



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:28 PM GMT

PDB ID : 3NYU  
Title : X-ray crystal structure of the Wbpe (WlbE) aminotransferase from pseudomonas aeruginosa as the PLP internal aldimine adduct with lysine 185  
Authors : Holden, H.M.; Thoden, J.B.  
Deposited on : 2010-07-15  
Resolution : 1.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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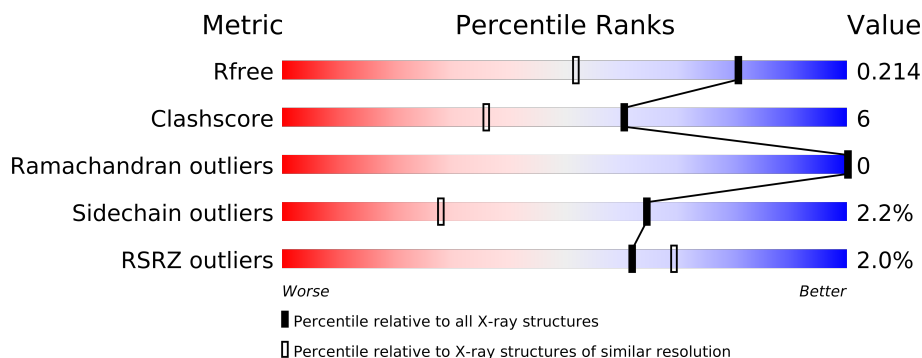
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.50 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))
$R_{free}$	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	
1	C	367	
1	D	367	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EDO	B	369	-	X
2	EDO	B	370	-	X
2	EDO	B	371	-	X
2	EDO	B	372	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12534 atoms, of which 0 are hydrogen and 0 are deuterium.

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 WbpE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	P	S	0	7	0
			2787	1769	475	530	1	12			
1	B	357	Total	C	N	O	P	S	0	5	0
			2758	1749	469	528	1	11			
1	C	357	Total	C	N	O	P	S	0	1	0
			2743	1740	469	522	1	11			
1	D	357	Total	C	N	O	P	S	0	0	0
			2735	1735	466	522	1	11			

There are 32 discrepancies between the modelled and reference sequences:

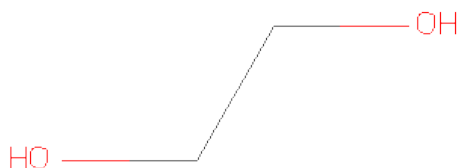
Chain	Residue	Modelled	Actual	Comment	Reference
A	360	LEU	-	EXPRESSION TAG	UNP Q9HZ76
A	361	GLU	-	EXPRESSION TAG	UNP Q9HZ76
A	362	HIS	-	EXPRESSION TAG	UNP Q9HZ76
A	363	HIS	-	EXPRESSION TAG	UNP Q9HZ76
A	364	HIS	-	EXPRESSION TAG	UNP Q9HZ76
A	365	HIS	-	EXPRESSION TAG	UNP Q9HZ76
A	366	HIS	-	EXPRESSION TAG	UNP Q9HZ76
A	367	HIS	-	EXPRESSION TAG	UNP Q9HZ76
B	360	LEU	-	EXPRESSION TAG	UNP Q9HZ76
B	361	GLU	-	EXPRESSION TAG	UNP Q9HZ76
B	362	HIS	-	EXPRESSION TAG	UNP Q9HZ76
B	363	HIS	-	EXPRESSION TAG	UNP Q9HZ76
B	364	HIS	-	EXPRESSION TAG	UNP Q9HZ76
B	365	HIS	-	EXPRESSION TAG	UNP Q9HZ76
B	366	HIS	-	EXPRESSION TAG	UNP Q9HZ76
B	367	HIS	-	EXPRESSION TAG	UNP Q9HZ76
C	360	LEU	-	EXPRESSION TAG	UNP Q9HZ76
C	361	GLU	-	EXPRESSION TAG	UNP Q9HZ76
C	362	HIS	-	EXPRESSION TAG	UNP Q9HZ76
C	363	HIS	-	EXPRESSION TAG	UNP Q9HZ76
C	364	HIS	-	EXPRESSION TAG	UNP Q9HZ76

