



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:03 PM UTC

PDB ID : 4YSN / pdb_00004ysn
Title : Structure of aminoacid racemase in complex with PLP
Authors : Sakuraba, H.; Mutaguchi, Y.; Hayashi, J.; Ohshima, T.
Deposited on : 2015-03-17
Resolution : 1.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

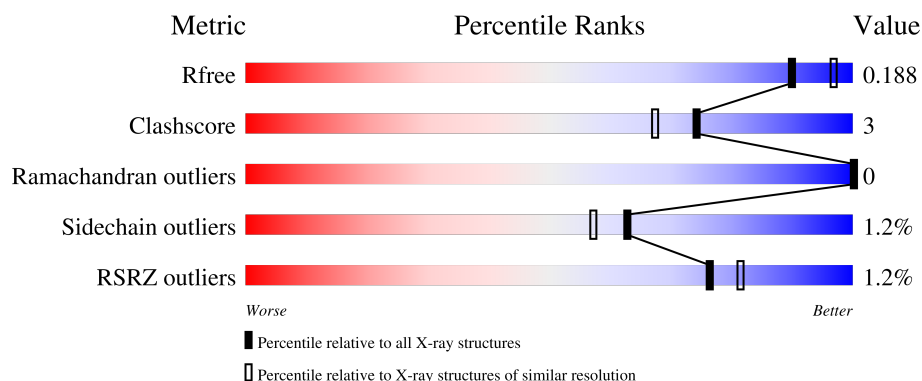
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

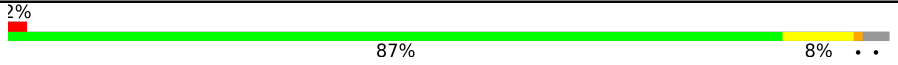
The reported resolution of this entry is 1.94 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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

Mol	Chain	Length	Quality of chain
1	A	462	
1	B	462	
1	C	462	
1	D	462	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15182 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 Putative 4-aminobutyrate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3451	2199	579	655	18			
1	B	443	Total	C	N	O	S	0	0	0
			3426	2183	574	652	17			
1	C	448	Total	C	N	O	S	0	0	0
			3468	2207	584	659	18			
1	D	442	Total	C	N	O	S	0	0	0
			3418	2177	573	651	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLY	-	expression tag	UNP M1GRN3
A	-10	SER	-	expression tag	UNP M1GRN3
A	-9	GLY	-	expression tag	UNP M1GRN3
A	-8	GLY	-	expression tag	UNP M1GRN3
A	-7	ILE	-	expression tag	UNP M1GRN3
A	-6	GLU	-	expression tag	UNP M1GRN3
A	-5	GLY	-	expression tag	UNP M1GRN3
A	-4	ARG	-	expression tag	UNP M1GRN3
A	-3	HIS	-	expression tag	UNP M1GRN3
A	-2	MET	-	expression tag	UNP M1GRN3
A	-1	GLU	-	expression tag	UNP M1GRN3
A	0	LEU	-	expression tag	UNP M1GRN3
B	-11	GLY	-	expression tag	UNP M1GRN3
B	-10	SER	-	expression tag	UNP M1GRN3
B	-9	GLY	-	expression tag	UNP M1GRN3
B	-8	GLY	-	expression tag	UNP M1GRN3
B	-7	ILE	-	expression tag	UNP M1GRN3
B	-6	GLU	-	expression tag	UNP M1GRN3
B	-5	GLY	-	expression tag	UNP M1GRN3
B	-4	ARG	-	expression tag	UNP M1GRN3
B	-3	HIS	-	expression tag	UNP M1GRN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP M1GRN3
B	-1	GLU	-	expression tag	UNP M1GRN3
B	0	LEU	-	expression tag	UNP M1GRN3
C	-11	GLY	-	expression tag	UNP M1GRN3
C	-10	SER	-	expression tag	UNP M1GRN3
C	-9	GLY	-	expression tag	UNP M1GRN3
C	-8	GLY	-	expression tag	UNP M1GRN3
C	-7	ILE	-	expression tag	UNP M1GRN3
C	-6	GLU	-	expression tag	UNP M1GRN3
C	-5	GLY	-	expression tag	UNP M1GRN3
C	-4	ARG	-	expression tag	UNP M1GRN3
C	-3	HIS	-	expression tag	UNP M1GRN3
C	-2	MET	-	expression tag	UNP M1GRN3
C	-1	GLU	-	expression tag	UNP M1GRN3
C	0	LEU	-	expression tag	UNP M1GRN3
D	-11	GLY	-	expression tag	UNP M1GRN3
D	-10	SER	-	expression tag	UNP M1GRN3
D	-9	GLY	-	expression tag	UNP M1GRN3
D	-8	GLY	-	expression tag	UNP M1GRN3
D	-7	ILE	-	expression tag	UNP M1GRN3
D	-6	GLU	-	expression tag	UNP M1GRN3
D	-5	GLY	-	expression tag	UNP M1GRN3
D	-4	ARG	-	expression tag	UNP M1GRN3
D	-3	HIS	-	expression tag	UNP M1GRN3
D	-2	MET	-	expression tag	UNP M1GRN3
D	-1	GLU	-	expression tag	UNP M1GRN3
D	0	LEU	-	expression tag	UNP M1GRN3

