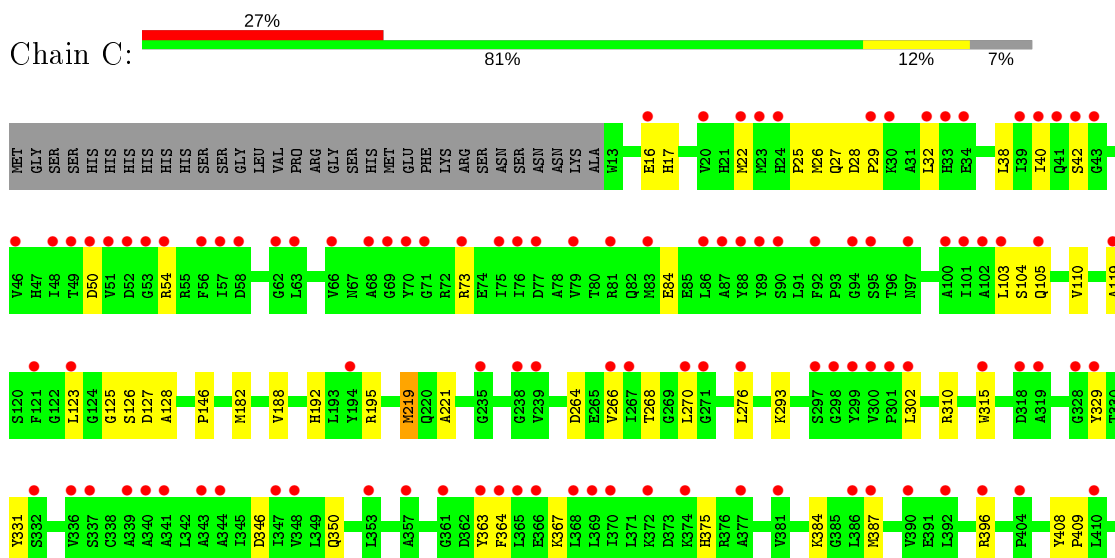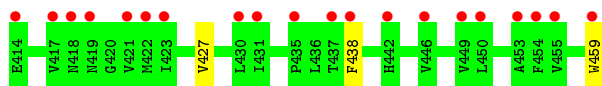
- Molecule 1: Aspartate aminotransferase family protein
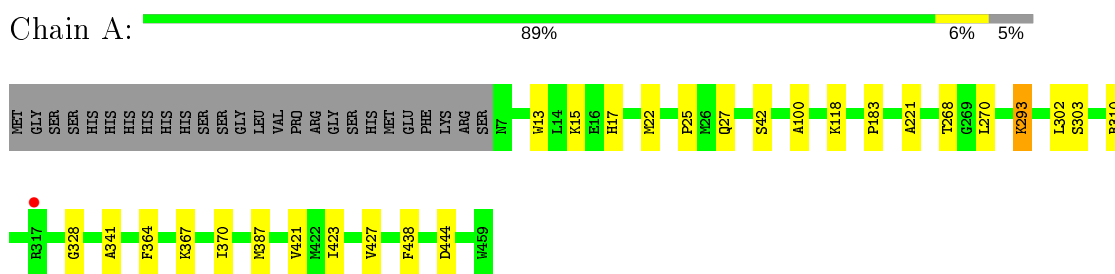
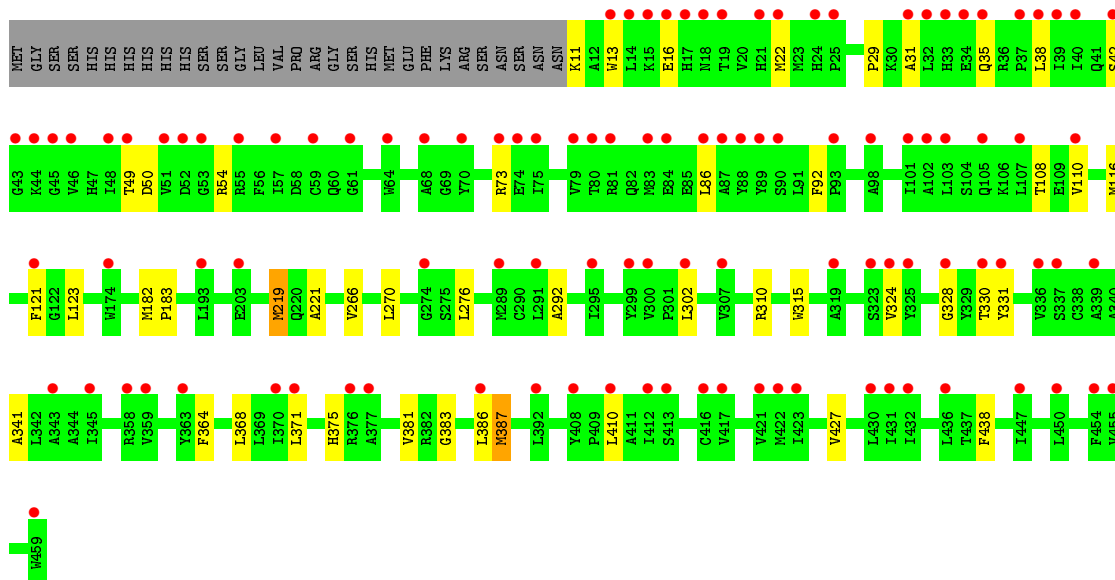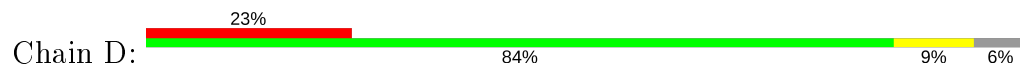- Molecule 1: Aspartate aminotransferase family protein

- Molecule 1: Aspartate aminotransferase family protein

• Molecule 1: Aspartate aminotransferase family protein

Chain D:
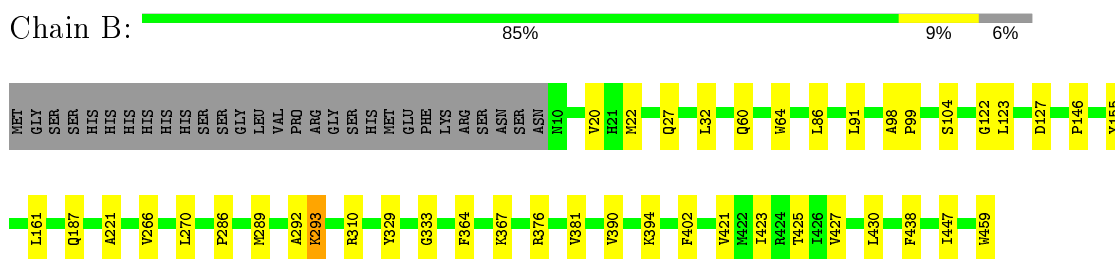
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.02Å 94.54Å 242.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.07 – 2.21 88.07 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (88.07-2.21) 99.8 (88.07-2.21)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.244 0.211 , 0.243	Depositor DCC
R_{free} test set	5323 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	1.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14248	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, SO4, PLP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.53	0/3570	0.67	0/4846
1	B	0.57	0/3548	0.66	0/4816
1	C	0.38	0/3511	0.58	0/4767
1	D	0.36	0/3529	0.57	0/4789
All	All	0.47	0/14158	0.62	0/19218

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	LEU	Peptide
1	B	270	LEU	Peptide
1	C	270	LEU	Peptide
1	D	270	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3489	0	3469	18	0
1	B	3467	0	3452	28	0
1	C	3432	0	3409	51	0
1	D	3450	0	3435	37	0
2	A	15	0	6	3	0
2	B	15	0	6	4	0
2	C	15	0	6	13	0
2	D	15	0	6	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	158	0	0	2	0
5	B	126	0	0	1	0
5	C	26	0	0	0	0
5	D	18	0	0	0	0
All	All	14248	0	13805	113	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 4.

