



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:47 AM UTC

PDB ID : 7YPM / pdb_00007ypm
Title : Crystal structure of transaminase CC1012 complexed with PLP and L-alanine
Authors : Yang, L.; Wang, H.; Wei, D.
Deposited on : 2022-08-03
Resolution : 1.98 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

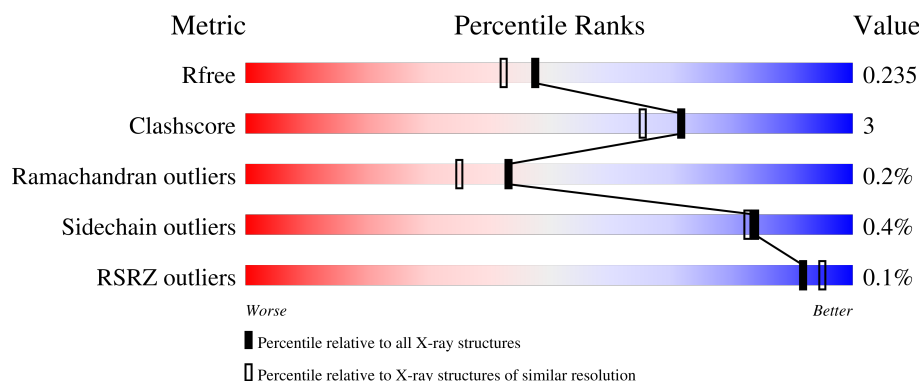
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	474	
1	B	474	
1	C	474	
1	D	474	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALA	B	503	-	X	-	-
3	ALA	C	503	-	X	-	-
3	ALA	D	503	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15347 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	454	Total	C	N	O	S	0	0	0
			3486	2218	616	636	16			
1	B	454	Total	C	N	O	S	0	0	0
			3486	2218	616	636	16			
1	C	454	Total	C	N	O	S	0	0	0
			3486	2218	616	636	16			
1	D	454	Total	C	N	O	S	0	1	0
			3494	2223	619	636	16			

There are 60 discrepancies between the modelled and reference sequences:

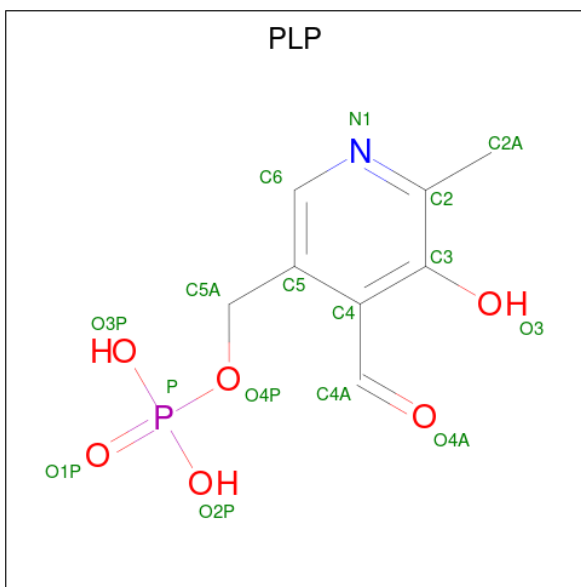
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A318BC23
A	-4	HIS	-	expression tag	UNP A0A318BC23
A	-3	HIS	-	expression tag	UNP A0A318BC23
A	-2	HIS	-	expression tag	UNP A0A318BC23
A	-1	HIS	-	expression tag	UNP A0A318BC23
A	0	HIS	-	expression tag	UNP A0A318BC23
A	1	HIS	-	expression tag	UNP A0A318BC23
A	44	GLU	ASP	engineered mutation	UNP A0A318BC23
A	138	PHE	TYR	engineered mutation	UNP A0A318BC23
A	192	GLN	PRO	engineered mutation	UNP A0A318BC23
A	377	VAL	THR	engineered mutation	UNP A0A318BC23
A	448	ARG	ALA	engineered mutation	UNP A0A318BC23
A	466	GLY	-	expression tag	UNP A0A318BC23
A	467	GLU	-	expression tag	UNP A0A318BC23
A	468	ASP	-	expression tag	UNP A0A318BC23
B	-5	MET	-	initiating methionine	UNP A0A318BC23
B	-4	HIS	-	expression tag	UNP A0A318BC23
B	-3	HIS	-	expression tag	UNP A0A318BC23
B	-2	HIS	-	expression tag	UNP A0A318BC23
B	-1	HIS	-	expression tag	UNP A0A318BC23
B	0	HIS	-	expression tag	UNP A0A318BC23