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		

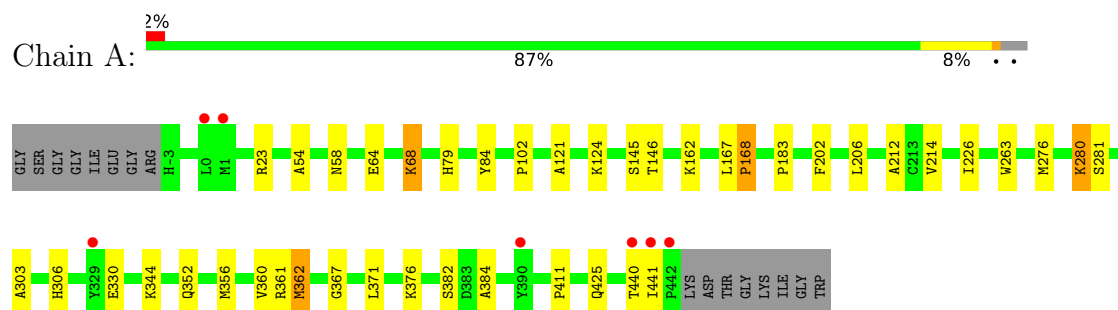
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	332	Total	O	0	0
			332	332		
3	B	338	Total	O	0	0
			338	338		
3	C	332	Total	O	0	0
			332	332		
3	D	357	Total	O	0	0
			357	357		

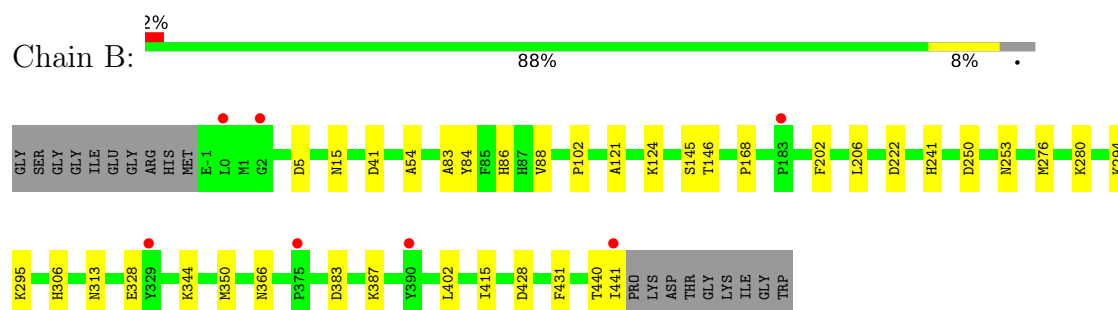
3 Residue-property plots

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.