All (113) 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:C:293:LYS:NZ	2:C:1001:PLP:C4A	1.77	1.46
1:C:293:LYS:HZ2	2:C:1001:PLP:C4A	1.45	1.19
1:A:293:LYS:NZ	2:A:501:PLP:C4A	2.07	1.18
1:A:293:LYS:HZ1	2:A:501:PLP:C4A	1.64	1.10
1:B:293:LYS:HZ1	2:B:501:PLP:C4A	1.70	1.04
1:B:293:LYS:NZ	2:B:501:PLP:C4A	2.21	1.03
1:C:293:LYS:HZ1	2:C:1001:PLP:C4A	1.52	1.02
1:A:293:LYS:HZ2	2:A:501:PLP:C4A	1.80	0.95
1:C:293:LYS:CE	2:C:1001:PLP:C4A	2.62	0.77
1:C:293:LYS:HZ2	2:C:1001:PLP:C4	1.98	0.76
1:C:50:ASP:OD2	1:C:54:ARG:NE	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:HIS:O	1:C:396:ARG:NH2	2.24	0.70
1:B:293:LYS:HZ2	2:B:501:PLP:C4A	2.02	0.70
1:B:376:ARG:NH1	1:B:459:TRP:O	2.25	0.70
1:C:119:ALA:HB3	1:D:22:MET:HE1	1.74	0.69
1:C:16:GLU:HG3	1:C:17:HIS:CD2	2.30	0.65
1:B:293:LYS:NZ	2:B:501:PLP:O3	2.32	0.63
1:D:31:ALA:O	1:D:35:GLN:HG2	2.01	0.61
1:C:119:ALA:HB3	1:D:22:MET:CE	2.31	0.60
1:D:38:LEU:HD22	1:D:54:ARG:HH22	1.69	0.58
1:C:126:SER:N	2:C:1001:PLP:H5A2	2.17	0.58
1:C:268:THR:HG22	1:C:387:MET:HE1	1.85	0.58
1:C:38:LEU:HD22	1:C:54:ARG:HH22	1.68	0.58
1:B:64:TRP:HB2	1:B:293:LYS:HD3	1.85	0.58
1:B:266:VAL:HG13	1:B:292:ALA:HB3	1.87	0.57
1:C:346:ASP:O	1:C:350:GLN:HG2	2.05	0.57
1:A:183:PRO:HG3	1:D:183:PRO:HG3	1.89	0.55
1:C:125:GLY:C	2:C:1001:PLP:H5A2	2.27	0.55
1:B:187:GLN:OE1	1:C:219:MET:HE1	2.08	0.53
1:C:123:LEU:N	1:C:127:ASP:OD2	2.27	0.52
1:D:368:LEU:HB3	1:D:381:VAL:HG11	1.91	0.51
1:D:31:ALA:HB1	1:D:35:GLN:NE2	2.26	0.51
1:C:266:VAL:HG12	1:C:293:LYS:HD2	1.91	0.51
2:C:1001:PLP:O1P	1:D:330:THR:HB	2.11	0.50
1:B:155:TYR:CE1	1:C:219:MET:HG3	2.46	0.50
1:A:268:THR:HG22	1:A:387:MET:HE1	1.92	0.50
1:A:118:LYS:HE2	1:B:20:VAL:O	2.11	0.50
1:C:22:MET:HE1	1:D:121:PHE:HE2	1.77	0.50
1:C:264:ASP:OD1	2:C:1001:PLP:H2A2	2.12	0.49
1:C:363:TYR:CZ	1:C:367:LYS:HE2	2.45	0.49
1:C:38:LEU:HD22	1:C:54:ARG:NH2	2.27	0.49
1:B:91:LEU:HD11	1:B:333:GLY:HA3	1.93	0.49
1:C:84:GLU:OE1	1:D:73:ARG:NH1	2.45	0.49
1:B:60:GLN:HG2	5:B:675:HOH:O	2.12	0.49
1:C:104:SER:OG	1:C:105:GLN:N	2.44	0.49
1:C:25:PRO:HB3	1:D:328:GLY:HA3	1.94	0.49
1:D:13:TRP:O	1:D:16:GLU:HG2	2.12	0.48