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Chain	Residue	Modelled	Actual	Comment	Reference
C	365	HIS	-	EXPRESSION TAG	UNP Q9HZ76
C	366	HIS	-	EXPRESSION TAG	UNP Q9HZ76
C	367	HIS	-	EXPRESSION TAG	UNP Q9HZ76
D	360	LEU	-	EXPRESSION TAG	UNP Q9HZ76
D	361	GLU	-	EXPRESSION TAG	UNP Q9HZ76
D	362	HIS	-	EXPRESSION TAG	UNP Q9HZ76
D	363	HIS	-	EXPRESSION TAG	UNP Q9HZ76
D	364	HIS	-	EXPRESSION TAG	UNP Q9HZ76
D	365	HIS	-	EXPRESSION TAG	UNP Q9HZ76
D	366	HIS	-	EXPRESSION TAG	UNP Q9HZ76
D	367	HIS	-	EXPRESSION TAG	UNP Q9HZ76

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	445	Total 445	O 445	0	0
4	B	387	Total 387	O 387	0	0
4	C	336	Total 336	O 336	0	0
4	D	321	Total 321	O 321	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

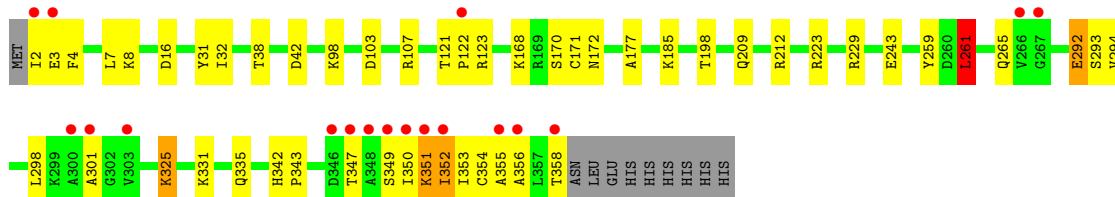
- Molecule 1: Aminotransferase WbpE

Chain A: 



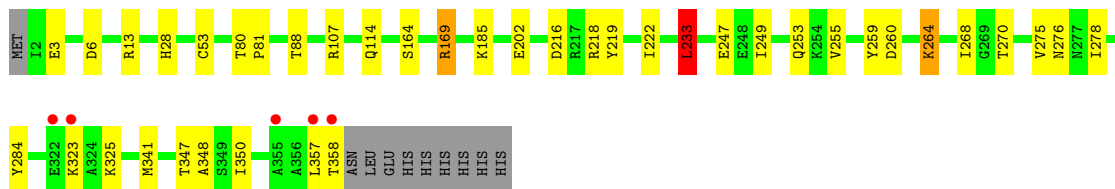
- Molecule 1: Aminotransferase WbpE

Chain B: 



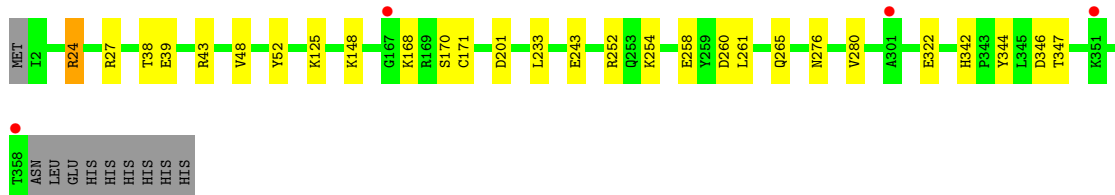
- Molecule 1: Aminotransferase WbpE

Chain C: 



- Molecule 1: Aminotransferase WbpE

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.63Å 54.07Å 150.90Å 84.26° 82.43° 64.93°	Depositor
Resolution (Å)	30.00 – 1.50 26.15 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-1.50) 93.0 (26.15-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.19 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.181 , 0.219 0.178 , 0.214	Depositor DCC
$R_{free}$ test set	10115 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 48.0	EDS
Estimated twinning fraction	0.017 for h,h-k,h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 200622 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: NA, LLP, EDO

