Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 08:48 pm GMT

PDB ID : 4A72

Title : Crystal structure of the omega transaminase from Chromobacterium violaceum in a mixture of apo and PLP-bound states

Authors : Logan, D.T.; Hakansson, M.; Yengo, K.; Svedendahl Humble, M.; Engelmark Cassimjee, K.; Walse, B.; Abedi, V.; Federsel, H.-J.; Berglund, P.

Deposited on : 2011-11-10

Resolution : 2.40 Å(reported)

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

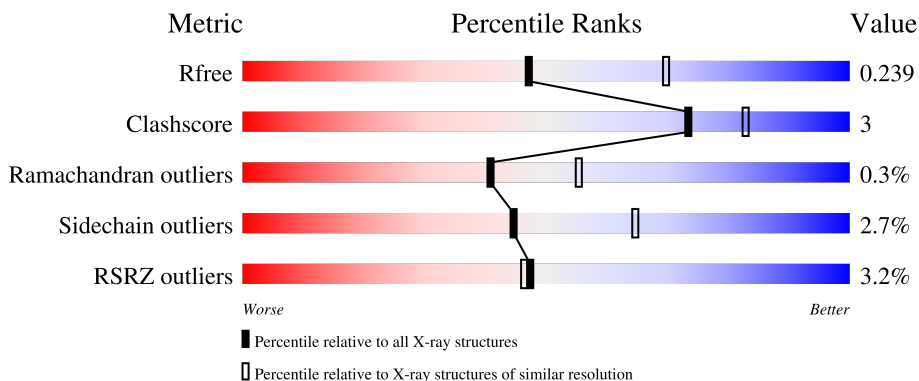|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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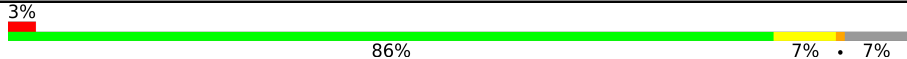*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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		0.239
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		2.7%
RSRZ outliers		3.2%

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	459	3% / 86% / 7% · 7%
1	B	459	6% / 85% / 7% 7%
1	C	459	% / 86% / 11% ··
1	D	459	2% / 90% / 7% ··

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14399 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 OMEGA TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3370	2154	589	607	20			
1	B	426	Total	C	N	O	S	0	0	0
			3339	2134	582	602	21			
1	C	453	Total	C	N	O	S	0	0	0
			3564	2271	628	644	21			
1	D	454	Total	C	N	O	S	0	0	0
			3568	2273	629	645	21			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
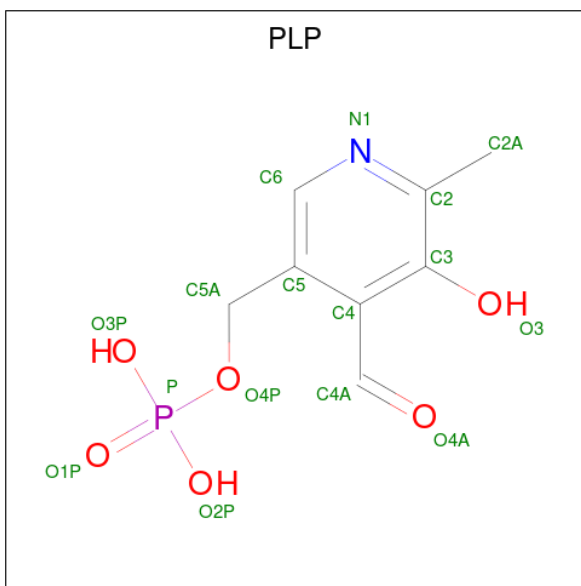
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total 111	O 111	0	0
3	B	111	Total 111	O 111	0	0
3	C	188	Total 188	O 188	0	0
3	D	118	Total 118	O 118	0	0