1:A:302:LEU:HD22	1:A:341:ALA:HB2	1.95	0.48
1:C:384:LYS:O	1:C:387:MET:HG2	2.13	0.48
1:D:50:ASP:OD2	1:D:54:ARG:NE	2.43	0.48
1:A:13:TRP:CE2	1:A:17:HIS:CD2	3.02	0.47
1:D:38:LEU:HD22	1:D:54:ARG:NH2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:VAL:HG12	1:B:423:ILE:HG13	1.97	0.47
1:C:16:GLU:HG3	1:C:17:HIS:HD2	1.77	0.47
1:C:125:GLY:HA3	2:C:1001:PLP:C5A	2.45	0.47
1:D:108:THR:HG23	1:D:116:MET:O	2.15	0.47
1:D:371:LEU:HD11	1:D:375:HIS:HD2	1.80	0.47
1:C:42:SER:HA	1:D:86:LEU:HB2	1.96	0.47
1:A:421:VAL:HG12	1:A:423:ILE:HG13	1.96	0.46
1:C:125:GLY:CA	2:C:1001:PLP:H5A2	2.44	0.46
1:B:122:GLY:C	1:B:123:LEU:HD22	2.35	0.46
1:C:127:ASP:OD1	1:C:128:ALA:N	2.49	0.46
1:A:370:ILE:HD11	5:A:742:HOH:O	2.15	0.46
1:C:125:GLY:HA3	2:C:1001:PLP:H5A2	1.98	0.45
1:A:328:GLY:O	1:B:161:LEU:CD1	2.65	0.45
1:D:371:LEU:CD1	1:D:375:HIS:HD2	2.30	0.45
1:B:155:TYR:CD1	1:C:219:MET:HG3	2.52	0.45
1:C:27:GLN:OE1	1:C:32:LEU:HD21	2.17	0.45
1:D:110:VAL:HG13	1:D:276:LEU:HD21	1.99	0.45
1:B:123:LEU:HD22	1:B:123:LEU:N	2.33	0.44
1:C:110:VAL:HG13	1:C:276:LEU:HD21	1.98	0.44
1:C:40:ILE:HA	1:C:50:ASP:HA	1.98	0.44
1:D:410:LEU:H	1:D:410:LEU:HD22	1.81	0.44
1:C:192:HIS:ND1	1:C:195:ARG:HB2	2.32	0.44
1:A:15:LYS:NZ	5:A:619:HOH:O	2.50	0.43
1:B:394:LYS:HG2	1:B:402:PHE:CE1	2.53	0.43
1:A:25:PRO:O	1:A:27:GLN:HG3	2.19	0.43
1:D:368:LEU:CB	1:D:381:VAL:HG11	2.49	0.43
1:C:408:TYR:CE2	1:C:459:TRP:HB2	2.53	0.43
1:B:367:LYS:HD3	1:B:447:ILE:HG13	2.00	0.42
1:D:266:VAL:HG13	1:D:292:ALA:HB3	2.01	0.42
1:B:27:GLN:NE2	1:B:32:LEU:HD21	2.34	0.42
1:C:28:ASP:HB2	1:D:324:VAL:HG22	2.00	0.42
1:C:293:LYS:HZ2	2:C:1001:PLP:C3	2.32	0.42
1:B:381:VAL:HG22	1:B:390:VAL:HG22	2.00	0.42
1:A:100:ALA:HB1	1:B:22:MET:HE1	2.01	0.42
1:C:103:LEU:HD21	1:C:302:LEU:HD21	2.01	0.42
1:C:29:PRO:CG	1:D:315:TRP:HB3	2.50	0.42
1:B:286:PRO:HG2	1:B:289:MET:HG2	2.01	0.41
1:C:408:TYR:HB3	1:C:409:PRO:HD3	2.02	0.41
1:A:42:SER:HA	1:B:86:LEU:HB2	2.03	0.41
1:B:98:ALA:HB3	1:B:99:PRO:HD3	2.03	0.41
1:D:123:LEU:HD11	1:D:331:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASP:HB2	1:B:329:TYR:CZ	2.55	0.41
1:C:127:ASP:HB2	1:C:329:TYR:CZ	2.56	0.41