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	0.54	0/2833	0.85	4/3850 (0.1%)
1	B	0.52	0/2798	0.84	3/3803 (0.1%)
1	C	0.50	1/2771 (0.0%)	0.79	2/3766 (0.1%)
1	D	0.45	0/2760	0.72	1/3752 (0.0%)
All	All	0.50	1/11162 (0.0%)	0.80	10/15171 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	CYS	CB-SG	-5.42	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	LEU	CA-CB-CG	8.54	134.95	115.30
1	A	252	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	B	212	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	C	341	MET	CG-SD-CE	-6.84	89.25	100.20
1	A	27	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	B	103	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	260	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	27	ARG	NE-CZ-NH2	5.66	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	D	260	ASP	CB-CG-OD1	5.41	123.17	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	ILE	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2787	0	2832	21	2
1	B	2758	0	2785	61	0
1	C	2743	0	2772	33	1
1	D	2735	0	2759	19	1
2	A	4	0	6	1	0
2	B	16	0	24	15	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	445	0	0	13	2
4	B	387	0	0	14	1
4	C	336	0	0	9	0
4	D	321	0	0	5	0
All	All	12534	0	11178	130	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (130) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:38[A]:THR:HG22	4:B:551:HOH:O	1.34	1.25
1:C:260:ASP:O	1:C:264:LYS:HD3	1.32	1.24
1:B:3:GLU:HA	4:B:813:HOH:O	1.43	1.13

