



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2021 – 02:09 PM JST

PDB ID : 7CWX
Title : Crystal structure of a tyrosine decarboxylase from *Enterococcus faecalis*
Authors : Yu, X.; Gong, M.; Huang, J.; Liu, W.; Chen, C.; Guo, R.
Deposited on : 2020-09-01
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

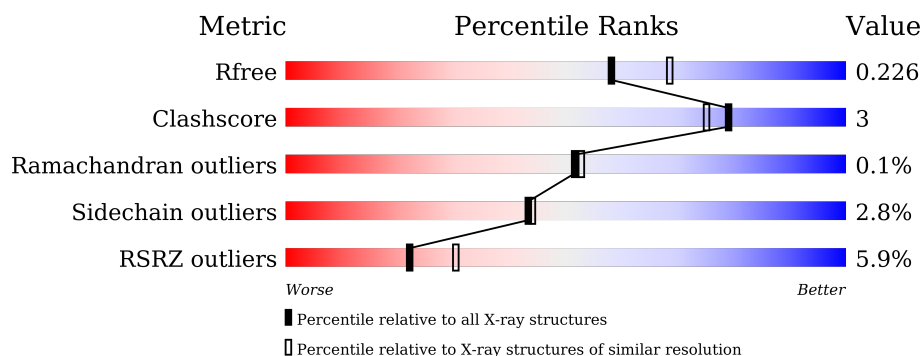
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	620	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> </div>
1	B	620	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
1	C	620	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14808 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.

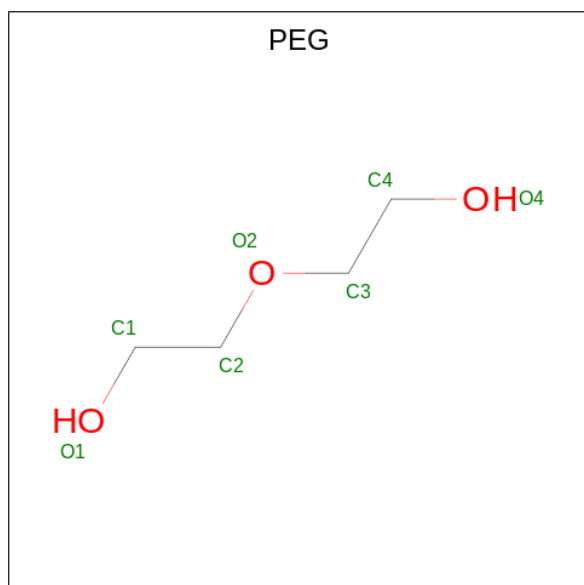
- Molecule 1 is a protein called Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4788	3059	793	915	21			
1	B	601	Total	C	N	O	S	0	0	0
			4784	3054	793	916	21			
1	C	582	Total	C	N	O	S	0	0	0
			4627	2953	770	883	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LYS	GLU	conflict	UNP Q8KXD2
B	62	LYS	GLU	conflict	UNP Q8KXD2
C	62	LYS	GLU	conflict	UNP Q8KXD2

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

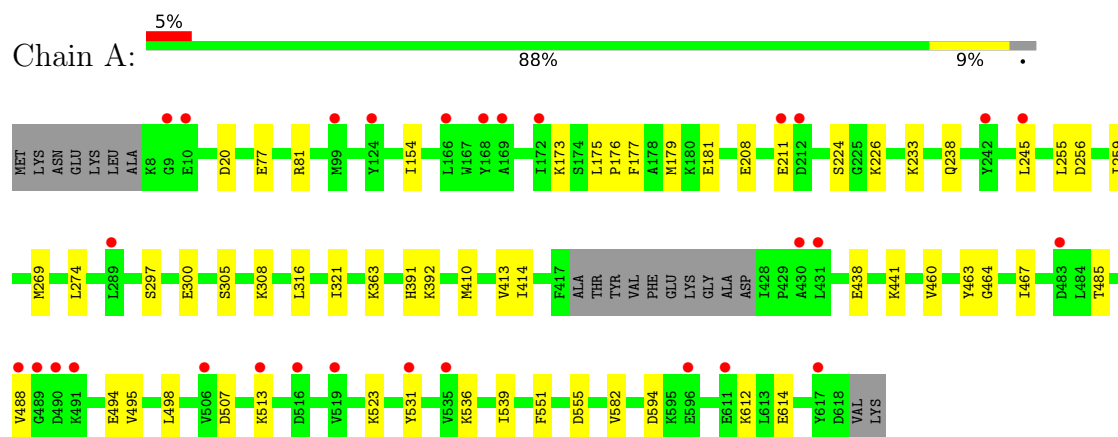
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	207	Total	O	0	0
			207	207		
4	B	201	Total	O	0	0
			201	201		
4	C	181	Total	O	0	0
			181	181		