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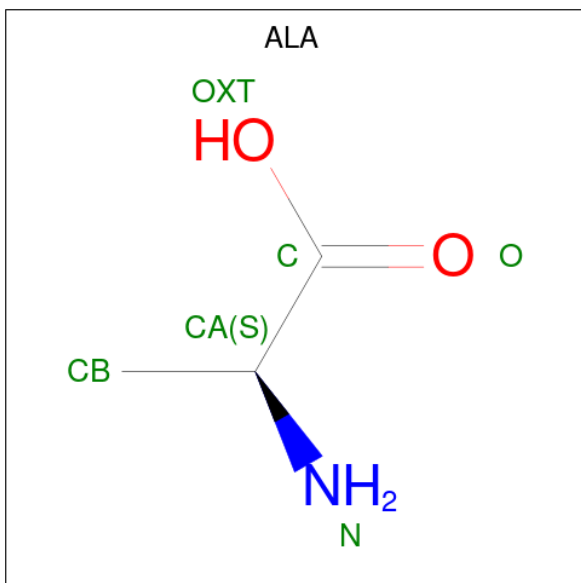
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	HIS	-	expression tag	UNP A0A318BC23
B	44	GLU	ASP	engineered mutation	UNP A0A318BC23
B	138	PHE	TYR	engineered mutation	UNP A0A318BC23
B	192	GLN	PRO	engineered mutation	UNP A0A318BC23
B	377	VAL	THR	engineered mutation	UNP A0A318BC23
B	448	ARG	ALA	engineered mutation	UNP A0A318BC23
B	466	GLY	-	expression tag	UNP A0A318BC23
B	467	GLU	-	expression tag	UNP A0A318BC23
B	468	ASP	-	expression tag	UNP A0A318BC23
C	-5	MET	-	initiating methionine	UNP A0A318BC23
C	-4	HIS	-	expression tag	UNP A0A318BC23
C	-3	HIS	-	expression tag	UNP A0A318BC23
C	-2	HIS	-	expression tag	UNP A0A318BC23
C	-1	HIS	-	expression tag	UNP A0A318BC23
C	0	HIS	-	expression tag	UNP A0A318BC23
C	1	HIS	-	expression tag	UNP A0A318BC23
C	44	GLU	ASP	engineered mutation	UNP A0A318BC23
C	138	PHE	TYR	engineered mutation	UNP A0A318BC23
C	192	GLN	PRO	engineered mutation	UNP A0A318BC23
C	377	VAL	THR	engineered mutation	UNP A0A318BC23
C	448	ARG	ALA	engineered mutation	UNP A0A318BC23
C	466	GLY	-	expression tag	UNP A0A318BC23
C	467	GLU	-	expression tag	UNP A0A318BC23
C	468	ASP	-	expression tag	UNP A0A318BC23
D	-5	MET	-	initiating methionine	UNP A0A318BC23
D	-4	HIS	-	expression tag	UNP A0A318BC23
D	-3	HIS	-	expression tag	UNP A0A318BC23
D	-2	HIS	-	expression tag	UNP A0A318BC23
D	-1	HIS	-	expression tag	UNP A0A318BC23
D	0	HIS	-	expression tag	UNP A0A318BC23
D	1	HIS	-	expression tag	UNP A0A318BC23
D	44	GLU	ASP	engineered mutation	UNP A0A318BC23
D	138	PHE	TYR	engineered mutation	UNP A0A318BC23
D	192	GLN	PRO	engineered mutation	UNP A0A318BC23
D	377	VAL	THR	engineered mutation	UNP A0A318BC23
D	448	ARG	ALA	engineered mutation	UNP A0A318BC23
D	466	GLY	-	expression tag	UNP A0A318BC23
D	467	GLU	-	expression tag	UNP A0A318BC23
D	468	ASP	-	expression tag	UNP A0A318BC23