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:229:ARG:HH22	2:B:372:EDO:H11	1.17	1.09
1:B:352:ILE:O	1:B:356:ALA:HB2	1.52	1.07
1:C:114:GLN:OE1	4:C:912:HOH:O	1.82	0.97
1:D:346:ASP:OD1	4:D:1413:HOH:O	1.80	0.97
1:A:185:LLP:OP1	2:B:372:EDO:H12	1.63	0.97
1:B:352:ILE:O	1:B:356:ALA:CB	2.15	0.95
1:D:38:THR:HG22	4:D:524:HOH:O	1.67	0.94
1:C:264:LYS:HE2	4:C:388:HOH:O	1.67	0.93
1:A:292[A]:GLU:OE1	4:A:1173:HOH:O	1.86	0.92
1:B:168:LYS:HE3	4:B:496:HOH:O	1.69	0.91
1:B:349:SER:O	1:B:353:ILE:HG13	1.71	0.90
1:B:38[A]:THR:HG23	4:B:605:HOH:O	1.70	0.90
1:B:4:PHE:N	4:B:813:HOH:O	2.04	0.89
1:D:38:THR:HG23	4:D:1376:HOH:O	1.71	0.89
1:B:3:GLU:CA	4:B:813:HOH:O	2.07	0.88
1:B:32:ILE:H	2:B:369:EDO:H11	1.40	0.87
1:A:16:ASP:HB2	4:A:1426:HOH:O	1.76	0.85
1:A:217:ARG:NE	4:A:525:HOH:O	2.10	0.84
1:B:107:ARG:HD3	4:B:509:HOH:O	1.79	0.83
1:B:350:ILE:O	1:B:354:CYS:N	2.13	0.82
1:A:42:ASP:OD1	4:A:909:HOH:O	2.01	0.77
1:A:24:ARG:NH2	4:A:973:HOH:O	2.17	0.77
1:D:322:GLU:CD	1:D:322:GLU:H	1.86	0.77
1:B:16:ASP:OD1	4:B:910:HOH:O	2.02	0.76
1:A:6:ASP:OD2	1:A:9:ASN:HB2	1.85	0.76
1:B:229:ARG:NH2	2:B:372:EDO:H11	1.98	0.76
1:B:349:SER:O	1:B:353:ILE:CG1	2.33	0.75
1:B:42[A]:ASP:OD1	4:B:1003:HOH:O	2.03	0.75
1:A:217:ARG:CD	4:A:525:HOH:O	2.35	0.74
1:A:186:PRO:HB2	4:A:961:HOH:O	1.87	0.73
1:B:351:LYS:HA	1:B:351:LYS:HE2	1.69	0.73
1:B:325:LYS:HE3	1:B:325:LYS:HA	1.70	0.73
1:B:32:ILE:N	2:B:369:EDO:H11	2.04	0.71
1:B:32:ILE:H	2:B:369:EDO:C1	2.02	0.71
1:A:289:ASP:OD2	4:A:1170:HOH:O	2.08	0.71
1:C:233:LEU:HD23	1:D:233:LEU:CD2	2.21	0.70
1:C:6:ASP:OD1	4:C:1271:HOH:O	2.09	0.70
1:C:247:GLU:HG3	4:C:975:HOH:O	1.91	0.70
1:C:260:ASP:O	1:C:264:LYS:CD	2.27	0.67
1:C:233:LEU:HD23	1:D:233:LEU:HD21	1.77	0.67
1:B:292[B]:GLU:OE1	4:B:1262:HOH:O	2.13	0.66
1:D:52:TYR:OH	1:D:201:ASP:OD1	2.07	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:202:GLU:HG3	4:C:698:HOH:O	1.97	0.63
1:B:294:VAL:O	1:B:298:LEU:HD13	1.99	0.62
1:D:39:GLU:OE1	1:D:43:ARG:NH2	2.25	0.62
1:B:32:ILE:HB	2:B:369:EDO:H12	1.83	0.60
1:C:275:VAL:O	1:C:276:ASN:HB2	2.02	0.59
1:B:351:LYS:HE2	1:B:351:LYS:CA	2.32	0.59
1:A:168:LYS:HE3	4:A:960:HOH:O	2.03	0.59
1:B:325:LYS:CA	1:B:325:LYS:HE3	2.34	0.58
1:A:217:ARG:NH2	4:A:1141:HOH:O	2.38	0.56
1:A:7:LEU:CD2	2:A:368:EDO:H22	2.36	0.56
1:B:301:ALA:O	1:B:352:ILE:HG21	2.06	0.55
1:B:31:TYR:N	2:B:369:EDO:H11	2.21	0.55
1:B:352:ILE:O	1:B:356:ALA:HB3	2.05	0.54
1:C:13:ARG:HD2	4:C:730:HOH:O	2.06	0.54
1:B:8:LYS:HG3	4:B:832:HOH:O	2.07	0.53
1:B:355:ALA:O	1:B:358:THR:HB	2.09	0.53
1:C:347:THR:HG22	1:C:348:ALA:N	2.23	0.53
1:A:217:ARG:HD2	4:A:525:HOH:O	2.05	0.53
1:C:268:ILE:HD13	1:C:357:LEU:HD13	1.91	0.52
1:A:88[B]:THR:HG22	1:A:156:ASP:OD2	2.10	0.52
1:B:351:LYS:CE	1:B:351:LYS:CA	2.88	0.52