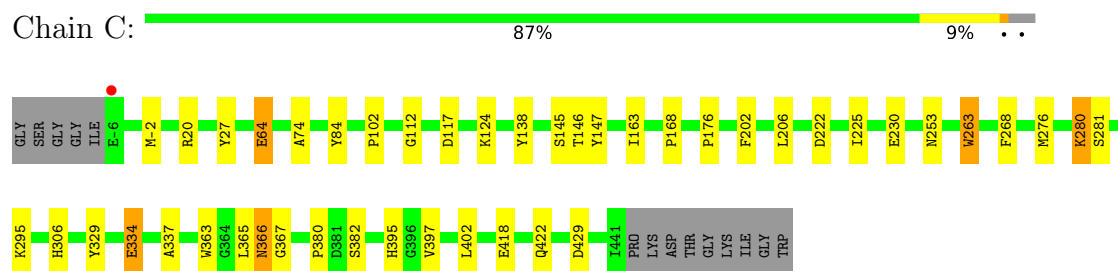
- Molecule 1: Putative 4-aminobutyrate aminotransferase



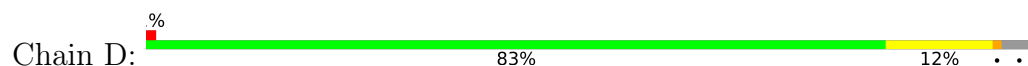
- Molecule 1: Putative 4-aminobutyrate aminotransferase