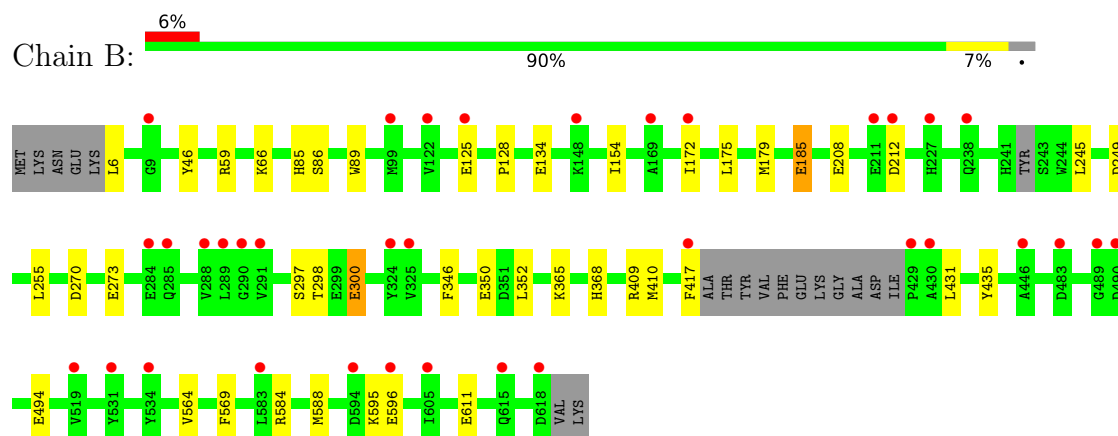
3 Residue-property plots

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.

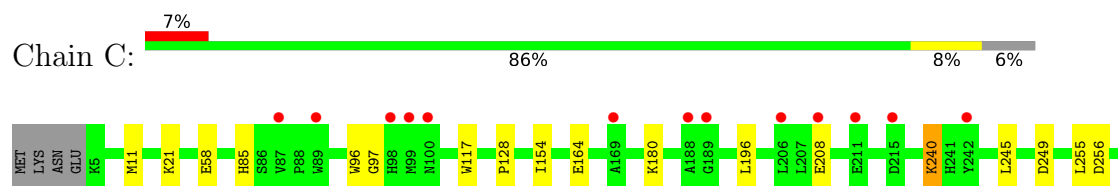
• Molecule 1: Decarboxylase

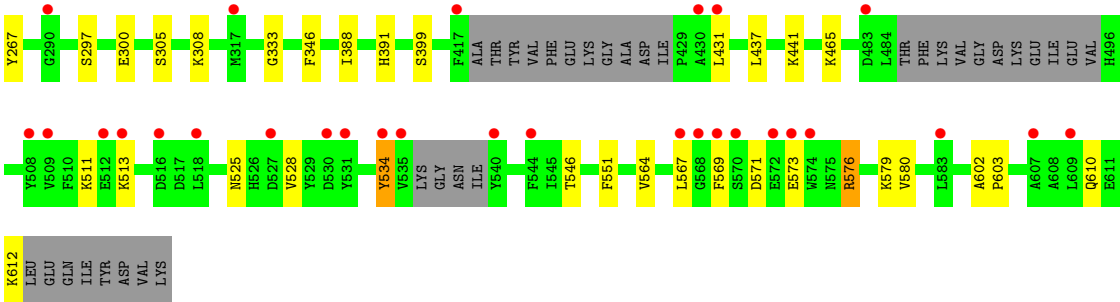


• Molecule 1: Decarboxylase



• Molecule 1: Decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.34Å 132.34Å 391.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.96 – 2.15 24.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.96-2.15) 95.9 (24.96-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.15Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.192 , 0.230 0.199 , 0.226	Depositor DCC
R_{free} test set	5515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.2	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	0.95	EDS
Total number of atoms	14808	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: GOL, 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	0.54	0/4906	0.69	0/6652
1	B	0.55	0/4900	0.70	0/6641
1	C	0.57	0/4740	0.73	0/6424
All	All	0.55	0/14546	0.71	0/19717

There are no bond length outliers.

There are no bond angle outliers.