1:C:26:MET:HG3	1:D:92:PHE:CE2	2.56	0.41
1:A:22:MET:HE2	1:B:104:SER:HB3	2.02	0.41
1:D:302:LEU:HD23	1:D:341:ALA:HB2	2.02	0.41
1:C:29:PRO:HG3	1:D:315:TRP:HB3	2.02	0.41
1:A:302:LEU:HG	1:A:303:SER:N	2.35	0.41
1:A:367:LYS:NZ	1:A:444:ASP:OD1	2.32	0.41
1:C:182:MET:SD	1:D:182:MET:HG2	2.60	0.41
1:B:425:THR:HG22	1:B:430:LEU:HD23	2.03	0.41
1:D:13:TRP:HA	1:D:16:GLU:HG2	2.01	0.40
1:C:123:LEU:HD11	1:C:331:TYR:HB2	2.04	0.40
1:D:219:MET:HE2	1:D:219:MET:HB3	1.88	0.40
1:D:387:MET:HE2	1:D:387:MET:HB2	1.74	0.40
1:D:42:SER:OG	1:D:49:THR:OG1	2.32	0.40
1:D:383:GLY:HA2	1:D:387:MET:O	2.21	0.40
3:B:502:GOL:O3	1:C:188:VAL:HA	2.22	0.40
1:C:315:TRP:HB3	1:D:29:PRO:HG2	2.02	0.40
1:D:35:GLN:O	1:D:35:GLN:HG3	2.22	0.40
1:D:386:LEU:HD23	1:D:386:LEU:HA	1.98	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	451/479 (94%)	434 (96%)	14 (3%)	3 (1%)	22	21
1	B	448/479 (94%)	431 (96%)	14 (3%)	3 (1%)	22	21
1	C	445/479 (93%)	427 (96%)	16 (4%)	2 (0%)	34	37
1	D	447/479 (93%)	430 (96%)	15 (3%)	2 (0%)	34	37
All	All	1791/1916 (94%)	1722 (96%)	59 (3%)	10 (1%)	25	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ALA
1	A	427	VAL
1	B	221	ALA
1	B	293	LYS
1	B	427	VAL
1	C	221	ALA
1	C	427	VAL
1	D	221	ALA
1	D	427	VAL
1	A	293	LYS

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	366/389 (94%)	363 (99%)	3 (1%)	81	89
1	B	363/389 (93%)	359 (99%)	4 (1%)	73	84
1	C	359/389 (92%)	353 (98%)	6 (2%)	60	73
1	D	361/389 (93%)	355 (98%)	6 (2%)	60	73
All	All	1449/1556 (93%)	1430 (99%)	19 (1%)	69	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	ARG
1	A	364	PHE
1	A	438	PHE
1	B	146	PRO
1	B	310	ARG
1	B	364	PHE
1	B	438	PHE
1	C	73	ARG
1	C	146	PRO
1	C	219	MET

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Mol	Chain	Res	Type
1	C	310	ARG
1	C	364	PHE
1	C	438	PHE
1	D	11	LYS
1	D	219	MET
1	D	310	ARG
1	D	364	PHE
1	D	387	MET
1	D	438	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	17	HIS
1	C	192	HIS
1	D	35	GLN
1	D	375	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	PLP	B	501	-	15,15,16	0.73	1 (6%)	20,22,23	0.62	0
3	GOL	A	502	-	5,5,5	0.10	0	5,5,5	0.32	0