1:B:3:GLU:CD	1:B:3:GLU:N	2.62	0.51
1:C:233:LEU:HD23	1:D:233:LEU:HD23	1.91	0.51
1:B:198:THR:HA	2:B:371:EDO:H21	1.92	0.51
1:B:351:LYS:O	1:B:352:ILE:C	2.48	0.50
1:D:170:SER:O	1:D:171:CYS:HB2	2.11	0.50
1:D:322:GLU:CD	1:D:322:GLU:N	2.61	0.50
1:B:121:THR:HB	1:B:122:PRO:HD2	1.93	0.50
1:A:185:LLP:OP1	2:B:372:EDO:C1	2.49	0.49
1:C:3:GLU:HG3	1:C:6:ASP:OD1	2.11	0.49
1:D:342:HIS:HD2	1:D:344:TYR:H	1.61	0.49
1:C:255:VAL:HG13	1:C:350:ILE:HD11	1.93	0.49
1:A:276:ASN:H	1:A:276:ASN:ND2	2.10	0.49
1:B:3:GLU:CD	1:B:3:GLU:H	2.16	0.49
1:D:258:GLU:OE1	1:D:347:THR:HG23	2.13	0.48
1:C:260:ASP:HA	1:C:270:THR:HG21	1.95	0.48
1:B:209:GLN:OE1	1:B:223[A]:ARG:NE	2.46	0.48
1:A:80[B]:THR:OG1	1:A:81:PRO:HD2	2.13	0.47
1:C:233:LEU:CD2	1:D:233:LEU:HD21	2.44	0.47
1:B:171:CYS:O	2:B:371:EDO:H22	2.14	0.47
1:C:169:ARG:HD2	1:C:169:ARG:HA	1.57	0.47
1:B:185:LLP:NZ	1:B:185:LLP:O3	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:301:ALA:O	1:B:352:ILE:CG2	2.63	0.46
1:A:30[B]:GLN:OE1	4:A:1075:HOH:O	2.21	0.46
1:C:275:VAL:HG12	4:C:711:HOH:O	2.15	0.46
1:C:264:LYS:HG3	4:C:457:HOH:O	2.16	0.46
1:B:7:LEU:CD2	2:B:370:EDO:H11	2.46	0.46
1:B:351:LYS:C	1:B:353:ILE:N	2.67	0.45
1:B:243:GLU:HG3	4:B:833:HOH:O	2.15	0.45
1:B:32:ILE:CB	2:B:369:EDO:H12	2.46	0.45
1:C:357:LEU:HD23	1:C:357:LEU:HA	1.84	0.45
1:B:123:ARG:NH2	4:B:1240:HOH:O	2.02	0.45
1:B:261:LEU:O	1:B:265:GLN:HG3	2.17	0.44
1:B:170:SER:O	1:B:171:CYS:HB2	2.17	0.44
1:C:114:GLN:NE2	4:C:862:HOH:O	2.31	0.44
1:B:356:ALA:C	1:B:358:THR:H	2.20	0.44
1:B:349:SER:O	1:B:353:ILE:CD1	2.66	0.43
1:B:198:THR:CA	2:B:371:EDO:H21	2.48	0.43
1:C:260:ASP:HB3	1:C:264:LYS:HE3	2.01	0.43
1:B:351:LYS:O	1:B:353:ILE:N	2.52	0.43
1:B:121:THR:HB	1:B:122:PRO:CD	2.47	0.43
1:D:252:ARG:HD3	1:D:280:VAL:O	2.19	0.43
1:B:3:GLU:C	4:B:813:HOH:O	2.27	0.43
1:B:342:HIS:HB2	1:B:343:PRO:CD	2.49	0.43
1:C:185:LLP:NZ	1:C:185:LLP:O3	2.51	0.43
1:C:80:THR:OG1	1:C:81:PRO:HD2	2.19	0.42
1:B:331:LYS:HZ3	1:B:335:GLN:NE2	2.17	0.42
1:B:350:ILE:HA	1:B:353:ILE:HB	2.02	0.42
1:B:171:CYS:HA	1:B:177:ALA:CB	2.50	0.42
1:C:325:LYS:HE2	1:C:325:LYS:HB2	1.86	0.42
1:D:148:LYS:HB3	1:D:148:LYS:HE2	1.71	0.42
1:B:3:GLU:CA	1:B:3:GLU:OE1	2.68	0.41
1:A:30[A]:GLN:NE2	4:A:1071:HOH:O	2.09	0.41
1:C:249:ILE:O	1:C:253:GLN:HG2	2.20	0.41
1:C:218:ARG:O	1:C:219:TYR:HB2	2.21	0.41
1:C:259:TYR:HB3	1:C:284:TYR:CZ	2.54	0.41
1:B:172:ASN:OD1	2:B:371:EDO:H12	2.21	0.41
1:D:243:GLU:HG3	4:D:971:HOH:O	2.21	0.41
1:C:216:ASP:OD1	1:C:222:ILE:HD13	2.21	0.41
1:D:27:ARG:HB3	4:D:858:HOH:O	2.21	0.41
1:C:323:LYS:HE2	1:C:323:LYS:HB2	1.79	0.41
1:C:164:SER:HB2	1:C:278:ILE:HB	2.03	0.41
1:A:111:LEU:HD23	1:A:111:LEU:C	2.41	0.41
1:D:261:LEU:O	1:D:265:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292[A]:GLU:H	1:B:292[A]:GLU:HG2	1.66	0.40

