



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:07 AM UTC

PDB ID : 6SNU / pdb_00006snu
Title : Crystal structure of the W60C mutant of the (S)-selective transaminase from *Chromobacterium violaceum*
Authors : Ruggieri, F.; Gustafsson, C.; Kimbung, R.Y.; Walse, B.; Logan, D.T.; Berglund, P.
Deposited on : 2019-08-27
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

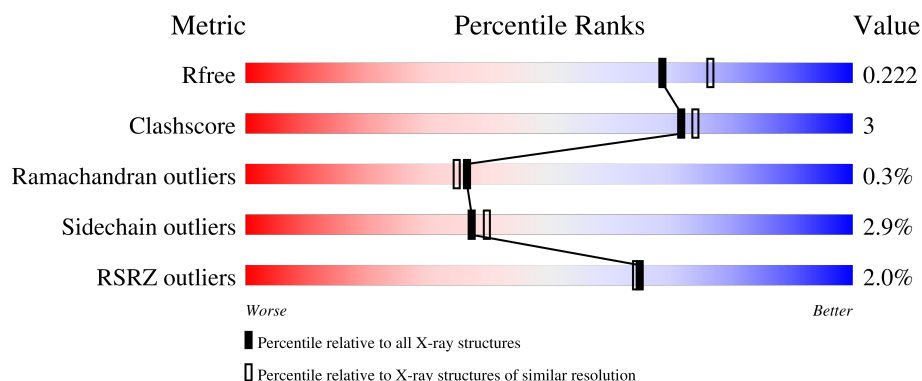
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	465	3% 87% 9% ..
1	B	465	3% 86% 11% ..
1	C	465	% 88% 9% ..
1	D	465	2% 87% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14564 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	452	Total	C	N	O	S	0	0	0
			3551	2257	626	646	22			
1	B	453	Total	C	N	O	S	0	0	0
			3555	2259	627	647	22			
1	C	455	Total	C	N	O	S	0	1	0
			3579	2274	633	650	22			
1	D	454	Total	C	N	O	S	0	1	0
			3574	2271	632	649	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP A0A1R0MXM9
A	-4	HIS	-	expression tag	UNP A0A1R0MXM9
A	-3	HIS	-	expression tag	UNP A0A1R0MXM9
A	-2	HIS	-	expression tag	UNP A0A1R0MXM9
A	-1	HIS	-	expression tag	UNP A0A1R0MXM9
A	0	HIS	-	expression tag	UNP A0A1R0MXM9
A	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9
B	-5	HIS	-	expression tag	UNP A0A1R0MXM9
B	-4	HIS	-	expression tag	UNP A0A1R0MXM9
B	-3	HIS	-	expression tag	UNP A0A1R0MXM9
B	-2	HIS	-	expression tag	UNP A0A1R0MXM9
B	-1	HIS	-	expression tag	UNP A0A1R0MXM9
B	0	HIS	-	expression tag	UNP A0A1R0MXM9
B	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9
C	-5	HIS	-	expression tag	UNP A0A1R0MXM9
C	-4	HIS	-	expression tag	UNP A0A1R0MXM9
C	-3	HIS	-	expression tag	UNP A0A1R0MXM9
C	-2	HIS	-	expression tag	UNP A0A1R0MXM9
C	-1	HIS	-	expression tag	UNP A0A1R0MXM9
C	0	HIS	-	expression tag	UNP A0A1R0MXM9
C	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9