4	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.42	0
4	SO4	B	503	-	4,4,4	0.20	0	6,6,6	0.12	0
2	PLP	C	1001	-	15,15,16	0.74	1 (6%)	20,22,23	0.61	0
2	PLP	D	801	1	15,15,16	0.73	1 (6%)	20,22,23	0.61	0
3	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.32	0
2	PLP	A	501	-	15,15,16	0.74	1 (6%)	20,22,23	0.61	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
2	PLP	B	501	-	-	2/6/6/8	0/1/1/1
3	GOL	A	502	-	-	2/4/4/4	-
2	PLP	C	1001	-	-	2/6/6/8	0/1/1/1
2	PLP	D	801	1	-	5/6/6/8	0/1/1/1
3	GOL	B	502	-	-	2/4/4/4	-
2	PLP	A	501	-	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	PLP	C4A-C4	-2.31	1.46	1.51
2	A	501	PLP	C4A-C4	-2.31	1.46	1.51
2	B	501	PLP	C4A-C4	-2.30	1.46	1.51
2	D	801	PLP	C4A-C4	-2.28	1.46	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C4-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C6-C5-C5A-O4P
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
2	C	1001	PLP	C4-C5-C5A-O4P
2	C	1001	PLP	C6-C5-C5A-O4P
3	B	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-O2
2	D	801	PLP	C5A-O4P-P-O3P
2	D	801	PLP	C4-C5-C5A-O4P
2	D	801	PLP	C5A-O4P-P-O1P
2	D	801	PLP	C6-C5-C5A-O4P
2	D	801	PLP	C5A-O4P-P-O2P

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PLP	4	0
2	C	1001	PLP	13	0
3	B	502	GOL	1	0
2	A	501	PLP	3	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 (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	453/479 (94%)	-0.06	1 (0%)	95	95	21, 34, 54, 94	0
1	B	450/479 (93%)	-0.10	0	100	100	23, 37, 60, 94	0
1	C	447/479 (93%)	1.26	128 (28%)	0	0	36, 94, 132, 149	0
1	D	449/479 (93%)	1.26	109 (24%)	0	0	36, 97, 131, 150	0
All	All	1799/1916 (93%)	0.59	238 (13%)	3	2	21, 53, 126, 150	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	ALA	8.3
1	D	17	HIS	8.2
1	D	87	ALA	8.0
1	D	14	LEU	7.8
1	D	299	TYR	7.7
1	D	22	MET	7.6
1	D	68	ALA	6.8
1	C	339	ALA	6.5
1	C	299	TYR	6.3
1	C	368	LEU	6.2
1	C	377	ALA	6.2
1	D	51	VAL	6.0
1	D	423	ILE	5.9
1	D	416	CYS	5.9
1	C	66	VAL	5.8
1	C	54	ARG	5.7
1	C	29	PRO	5.7
1	C	70	TYR	5.6
1	D	328	GLY	5.6
1	D	345	ILE	5.6
1	D	454	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	51	VAL	5.4
