



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2025 – 08:29 AM EDT

PDB ID : 4EMY  
Title : Crystal structure of aminotransferase from anaerococcus prevotii dsm 20548.  
Authors : Chang, C.; Tesar, C.; Bearden, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2012-04-12  
Resolution : 2.86 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

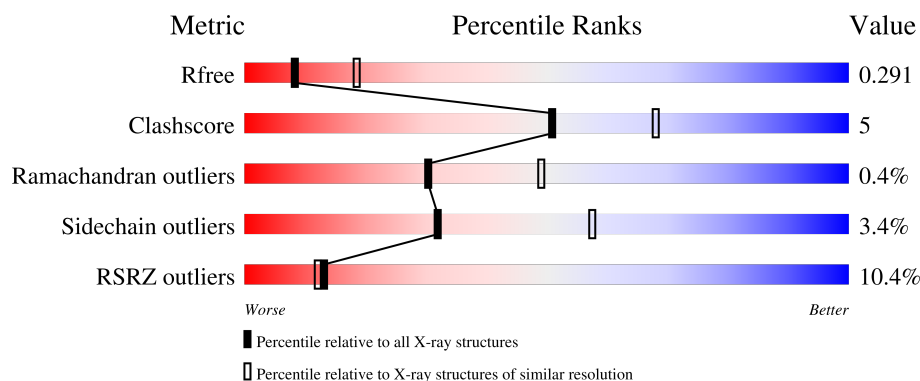
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.86 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))
$R_{free}$	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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  $\geq 3$ , 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	413	
1	B	413	
1	C	413	
1	D	413	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13055 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 class I and II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	Se	0	0	0
			3249	2080	538	621	4	6			
1	B	409	Total	C	N	O	S	Se	0	0	0
			3249	2080	538	621	4	6			
1	C	407	Total	C	N	O	S	Se	0	0	0
			3230	2065	536	619	4	6			
1	D	407	Total	C	N	O	S	Se	0	0	0
			3235	2073	536	616	4	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP C7REB0
A	-1	ASN	-	expression tag	UNP C7REB0
A	0	ALA	-	expression tag	UNP C7REB0
B	-2	SER	-	expression tag	UNP C7REB0
B	-1	ASN	-	expression tag	UNP C7REB0
B	0	ALA	-	expression tag	UNP C7REB0
C	-2	SER	-	expression tag	UNP C7REB0
C	-1	ASN	-	expression tag	UNP C7REB0
C	0	ALA	-	expression tag	UNP C7REB0
D	-2	SER	-	expression tag	UNP C7REB0
D	-1	ASN	-	expression tag	UNP C7REB0
D	0	ALA	-	expression tag	UNP C7REB0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

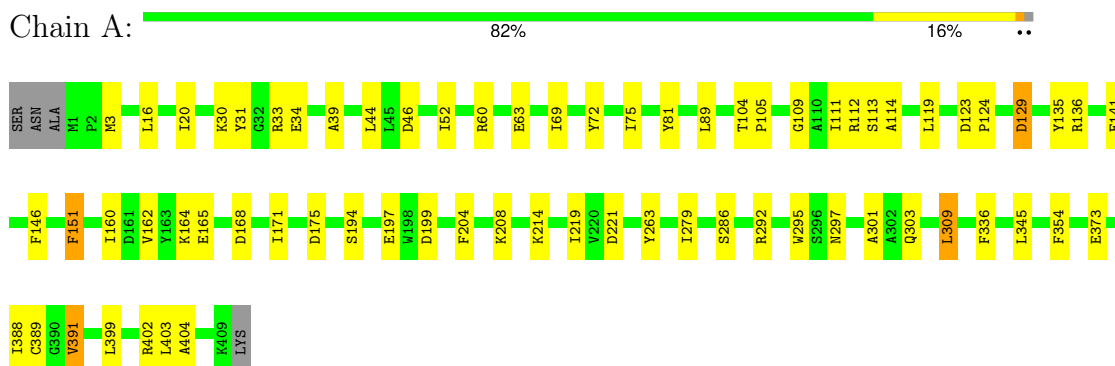
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	10	Total	O	0	0
			10	10		
3	C	4	Total	O	0	0
			4	4		
3	D	7	Total	O	0	0
			7	7		