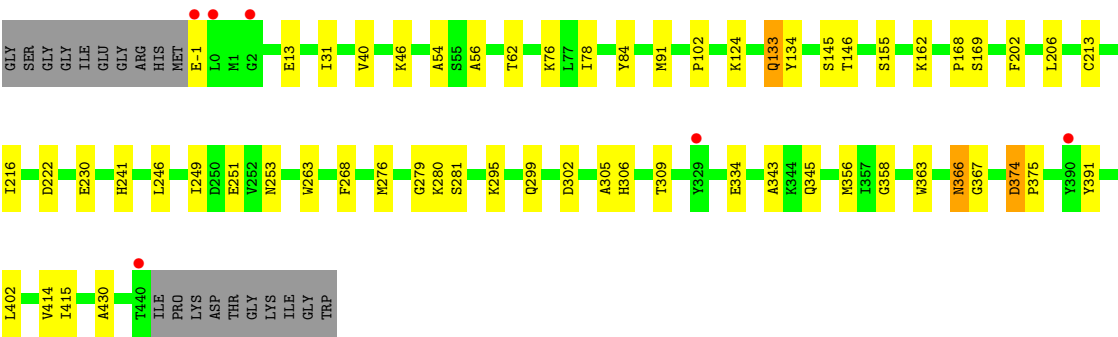


- Molecule 1: Putative 4-aminobutyrate aminotransferase



- Molecule 1: Putative 4-aminobutyrate aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.03Å 169.02Å 178.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.94 50.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-1.94) 99.4 (50.00-1.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.83 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.147 , 0.188 0.150 , 0.188	Depositor DCC
R_{free} test set	6663 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15182	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.33	14/3531 (0.4%)	1.09	4/4787 (0.1%)
1	B	1.31	9/3504 (0.3%)	1.07	2/4750 (0.0%)
1	C	1.37	17/3547 (0.5%)	1.11	5/4806 (0.1%)
1	D	1.37	13/3496 (0.4%)	1.12	8/4739 (0.2%)
All	All	1.34	53/14078 (0.4%)	1.10	19/19082 (0.1%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	329	TYR	C-O	7.12	1.33	1.24
1	A	330	GLU	C-O	-6.58	1.15	1.24
1	C	27	TYR	CA-C	-6.42	1.44	1.52
1	A	360	VAL	C-O	-6.33	1.17	1.24
1	A	281	SER	C-O	-6.22	1.16	1.24
1	B	88	VAL	CA-C	6.13	1.57	1.52
1	B	86	HIS	C-O	-6.07	1.16	1.23
1	B	313	ASN	CA-C	5.99	1.59	1.53
1	B	83	ALA	C-O	-5.96	1.16	1.24
1	A	212	ALA	C-O	-5.96	1.17	1.24
1	C	281	SER	C-O	-5.92	1.16	1.24
1	D	366	ASN	C-O	-5.87	1.16	1.24
1	A	58	ASN	C-O	-5.83	1.17	1.24
1	C	176	PRO	CA-C	-5.80	1.46	1.52
1	C	395	HIS	C-O	-5.80	1.16	1.23
1	D	305	ALA	C-O	-5.79	1.16	1.24
1	B	328	GLU	C-O	-5.78	1.17	1.24
1	A	362	MET	C-O	-5.71	1.17	1.23
1	C	263	TRP	CA-C	-5.70	1.45	1.52
1	D	134	TYR	C-O	-5.58	1.17	1.23
1	A	280	LYS	C-O	-5.58	1.17	1.24
1	C	337	ALA	C-O	-5.57	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	C-O	-5.51	1.17	1.23
1	B	84	TYR	C-O	-5.50	1.16	1.23
1	C	365	LEU	C-O	-5.49	1.17	1.23
1	B	366	ASN	C-O	-5.48	1.17	1.24
1	D	356	MET	C-O	-5.48	1.17	1.24
1	A	214	VAL	C-O	-5.47	1.18	1.24
1	C	74	ALA	N-CA	-5.46	1.39	1.46
1	C	397	VAL	C-O	5.43	1.29	1.24
1	C	429	ASP	C-O	-5.43	1.17	1.24
1	C	382	SER	C-O	-5.40	1.17	1.24
1	A	84	TYR	C-O	-5.38	1.16	1.24
1	C	380	PRO	C-O	-5.37	1.17	1.23
1	D	155	SER	C-O	-5.34	1.17	1.24
1	D	76	LYS	C-O	-5.29	1.17	1.23
1	B	88	VAL	CA-CB	5.28	1.57	1.53
1	A	23	ARG	C-O	-5.27	1.18	1.23
1	D	246	LEU	C-O	5.24	1.30	1.23
1	D	78	ILE	C-O	-5.22	1.18	1.24
1	A	183	PRO	N-CA	5.20	1.53	1.47
1	A	361	ARG	C-O	-5.20	1.17	1.24
1	D	62	THR	C-O	-5.19	1.17	1.23
1	D	279	GLY	C-O	-5.18	1.18	1.23
1	D	31	ILE	C-O	5.18	1.30	1.24
1	D	91	MET	C-O	-5.17	1.18	1.24
1	B	415	ILE	CA-C	5.10	1.58	1.52
1	C	366	ASN	C-O	-5.07	1.17	1.24
1	D	84	TYR	C-O	-5.03	1.17	1.24
1	C	84	TYR	C-O	-5.03	1.17	1.24
1	A	303	ALA	C-O	-5.02	1.17	1.23
1	C	280	LYS	C-O	-5.02	1.17	1.24
1	C	225	ILE	C-O	-5.01	1.18	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASN	N-CA-C	6.20	119.94	112.38
1	D	358	GLY	N-CA-C	5.84	119.56	112.49
1	A	79	HIS	N-CA-C	5.79	117.92	108.55
1	D	374	ASP	CA-C-N	5.73	125.27	119.19
1	D	374	ASP	C-N-CA	5.73	125.27	119.19
1	B	41	ASP	N-CA-C	5.67	117.85	110.53
1	C	147	TYR	N-CA-C	5.66	118.22	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	ILE	N-CA-C	5.64	118.31	112.90
1	D	213	CYS	N-CA-C	5.45	117.13	108.79
1	C	138	TYR	N-CA-C	5.43	118.34	109.59
1	C	334	GLU	CB-CG-CD	5.38	121.74	112.60
1	D	133	GLN	N-CA-C	5.35	119.93	113.41
1	A	425	GLN	N-CA-C	-5.29	105.59	111.36
1	D	367	GLY	N-CA-C	5.23	118.75	110.96
1	A	411	PRO	N-CA-C	5.11	116.93	110.70
1	D	216	ILE	N-CA-C	5.08	116.03	108.46
1	C	367	GLY	N-CA-C	5.02	118.58	110.90
1	D	343	ALA	N-CA-C	5.01	116.74	111.28
1	A	367	GLY	N-CA-C	5.00	118.89	111.18