All (4) 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	Distance(Å)	Clash(Å)
1:C:107[A]:ARG:NH1	4:B:509:HOH:O[1_554]	1.64	0.56
1:D:24:ARG:NH1	1:D:322:GLU:OE2[1_545]	1.93	0.27
1:A:292[A]:GLU:OE1	4:A:1135:HOH:O[1_455]	1.96	0.24
1:A:322:GLU:OE2	4:A:737:HOH:O[1_465]	2.11	0.09

## 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	363/367 (99%)	357 (98%)	6 (2%)	0	100	100
1	B	359/367 (98%)	347 (97%)	12 (3%)	0	100	100
1	C	355/367 (97%)	345 (97%)	10 (3%)	0	100	100
1	D	354/367 (96%)	345 (98%)	9 (2%)	0	100	100
All	All	1431/1468 (98%)	1394 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	296/298 (99%)	292 (99%)	4 (1%)	78	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	292/298 (98%)	281 (96%)	11 (4%)	44	11
1	C	289/298 (97%)	283 (98%)	6 (2%)	66	30
1	D	288/298 (97%)	282 (98%)	6 (2%)	66	30
All	All	1165/1192 (98%)	1138 (98%)	27 (2%)	64	26

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LYS
1	A	218	ARG
1	A	276	ASN
1	A	351	LYS
1	B	98	LYS
1	B	259	TYR
1	B	261	LEU
1	B	292[A]	GLU
1	B	292[B]	GLU
1	B	293[A]	SER
1	B	293[B]	SER
1	B	325	LYS
1	B	347	THR
1	B	351	LYS
1	B	352	ILE
1	C	28	HIS
1	C	88	THR
1	C	169	ARG
1	C	233	LEU
1	C	264	LYS
1	C	358	THR
1	D	24	ARG
1	D	48	VAL
1	D	125	LYS
1	D	168	LYS
1	D	254	LYS
1	D	276	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN

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Mol	Chain	Res	Type
1	A	265	GLN
1	A	276	ASN
1	A	283	GLN
1	B	30	GLN
1	B	64	GLN
1	B	265	GLN
1	B	283	GLN
1	C	9	ASN
1	C	30	GLN
1	C	64	GLN
1	C	265	GLN
1	C	283	GLN
1	C	342	HIS
1	D	30	GLN
1	D	64	GLN
1	D	114	GLN
1	D	276	ASN
1	D	283	GLN
1	D	342	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	A	185	1	24,24,25	4.48	9 (37%)	30,32,34	2.84	13 (43%)
1	LLP	B	185	1	24,24,25	4.17	6 (25%)	30,32,34	2.76	11 (36%)
1	LLP	C	185	1	24,24,25	4.37	6 (25%)	30,32,34	2.61	10 (33%)
1	LLP	D	185	1	24,24,25	4.34	7 (29%)	30,32,34	2.57	11 (36%)