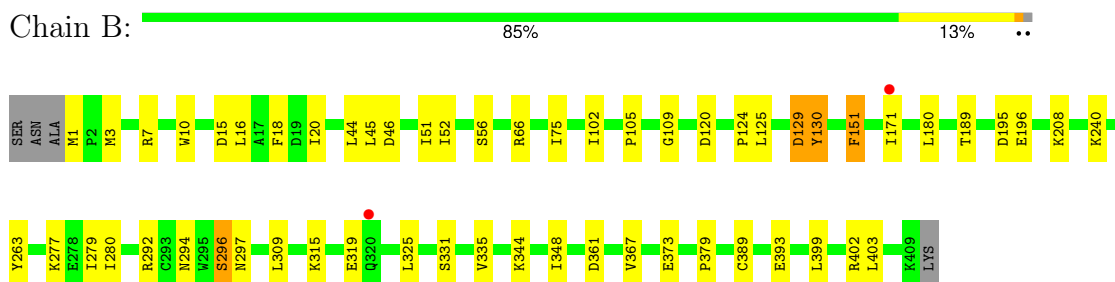
### 3 Residue-property plots [i](#)

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

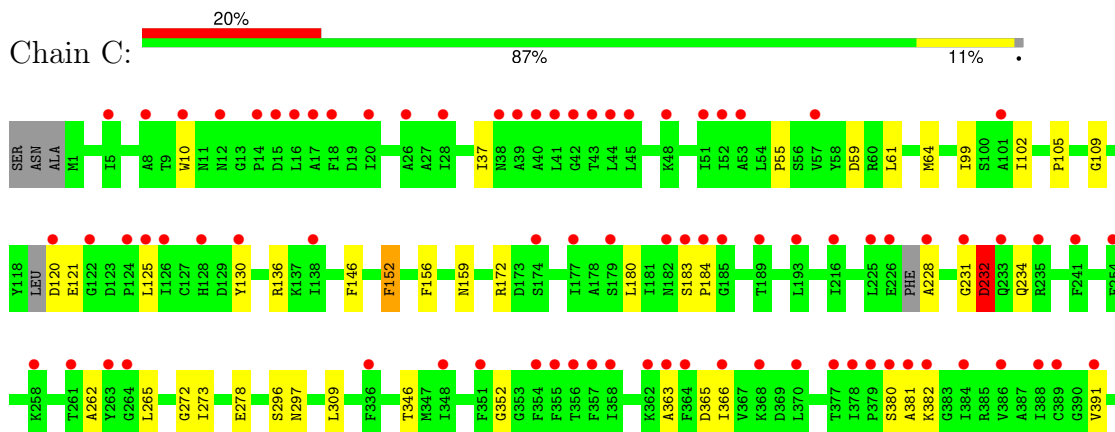
#### • Molecule 1: Aminotransferase class I and II