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



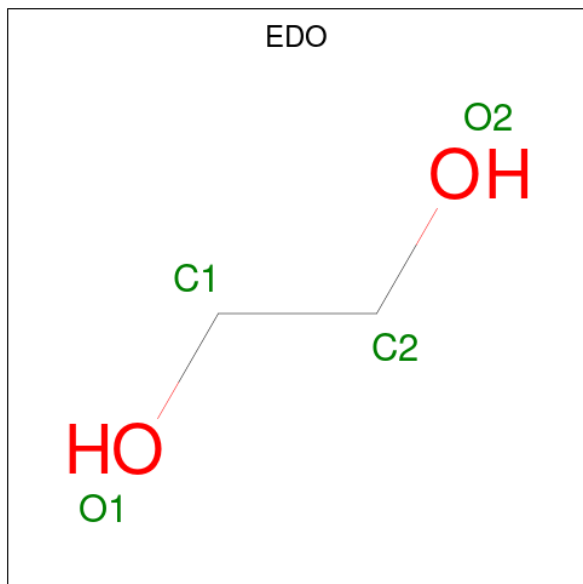
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



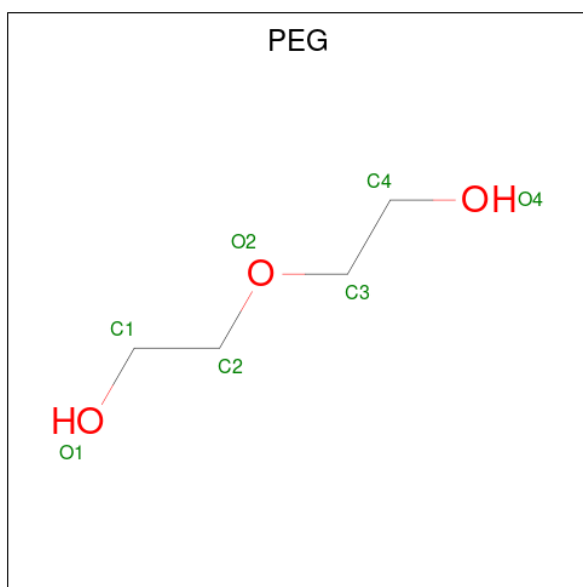
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 6 3 1 2	0	0
3	B	1	Total C N O 6 3 1 2	0	0
3	B	1	Total C N O 6 3 1 2	0	0
3	C	1	Total C N O 6 3 1 2	0	0
3	D	1	Total C N O 6 3 1 2	0	0
3	D	1	Total C N O 6 3 1 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		

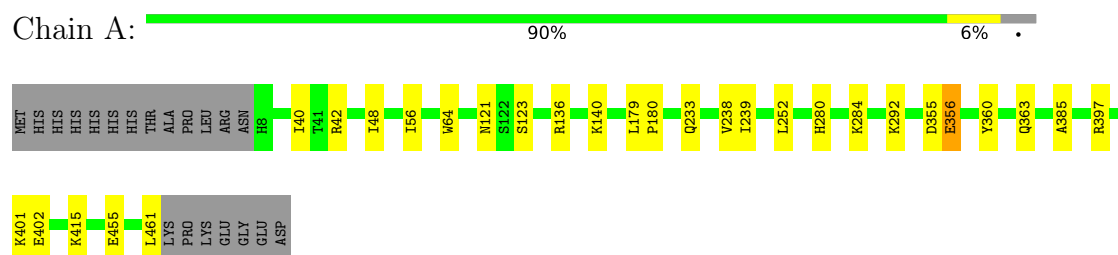
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	309	Total	O	0	0
			309	309		
6	B	314	Total	O	0	0
			314	314		
6	C	333	Total	O	0	0
			333	333		
6	D	332	Total	O	0	0
			332	332		