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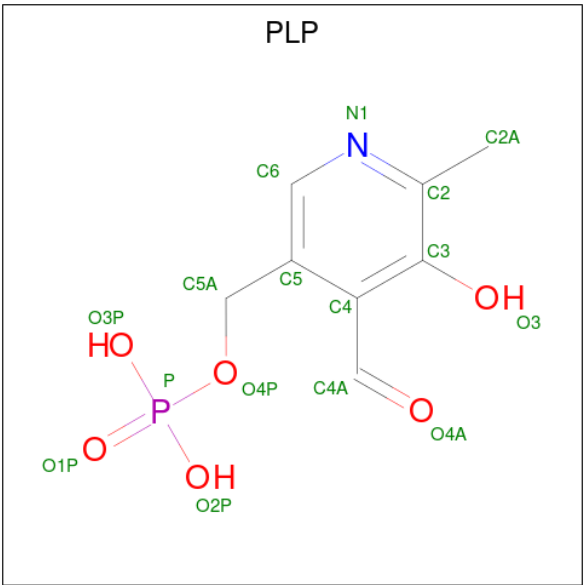
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP A0A1R0MXM9
D	-4	HIS	-	expression tag	UNP A0A1R0MXM9
D	-3	HIS	-	expression tag	UNP A0A1R0MXM9
D	-2	HIS	-	expression tag	UNP A0A1R0MXM9
D	-1	HIS	-	expression tag	UNP A0A1R0MXM9
D	0	HIS	-	expression tag	UNP A0A1R0MXM9
D	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9

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



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		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).

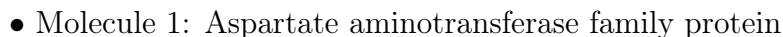
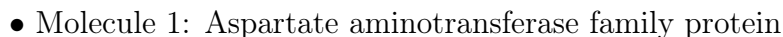
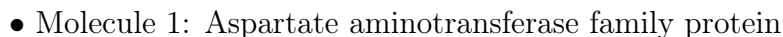


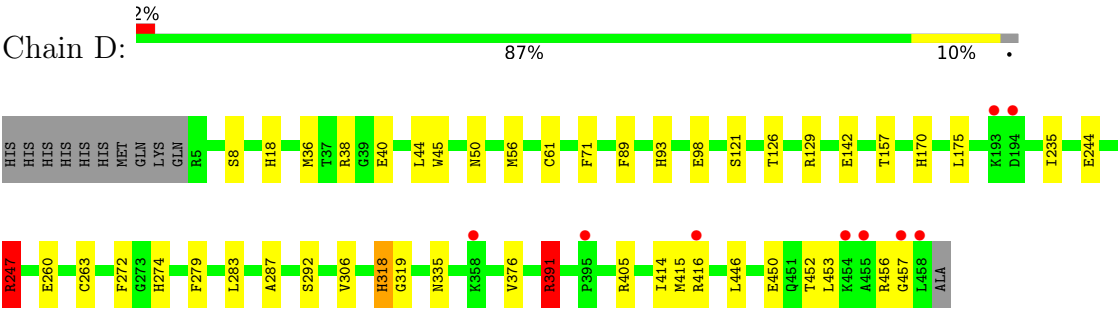
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	57	Total	O	0	0
			57	57		
4	C	78	Total	O	0	0
			78	78		
4	D	58	Total	O	0	0
			58	58		

- Molecule 1: Aspartate aminotransferase family protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.22Å 62.20Å 118.42Å 75.03° 81.31° 75.30°	Depositor
Resolution (Å)	48.28 – 2.00 48.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.28-2.00) 96.2 (48.28-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.181 , 0.215 0.190 , 0.222	Depositor DCC
R_{free} test set	5299 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14564	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 10.27% 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: EDO, PLP, OCS

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	1.19	6/3633 (0.2%)	1.40	10/4915 (0.2%)
1	B	1.20	7/3637 (0.2%)	1.38	8/4920 (0.2%)
1	C	1.22	7/3661 (0.2%)	1.41	11/4952 (0.2%)
1	D	1.16	3/3656 (0.1%)	1.40	12/4945 (0.2%)
All	All	1.19	23/14587 (0.2%)	1.40	41/19732 (0.2%)

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	C	0	1
1	D	0	1
All	All	0	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	276	HIS	CE1-NE2	6.84	1.39	1.32
1	C	18	HIS	CE1-NE2	6.58	1.39	1.32
1	B	210	GLU	CD-OE2	6.57	1.37	1.25
1	B	429	VAL	C-O	-6.29	1.17	1.24
1	B	170	HIS	CE1-NE2	6.21	1.38	1.32