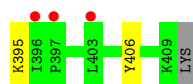


#### • Molecule 1: Aminotransferase class I and II

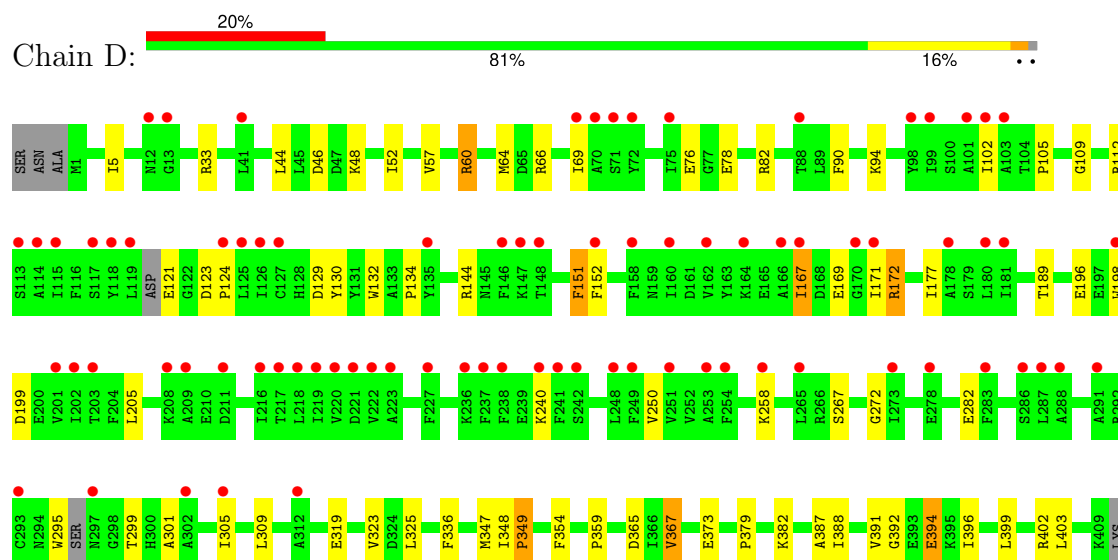


#### • Molecule 1: Aminotransferase class I and II





● Molecule 1: Aminotransferase class I and II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.30Å 131.18Å 239.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.86 50.00 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.86) 99.8 (50.00-2.86)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.245 , 0.290 0.246 , 0.291	Depositor DCC
$R_{free}$ test set	2418 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.4	Xtriage
Anisotropy	0.960	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.42	0/3315	0.55	0/4470
1	B	0.40	0/3315	0.54	0/4470
1	C	0.41	1/3293 (0.0%)	0.51	0/4437
1	D	0.41	1/3299 (0.0%)	0.51	0/4445
All	All	0.41	2/13222 (0.0%)	0.53	0/17822

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	TRP	CD2-CE2	5.11	1.47	1.41
1	D	198	TRP	CD2-CE2	5.05	1.47	1.41

There are no bond angle outliers.

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	3249	0	3200	46	0
1	B	3249	0	3200	32	0
1	C	3230	0	3178	21	0
1	D	3235	0	3189	40	0
2	A	16	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	8	0	0
2	C	16	0	8	0	0
2	D	16	0	8	2	0
3	A	7	0	0	1	0
3	B	10	0	0	1	0
3	C	4	0	0	0	0
3	D	7	0	0	0	0
All	All	13055	0	12798	132	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 5.