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	4788	0	4626	33	0
1	B	4784	0	4624	24	0
1	C	4627	0	4466	27	0
2	A	7	0	10	0	0
2	B	7	0	10	1	0
3	B	6	0	8	0	0
4	A	207	0	0	3	0
4	B	201	0	0	1	0
4	C	181	0	0	1	0
All	All	14808	0	13744	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (77) 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:125:GLU:HA	1:C:534:TYR:HE2	1.47	0.79
1:A:498:LEU:HD21	1:A:551:PHE:CE2	2.29	0.67
1:B:85:HIS:HB3	1:C:128:PRO:HB2	1.79	0.64
1:C:534:TYR:HD1	1:C:534:TYR:O	1.82	0.63
1:A:77:GLU:OE2	1:A:81:ARG:HD2	2.02	0.59
1:A:245:LEU:HB3	1:A:255:LEU:CD2	2.35	0.57
1:B:564:VAL:HG13	1:B:569:PHE:HB2	1.86	0.57
1:C:564:VAL:HG13	1:C:569:PHE:HB2	1.86	0.57
1:A:256:ASP:N	1:A:256:ASP:OD1	2.37	0.57
1:B:368:HIS:HD2	4:B:1013:HOH:O	1.86	0.57
1:B:46:TYR:O	1:C:21:LYS:NZ	2.38	0.56
1:C:441:LYS:HE2	4:C:714:HOH:O	2.05	0.56
1:C:534:TYR:O	1:C:534:TYR:CD1	2.59	0.55
1:A:154:ILE:O	1:A:441:LYS:NZ	2.30	0.55
1:C:551:PHE:HB2	1:C:580:VAL:HG13	1.88	0.55
1:A:531:TYR:CE1	1:A:536:LYS:HD3	2.42	0.54
1:C:154:ILE:O	1:C:441:LYS:NZ	2.40	0.54
1:A:238:GLN:HG2	1:A:555:ASP:O	2.08	0.54
1:A:363:LYS:HE2	1:A:594:ASP:HB2	1.90	0.53
1:C:602:ALA:HB3	1:C:603:PRO:HD3	1.90	0.53
1:B:172:ILE:HD11	1:B:410:MET:HE3	1.91	0.52
1:C:267:TYR:HB2	1:C:300:GLU:HG3	1.90	0.52
1:C:164:GLU:HG3	1:C:437:LEU:HB2	1.93	0.51
1:C:245:LEU:HB3	1:C:255:LEU:HD22	1.92	0.51
1:C:297:SER:OG	1:C:300:GLU:HG2	2.11	0.50
1:B:417:PHE:HZ	1:B:435:TYR:CZ	2.30	0.50
1:A:413:VAL:HG23	1:A:414:ILE:HG23	1.95	0.49
1:A:531:TYR:O	1:A:612:LYS:HE3	2.12	0.49
1:B:297:SER:OG	1:B:300:GLU:HG2	2.12	0.49
1:A:233:LYS:HD2	1:A:259:ILE:HD11	1.95	0.49
1:A:316:LEU:HB3	1:A:321:ILE:HB	1.95	0.49
1:A:305:SER:HB3	1:A:308:LYS:HD3	1.96	0.48
1:B:417:PHE:HZ	1:B:435:TYR:CE1	2.31	0.48
1:A:438:GLU:HG2	4:A:935:HOH:O	2.13	0.48
2:B:801:PEG:H12	2:B:801:PEG:H32	1.43	0.47
1:A:175:LEU:O	1:A:179:MET:HG3	2.14	0.47
1:B:245:LEU:HB3	1:B:255:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:ASN:HA	1:C:528:VAL:HG22	1.97	0.46
1:A:20:ASP:N	1:A:20:ASP:OD1	2.49	0.46
1:A:441:LYS:HE2	4:A:865:HOH:O	2.15	0.46
1:A:269:MET:HE3	1:A:274:LEU:HD22	1.97	0.45
1:A:494:GLU:HG2	1:A:495:VAL:H	1.81	0.45
1:A:245:LEU:HB3	1:A:255:LEU:HD22	1.99	0.45
1:B:270:ASP:HB3	1:B:273:GLU:HB2	1.97	0.45
1:A:177:PHE:O	1:A:181:GLU:HG3	2.17	0.45
1:A:224:SER:OG	1:A:226:LYS:HD3	2.16	0.45
1:B:6:LEU:HD23	1:B:6:LEU:HA	1.88	0.45
1:A:488:VAL:HG23	1:A:614:GLU:HG2	1.99	0.45
1:B:128:PRO:HB2	1:C:85:HIS:HB3	1.99	0.45
1:B:208:GLU:HG3	1:B:409:ARG:HD2	1.99	0.44
1:C:333:GLY:HA3	1:C:388:ILE:HG13	1.99	0.44
1:B:125:GLU:HG2	1:C:534:TYR:CE2	2.52	0.44
1:C:240:LYS:HB3	1:C:240:LYS:HE2	1.58	0.44
1:C:610:GLN:C	1:C:612:LYS:H	2.20	0.44
1:A:507:ASP:HB3	1:A:582:VAL:HG11	1.99	0.43
1:A:410:MET:O	1:A:413:VAL:HG22	2.19	0.43
1:A:513:LYS:HE3	1:A:513:LYS:HB3	1.84	0.43
1:A:523:LYS:HD2	4:A:1000:HOH:O	2.17	0.43
1:C:576:ARG:HE	1:C:576:ARG:HB2	1.36	0.43
1:A:498:LEU:HD21	1:A:551:PHE:HE2	1.80	0.43
1:B:588:MET:HE3	1:B:588:MET:HB3	1.90	0.42
1:B:297:SER:HG	1:B:300:GLU:HG2	1.83	0.42
1:B:125:GLU:HA	1:C:534:TYR:CE2	2.38	0.42
1:B:85:HIS:O	1:C:128:PRO:HD2	2.20	0.42
1:C:11:MET:O	1:C:465:LYS:NZ	2.43	0.42
1:A:173:LYS:O	1:A:176:PRO:HD2	2.20	0.42
1:A:463:TYR:O	1:A:467:ILE:HG12	2.20	0.42
1:B:352:LEU:HD12	1:B:352:LEU:HA	1.91	0.42
1:A:494:GLU:HG2	1:A:495:VAL:N	2.36	0.41
1:B:185:GLU:H	1:B:185:GLU:HG3	1.45	0.41
1:A:297:SER:OG	1:A:300:GLU:HG2	2.21	0.41
1:B:86:SER:HB3	1:C:117:TRP:CD1	2.56	0.41
1:B:175:LEU:O	1:B:179:MET:HG3	2.21	0.41
1:B:134:GLU:HG3	1:B:154:ILE:HD12	2.02	0.41
1:A:460:VAL:HA	1:A:464:GLY:HA3	2.03	0.40
1:C:305:SER:HB3	1:C:308:LYS:HG3	2.04	0.40
1:C:96:TRP:O	1:C:546:THR:HA	2.21	0.40