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ASP	CA-CB-CG	7.65	120.25	112.60
1	D	247	ARG	CG-CD-NE	-6.87	96.89	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	PHE	CA-CB-CG	6.25	120.05	113.80
1	D	38	ARG	CG-CD-NE	6.15	125.54	112.00
1	B	416	ARG	CB-CG-CD	6.05	125.21	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	192	GLY	Peptide
1	D	457	GLY	Peptide

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	3551	0	3446	18	1
1	B	3555	0	3449	31	0
1	C	3579	0	3478	23	0
1	D	3574	0	3472	27	0
2	A	4	0	6	0	0
2	B	12	0	18	0	0
3	A	15	0	6	1	0
3	B	15	0	6	0	0
3	C	15	0	6	1	0
3	D	15	0	6	1	0
4	A	36	0	0	2	0
4	B	57	0	0	1	0
4	C	78	0	0	4	0
4	D	58	0	0	1	0
All	All	14564	0	13893	93	1

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.

The worst 5 of 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:B:21:PRO:O	1:B:23:THR:HG23	1.63	0.99
1:A:21:PRO:O	1:A:23:THR:HG23	1.66	0.95
1:D:391:ARG:O	1:D:391:ARG:HG2	1.79	0.81
1:C:416[B]:ARG:CZ	4:C:601:HOH:O	2.31	0.78
3:C:501:PLP:P	4:C:603:HOH:O	2.42	0.77

All (1) 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)
1:A:38:ARG:NH1	1:A:142:GLU:OE2[1_565]	2.18	0.02

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	449/465 (97%)	435 (97%)	12 (3%)	2 (0%)	30	27
1	B	450/465 (97%)	433 (96%)	16 (4%)	1 (0%)	43	42
1	C	453/465 (97%)	438 (97%)	14 (3%)	1 (0%)	43	42
1	D	452/465 (97%)	435 (96%)	16 (4%)	1 (0%)	43	42
All	All	1804/1860 (97%)	1741 (96%)	58 (3%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	ALA
1	A	287	ALA
1	C	287	ALA
1	D	287	ALA
1	A	58	GLY

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	362/373 (97%)	351 (97%)	11 (3%)	36	38
1	B	362/373 (97%)	349 (96%)	13 (4%)	31	31
1	C	364/373 (98%)	357 (98%)	7 (2%)	50	56
1	D	364/373 (98%)	353 (97%)	11 (3%)	36	38
All	All	1452/1492 (97%)	1410 (97%)	42 (3%)	37	40

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	405	ARG
1	D	376	VAL
1	C	444	ARG
1	D	40	GLU
1	D	414	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	369	HIS
1	D	318	HIS
1	D	335	ASN
1	D	274	HIS
1	B	318	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	OCS	B	263	1	6,8,9	0.66	0	7,11,13	1.68	1 (14%)
1	OCS	A	263	1	6,8,9	1.25	1 (16%)	7,11,13	1.28	1 (14%)
1	OCS	C	263	1	6,8,9	1.21	1 (16%)	7,11,13	1.80	3 (42%)
1	OCS	D	263	1	6,8,9	1.18	1 (16%)	7,11,13	2.99	2 (28%)

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	OCS	B	263	1	-	3/4/7/9	-
1	OCS	A	263	1	-	3/4/7/9	-
1	OCS	C	263	1	-	3/4/7/9	-
1	OCS	D	263	1	-	3/4/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	OCS	OD3-SG	2.68	1.52	1.45
1	D	263	OCS	OD3-SG	2.50	1.52	1.45
1	C	263	OCS	CB-CA	2.09	1.55	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	OCS	OD3-SG-CB	-6.49	97.07	106.76
1	D	263	OCS	OD2-SG-OD1	4.16	121.80	111.40
1	B	263	OCS	OD3-SG-CB	-3.86	101.00	106.76
1	C	263	OCS	OD1-SG-CB	2.83	110.98	106.76
1	C	263	OCS	OD2-SG-CB	-2.51	101.12	105.97