All (132) 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:228:ALA:HA	1:C:352:GLY:HA3	1.46	0.94
1:A:112:ARG:HD2	1:B:294:ASN:HA	1.64	0.78
1:D:394:GLU:CD	1:D:394:GLU:H	1.89	0.75
1:A:111:ILE:HD13	1:A:135:TYR:HE1	1.57	0.70
1:B:105:PRO:HD2	1:B:109:GLY:HA3	1.74	0.69
1:D:33:ARG:HD2	1:D:48:LYS:O	1.94	0.67
1:C:231:GLY:O	1:C:232:ASP:HB3	1.94	0.66
1:A:373:GLU:OE1	1:A:402:ARG:HD3	1.96	0.66
1:A:204:PHE:CZ	1:A:208:LYS:HE2	2.32	0.64
1:A:114:ALA:HB1	1:A:219:ILE:CD1	2.28	0.64
1:C:130:TYR:HE2	1:C:152:PHE:CZ	2.16	0.64
1:D:258:LYS:HE3	2:D:501:PLP:H4A	1.81	0.63
1:A:44:LEU:HG	1:A:354:PHE:CZ	2.34	0.63
1:D:367:VAL:HG11	1:D:379:PRO:HG3	1.81	0.62
1:A:399:LEU:O	1:A:403:LEU:HB2	2.00	0.62
1:D:373:GLU:OE1	1:D:402:ARG:HD3	2.00	0.62
1:A:75:ILE:HD12	1:A:292:ARG:HD3	1.82	0.61
1:A:168:ASP:OD1	1:A:208:LYS:HE3	2.00	0.61
1:A:129:ASP:HB2	1:A:151:PHE:H	1.65	0.61
1:B:373:GLU:OE1	1:B:402:ARG:HD3	2.01	0.61
1:D:46:ASP:HB3	1:D:52:ILE:HD11	1.84	0.60
1:D:121:GLU:O	1:D:144:ARG:HA	2.03	0.59
1:C:37:ILE:HG23	1:C:391:VAL:HG11	1.84	0.59
1:B:125:LEU:HD11	1:B:180:LEU:HB2	1.86	0.57
1:D:66:ARG:HA	1:D:69:ILE:HD12	1.87	0.57
1:B:367:VAL:HG23	3:B:607:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LEU:O	1:B:403:LEU:HB2	2.05	0.56
1:D:129:ASP:HB2	1:D:151:PHE:H	1.70	0.56
1:B:129:ASP:HB2	1:B:151:PHE:H	1.70	0.55
1:B:46:ASP:HB3	1:B:52:ILE:HD11	1.88	0.55
1:B:195:ASP:O	1:B:240:LYS:HE3	2.06	0.55
1:A:336:PHE:HB2	1:A:388:ILE:HD11	1.90	0.54
1:C:184:PRO:HB2	1:C:228:ALA:CB	2.36	0.54
1:A:279:ILE:HD12	1:B:3:MSE:HG2	1.90	0.54
1:C:105:PRO:HD2	1:C:109:GLY:HA3	1.89	0.54
1:B:44:LEU:HD23	1:B:389:CYS:HB2	1.89	0.53
1:D:347:MSE:HA	1:D:359:PRO:HD2	1.90	0.53
1:C:152:PHE:HA	1:C:159:ASN:HB2	1.91	0.52
1:A:114:ALA:HB1	1:A:219:ILE:HD12	1.91	0.52
1:A:171:ILE:CG2	1:A:171:ILE:O	2.58	0.52
1:A:160:ILE:HG13	1:A:164:LYS:HE3	1.92	0.51
1:A:194:SER:OG	1:A:197:GLU:HG3	2.10	0.51
1:D:52:ILE:HG21	1:D:325:LEU:HD13	1.92	0.51
1:D:105:PRO:HD3	1:D:295:TRP:CE2	2.46	0.51
1:D:392:GLY:O	1:D:396:ILE:HG12	2.10	0.51
1:A:112:ARG:HG3	1:A:113:SER:N	2.26	0.51
1:D:76:GLU:HA	1:D:102:ILE:HG23	1.92	0.51
1:A:3:MSE:HG2	1:B:279:ILE:HD12	1.94	0.50
1:A:16:LEU:O	1:A:20:ILE:HG12	2.11	0.50
1:A:75:ILE:CD1	1:A:292:ARG:HD3	2.41	0.49
1:B:367:VAL:HG11	1:B:379:PRO:HG3	1.94	0.49
1:A:114:ALA:CB	1:A:219:ILE:HD12	2.42	0.49
1:D:199:ASP:OD1	1:D:240:LYS:HE3	2.13	0.49
1:D:171:ILE:HG22	1:D:171:ILE:O	2.13	0.48
1:D:64:MSE:HE1	1:D:305:ILE:HG13	1.95	0.48
1:B:75:ILE:HD12	1:B:292:ARG:HD3	1.95	0.48
1:D:152:PHE:HE2	1:D:189:THR:HG21	1.79	0.48
1:D:399:LEU:O	1:D:403:LEU:HB2	2.12	0.48
1:D:250:VAL:O	1:D:272:GLY:HA2	2.14	0.48
1:B:171:ILE:HD13	1:B:208:LYS:HB3	1.96	0.48
1:D:69:ILE:HG23	1:D:301:ALA:HB2	1.95	0.48
1:A:286:SER:HA	1:B:10:TRP:HD1	1.79	0.47
1:A:69:ILE:HG23	1:A:301:ALA:HB2	1.96	0.47
1:B:1:MSE:H1	1:B:1:MSE:HE2	1.79	0.47
1:B:292:ARG:HA	1:B:292:ARG:HD2	1.71	0.47
1:A:292:ARG:HA	1:A:292:ARG:HD2	1.61	0.47
1:C:125:LEU:HD11	1:C:180:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:PHE:CE2	1:D:189:THR:HG21	2.49	0.47
1:D:60:ARG:O	1:D:64:MSE:HB2	2.15	0.47
1:B:1:MSE:HE2	1:B:1:MSE:N	2.31	0.47