3 Residue-property plots ⓘ

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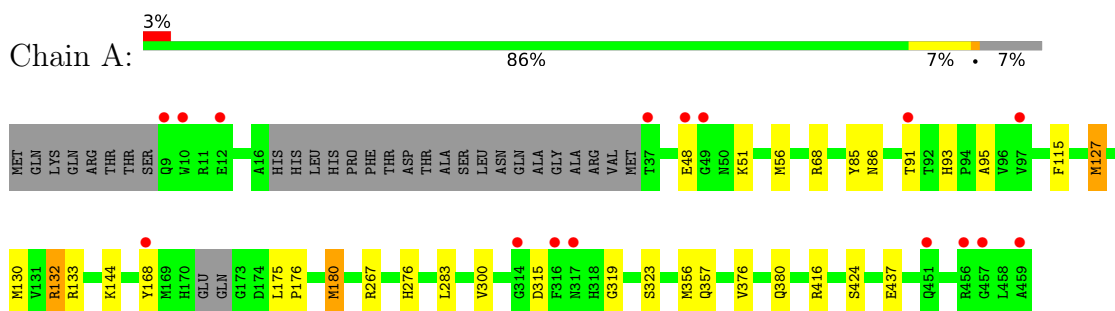
Chain A:

• Molecule 1: OMEGA TRANSAMINASE

Chain B:

• Molecule 1: OMEGA TRANSAMINASE

Chain C:

• Molecule 1: OMEGA TRANSAMINASE

Chain D:
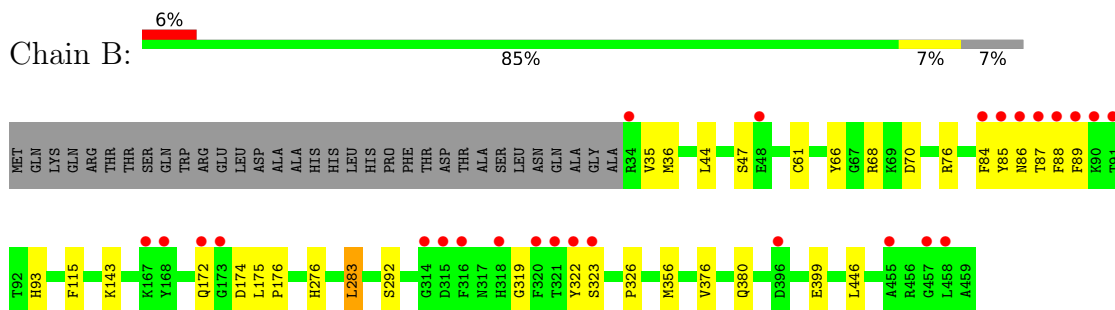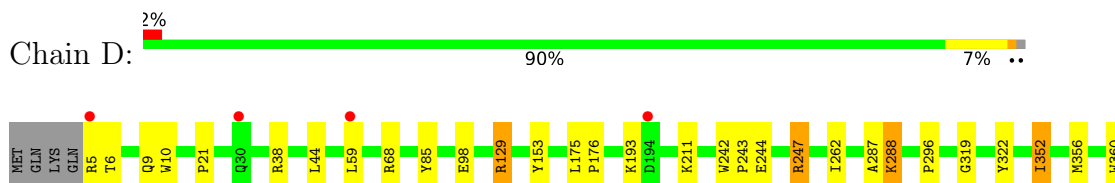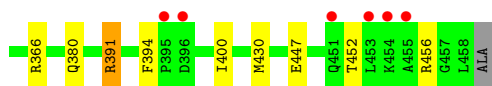
4 Data and refinement statistics ⓘ