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	263	OCS	CA-CB-SG-OD1
1	B	263	OCS	CA-CB-SG-OD1
1	B	263	OCS	CA-CB-SG-OD2
1	B	263	OCS	CA-CB-SG-OD3
1	C	263	OCS	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	EDO	B	501	-	3,3,3	0.53	0	2,2,2	0.39	0
3	PLP	D	501	1	15,15,16	1.52	1 (6%)	21,22,23	2.84	8 (38%)
3	PLP	C	501	1	15,15,16	1.61	1 (6%)	21,22,23	2.90	8 (38%)
2	EDO	B	502	-	3,3,3	0.36	0	2,2,2	0.48	0
3	PLP	B	504	1	15,15,16	1.17	2 (13%)	21,22,23	2.45	6 (28%)
2	EDO	B	503	-	3,3,3	0.16	0	2,2,2	0.27	0
3	PLP	A	502	1	15,15,16	1.42	1 (6%)	21,22,23	2.51	6 (28%)
2	EDO	A	501	-	3,3,3	0.26	0	2,2,2	0.41	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	B	501	-	-	1/1/1/1	-
3	PLP	D	501	1	-	0/6/6/8	0/1/1/1
3	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	EDO	B	502	-	-	1/1/1/1	-
3	PLP	B	504	1	-	0/6/6/8	0/1/1/1
2	EDO	B	503	-	-	1/1/1/1	-
3	PLP	A	502	1	-	0/6/6/8	0/1/1/1
2	EDO	A	501	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	PLP	P-O4P	5.32	1.77	1.60
3	D	501	PLP	P-O4P	4.47	1.74	1.60
3	A	502	PLP	P-O4P	4.45	1.74	1.60
3	B	504	PLP	P-O4P	2.34	1.67	1.60
3	B	504	PLP	P-O1P	2.05	1.56	1.50

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PLP	O4P-C5A-C5	7.48	123.39	109.36
3	D	501	PLP	O4P-C5A-C5	7.07	122.60	109.36
3	D	501	PLP	O4P-P-O1P	-6.73	88.25	106.44
3	B	504	PLP	O4P-C5A-C5	6.62	121.76	109.36
3	C	501	PLP	O3P-P-O4P	-6.47	89.79	106.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EDO	O1-C1-C2-O2
2	B	503	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2
2	B	502	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	PLP	1	0
3	C	501	PLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	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 [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	451/465 (96%)	0.15	13 (2%) 53 52	12, 25, 44, 67	0
1	B	452/465 (97%)	-0.02	12 (2%) 56 55	10, 21, 40, 62	0
1	C	454/465 (97%)	-0.37	3 (0%) 84 84	7, 15, 28, 50	1 (0%)
1	D	453/465 (97%)	-0.11	9 (1%) 65 64	10, 19, 38, 63	1 (0%)
All	All	1810/1860 (97%)	-0.09	37 (2%) 65 64	7, 19, 40, 67	2 (0%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	LEU	7.0
1	B	6	THR	4.0
1	A	455	ALA	3.6
1	B	5	ARG	3.5
1	A	453	LEU	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	D	263	9/10	0.93	0.11	19,21,30,31	0
1	OCS	C	263	9/10	0.96	0.08	14,15,23,23	0
1	OCS	A	263	9/10	0.96	0.07	23,25,31,32	0
1	OCS	B	263	9/10	0.97	0.07	17,19,21,23	0

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	EDO	B	502	4/4	0.84	0.15	39,39,40,41	0
2	EDO	B	503	4/4	0.85	0.17	41,42,43,43	0
2	EDO	A	501	4/4	0.86	0.17	36,36,37,38	0
2	EDO	B	501	4/4	0.86	0.13	37,37,39,39	0
3	PLP	B	504	15/16	0.90	0.10	27,29,34,35	0
3	PLP	D	501	15/16	0.93	0.08	16,18,22,23	0
3	PLP	C	501	15/16	0.94	0.08	12,15,19,22	0
3	PLP	A	502	15/16	0.94	0.07	20,22,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.