1	C	417	VAL	5.3
1	C	119	ALA	5.1
1	D	417	VAL	5.1
1	C	422	MET	5.1
1	C	319	ALA	5.1
1	C	68	ALA	4.9
1	D	38	LEU	4.9
1	D	75	ILE	4.8
1	D	70	TYR	4.8
1	D	102	ALA	4.7
1	C	270	LEU	4.7
1	C	22	MET	4.6
1	C	421	VAL	4.6
1	C	56	PHE	4.4
1	C	69	GLY	4.4
1	C	386	LEU	4.4
1	D	174	TRP	4.4
1	C	392	LEU	4.3
1	C	361	GLY	4.3
1	D	339	ALA	4.2
1	C	418	ASN	4.2
1	C	336	VAL	4.2
1	D	331	TYR	4.1
1	D	32	LEU	4.1
1	D	64	TRP	4.1
1	D	81	ARG	4.1
1	C	32	LEU	4.1
1	C	344	ALA	4.0
1	C	454	PHE	4.0
1	C	348	VAL	4.0
1	C	390	VAL	4.0
1	C	459	TRP	3.9
1	C	438	PHE	3.9
1	D	59	CYS	3.8
1	C	43	GLY	3.8
1	D	34	GLU	3.8
1	C	446	VAL	3.8
1	D	412	ILE	3.8
1	C	271	GLY	3.8
1	D	24	HIS	3.8
1	C	435	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	364	PHE	3.7
1	C	302	LEU	3.6
1	C	450	LEU	3.6
1	C	63	LEU	3.6
1	C	73	ARG	3.6
1	C	370	ILE	3.5
1	D	121	PHE	3.5
1	C	76	ILE	3.5
1	C	102	ALA	3.5
1	D	363	TYR	3.5
1	D	376	ARG	3.5
1	C	300	VAL	3.5
1	D	101	ILE	3.5
1	C	16	GLU	3.5
1	C	94	GLY	3.4
1	D	52	ASP	3.4
1	C	30	LYS	3.4
1	C	88	TYR	3.4
1	D	37	PRO	3.4
1	C	52	ASP	3.4
1	C	57	ILE	3.4
1	C	20	VAL	3.3
1	C	238	GLY	3.3
1	D	86	LEU	3.3
1	D	300	VAL	3.3
1	C	332	SER	3.3
1	D	422	MET	3.3
1	C	423	ILE	3.3
1	D	35	GLN	3.2
1	D	274	GLY	3.2
1	D	413	SER	3.2
1	D	88	TYR	3.2
1	D	46	VAL	3.2
1	C	366	GLU	3.2
1	D	43	GLY	3.2
1	D	377	ALA	3.2
1	D	42	SER	3.2
1	C	328	GLY	3.2
1	D	421	VAL	3.2
1	C	89	TYR	3.1
1	D	450	LEU	3.1
1	D	33	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	89	TYR	3.1
1	C	46	VAL	3.0
1	D	21	HIS	3.0
1	D	193	LEU	3.0
1	C	301	PRO	3.0
1	D	93	PRO	3.0
1	C	315	TRP	3.0
1	D	13	TRP	3.0
1	D	432	ILE	3.0
1	D	53	GLY	3.0
1	D	370	ILE	3.0
1	C	404	PRO	3.0
1	A	317	ARG	3.0
1	D	319	ALA	2.9
1	D	302	LEU	2.9
1	D	386	LEU	2.9
1	D	31	ALA	2.9
1	C	50	ASP	2.9
1	C	410	LEU	2.9
1	D	79	VAL	2.9
1	C	39	ILE	2.9
1	C	95	SER	2.9
1	D	323	SER	2.9
1	D	291	LEU	2.8
1	D	16	GLU	2.8
1	D	105	GLN	2.8
1	C	381	VAL	2.8
1	C	23	MET	2.8
1	D	430	LEU	2.8
1	D	19	THR	2.8
1	C	105	GLN	2.8
1	D	436	LEU	2.8
1	C	81	ARG	2.8
1	C	40	ILE	2.8
1	C	343	ALA	2.8
1	D	359	VAL	2.8
1	C	365	LEU	2.8
1	C	329	TYR	2.8
1	C	442	HIS	2.7
1	D	408	TYR	2.7
1	C	123	LEU	2.7
