



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:26 PM UTC

PDB ID : 3PXP / pdb_00003pxp
Title : Crystal structure of a PAS and DNA binding domain containing protein (Caur_2278) from CHLOROFLEXUS AURANTIACUS J-10-FL at 2.30 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-12-10
Resolution : 2.30 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

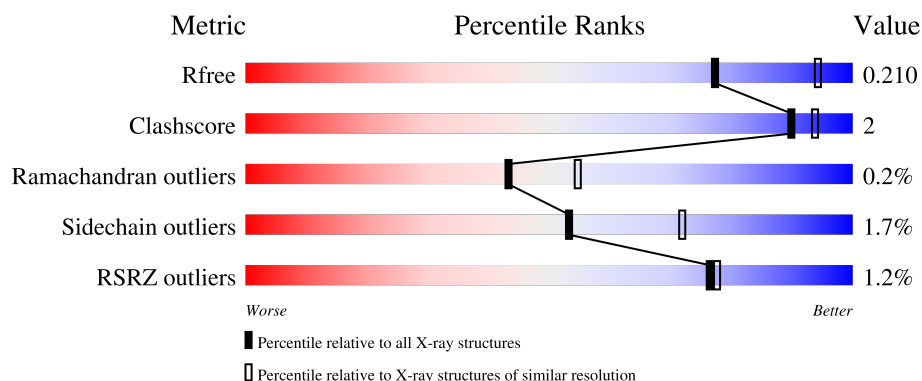
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	292	2% 95% 5%
1	B	292	91% 7% ..
1	C	292	% 93% 5% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7917 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.

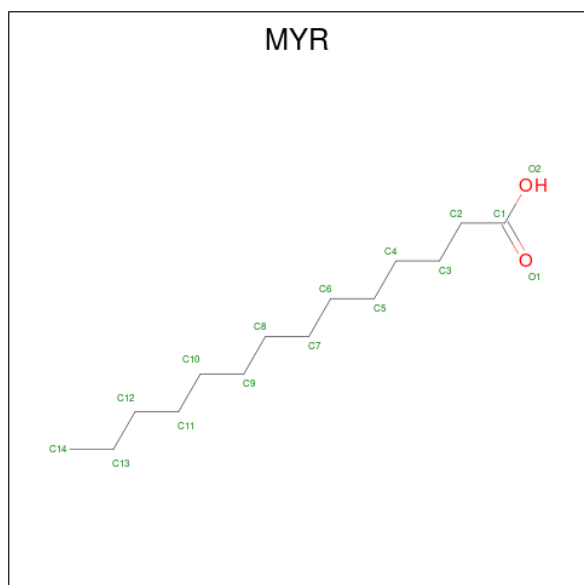
- Molecule 1 is a protein called Helix-turn-helix domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	Se	0	7	0
			2423	1548	429	435	11			
1	B	289	Total	C	N	O	Se	0	5	0
			2384	1528	419	425	12			
1	C	289	Total	C	N	O	Se	0	7	0
			2406	1546	419	430	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A9WGF5
B	0	GLY	-	expression tag	UNP A9WGF5
C	0	GLY	-	expression tag	UNP A9WGF5

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).

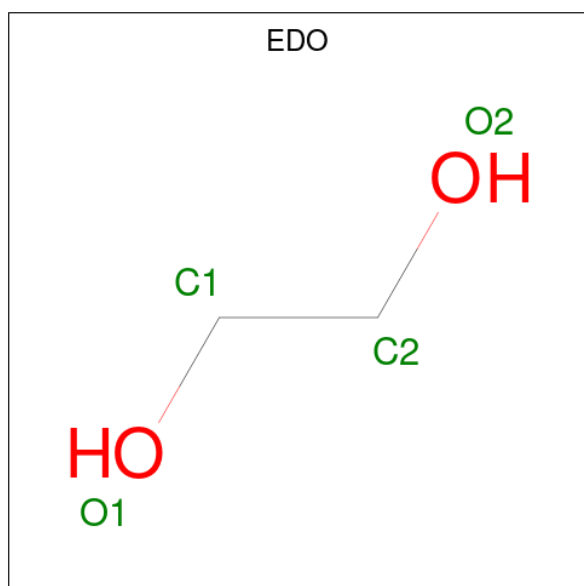


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	C	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