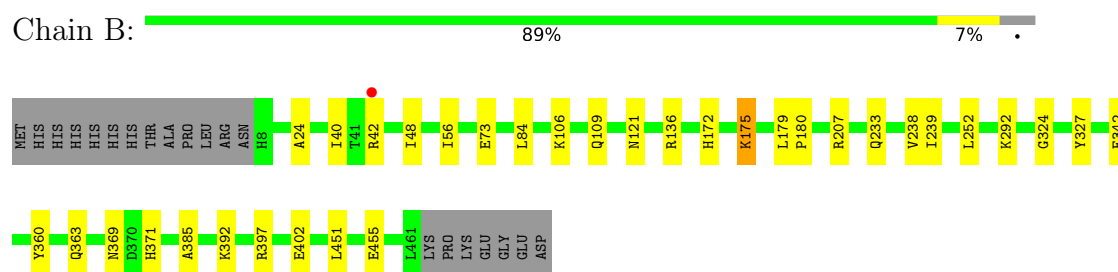
3 Residue-property plots

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.

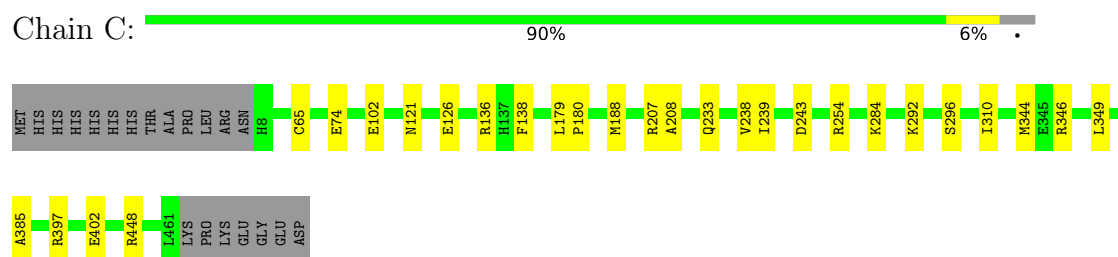
- Molecule 1: Aspartate aminotransferase family protein



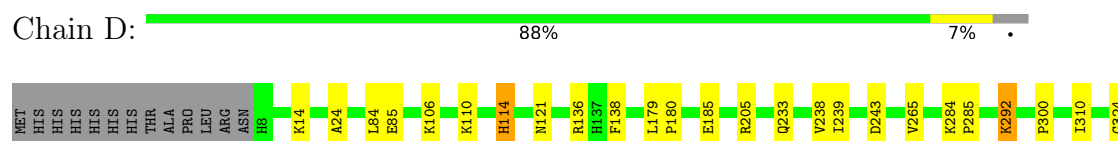
- Molecule 1: Aspartate aminotransferase family protein



- Molecule 1: Aspartate aminotransferase family protein



- Molecule 1: Aspartate aminotransferase family protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.97Å 79.27Å 173.84Å 90.00° 100.31° 90.00°	Depositor
Resolution (Å)	46.61 – 1.98 46.61 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.61-1.98) 98.7 (46.61-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.216 , 0.237 0.215 , 0.235	Depositor DCC
R_{free} test set	5925 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15347	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 93.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0866e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.16	0/3567	0.48	5/4832 (0.1%)
1	B	0.17	0/3567	0.44	3/4832 (0.1%)
1	C	0.13	0/3567	0.37	0/4832
1	D	0.13	0/3578	0.38	0/4846
All	All	0.15	0/14279	0.42	8/19342 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	LYS	CB-CG-CD	-10.12	88.03	111.30
1	A	42	ARG	CB-CG-CD	-8.14	92.59	111.30
1	B	175	LYS	CG-CD-CE	6.73	126.77	111.30
1	A	415	LYS	CD-CE-NZ	-6.57	90.88	111.90
1	B	175	LYS	CD-CE-NZ	-6.43	91.32	111.90
1	B	252	LEU	CB-CG-CD2	-5.85	93.14	110.70
1	A	356	GLU	CA-CB-CG	-5.41	103.28	114.10
1	A	42	ARG	CG-CD-NE	5.37	123.81	112.00