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	3451	0	3413	22	0
1	B	3426	0	3389	23	0
1	C	3468	0	3427	20	0
1	D	3418	0	3378	28	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
2	C	15	0	6	1	0
2	D	15	0	6	1	0
3	A	332	0	0	3	0
3	B	338	0	0	6	0
3	C	332	0	0	5	0
3	D	357	0	0	4	0
All	All	15182	0	13631	86	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 (86) 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:352:GLN:HG3	3:A:1311:HOH:O	1.63	0.99
1:A:356:MET:HE2	1:A:371:LEU:HD13	1.69	0.75
1:B:350:MET:HE3	1:B:428:ASP:HA	1.70	0.74
1:A:356:MET:CE	1:A:384:ALA:HB1	2.21	0.69
1:D:-1:GLU:HB3	3:D:1404:HOH:O	1.95	0.67
1:B:241:HIS:HE1	3:B:1324:HOH:O	1.78	0.66
1:C:334:GLU:CD	3:C:1121:HOH:O	2.41	0.64
1:A:356:MET:HE1	1:A:384:ALA:HB1	1.79	0.63
1:B:124:LYS:NZ	1:B:306:HIS:HD2	1.98	0.61
1:B:350:MET:CE	1:B:431:PHE:CD2	2.86	0.59
1:D:102:PRO:HD2	1:D:276:MET:SD	2.43	0.59
1:D:334:GLU:HG3	3:D:1432:HOH:O	2.03	0.58
1:C:124:LYS:NZ	1:C:306:HIS:HD2	2.01	0.57
1:A:124:LYS:NZ	1:A:306:HIS:HD2	2.03	0.57
1:B:350:MET:HE2	1:B:431:PHE:CE2	2.39	0.56
1:B:344:LYS:NZ	3:B:1103:HOH:O	2.37	0.56
1:B:102:PRO:HD2	1:B:276:MET:SD	2.47	0.55
1:B:121:ALA:HB2	1:B:306:HIS:CE1	2.41	0.55
1:A:168:PRO:HG3	1:B:168:PRO:HG3	1.89	0.55
1:C:124:LYS:HZ1	1:C:306:HIS:HD2	1.55	0.54
1:B:350:MET:CE	1:B:431:PHE:CE2	2.90	0.54
1:D:124:LYS:NZ	1:D:306:HIS:HD2	2.04	0.54
1:C:64:GLU:HG2	3:C:1285:HOH:O	2.08	0.54
1:D:253:ASN:HB2	2:D:1001:PLP:O3	2.09	0.53
1:A:344:LYS:HE3	3:A:1298:HOH:O	2.10	0.51
1:D:202:PHE:HA	1:D:206:LEU:O	2.12	0.50
1:C:202:PHE:HA	1:C:206:LEU:O	2.12	0.50
1:A:68:LYS:N	1:A:68:LYS:HD3	2.26	0.50
1:D:295:LYS:HE2	1:D:299:GLN:NE2	2.26	0.50
1:C:280:LYS:HE3	1:D:309:THR:OG1	2.11	0.50
1:B:124:LYS:HZ1	1:B:306:HIS:HD2	1.58	0.50
1:B:295:LYS:NZ	3:B:1110:HOH:O	2.45	0.49
1:B:222:ASP:HA	1:B:402:LEU:HD22	1.95	0.49
1:C:20:ARG:NE	1:D:302:ASP:OD1	2.37	0.49
1:D:241:HIS:HD2	3:D:1271:HOH:O	1.95	0.49
1:C:222:ASP:HA	1:C:402:LEU:HD22	1.95	0.48
1:D:133:GLN:NE2	1:D:169:SER:OG	2.43	0.48
1:B:350:MET:HE2	1:B:431:PHE:CD2	2.48	0.48
1:A:124:LYS:HZ1	1:A:306:HIS:HD2	1.62	0.48
1:B:350:MET:CE	1:B:431:PHE:HD2	2.25	0.48
1:C:168:PRO:HG3	1:D:168:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:HD2	1:A:276:MET:SD	2.54	0.47
1:C:112:GLY:HA3	1:C:117:ASP:OD1	2.14	0.47
1:C:102:PRO:HD2	1:C:276:MET:SD	2.55	0.47
1:A:146:THR:HG21	1:B:146:THR:HG21	1.96	0.47