1:D:121:GLU:C	1:D:123:ASP:H	2.18	0.47
1:B:16:LEU:O	1:B:20:ILE:HG12	2.15	0.46
1:C:61:LEU:HA	1:C:64:MSE:HE3	1.98	0.46
1:B:335:VAL:HG21	1:B:393:GLU:HG2	1.98	0.46
1:D:130:TYR:CE2	1:D:382:LYS:HB3	2.51	0.45
1:D:57:VAL:HG13	1:D:305:ILE:HG21	1.99	0.45
1:A:60:ARG:HG3	1:A:309:LEU:CD1	2.46	0.45
1:B:315:LYS:O	1:B:319:GLU:HG2	2.15	0.45
1:D:44:LEU:HG	1:D:354:PHE:CZ	2.51	0.45
1:A:105:PRO:HD2	1:A:109:GLY:HA3	1.99	0.45
1:B:56:SER:O	1:B:309:LEU:HD21	2.16	0.45
1:D:319:GLU:O	1:D:323:VAL:HG23	2.16	0.45
1:A:105:PRO:HD3	1:A:295:TRP:CE2	2.52	0.45
1:A:39:ALA:HB2	1:A:391:VAL:HG11	1.98	0.45
1:C:380:SER:C	1:C:382:LYS:H	2.20	0.44
1:A:175:ASP:HA	1:A:214:LYS:HD3	1.99	0.44
1:A:81:TYR:CD1	1:A:303:GLN:HA	2.52	0.44
1:A:119:LEU:HD22	1:A:123:ASP:HB3	1.99	0.44
1:A:72:TYR:CZ	1:B:263:TYR:HB3	2.52	0.44
1:A:111:ILE:HD13	1:A:135:TYR:CE1	2.46	0.44
1:B:44:LEU:HD13	1:B:325:LEU:HD11	2.00	0.44
1:A:221:ASP:OD2	2:A:501:PLP:N1	2.51	0.44
1:A:72:TYR:CE1	1:B:263:TYR:HB3	2.53	0.44
1:B:130:TYR:CD2	1:B:130:TYR:N	2.86	0.43
1:C:231:GLY:H	1:C:234:GLN:HE22	1.67	0.43
1:D:132:TRP:CE2	1:D:134:PRO:HG2	2.53	0.43
1:A:345:LEU:HD13	1:A:404:ALA:HA	2.00	0.43
1:B:189:THR:HB	1:B:348:ILE:HG21	1.99	0.43
1:A:136:ARG:HG3	1:A:146:PHE:CD2	2.54	0.43
1:B:15:ASP:HB3	1:B:18:PHE:HB3	2.00	0.43
1:A:104:THR:HB	1:A:109:GLY:HA3	1.99	0.43
1:A:162:VAL:HA	1:A:165:GLU:HG2	2.00	0.43
1:C:37:ILE:HG12	1:C:395:LYS:HD3	2.00	0.43
1:C:136:ARG:HG3	1:C:146:PHE:CD2	2.54	0.43
1:D:167:ILE:HD12	1:D:205:LEU:HD21	2.00	0.43
1:B:277:LYS:O	1:B:280:ILE:HG22	2.19	0.43
1:D:258:LYS:CE	2:D:501:PLP:H4A	2.48	0.43
1:C:366:ILE:HG23	1:C:406:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PHE:HB3	1:D:94:LYS:HA	2.00	0.42
1:D:78:GLU:O	1:D:82:ARG:HG3	2.18	0.42
1:A:30:LYS:HD2	1:A:31:TYR:CZ	2.54	0.42
1:C:120:ASP:HB2	1:D:5:ILE:HG21	2.00	0.42
1:B:7:ARG:O	1:B:10:TRP:CZ2	2.72	0.42
1:D:169:GLU:HA	1:D:172:ARG:HD3	2.02	0.42
1:D:336:PHE:HB2	1:D:388:ILE:HD11	2.01	0.42
1:C:55:PRO:O	1:C:59:ASP:HB2	2.20	0.42
1:A:60:ARG:HG3	1:A:309:LEU:HD13	2.02	0.41
1:C:363:ALA:C	1:C:365:ASP:H	2.23	0.41
1:D:348:ILE:HA	1:D:349:PRO:HD2	1.92	0.41
1:A:60:ARG:NH1	1:A:63:GLU:OE1	2.53	0.41
1:B:45:LEU:HD23	1:B:51:ILE:HA	2.01	0.41
1:C:99:ILE:HA	1:C:272:GLY:O	2.20	0.41
1:C:120:ASP:OD1	1:C:121:GLU:N	2.53	0.41
1:C:152:PHE:CE2	1:C:156:PHE:CD1	3.09	0.41
1:D:105:PRO:HD2	1:D:109:GLY:HA3	2.02	0.41
1:A:44:LEU:HD23	1:A:389:CYS:HB2	2.03	0.41
1:A:112:ARG:NH1	3:A:606:HOH:O	2.53	0.41
1:A:123:ASP:HA	1:A:124:PRO:HD3	1.93	0.41
1:D:391:VAL:HG23	1:D:396:ILE:CD1	2.51	0.41
1:C:262:ALA:HB1	1:C:265:LEU:HD12	2.03	0.41
1:A:46:ASP:HB3	1:A:52:ILE:HD11	2.03	0.40
1:D:124:PRO:HG2	1:D:177:ILE:HG22	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	407/413 (98%)	386 (95%)	20 (5%)	1 (0%)	44 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	407/413 (98%)	391 (96%)	14 (3%)	2 (0%)	25	43
1	C	401/413 (97%)	370 (92%)	29 (7%)	2 (0%)	25	43
1	D	401/413 (97%)	375 (94%)	24 (6%)	2 (0%)	25	43
All	All	1616/1652 (98%)	1522 (94%)	87 (5%)	7 (0%)	30	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	C	381	ALA
1	B	296	SER
1	D	172	ARG
1	D	387	ALA
1	C	232	ASP
1	B	124	PRO