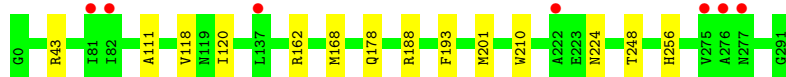
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total 231	O 231	0	1
5	B	194	Total 196	O 196	0	2
5	C	184	Total 184	O 184	0	0

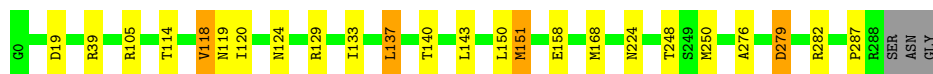
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

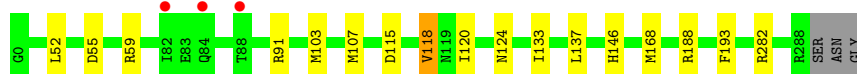
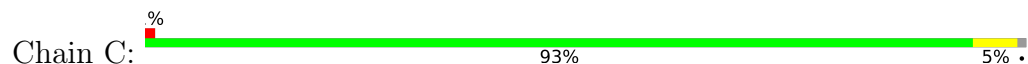
- Molecule 1: Helix-turn-helix domain protein



- Molecule 1: Helix-turn-helix domain protein



- Molecule 1: Helix-turn-helix domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.81Å 83.57Å 54.52Å 90.00° 103.12° 90.00°	Depositor
Resolution (Å)	29.75 – 2.30 29.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.75-2.30) 99.4 (29.75-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.31Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.168 , 0.206 0.170 , 0.210	Depositor DCC
R_{free} test set	2235 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7917	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

5.1 Standard geometry

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

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	0.85	0/2489	1.20	1/3355 (0.0%)
1	B	0.83	1/2443 (0.0%)	1.20	4/3294 (0.1%)
1	C	0.84	0/2471	1.17	6/3330 (0.2%)
All	All	0.84	1/7403 (0.0%)	1.19	11/9979 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	MSE	SE-CE	-7.89	1.71	1.95

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	LEU	CA-C-N	6.16	129.59	120.90
1	C	52	LEU	C-N-CA	6.16	129.59	120.90
1	C	115	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	224	ASN	CA-CB-CG	5.54	118.14	112.60
1	B	124	ASN	CA-CB-CG	5.32	117.92	112.60
1	B	224	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	146	HIS	CA-C-N	5.25	125.91	120.03
1	C	146	HIS	C-N-CA	5.25	125.91	120.03
1	B	279	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	124	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	19	ASP	CA-CB-CG	5.06	117.66	112.60