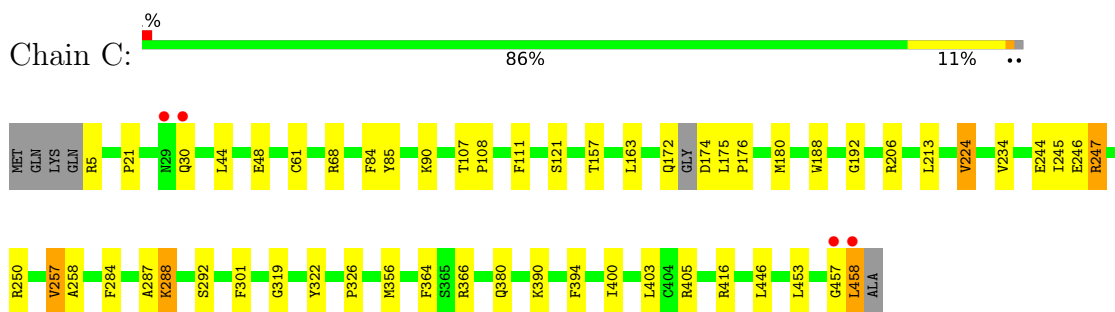| Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.35Å 62.12Å 119.24Å 105.27° 90.66° 104.43°	Depositor
Resolution (Å)	26.39 – 2.40 29.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (26.39-2.40) 96.4 (29.61-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.173 , 0.239 0.176 , 0.239	Depositor DCC
R_{free} test set	3141 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14399	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.21	0/3457	0.39	0/4675
1	B	0.22	0/3426	0.39	0/4635
1	C	0.22	0/3657	0.41	0/4949
1	D	0.24	0/3662	0.40	0/4957
All	All	0.22	0/14202	0.40	0/19216

There are no bond length outliers.

There are no bond angle outliers.

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	3370	0	3280	21	0
1	B	3339	0	3254	17	0
1	C	3564	0	3462	38	0
1	D	3568	0	3466	25	0
2	C	15	0	6	0	0
2	D	15	0	6	2	0
3	A	111	0	0	1	0
3	B	111	0	0	1	0
3	C	188	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	118	0	0	0	0
All	All	14399	0	13474	90	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 3.