### 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	344/341 (101%)	334 (97%)	10 (3%)	37	63
1	B	344/341 (101%)	332 (96%)	12 (4%)	31	57
1	C	342/341 (100%)	331 (97%)	11 (3%)	34	60
1	D	342/341 (100%)	329 (96%)	13 (4%)	28	54
All	All	1372/1364 (101%)	1326 (97%)	46 (3%)	32	57

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	89	LEU
1	A	129	ASP
1	A	141	GLU

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Mol	Chain	Res	Type
1	A	151	PHE
1	A	199	ASP
1	A	263	TYR
1	A	297	ASN
1	A	309	LEU
1	A	391	VAL
1	B	66	ARG
1	B	102	ILE
1	B	120	ASP
1	B	129	ASP
1	B	130	TYR
1	B	151	PHE
1	B	196	GLU
1	B	296	SER
1	B	297	ASN
1	B	331	SER
1	B	344	LYS
1	B	361	ASP
1	C	102	ILE
1	C	152	PHE
1	C	172	ARG
1	C	183	SER
1	C	232	ASP
1	C	273	ILE
1	C	278	GLU
1	C	296	SER
1	C	297	ASN
1	C	309	LEU
1	C	346	THR
1	D	60	ARG
1	D	112	ARG
1	D	151	PHE
1	D	167	ILE
1	D	196	GLU
1	D	267	SER
1	D	282	GLU
1	D	299	THR
1	D	309	LEU
1	D	349	PRO
1	D	365	ASP
1	D	367	VAL
1	D	394	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

4 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	A	501	-	16,16,16	1.30	1 (6%)	20,23,23	1.29	3 (15%)
2	PLP	C	501	-	16,16,16	1.28	2 (12%)	20,23,23	1.24	3 (15%)
2	PLP	D	501	-	16,16,16	1.26	2 (12%)	20,23,23	1.39	2 (10%)
2	PLP	B	501	-	16,16,16	1.30	1 (6%)	20,23,23	1.44	4 (20%)