1	C	414	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	396	ARG	2.7
1	D	44	LYS	2.7
1	D	459	TRP	2.7
1	C	75	ILE	2.6
1	D	57	ILE	2.6
1	D	39	ILE	2.6
1	C	318	ASP	2.6
1	D	325	TYR	2.6
1	D	371	LEU	2.6
1	C	71	GLY	2.6
1	D	45	GLY	2.6
1	D	55	ARG	2.5
1	C	79	VAL	2.5
1	C	449	VAL	2.5
1	D	455	VAL	2.5
1	C	453	ALA	2.5
1	D	90	SER	2.5
1	D	40	ILE	2.5
1	C	353	LEU	2.5
1	C	100	ALA	2.5
1	C	341	ALA	2.5
1	D	15	LYS	2.5
1	C	83	MET	2.4
1	D	336	VAL	2.4
1	C	419	ASN	2.4
1	D	84	GLU	2.4
1	C	53	GLY	2.4
1	D	447	ILE	2.4
1	C	103	LEU	2.4
1	D	80	THR	2.4
1	C	340	ALA	2.3
1	D	107	LEU	2.3
1	C	235	GLY	2.3
1	D	74	GLU	2.3
1	D	203	GLU	2.3
1	D	431	ILE	2.3
1	C	92	PHE	2.3
1	C	276	LEU	2.3
1	C	363	TYR	2.3
1	C	347	ILE	2.3
1	D	48	ILE	2.3
1	C	34	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	337	SER	2.3
1	C	239	VAL	2.3
1	D	324	VAL	2.3
1	D	295	ILE	2.3
1	D	18	ASN	2.3
1	C	369	LEU	2.2
1	C	194	TYR	2.2
1	D	83	MET	2.2
1	C	266	VAL	2.2
1	D	73	ARG	2.2
1	D	392	LEU	2.2
1	D	289	MET	2.2
1	D	49	THR	2.2
1	D	337	SER	2.2
1	D	343	ALA	2.2
1	C	101	ILE	2.2
1	C	374	LYS	2.2
1	C	49	THR	2.2
1	C	48	ILE	2.2
1	C	431	ILE	2.2
1	C	97	ASN	2.2
1	C	33	HIS	2.2
1	C	437	THR	2.2
1	C	42	SER	2.2
1	C	298	GLY	2.2
1	C	86	LEU	2.1
1	D	307	VAL	2.1
1	C	357	ALA	2.1
1	D	25	PRO	2.1
1	C	62	GLY	2.1
1	C	121	PHE	2.1
1	D	330	THR	2.1
1	C	90	SER	2.1
1	C	58	ASP	2.1
1	C	430	LEU	2.0
1	D	103	LEU	2.0
1	C	372	LYS	2.0
1	C	387	MET	2.0
1	D	98	ALA	2.0
1	C	41	GLN	2.0
1	C	455	VAL	2.0
1	C	24	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	61	GLY	2.0
1	D	110	VAL	2.0
1	C	267	ILE	2.0
1	D	410	LEU	2.0
1	C	77	ASP	2.0
1	C	297	SER	2.0
1	D	358	ARG	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. 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	PLP	D	801	15/16	0.85	0.23	79,97,106,109	0
2	PLP	C	1001	15/16	0.87	0.18	57,69,89,95	0
3	GOL	A	502	6/6	0.92	0.17	49,54,57,59	0
2	PLP	B	501	15/16	0.94	0.14	18,26,33,34	0
3	GOL	B	502	6/6	0.94	0.20	39,58,61,62	0
4	SO4	B	503	5/5	0.97	0.14	49,55,57,74	0
4	SO4	A	503	5/5	0.97	0.14	55,58,61,66	0
2	PLP	A	501	15/16	0.97	0.16	15,26,31,40	0

6.5 Other polymers (i)

There are no such residues in this entry.