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	3486	0	3461	16	1
1	B	3486	0	3461	31	0
1	C	3486	0	3460	17	1
1	D	3494	0	3474	33	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
2	C	15	0	7	0	0
2	D	15	0	7	1	0
3	A	6	0	4	1	0
3	B	12	0	8	2	0
3	C	6	0	4	2	0
3	D	12	0	8	5	0
4	A	4	0	6	0	0
5	C	7	0	10	0	0
6	A	309	0	0	4	1
6	B	314	0	0	6	0
6	C	333	0	0	5	1
6	D	332	0	0	6	0
All	All	15347	0	13924	93	2

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 (93) 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:D:185:GLU:OE2	6:D:601:HOH:O	1.85	0.91
1:B:402:GLU:OE2	6:B:601:HOH:O	1.94	0.85
1:D:14:LYS:NZ	6:D:604:HOH:O	2.14	0.80
3:D:502:ALA:O	6:D:602:HOH:O	2.01	0.78
1:B:172:HIS:HD2	1:B:175:LYS:NZ	1.82	0.76
1:B:342:GLU:OE2	6:B:602:HOH:O	2.08	0.70
1:B:106:LYS:NZ	6:B:604:HOH:O	2.24	0.70
1:D:442:GLU:OE1	6:D:603:HOH:O	2.11	0.68
1:D:136:ARG:HH12	3:D:503:ALA:CB	2.06	0.68
1:A:455:GLU:OE1	6:A:601:HOH:O	2.12	0.67
1:B:455:GLU:OE1	6:B:603:HOH:O	2.12	0.67
1:A:401:LYS:HZ3	1:A:401:LYS:HB2	1.62	0.65
1:D:347:GLU:HB2	1:D:349:LEU:CD1	2.27	0.65
1:B:172:HIS:HD2	1:B:175:LYS:HZ2	1.44	0.65
1:B:172:HIS:CD2	1:B:175:LYS:HZ2	2.15	0.64
1:B:109:GLN:OE1	6:B:604:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LYS:HE2	6:D:695:HOH:O	1.98	0.64
1:D:347:GLU:HB2	1:D:349:LEU:HD13	1.80	0.63
1:A:461:LEU:O	6:A:602:HOH:O	2.16	0.62
1:B:397:ARG:HG3	1:B:402:GLU:HG3	1.81	0.61
1:C:397:ARG:HG3	1:C:402:GLU:HG3	1.80	0.61
1:D:136:ARG:HH12	3:D:503:ALA:HB2	1.64	0.61
1:C:254:ARG:NH1	6:C:601:HOH:O	1.98	0.58
1:B:136:ARG:NH1	3:B:503:ALA:HB2	2.20	0.56
1:D:233:GLN:HB2	1:D:239:ILE:HB	1.87	0.56
1:B:40:ILE:HD12	1:B:48:ILE:HD13	1.88	0.55
1:D:110:LYS:NZ	1:D:345:GLU:OE2	2.40	0.55
1:A:397:ARG:HG3	1:A:402:GLU:HG3	1.88	0.54
1:B:24:ALA:HB1	1:D:324:GLY:HA3	1.90	0.54
1:D:179:LEU:HB3	1:D:180:PRO:HA	1.89	0.54
1:A:64:TRP:NE1	3:A:502:ALA:O	2.42	0.53
1:B:324:GLY:HA3	1:D:24:ALA:HB1	1.89	0.53
1:D:347:GLU:CB	1:D:349:LEU:CD1	2.87	0.53
1:D:397:ARG:HG3	1:D:402:GLU:HG3	1.90	0.52
1:C:102:GLU:OE2	6:C:602:HOH:O	2.19	0.52
1:C:74:GLU:OE2	1:C:346:ARG:NH2	2.34	0.51
1:B:172:HIS:HD2	1:B:175:LYS:HZ1	1.56	0.51
1:D:421[B]:ARG:HG3	1:D:421[B]:ARG:HH21	1.76	0.50
1:A:233:GLN:HB2	1:A:239:ILE:HB	1.92	0.50
1:B:136:ARG:HH12	3:B:503:ALA:HB2	1.77	0.50
1:C:284:LYS:HD3	6:C:682:HOH:O	2.12	0.50
1:D:344:MET:HA	1:D:349:LEU:HD22	1.93	0.50