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	2423	0	2410	7	0
1	B	2384	0	2378	11	0
1	C	2406	0	2405	8	0
2	A	16	0	27	1	0
2	B	16	0	27	2	0
2	C	16	0	28	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	1	0
4	A	16	0	24	1	0
4	B	12	0	18	0	0
4	C	12	0	18	0	0
5	A	231	0	0	1	0
5	B	196	0	0	0	0
5	C	184	0	0	0	0
All	All	7917	0	7335	26	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 2.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HD2	3:C:303:CL:CL	2.31	0.67
1:C:120:ILE:HD13	2:C:301:MYR:H72	1.79	0.65
1:C:133:ILE:HD12	2:C:301:MYR:H81	1.79	0.64
1:B:120:ILE:HD13	2:B:301:MYR:H71	1.80	0.63
1:B:133:ILE:HG13	2:B:301:MYR:H91	1.82	0.62
1:B:150:LEU:HD22	1:B:151:MSE:HE2	1.86	0.57
1:A:162:ARG:H	4:A:313:EDO:H21	1.70	0.57
1:A:201:MSE:HE1	1:A:210:TRP:CD1	2.41	0.56
1:B:150:LEU:HD22	1:B:151:MSE:CE	2.38	0.53
1:C:103:MSE:HG2	1:C:107:MSE:HE3	1.91	0.52
1:A:120:ILE:HD13	2:A:301:MYR:H72	1.93	0.50
1:C:133:ILE:CD1	2:C:301:MYR:H81	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:NH1	1:B:279:ASP:OD1	2.48	0.47
1:B:250:MSE:HB3	1:B:287:PRO:HB3	1.97	0.46
1:C:120:ILE:HD13	2:C:301:MYR:H92	1.99	0.45
1:B:140:THR:O	1:B:143[B]:LEU:HG	2.17	0.44
1:A:178:GLN:HG2	5:A:592:HOH:O	2.18	0.43
1:A:188:ARG:HD2	1:A:193:PHE:CE2	2.53	0.42
1:B:114:THR:HA	1:B:119:ASN:O	2.20	0.42
1:B:137:LEU:HD11	1:B:158:GLU:HB3	2.01	0.42
1:B:129:ARG:HG3	1:B:276:ALA:HB2	2.01	0.41
1:B:150:LEU:CD2	1:B:151:MSE:HE2	2.50	0.41
1:C:188:ARG:HD2	1:C:193:PHE:CE2	2.56	0.41
1:A:111:ALA:HA	1:A:256:HIS:O	2.21	0.40
1:C:55:ASP:O	1:C:59:ARG:HG3	2.21	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	297/292 (102%)	290 (98%)	7 (2%)	0	100	100
1	B	292/292 (100%)	289 (99%)	2 (1%)	1 (0%)	36	46
1	C	294/292 (101%)	291 (99%)	2 (1%)	1 (0%)	36	46
All	All	883/876 (101%)	870 (98%)	11 (1%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	VAL
1	C	118	VAL

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	258/244 (106%)	255 (99%)	3 (1%)	63	79
1	B	253/244 (104%)	247 (98%)	6 (2%)	43	62
1	C	256/244 (105%)	252 (98%)	4 (2%)	55	73
All	All	767/732 (105%)	754 (98%)	13 (2%)	53	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
1	A	168	MSE
1	A	248	THR
1	B	39	ARG
1	B	118	VAL
1	B	137	LEU
1	B	168	MSE
1	B	248	THR
1	B	282	ARG
1	C	118	VAL
1	C	137	LEU
1	C	168	MSE
1	C	282	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	106	ASN
1	A	176	ASN
1	A	202	GLN
1	B	35	GLN
1	B	106	ASN
1	B	116	GLN
1	B	176	ASN

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Mol	Chain	Res	Type
1	C	51	HIS
1	C	106	ASN
1	C	132	ASN

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](#)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	$\# Z > 2$
4	EDO	C	309	-	3,3,3	0.27	0	2,2,2	0.73	0
4	EDO	C	314	-	3,3,3	0.42	0	2,2,2	0.24	0
4	EDO	A	310	-	3,3,3	0.56	0	2,2,2	0.03	0
2	MYR	B	301	-	15,15,15	0.69	0	15,15,15	0.97	1 (6%)
2	MYR	A	301	-	15,15,15	0.69	0	15,15,15	1.37	1 (6%)
4	EDO	C	315	-	3,3,3	0.40	0	2,2,2	0.39	0
4	EDO	A	307	-	3,3,3	0.40	0	2,2,2	0.51	0
4	EDO	B	316	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	A	311	-	3,3,3	0.44	0	2,2,2	0.30	0
4	EDO	B	312	-	3,3,3	0.50	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYR	C	301	-	15,15,15	1.34	2 (13%)	15,15,15	1.10	2 (13%)
4	EDO	A	313	-	3,3,3	0.50	0	2,2,2	0.19	0
4	EDO	B	308	-	3,3,3	0.47	0	2,2,2	0.23	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
4	EDO	C	309	-	-	1/1/1/1	-
4	EDO	C	314	-	-	0/1/1/1	-
4	EDO	A	310	-	-	1/1/1/1	-
2	MYR	B	301	-	-	9/13/13/13	-
2	MYR	A	301	-	-	6/13/13/13	-
4	EDO	C	315	-	-	1/1/1/1	-
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	B	316	-	-	0/1/1/1	-
4	EDO	A	311	-	-	0/1/1/1	-
4	EDO	B	312	-	-	0/1/1/1	-
2	MYR	C	301	-	-	5/13/13/13	-
4	EDO	A	313	-	-	1/1/1/1	-
4	EDO	B	308	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	MYR	C2-C1	3.57	1.58	1.50
2	C	301	MYR	O2-C1	2.69	1.39	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MYR	O2-C1-O1	-3.92	113.24	123.33
2	C	301	MYR	O2-C1-O1	-2.49	116.92	123.33
2	C	301	MYR	O2-C1-C2	2.35	121.42	114.00
2	B	301	MYR	O2-C1-O1	-2.01	118.15	123.33