1:C:295:LYS:CE	3:C:1137:HOH:O	2.63	0.46
1:A:162:LYS:HD2	3:B:1209:HOH:O	2.16	0.46
1:A:121:ALA:HB2	1:A:306:HIS:CE1	2.51	0.45
1:A:356:MET:HE3	1:A:384:ALA:HB1	1.97	0.45
1:C:102:PRO:HD3	1:C:263:TRP:CD1	2.52	0.45
1:D:222:ASP:HA	1:D:402:LEU:HD22	1.98	0.45
1:C:20:ARG:NH2	1:D:302:ASP:OD1	2.49	0.44
1:B:202:PHE:HA	1:B:206:LEU:O	2.18	0.44
1:D:102:PRO:HD3	1:D:263:TRP:CD1	2.53	0.44
1:A:54:ALA:O	1:A:280:LYS:HD3	2.18	0.44
1:D:306:HIS:HE1	3:D:1166:HOH:O	2.01	0.43
1:D:414:VAL:O	1:D:415:ILE:C	2.61	0.43
1:B:253:ASN:HB2	2:B:1001:PLP:O3	2.18	0.43
1:C:418:GLU:O	1:C:422:GLN:HG3	2.17	0.43
1:D:374:ASP:HA	1:D:375:PRO:HD3	1.85	0.43
1:D:230:GLU:OE1	1:D:268:PHE:HA	2.18	0.43
1:A:362:MET:HE2	1:A:362:MET:HB2	1.98	0.43
1:A:102:PRO:HD3	1:A:263:TRP:CD1	2.54	0.43
1:D:249:ILE:O	1:D:276:MET:HA	2.18	0.43
1:B:344:LYS:HE3	3:B:1272:HOH:O	2.18	0.42
1:C:146:THR:HG21	1:D:146:THR:HG21	2.01	0.42
1:B:294:LYS:NZ	3:B:1117:HOH:O	2.51	0.42
1:D:54:ALA:O	1:D:280:LYS:HD3	2.19	0.42
1:C:253:ASN:HB2	2:C:1001:PLP:O3	2.19	0.42
1:D:251:GLU:HG3	1:D:276:MET:HE3	2.02	0.42
3:C:1425:HOH:O	1:D:13:GLU:HG2	2.20	0.42
1:C:363:TRP:O	1:C:366:ASN:HB3	2.18	0.42
1:A:167:LEU:HA	1:A:168:PRO:HD3	1.83	0.42
1:C:230:GLU:OE1	1:C:268:PHE:HA	2.20	0.42
1:B:54:ALA:O	1:B:280:LYS:HD3	2.20	0.41
1:B:250:ASP:C	1:B:250:ASP:OD1	2.64	0.41
1:A:202:PHE:HA	1:A:206:LEU:O	2.20	0.41
1:D:40:VAL:HG22	1:D:46:LYS:HG2	2.02	0.41
1:A:306:HIS:HE1	3:A:1210:HOH:O	2.03	0.41
1:A:124:LYS:NZ	1:A:306:HIS:CD2	2.88	0.40
1:C:306:HIS:HE1	3:C:1131:HOH:O	2.04	0.40
1:D:56:ALA:O	1:D:281:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ASP:OD2	1:B:387:LYS:HE2	2.21	0.40
1:D:391:TYR:CD1	1:D:430:ALA:HB2	2.57	0.40
1:D:363:TRP:O	1:D:366:ASN:HB3	2.22	0.40
1:A:64:GLU:HB2	1:A:68:LYS:HE2	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	444/462 (96%)	430 (97%)	14 (3%)	0	100	100
1	B	441/462 (96%)	428 (97%)	13 (3%)	0	100	100
1	C	446/462 (96%)	431 (97%)	15 (3%)	0	100	100
1	D	440/462 (95%)	426 (97%)	14 (3%)	0	100	100
All	All	1771/1848 (96%)	1715 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	369/379 (97%)	362 (98%)	7 (2%)	50	40
1	B	366/379 (97%)	362 (99%)	4 (1%)	65	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	370/379 (98%)	367 (99%)	3 (1%)	73	71
1	D	365/379 (96%)	362 (99%)	3 (1%)	73	71
All	All	1470/1516 (97%)	1453 (99%)	17 (1%)	63	57