1:B:179:LEU:HB3	1:B:180:PRO:HA	1.95	0.49
1:B:360:TYR:O	1:B:363:GLN:HG3	2.12	0.49
1:B:172:HIS:CD2	1:B:175:LYS:NZ	2.70	0.48
1:C:179:LEU:HB3	1:C:180:PRO:HA	1.95	0.48
1:A:179:LEU:HB3	1:A:180:PRO:HA	1.96	0.48
1:A:48:ILE:HD11	1:A:56:ILE:HB	1.96	0.47
1:A:355:ASP:C	1:A:356:GLU:HG2	2.37	0.47
1:B:73:GLU:HG2	1:D:84:LEU:HD21	1.95	0.47
1:C:188:MET:SD	1:C:208:ALA:HA	2.55	0.47
1:C:243:ASP:OD1	6:C:603:HOH:O	2.20	0.47
1:D:106:LYS:HD2	1:D:110:LYS:HE2	1.97	0.47
1:A:280:HIS:HD2	6:A:664:HOH:O	1.96	0.46
1:B:238:VAL:HB	1:B:385:ALA:HB2	1.97	0.46
1:B:233:GLN:HB2	1:B:239:ILE:HB	1.96	0.46
1:C:136:ARG:HH12	3:C:503:ALA:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TYR:O	1:A:363:GLN:HG3	2.16	0.46
1:B:207:ARG:HG2	6:B:855:HOH:O	2.16	0.46
1:D:136:ARG:HH12	3:D:503:ALA:N	2.14	0.46
1:A:48:ILE:CD1	1:A:56:ILE:HB	2.47	0.45
1:D:238:VAL:HB	1:D:385:ALA:HB2	1.98	0.45
1:C:188:MET:HE1	1:C:207:ARG:NH1	2.32	0.45
1:D:205:ARG:HD3	1:D:243:ASP:O	2.17	0.45
1:C:138:PHE:CE1	1:C:310:ILE:HD13	2.51	0.44
1:D:138:PHE:CE1	1:D:310:ILE:HD13	2.52	0.44
1:A:136:ARG:O	1:A:140:LYS:HG2	2.18	0.44
1:B:48:ILE:HD11	1:B:56:ILE:HB	2.00	0.44
1:D:265:VAL:HG12	1:D:292:LYS:HD2	2.00	0.44
1:D:114:HIS:HE1	1:D:285:PRO:O	2.00	0.44
1:B:371:HIS:CE1	1:B:451:LEU:HB3	2.53	0.44
1:B:42:ARG:HD3	1:D:85:GLU:CD	2.43	0.43
1:C:233:GLN:HB2	1:C:239:ILE:HB	2.00	0.43
1:D:371:HIS:CE1	1:D:451:LEU:HB3	2.54	0.43
1:D:136:ARG:NH1	3:D:503:ALA:HB2	2.33	0.43
1:B:369:ASN:O	1:B:392:LYS:NZ	2.52	0.42
1:C:238:VAL:HB	1:C:385:ALA:HB2	2.01	0.42
1:C:65:CYS:O	1:C:296:SER:HA	2.20	0.42
1:D:292:LYS:NZ	2:D:501:PLP:O3	2.52	0.42
1:A:284:LYS:NZ	6:A:619:HOH:O	2.51	0.42
1:D:347:GLU:HB2	1:D:349:LEU:HD11	2.02	0.42
1:D:448:ARG:NH1	6:D:618:HOH:O	2.51	0.42
1:A:238:VAL:HB	1:A:385:ALA:HB2	2.01	0.42
1:B:48:ILE:CD1	1:B:56:ILE:HB	2.50	0.42
1:B:48:ILE:HD11	1:B:56:ILE:HD12	2.01	0.42
1:B:48:ILE:C	1:B:48:ILE:HD12	2.45	0.41
1:B:327:TYR:CE2	1:D:300:PRO:HA	2.55	0.41
1:C:344:MET:HA	1:C:349:LEU:HD22	2.01	0.41
1:B:84:LEU:HD23	1:B:84:LEU:HA	1.92	0.41
1:A:40:ILE:HD12	1:A:48:ILE:HD13	2.03	0.41
1:D:84:LEU:HD23	1:D:84:LEU:HA	1.79	0.40
1:C:136:ARG:HH12	3:C:503:ALA:N	2.18	0.40
1:C:448:ARG:NH1	6:C:619:HOH:O	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:862:HOH:O	6:C:660:HOH:O[1_455]	2.09	0.11
1:A:123:SER:OG	1:C:126:GLU:OE2[1_455]	2.18	0.02