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MYR	C9-C10-C11-C12
2	A	301	MYR	C1-C2-C3-C4
2	A	301	MYR	C6-C7-C8-C9
2	B	301	MYR	C2-C3-C4-C5
2	B	301	MYR	C4-C5-C6-C7
2	C	301	MYR	C6-C7-C8-C9
2	B	301	MYR	C3-C4-C5-C6
4	A	313	EDO	O1-C1-C2-O2
2	A	301	MYR	C3-C4-C5-C6
2	A	301	MYR	C2-C3-C4-C5
2	C	301	MYR	C2-C3-C4-C5
2	C	301	MYR	C7-C8-C9-C10
2	B	301	MYR	C10-C11-C12-C13
4	B	308	EDO	O1-C1-C2-O2
2	B	301	MYR	C9-C10-C11-C12
2	B	301	MYR	C6-C7-C8-C9
4	C	315	EDO	O1-C1-C2-O2
2	C	301	MYR	C3-C4-C5-C6
4	C	309	EDO	O1-C1-C2-O2
2	B	301	MYR	O2-C1-C2-C3
2	A	301	MYR	C5-C6-C7-C8
2	B	301	MYR	O1-C1-C2-C3
2	B	301	MYR	C11-C10-C9-C8
4	A	310	EDO	O1-C1-C2-O2
2	C	301	MYR	C10-C11-C12-C13

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	MYR	2	0
2	A	301	MYR	1	0
2	C	301	MYR	4	0
4	A	313	EDO	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	281/292 (96%)	-0.28	7 (2%) 58 60	16, 31, 64, 102	7 (2%)
1	B	278/292 (95%)	-0.24	0 100 100	19, 36, 64, 80	4 (1%)
1	C	278/292 (95%)	-0.23	3 (1%) 78 79	13, 35, 67, 102	7 (2%)
All	All	837/876 (95%)	-0.25	10 (1%) 76 77	13, 34, 66, 102	18 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ALA	4.4
1	A	277	ASN	3.9
1	A	275	VAL	2.9
1	C	88	THR	2.7
1	A	81	ILE	2.6
1	A	222	ALA	2.5
1	A	82	ILE	2.2
1	C	84	GLN	2.2
1	A	137	LEU	2.2
1	C	82	ILE	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

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
4	EDO	C	315	4/4	0.73	0.15	71,71,72,77	0
4	EDO	B	312	4/4	0.81	0.17	62,63,63,67	0
3	CL	C	303	1/1	0.83	0.12	80,80,80,80	0
4	EDO	C	309	4/4	0.85	0.16	45,48,50,52	0
4	EDO	A	313	4/4	0.86	0.16	56,59,59,65	0
4	EDO	B	316	4/4	0.86	0.12	46,47,50,55	0
4	EDO	B	308	4/4	0.89	0.12	47,48,48,56	0
2	MYR	B	301	16/16	0.90	0.11	43,45,48,48	0
2	MYR	A	301	16/16	0.90	0.11	37,39,43,44	0
3	CL	C	305	1/1	0.90	0.23	86,86,86,86	0
3	CL	C	304	1/1	0.91	0.12	63,63,63,63	0
2	MYR	C	301	16/16	0.92	0.10	40,42,45,45	0
4	EDO	A	307	4/4	0.93	0.14	47,49,49,53	0
4	EDO	A	310	4/4	0.93	0.12	38,39,41,42	0
4	EDO	C	314	4/4	0.94	0.08	48,49,51,53	0
4	EDO	A	311	4/4	0.95	0.10	32,38,41,44	0
3	CL	A	302	1/1	0.95	0.07	64,64,64,64	0
3	CL	B	306	1/1	0.96	0.12	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.