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	A	501	-	-	5/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	501	-	-	2/8/8/8	0/1/1/1
2	PLP	D	501	-	-	2/8/8/8	0/1/1/1
2	PLP	B	501	-	-	4/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	PLP	C2-N1	3.14	1.39	1.33
2	C	501	PLP	C2-N1	3.06	1.39	1.33
2	B	501	PLP	C2-N1	2.97	1.39	1.33
2	A	501	PLP	C2-N1	2.84	1.38	1.33
2	D	501	PLP	C6-N1	2.33	1.39	1.34
2	C	501	PLP	C6-N1	2.31	1.39	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLP	C5-C6-N1	-2.80	119.27	123.83
2	D	501	PLP	C3-C4-C5	2.80	120.52	118.28
2	D	501	PLP	C5-C6-N1	-2.76	119.34	123.83
2	A	501	PLP	C3-C4-C4A	-2.65	116.20	119.84
2	C	501	PLP	C3-C4-C5	2.43	120.23	118.28
2	C	501	PLP	C5-C6-N1	-2.38	119.95	123.83
2	A	501	PLP	C5-C6-N1	-2.35	120.01	123.83
2	B	501	PLP	O4A-C4A-C4	-2.26	119.43	124.80
2	B	501	PLP	C3-C4-C5	2.11	119.97	118.28
2	A	501	PLP	O4P-C5A-C5	2.06	113.22	109.36
2	C	501	PLP	O4A-C4A-C4	-2.01	120.03	124.80
2	B	501	PLP	O3-C3-C2	2.00	121.73	117.58

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C3-C4-C4A-O4A
2	A	501	PLP	C5A-O4P-P-O1P
2	A	501	PLP	C5A-O4P-P-O2P
2	B	501	PLP	C3-C4-C4A-O4A
2	B	501	PLP	C5A-O4P-P-O3P
2	C	501	PLP	C3-C4-C4A-O4A