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	452/474 (95%)	431 (95%)	20 (4%)	1 (0%)	43	35
1	B	452/474 (95%)	432 (96%)	19 (4%)	1 (0%)	43	35
1	C	452/474 (95%)	432 (96%)	19 (4%)	1 (0%)	43	35
1	D	453/474 (96%)	434 (96%)	18 (4%)	1 (0%)	43	35
All	All	1809/1896 (95%)	1729 (96%)	76 (4%)	4 (0%)	43	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	LYS
1	B	292	LYS
1	C	292	LYS
1	D	292	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	358/376 (95%)	356 (99%)	2 (1%)	78	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	358/376 (95%)	357 (100%)	1 (0%)	86	86
1	C	358/376 (95%)	357 (100%)	1 (0%)	86	86
1	D	359/376 (96%)	357 (99%)	2 (1%)	78	76
All	All	1433/1504 (95%)	1427 (100%)	6 (0%)	84	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	252	LEU
1	B	121	ASN
1	C	121	ASN
1	D	114	HIS
1	D	121	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	34	GLN
1	A	49	HIS
1	A	280	HIS
1	B	34	GLN
1	B	49	HIS
1	B	172	HIS
1	B	280	HIS
1	C	34	GLN
1	C	114	HIS
1	C	172	HIS
1	C	340	ASN
1	D	34	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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
3	ALA	D	503	-	5,5,5	1.25	1 (20%)	6,6,6	1.46	2 (33%)
2	PLP	C	501	1	15,15,16	1.06	1 (6%)	21,22,23	1.25	3 (14%)
2	PLP	D	501	1	15,15,16	1.06	1 (6%)	21,22,23	1.25	2 (9%)
3	ALA	B	503	-	5,5,5	1.21	1 (20%)	6,6,6	1.49	2 (33%)
2	PLP	B	501	1	15,15,16	1.02	1 (6%)	21,22,23	1.08	2 (9%)
5	PEG	C	502	-	6,6,6	0.49	0	5,5,5	0.27	0
3	ALA	B	502	-	5,5,5	1.17	1 (20%)	6,6,6	1.43	1 (16%)
3	ALA	D	502	-	5,5,5	1.23	1 (20%)	6,6,6	1.40	2 (33%)
4	EDO	A	503	-	3,3,3	0.42	0	2,2,2	0.41	0
3	ALA	A	502	-	5,5,5	1.21	1 (20%)	6,6,6	1.47	2 (33%)
3	ALA	C	503	-	5,5,5	1.35	1 (20%)	6,6,6	1.28	1 (16%)
2	PLP	A	501	1	15,15,16	1.07	1 (6%)	21,22,23	1.12	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ALA	D	503	-	-	3/4/4/4	-
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1
3	ALA	B	503	-	-	4/4/4/4	-
2	PLP	B	501	1	-	3/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	502	-	-	1/4/4/4	-
3	ALA	B	502	-	-	2/4/4/4	-
3	ALA	D	502	-	-	1/4/4/4	-
4	EDO	A	503	-	-	1/1/1/1	-
3	ALA	A	502	-	-	0/4/4/4	-
3	ALA	C	503	-	-	4/4/4/4	-
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C2-N1	2.50	1.38	1.33
2	D	501	PLP	C2-N1	2.49	1.38	1.33
2	C	501	PLP	C2-N1	2.46	1.38	1.33
2	B	501	PLP	C2-N1	2.41	1.38	1.33
3	C	503	ALA	OXT-C	-2.23	1.23	1.30
3	B	503	ALA	OXT-C	-2.22	1.23	1.30
3	B	502	ALA	OXT-C	-2.21	1.23	1.30
3	D	502	ALA	OXT-C	-2.21	1.23	1.30
3	A	502	ALA	OXT-C	-2.21	1.23	1.30
3	D	503	ALA	OXT-C	-2.14	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	PLP	C4A-C4-C3	-3.08	115.39	120.52