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
1	LLP	A	185	1	-	0/15/17/19	0/1/1/1
1	LLP	B	185	1	-	0/15/17/19	0/1/1/1
1	LLP	C	185	1	-	0/15/17/19	0/1/1/1
1	LLP	D	185	1	-	0/15/17/19	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	LLP	O-C	20.00	1.25	1.11
1	C	185	LLP	O-C	19.63	1.24	1.11
1	D	185	LLP	O-C	18.91	1.24	1.11
1	B	185	LLP	O-C	18.67	1.24	1.11
1	D	185	LLP	O3-C3	-5.25	1.24	1.37
1	A	185	LLP	O3-C3	-5.18	1.24	1.37
1	B	185	LLP	O3-C3	-4.68	1.25	1.37
1	C	185	LLP	O3-C3	-4.64	1.25	1.37
1	D	185	LLP	CB-CA	3.76	1.56	1.53
1	C	185	LLP	CE-NZ	3.47	1.58	1.46
1	A	185	LLP	CE-NZ	3.45	1.58	1.46
1	B	185	LLP	CE-NZ	3.44	1.58	1.46
1	D	185	LLP	CA-C	3.37	1.54	1.48
1	D	185	LLP	CE-NZ	3.12	1.57	1.46
1	A	185	LLP	CA-C	2.87	1.53	1.48
1	C	185	LLP	CB-CA	2.80	1.55	1.53
1	C	185	LLP	C2-N1	2.71	1.38	1.33
1	A	185	LLP	P-OP3	-2.65	1.45	1.54
1	B	185	LLP	CA-C	2.64	1.53	1.48
1	C	185	LLP	CA-C	2.45	1.52	1.48
1	A	185	LLP	C3-C2	-2.43	1.39	1.40
1	B	185	LLP	C2-N1	2.41	1.38	1.33
1	B	185	LLP	CD-CE	2.41	1.62	1.51
1	D	185	LLP	P-OP2	-2.40	1.45	1.54
1	A	185	LLP	P-OP2	-2.34	1.46	1.54
1	D	185	LLP	CD-CE	2.17	1.60	1.51
1	A	185	LLP	CD-CE	2.15	1.60	1.51
1	A	185	LLP	C2-N1	2.02	1.37	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LLP	C4'-C4-C5	8.68	127.66	119.70
1	C	185	LLP	C4'-C4-C5	7.83	126.88	119.70
1	B	185	LLP	C4'-C4-C5	7.10	126.22	119.70
1	B	185	LLP	CD-CE-NZ	6.75	130.03	112.09
1	D	185	LLP	C4'-C4-C5	6.72	125.87	119.70
1	B	185	LLP	C6-C5-C4	6.30	122.88	118.10
1	C	185	LLP	CD-CE-NZ	6.08	128.24	112.09
1	A	185	LLP	C-CA-N	-5.45	108.39	113.83
1	A	185	LLP	CD-CE-NZ	5.42	126.50	112.09
1	D	185	LLP	C6-C5-C4	4.98	121.88	118.10
1	A	185	LLP	C4'-C4-C3	-4.60	114.46	120.31
1	C	185	LLP	C6-C5-C4	4.53	121.54	118.10
1	D	185	LLP	C4-C4'-NZ	-4.49	103.17	111.52
1	B	185	LLP	C5'-C5-C6	-4.29	111.16	119.28
1	D	185	LLP	CD-CE-NZ	4.26	123.41	112.09
1	B	185	LLP	C-CA-N	-4.07	109.76	113.83
1	A	185	LLP	C5'-C5-C6	-4.03	111.64	119.28
1	D	185	LLP	OP4-C5'-C5	3.87	117.12	109.26
1	C	185	LLP	C-CA-N	-3.76	110.08	113.83
1	D	185	LLP	C-CA-N	-3.69	110.14	113.83
1	C	185	LLP	OP4-C5'-C5	3.59	116.56	109.26
1	D	185	LLP	C4'-NZ-CE	3.45	126.15	113.47
1	C	185	LLP	OP2-P-OP4	-3.41	97.23	106.65
1	A	185	LLP	C4'-NZ-CE	3.32	125.67	113.47
1	A	185	LLP	C4-C4'-NZ	-3.21	105.55	111.52
1	C	185	LLP	C5'-C5-C6	-3.13	113.35	119.28
1	D	185	LLP	OP2-P-OP4	-3.07	98.18	106.65
1	A	185	LLP	C6-C5-C4	3.01	120.38	118.10
1	B	185	LLP	OP4-C5'-C5	2.94	115.25	109.26
1	D	185	LLP	C5'-C5-C6	-2.92	113.75	119.28
1	B	185	LLP	O3-C3-C2	2.92	122.80	117.61
1	B	185	LLP	C5-C6-N1	-2.86	118.70	123.86