All (90) 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:172:GLN:O	1:D:129:ARG:NH1	2.07	0.88
1:C:5:ARG:NH1	1:D:98:GLU:OE2	2.17	0.78
1:B:89:PHE:O	1:B:322:TYR:OH	2.11	0.68
1:B:85:TYR:O	3:B:2013:HOH:O	2.10	0.68
1:C:458:LEU:C	1:C:458:LEU:HD22	2.16	0.66
1:B:319:GLY:O	1:B:323:SER:OG	2.09	0.64
1:A:85:TYR:OH	1:A:91:THR:OG1	2.16	0.61
1:A:133:ARG:NE	1:A:315:ASP:OD2	2.35	0.60
1:C:458:LEU:C	1:C:458:LEU:CD2	2.70	0.60
1:D:5:ARG:N	1:D:9:GLN:OE1	2.35	0.59
1:C:175:LEU:HB3	1:C:176:PRO:HA	1.85	0.59
1:C:174:ASP:N	3:C:2090:HOH:O	2.34	0.58
1:A:319:GLY:O	1:A:323:SER:OG	2.19	0.56
1:C:224:VAL:HB	1:C:257:VAL:HG22	1.85	0.56
1:D:244:GLU:OE2	1:D:247:ARG:NH1	2.38	0.56
3:C:2084:HOH:O	1:D:129:ARG:NE	2.38	0.55
1:A:56:MET:CE	1:A:424:SER:HA	2.38	0.53
1:B:35:VAL:O	1:B:47:SER:N	2.42	0.53
1:A:356:MET:HG2	1:A:380:GLN:NE2	2.24	0.53
1:B:115:PHE:CE2	1:B:319:GLY:HA3	2.44	0.52
1:D:175:LEU:HB3	1:D:176:PRO:HA	1.91	0.52
1:A:51:LYS:NZ	1:A:437:GLU:OE2	2.27	0.51
1:C:107:THR:HG23	1:C:108:PRO:HD2	1.93	0.50
1:C:284:PHE:CE1	1:C:301:PHE:CD2	3.00	0.50
1:A:132:ARG:NH1	1:A:144:LYS:O	2.45	0.49
1:A:180:MET:HE3	1:A:180:MET:HA	1.94	0.49
1:A:132:ARG:O	1:A:144:LYS:NZ	2.46	0.48
1:B:86:ASN:OD1	1:B:87:THR:N	2.47	0.48
1:B:175:LEU:HB3	1:B:176:PRO:HA	1.94	0.48
1:C:84:PHE:HA	1:C:326:PRO:HG2	1.95	0.48
1:C:394:PHE:CG	1:C:400:ILE:HG13	2.49	0.48
1:C:457:GLY:O	1:C:458:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TYR:CE1	1:B:36:MET:HB3	2.49	0.47
1:C:246:GLU:O	1:C:247:ARG:CB	2.63	0.47
1:C:356:MET:HG2	1:C:380:GLN:NE2	2.30	0.47
1:C:453:LEU:O	1:C:458:LEU:HA	2.14	0.46
1:C:390:LYS:NZ	3:C:2167:HOH:O	2.43	0.46
1:C:188:TRP:CE3	1:C:192:GLY:HA3	2.50	0.46
1:B:356:MET:HG2	1:B:380:GLN:NE2	2.31	0.45
1:C:246:GLU:O	1:C:247:ARG:CG	2.64	0.45
1:D:352:ILE:HD12	1:D:430:MET:O	2.17	0.45
1:C:107:THR:HG22	1:C:111:PHE:HB2	1.98	0.45
1:C:322:TYR:OH	1:D:288:LYS:HA	2.17	0.45
1:C:234:VAL:HG12	1:C:234:VAL:O	2.17	0.45
1:B:276:HIS:CE1	1:B:376:VAL:HG21	2.52	0.45
1:A:130:MET:HE1	1:A:300:VAL:HG11	1.98	0.44
1:D:356:MET:HG2	1:D:380:GLN:NE2	2.32	0.44
1:C:107:THR:CG2	1:C:111:PHE:HB2	2.47	0.44
1:D:6:THR:O	1:D:10:TRP:CD1	2.70	0.44
1:D:366:ARG:NH2	1:D:447:GLU:OE2	2.50	0.44
1:D:193:LYS:O	1:D:391:ARG:NH2	2.51	0.44
1:B:87:THR:HA	1:B:322:TYR:CE1	2.53	0.43
1:C:288:LYS:HA	1:D:322:TYR:OH	2.18	0.43
3:C:2084:HOH:O	1:D:129:ARG:NH2	2.51	0.43
1:A:283:LEU:N	1:A:283:LEU:HD23	2.33	0.43
1:D:242:TRP:N	1:D:243:PRO:CD	2.81	0.43
1:A:276:HIS:CE1	1:A:376:VAL:HG21	2.54	0.43
1:C:61:CYS:O	1:C:292:SER:HA	2.18	0.43
1:D:262:ILE:HG13	2:D:1288:PLP:O3	2.18	0.43
1:A:127:MET:C	1:A:127:MET:SD	2.97	0.43
1:B:88:PHE:C	1:B:88:PHE:CD1	2.91	0.43
1:A:130:MET:CE	1:A:300:VAL:HG11	2.48	0.43
1:C:121:SER:HB3	1:C:157:THR:HG23	1.99	0.43
1:C:44:LEU:HD11	1:D:85:TYR:CE1	2.54	0.42
1:B:61:CYS:O	1:B:292:SER:HA	2.20	0.42
1:B:283:LEU:HD12	1:B:283:LEU:N	2.34	0.42
1:A:93:HIS:CD2	1:A:95:ALA:HB3	2.55	0.42
1:A:86:ASN:ND2	3:A:2008:HOH:O	2.47	0.42
1:C:163:LEU:HD21	1:C:224:VAL:HG11	2.01	0.42
1:B:93:HIS:CE1	1:B:326:PRO:HB3	2.54	0.41
1:C:245:ILE:HG22	1:C:246:GLU:N	2.33	0.41
1:D:394:PHE:CG	1:D:400:ILE:HG13	2.55	0.41
1:D:452:THR:O	1:D:456:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLU:O	1:C:247:ARG:HG3	2.19	0.41
1:A:115:PHE:CE2	1:A:319:GLY:HA3	2.55	0.41
1:C:21:PRO:HB3	1:D:319:GLY:HA3	2.02	0.41
1:C:258:ALA:O	1:C:284:PHE:HA	2.21	0.41
1:B:68:ARG:HG3	1:B:70:ASP:OD1	2.20	0.41
1:C:364:PHE:CD1	1:C:446:LEU:HD12	2.55	0.41
1:D:153:TYR:O	2:D:1288:PLP:H2A3	2.21	0.41
1:A:357:GLN:NE2	1:A:357:GLN:HA	2.35	0.41
1:C:21:PRO:CB	1:D:319:GLY:HA3	2.51	0.41
1:B:44:LEU:HD21	1:B:66:TYR:CE2	2.55	0.41
1:C:322:TYR:CD2	1:D:296:PRO:HA	2.56	0.41
1:A:56:MET:HE1	1:A:424:SER:HA	2.03	0.41
1:A:175:LEU:HB3	1:A:176:PRO:HA	2.01	0.41
1:C:319:GLY:HA3	1:D:21:PRO:HB3	2.03	0.40
1:C:85:TYR:CE1	1:D:44:LEU:HD11	2.57	0.40
1:C:107:THR:CG2	1:C:108:PRO:HD2	2.51	0.40
1:C:206:ARG:NH1	1:C:244:GLU:OE2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/459 (92%)	407 (96%)	16 (4%)	0	100	100
1	B	424/459 (92%)	404 (95%)	20 (5%)	0	100	100
1	C	449/459 (98%)	430 (96%)	16 (4%)	3 (1%)	22	32
1	D	452/459 (98%)	431 (95%)	18 (4%)	3 (1%)	22	32
All	All	1748/1836 (95%)	1672 (96%)	70 (4%)	6 (0%)	41	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	287	ALA
1	D	288	LYS
1	C	247	ARG
1	C	287	ALA
1	C	288	LYS
1	D	68	ARG