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	145	SER
1	A	226	ILE
1	A	376	LYS
1	A	382	SER
1	A	440	THR
1	A	441	ILE
1	B	5	ASP
1	B	145	SER
1	B	440	THR
1	B	441	ILE
1	C	-2	MET
1	C	64	GLU
1	C	145	SER
1	D	145	SER
1	D	162	LYS
1	D	345	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	45	ASN
1	A	104	ASN
1	A	119	ASN
1	A	133	GLN
1	A	306	HIS
1	B	25	ASN
1	B	113	ASN
1	B	119	ASN
1	B	241	HIS
1	B	243	HIS
1	B	306	HIS

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Mol	Chain	Res	Type
1	C	25	ASN
1	C	104	ASN
1	C	119	ASN
1	C	306	HIS
1	C	345	GLN
1	C	352	GLN
1	D	25	ASN
1	D	119	ASN
1	D	133	GLN
1	D	243	HIS
1	D	306	HIS
1	D	351	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	1001	1	15,15,16	2.50	6 (40%)	21,22,23	1.26	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	C	1001	1	15,15,16	2.12	6 (40%)	21,22,23	1.60	7 (33%)
2	PLP	B	1001	1	15,15,16	1.99	4 (26%)	21,22,23	1.92	6 (28%)
2	PLP	A	1001	1	15,15,16	2.58	5 (33%)	21,22,23	1.99	5 (23%)