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Mol	Chain	Res	Type	Atoms
2	D	501	PLP	C3-C4-C4A-O4A
2	A	501	PLP	C5-C4-C4A-O4A
2	B	501	PLP	C5-C4-C4A-O4A
2	D	501	PLP	C5-C4-C4A-O4A
2	C	501	PLP	C5-C4-C4A-O4A
2	B	501	PLP	C5A-O4P-P-O2P
2	A	501	PLP	C5A-O4P-P-O3P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	1	0
2	D	501	PLP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	403/413 (97%)	-0.36	0 100 100	34, 48, 64, 86	0
1	B	403/413 (97%)	-0.35	2 (0%) 87 86	33, 46, 70, 96	0
1	C	401/413 (97%)	1.27	84 (20%) 3 3	61, 108, 144, 233	0
1	D	401/413 (97%)	1.17	81 (20%) 3 4	50, 95, 130, 220	0
All	All	1608/1652 (97%)	0.43	167 (10%) 13 12	33, 67, 136, 233	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	384	ILE	7.2
1	D	70	ALA	7.2
1	C	17	ALA	5.4
1	D	241	PHE	5.0
1	C	363	ALA	4.4
1	C	44	LEU	4.4
1	D	293	CYS	4.4
1	C	377	THR	4.4
1	C	40	ALA	4.4
1	C	356	THR	4.3
1	D	236	LYS	4.2
1	D	219	ILE	4.1
1	C	261	THR	4.0
1	D	171	ILE	4.0
1	D	69	ILE	4.0
1	C	122	GLY	4.0
1	C	193	LEU	4.0
1	D	170	GLY	4.0
1	D	126	ILE	3.9
1	C	52	ILE	3.9
1	D	242	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	178	ALA	3.8
1	C	354	PHE	3.7
1	C	16	LEU	3.7
1	C	5	ILE	3.7
1	C	386	VAL	3.7
1	D	238	PHE	3.6
1	C	366	ILE	3.6
1	D	72	TYR	3.6
1	C	388	ILE	3.6
1	D	305	ILE	3.6
1	D	216	ILE	3.6
1	C	179	SER	3.5
1	C	26	ALA	3.5
1	C	381	ALA	3.5
1	D	227	PHE	3.5
1	C	364	PHE	3.4
1	C	8	ALA	3.3
1	C	138	ILE	3.3
1	D	102	ILE	3.3
1	D	202	ILE	3.3
1	D	115	ILE	3.2
1	D	158	PHE	3.2
1	D	218	LEU	3.2
1	D	101	ALA	3.2
1	D	223	ALA	3.2
1	D	253	ALA	3.2
1	D	119	LEU	3.2
1	C	403	LEU	3.2
1	D	248	LEU	3.2
1	D	209	ALA	3.1
1	D	167	ILE	3.1
1	C	120	ASP	3.1
1	D	135	TYR	3.1
1	C	182	ASN	3.1
1	D	71	SER	3.1
1	C	101	ALA	3.1
1	C	57	VAL	3.1
1	D	203	THR	3.0
1	D	237	PHE	3.0
1	D	249	PHE	3.0
1	C	225	LEU	3.0
1	C	355	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	283	PHE	2.9
1	C	51	ILE	2.9
1	C	378	ILE	2.9
1	C	362	LYS	2.9
1	D	198	TRP	2.9
1	C	12	ASN	2.9
1	C	41	LEU	2.8
1	C	14	PRO	2.8
1	D	201	VAL	2.8
1	D	103	ALA	2.8
1	D	211	ASP	2.8
1	C	263	TYR	2.8
1	B	320	GLN	2.8
1	C	38	ASN	2.7
1	D	113	SER	2.7
1	D	180	LEU	2.7
1	D	265	LEU	2.7
1	C	382	LYS	2.7
1	C	391	VAL	2.7
1	D	288	ALA	2.7
1	C	226	GLU	2.7
1	C	379	PRO	2.7
1	D	152	PHE	2.6
1	D	297	ASN	2.6
1	D	166	ALA	2.6
1	C	10	TRP	2.6
1	C	357	PHE	2.6
1	C	189	THR	2.5
1	D	302	ALA	2.5
1	C	124	PRO	2.5
1	C	348	ILE	2.5
1	C	130	TYR	2.5
1	D	291	ALA	2.5
1	C	42	GLY	2.5
1	D	147	LYS	2.4
1	C	235	ARG	2.4
1	C	128	HIS	2.4
1	C	185	GLY	2.4
1	D	181	ILE	2.4
1	D	146	PHE	2.4
1	C	264	GLY	2.4
1	C	258	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	254	PHE	2.4
1	D	88	THR	2.4
1	D	125	LEU	2.3
1	D	258	LYS	2.3
1	D	312	ALA	2.3
1	C	183	SER	2.3
1	C	43	THR	2.3
1	D	12	ASN	2.3
1	C	216	ILE	2.3
1	D	13	GLY	2.3
1	C	174	SER	2.3
1	D	287	LEU	2.3
1	D	148	THR	2.3
1	D	75	ILE	2.2
1	D	220	VAL	2.2
1	D	221	ASP	2.2
1	C	368	LYS	2.2
1	C	396	ILE	2.2
1	C	18	PHE	2.2
1	C	39	ALA	2.2
1	D	273	ILE	2.2
1	C	231	GLY	2.2
1	D	118	TYR	2.2
1	C	241	PHE	2.2
1	C	336	PHE	2.2
1	C	228	ALA	2.2
1	D	208	LYS	2.2
1	D	124	PRO	2.2
1	C	28	ILE	2.2
1	C	126	ILE	2.2
1	D	162	VAL	2.2
1	C	351	PHE	2.2
1	C	184	PRO	2.2
1	C	15	ASP	2.2
1	C	177	ILE	2.2
1	D	99	ILE	2.2
1	D	251	VAL	2.2
1	D	98	TYR	2.1
1	C	48	LYS	2.1
1	C	125	LEU	2.1
1	C	20	ILE	2.1
1	D	117	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	217	THR	2.1
1	D	41	LEU	2.1
1	D	240	LYS	2.1
1	C	397	PRO	2.1
1	C	45	LEU	2.1
1	C	370	LEU	2.1
1	D	114	ALA	2.1
1	C	389	CYS	2.1
1	D	127	CYS	2.1
1	D	160	ILE	2.1
1	D	286	SER	2.1
1	D	278	GLU	2.1
1	D	164	LYS	2.1
1	C	254	PHE	2.1
1	C	233	GLN	2.0
1	C	380	SER	2.0
1	C	53	ALA	2.0
1	B	171	ILE	2.0
1	C	358	ILE	2.0
1	D	222	VAL	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PLP	C	501	16/16	0.79	0.14	59,68,74,79	0
2	PLP	D	501	16/16	0.88	0.10	38,46,57,57	0
2	PLP	A	501	16/16	0.96	0.09	23,28,33,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	B	501	16/16	0.96	0.09	30,37,43,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.