5.3.2   Protein sidechains   ⓘ

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	342/368 (93%)	334 (98%)	8 (2%)	50	70
1	B	340/368 (92%)	332 (98%)	8 (2%)	49	68
1	C	364/368 (99%)	350 (96%)	14 (4%)	33	51
1	D	364/368 (99%)	356 (98%)	8 (2%)	52	71
All	All	1410/1472 (96%)	1372 (97%)	38 (3%)	44	65

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	68	ARG
1	A	127	MET
1	A	132	ARG
1	A	168	TYR
1	A	180	MET
1	A	267	ARG
1	A	416	ARG
1	B	76	ARG
1	B	84	PHE
1	B	143	LYS
1	B	172	GLN
1	B	174	ASP
1	B	283	LEU
1	B	399	GLU
1	B	446	LEU

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Mol	Chain	Res	Type
1	C	30	GLN
1	C	48	GLU
1	C	68	ARG
1	C	90	LYS
1	C	180	MET
1	C	213	LEU
1	C	224	VAL
1	C	250	ARG
1	C	257	VAL
1	C	366	ARG
1	C	403	LEU
1	C	405	ARG
1	C	416	ARG
1	C	458	LEU
1	D	38	ARG
1	D	59	LEU
1	D	129	ARG
1	D	211	LYS
1	D	247	ARG
1	D	352	ILE
1	D	360	TRP
1	D	391	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	GLN
1	A	369	HIS
1	A	380	GLN
1	B	78	GLN
1	B	380	GLN
1	B	421	HIS
1	C	154	HIS
1	C	380	GLN
1	D	318	HIS
1	D	380	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	C	1288	1	15,15,16	3.10	3 (20%)	20,22,23	1.41	3 (15%)
2	PLP	D	1288	1	15,15,16	3.06	3 (20%)	20,22,23	1.38	2 (10%)