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	D	1001	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1001	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1001	1	-	0/6/6/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PLP	C3-C2	7.03	1.48	1.41
2	D	1001	PLP	C3-C4	4.76	1.49	1.40
2	B	1001	PLP	C3-C4	4.65	1.49	1.40
2	D	1001	PLP	C5-C4	4.57	1.45	1.40
2	D	1001	PLP	C4A-C4	-4.28	1.43	1.51
2	C	1001	PLP	C3-C4	4.26	1.48	1.40
2	A	1001	PLP	C5-C4	3.99	1.45	1.40
2	D	1001	PLP	C3-C2	3.84	1.45	1.41
2	A	1001	PLP	C3-C4	3.67	1.47	1.40
2	C	1001	PLP	C3-C2	3.66	1.44	1.41
2	B	1001	PLP	C4A-C4	-3.25	1.45	1.51
2	C	1001	PLP	C5-C4	3.24	1.44	1.40
2	A	1001	PLP	O3-C3	-3.04	1.29	1.36
2	D	1001	PLP	C2A-C2	2.78	1.54	1.50
2	B	1001	PLP	C5-C4	2.69	1.43	1.40
2	B	1001	PLP	C3-C2	2.68	1.43	1.41
2	C	1001	PLP	C4A-C4	-2.44	1.46	1.51
2	C	1001	PLP	C2A-C2	2.42	1.54	1.50
2	A	1001	PLP	C4A-C4	-2.22	1.47	1.51
2	D	1001	PLP	C2-N1	2.15	1.37	1.33
2	C	1001	PLP	P-O3P	-2.12	1.46	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	PLP	O4P-C5A-C5	4.81	118.38	109.36
2	B	1001	PLP	O4P-C5A-C5	4.30	117.41	109.36
2	A	1001	PLP	C3-C4-C5	-3.79	114.04	118.59
2	B	1001	PLP	C6-N1-C2	3.58	125.68	119.20
2	B	1001	PLP	C3-C2-N1	-3.45	116.61	120.96
2	A	1001	PLP	O4P-P-O1P	-3.16	97.89	106.44
2	B	1001	PLP	O4P-P-O1P	-3.14	97.95	106.44
2	A	1001	PLP	C3-C2-N1	-2.94	117.25	120.96
2	B	1001	PLP	C2A-C2-N1	2.78	122.88	117.64
2	C	1001	PLP	O2P-P-O4P	-2.62	99.83	106.67
2	C	1001	PLP	C3-C2-N1	-2.51	117.79	120.96
2	C	1001	PLP	C3-C4-C5	-2.49	115.61	118.59
2	C	1001	PLP	C6-N1-C2	2.43	123.61	119.20
2	A	1001	PLP	O3P-P-O2P	2.41	116.85	107.80
2	C	1001	PLP	O3-C3-C2	2.35	122.46	117.58
2	C	1001	PLP	O3P-P-O2P	2.32	116.49	107.80
2	B	1001	PLP	C4A-C4-C5	2.24	123.25	120.94
2	D	1001	PLP	O3P-P-O2P	2.24	116.19	107.80
2	D	1001	PLP	O4P-C5A-C5	2.22	113.53	109.36
2	C	1001	PLP	O4P-C5A-C5	2.17	113.42	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	PLP	1	0
2	C	1001	PLP	1	0
2	B	1001	PLP	1	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, 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	446/462 (96%)	-0.30	7 (1%) 70 77	12, 21, 35, 80	0
1	B	443/462 (95%)	-0.17	7 (1%) 70 77	13, 22, 42, 82	0
1	C	448/462 (96%)	-0.51	1 (0%) 91 94	11, 17, 30, 69	0
1	D	442/462 (95%)	-0.46	6 (1%) 73 79	11, 17, 32, 73	0
All	All	1779/1848 (96%)	-0.36	21 (1%) 76 81	11, 19, 36, 82	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	TYR	5.1
1	A	329	TYR	4.2
1	B	441	ILE	4.2
1	B	2	GLY	3.6
1	A	0	LEU	3.6
1	A	1	MET	3.5
1	D	440	THR	3.4
1	B	0	LEU	3.3
1	A	442	PRO	3.1
1	D	329	TYR	3.0
1	C	-6	GLU	2.9
1	D	2	GLY	2.9
1	A	441	ILE	2.9
1	A	390	TYR	2.8
1	D	390	TYR	2.7
1	B	390	TYR	2.7
1	D	0	LEU	2.7
1	D	-1	GLU	2.6
1	B	183	PRO	2.4
1	B	375	PRO	2.2
1	A	440	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	B	1001	15/16	0.98	0.04	16,18,22,22	0
2	PLP	D	1001	15/16	0.98	0.04	11,13,16,17	0
2	PLP	C	1001	15/16	0.99	0.04	12,13,18,19	0
2	PLP	A	1001	15/16	0.99	0.04	14,16,20,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.