3	B	503	ALA	OXT-C-O	-2.81	117.71	124.08
2	C	501	PLP	C6-C5-C4	2.80	120.39	118.10
3	A	502	ALA	OXT-C-O	-2.71	117.94	124.08
3	B	502	ALA	OXT-C-O	-2.69	117.98	124.08
2	A	501	PLP	C6-C5-C4	2.58	120.21	118.10
3	D	502	ALA	OXT-C-O	-2.57	118.24	124.08
2	D	501	PLP	C6-C5-C4	2.56	120.19	118.10
2	B	501	PLP	C4A-C4-C3	-2.46	116.41	120.52
3	C	503	ALA	OXT-C-O	-2.37	118.70	124.08
2	B	501	PLP	C6-C5-C4	2.36	120.03	118.10
3	D	503	ALA	OXT-C-CA	2.35	121.89	113.79
3	D	503	ALA	OXT-C-O	-2.34	118.78	124.08
2	C	501	PLP	C4A-C4-C3	-2.33	116.64	120.52
3	A	502	ALA	OXT-C-CA	2.17	121.28	113.79
2	A	501	PLP	C4A-C4-C3	-2.14	116.95	120.52
3	B	503	ALA	OXT-C-CA	2.08	120.94	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	ALA	OXT-C-CA	2.06	120.89	113.79
2	C	501	PLP	C5-C6-N1	-2.04	120.51	123.83
2	A	501	PLP	C5-C6-N1	-2.00	120.57	123.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	ALA	O-C-CA-CB
3	C	503	ALA	OXT-C-CA-CB
3	B	502	ALA	OXT-C-CA-N
3	C	503	ALA	OXT-C-CA-N
3	B	503	ALA	O-C-CA-CB
3	B	503	ALA	OXT-C-CA-CB
3	D	503	ALA	O-C-CA-CB
3	D	503	ALA	OXT-C-CA-CB
3	D	503	ALA	OXT-C-CA-N
5	C	502	PEG	C1-C2-O2-C3
3	B	502	ALA	O-C-CA-N
3	C	503	ALA	O-C-CA-N
2	B	501	PLP	C5A-O4P-P-O1P
3	B	503	ALA	OXT-C-CA-N
3	D	502	ALA	OXT-C-CA-N
4	A	503	EDO	O1-C1-C2-O2
2	B	501	PLP	C5A-O4P-P-O2P
2	B	501	PLP	C5A-O4P-P-O3P
3	B	503	ALA	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	ALA	4	0
2	D	501	PLP	1	0
3	B	503	ALA	2	0
3	D	502	ALA	1	0
3	A	502	ALA	1	0
3	C	503	ALA	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 [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	454/474 (95%)	-0.28	0 100 100	18, 25, 35, 51	0
1	B	454/474 (95%)	-0.31	1 (0%) 91 94	18, 25, 33, 43	0
1	C	454/474 (95%)	-0.34	0 100 100	18, 25, 34, 48	0
1	D	454/474 (95%)	-0.34	0 100 100	17, 24, 33, 42	1 (0%)
All	All	1816/1896 (95%)	-0.32	1 (0%) 92 95	17, 25, 34, 51	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ARG	2.1

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(Å ²)	Q<0.9
3	ALA	C	503	6/6	0.58	0.24	29,34,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ALA	A	502	6/6	0.64	0.19	33,38,41,42	0
3	ALA	B	502	6/6	0.70	0.17	33,38,41,48	0
3	ALA	D	503	6/6	0.72	0.20	23,34,38,42	0
5	PEG	C	502	7/7	0.77	0.14	32,33,41,42	0
3	ALA	D	502	6/6	0.79	0.13	33,38,39,45	0
4	EDO	A	503	4/4	0.82	0.17	38,41,46,47	0
3	ALA	B	503	6/6	0.82	0.13	26,34,41,42	0
2	PLP	B	501	15/16	0.97	0.06	17,22,27,29	0
2	PLP	C	501	15/16	0.97	0.06	19,20,27,30	0
2	PLP	A	501	15/16	0.98	0.05	18,21,26,29	0
2	PLP	D	501	15/16	0.98	0.05	18,19,24,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.