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	C	1288	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1288	1	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1288	PLP	C5-C4	8.01	1.49	1.40
2	D	1288	PLP	C5-C4	7.89	1.49	1.40
2	C	1288	PLP	C3-C2	7.68	1.48	1.40
2	D	1288	PLP	C3-C2	7.59	1.48	1.40
2	C	1288	PLP	C3-C4	4.04	1.48	1.40
2	D	1288	PLP	C3-C4	3.99	1.48	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1288	PLP	C4A-C4-C5	2.86	123.88	120.94
2	C	1288	PLP	C4A-C4-C5	2.74	123.76	120.94
2	D	1288	PLP	C6-N1-C2	2.24	123.32	119.17
2	C	1288	PLP	C6-N1-C2	2.21	123.27	119.17
2	C	1288	PLP	C3-C4-C5	-2.07	116.50	118.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1288	PLP	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	429/459 (93%)	-0.26	16 (3%)	41	41	14, 34, 74, 104	8 (1%)
1	B	426/459 (92%)	-0.25	26 (6%)	21	20	14, 32, 73, 124	8 (1%)
1	C	453/459 (98%)	-0.46	4 (0%)	84	82	12, 28, 55, 79	0
1	D	454/459 (98%)	-0.14	10 (2%)	62	60	14, 36, 74, 97	0
All	All	1762/1836 (95%)	-0.28	56 (3%)	47	46	12, 32, 71, 124	16 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	TYR	4.9
1	B	85	TYR	4.3
1	D	453	LEU	4.1
1	B	89	PHE	4.0
1	B	321	THR	4.0
1	B	172	GLN	3.9
1	B	458	LEU	3.8
1	A	10	TRP	3.6
1	A	168	TYR	3.5
1	A	457	GLY	3.4
1	D	30	GLN	3.4
1	C	458	LEU	3.4
1	A	91	THR	3.3
1	A	37	THR	3.2
1	B	320	PHE	3.2
1	B	457	GLY	3.2
1	B	314	GLY	3.2
1	A	459	ALA	3.2
1	B	167	LYS	3.2
1	B	322	TYR	3.0
1	D	455	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	91	THR	2.9
1	B	87	THR	2.9
1	D	395	PRO	2.8
1	B	48	GLU	2.8
1	D	454	LYS	2.6
1	A	317	ASN	2.6
1	A	12	GLU	2.6
1	B	88	PHE	2.6
1	A	9	GLN	2.6
1	B	316	PHE	2.5
1	B	323	SER	2.5
1	A	456	ARG	2.5
1	B	396	ASP	2.5
1	A	49	GLY	2.5
1	C	30	GLN	2.4
1	B	34	ARG	2.4
1	B	455	ALA	2.4
1	B	173	GLY	2.4
1	A	451	GLN	2.4
1	C	29	ASN	2.3
1	A	97	VAL	2.3
1	A	314	GLY	2.2
1	B	315	ASP	2.2
1	C	457	GLY	2.2
1	B	84	PHE	2.2
1	B	318	HIS	2.2
1	A	316	PHE	2.2
1	A	48	GLU	2.2
1	D	396	ASP	2.1
1	D	59	LEU	2.1
1	D	194	ASP	2.1
1	D	451	GLN	2.1
1	B	86	ASN	2.0
1	D	5	ARG	2.0
1	B	90	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	1288	15/16	0.93	0.22	29,52,68,69	0
2	PLP	C	1288	15/16	0.96	0.17	25,47,63,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.