1	B	185	LLP	C4'-NZ-CE	2.83	123.89	113.47
1	C	185	LLP	C4'-C4-C3	-2.70	116.88	120.31
1	D	185	LLP	C4'-C4-C3	-2.62	116.98	120.31
1	D	185	LLP	C5-C6-N1	-2.62	119.14	123.86
1	C	185	LLP	C4'-NZ-CE	2.59	123.02	113.47
1	C	185	LLP	C3-C4-C5	-2.47	116.12	118.74
1	A	185	LLP	CD-CG-CB	2.36	122.25	113.64
1	A	185	LLP	C5'-C5-C4	2.34	127.91	123.02
1	A	185	LLP	C5-C6-N1	-2.32	119.67	123.86
1	B	185	LLP	C3-C4-C5	-2.29	116.31	118.74
1	B	185	LLP	C4'-C4-C3	-2.24	117.46	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LLP	C2'-C2-C3	2.19	123.67	121.02
1	A	185	LLP	OP4-C5'-C5	2.07	113.46	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	EDO	A	368	-	3,3,3	0.66	0	2,2,2	0.29	0
2	EDO	B	369	-	3,3,3	0.57	0	2,2,2	0.72	0
2	EDO	B	370	-	3,3,3	0.57	0	2,2,2	0.54	0
2	EDO	B	371	-	3,3,3	0.55	0	2,2,2	0.67	0
2	EDO	B	372	-	3,3,3	0.67	0	2,2,2	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	368	-	-	0/1/1/1	0/0/0/0
2	EDO	B	369	-	-	0/1/1/1	0/0/0/0
2	EDO	B	370	-	-	0/1/1/1	0/0/0/0
2	EDO	B	371	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	372	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	359/367 (97%)	-0.22	2 (0%) 86 91	5, 11, 23, 40	0
1	B	357/367 (97%)	0.10	18 (5%) 28 31	5, 13, 29, 42	0
1	C	357/367 (97%)	0.23	5 (1%) 72 79	10, 16, 27, 43	0
1	D	357/367 (97%)	0.02	4 (1%) 77 84	10, 16, 27, 39	0
All	All	1430/1468 (97%)	0.03	29 (2%) 62 69	5, 14, 27, 43	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	ILE	7.7
1	B	2	ILE	6.0
1	B	348	ALA	5.4
1	B	358	THR	5.0
1	C	358	THR	5.0
1	B	300	ALA	3.6
1	B	303	VAL	3.6
1	C	355	ALA	3.5
1	D	358	THR	3.5
1	B	350	ILE	3.4
1	B	355	ALA	3.4
1	C	357	LEU	3.2
1	C	322	GLU	3.0
1	B	266	VAL	2.7
1	B	347	THR	2.6
1	B	351	LYS	2.6
1	A	358	THR	2.6
1	B	356	ALA	2.5
1	C	323	LYS	2.5
1	B	3	GLU	2.4
1	A	88[A]	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	351	LYS	2.3
1	B	346	ASP	2.2
1	B	349	SER	2.1
1	B	301	ALA	2.0
1	B	267	GLY	2.0
1	B	122	PRO	2.0
1	D	301	ALA	2.0
1	D	167	GLY	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	B	185	24/25	0.08	0.66	6,8,21,25	0
1	LLP	C	185	24/25	0.09	0.14	9,15,21,27	0
1	LLP	D	185	24/25	0.08	0.04	10,14,25,32	0
1	LLP	A	185	24/25	0.07	-0.19	6,8,23,27	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	B	369	4/4	0.17	6.47	22,23,24,33	0
2	EDO	B	372	4/4	0.11	6.11	17,21,24,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	371	4/4	0.12	4.24	23,26,27,28	0
2	EDO	B	370	4/4	0.12	2.54	19,20,24,24	0
2	EDO	A	368	4/4	0.08	0.30	15,16,16,18	0
3	NA	C	368	1/1	0.05	-3.48	11,11,11,11	0
3	NA	B	368	1/1	0.04	-4.07	4,4,4,4	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.