There are no symmetry-related clashes.

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	597/620 (96%)	577 (97%)	20 (3%)	0	100	100
1	B	595/620 (96%)	577 (97%)	18 (3%)	0	100	100
1	C	574/620 (93%)	551 (96%)	22 (4%)	1 (0%)	47	46
All	All	1766/1860 (95%)	1705 (96%)	60 (3%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	GLY

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	509/525 (97%)	503 (99%)	6 (1%)	71	76
1	B	509/525 (97%)	492 (97%)	17 (3%)	38	37
1	C	491/525 (94%)	472 (96%)	19 (4%)	32	30
All	All	1509/1575 (96%)	1467 (97%)	42 (3%)	43	44

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	GLU
1	A	211	GLU

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Mol	Chain	Res	Type
1	A	391	HIS
1	A	392	LYS
1	A	485	THR
1	A	539	ILE
1	B	59	ARG
1	B	66	LYS
1	B	89	TRP
1	B	185	GLU
1	B	212	ASP
1	B	249	ASP
1	B	298	THR
1	B	300	GLU
1	B	346	PHE
1	B	350	GLU
1	B	365	LYS
1	B	431	LEU
1	B	494	GLU
1	B	584	ARG
1	B	595	LYS
1	B	596	GLU
1	B	611	GLU
1	C	58	GLU
1	C	180	LYS
1	C	196	LEU
1	C	208	GLU
1	C	240	LYS
1	C	249	ASP
1	C	256	ASP
1	C	346	PHE
1	C	391	HIS
1	C	399	SER
1	C	431	LEU
1	C	511	LYS
1	C	513	LYS
1	C	534	TYR
1	C	567	LEU
1	C	571	ASP
1	C	573	GLU
1	C	576	ARG
1	C	579	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	PEG	B	801	-	6,6,6	0.14	0	5,5,5	0.17	0
3	GOL	B	802	-	5,5,5	1.07	0	5,5,5	1.30	0
2	PEG	A	701	-	6,6,6	0.10	0	5,5,5	0.09	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	PEG	B	801	-	-	3/4/4/4	-
3	GOL	B	802	-	-	4/4/4/4	-
2	PEG	A	701	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	PEG	C1-C2-O2-C3
3	B	802	GOL	O1-C1-C2-O2
2	A	701	PEG	O1-C1-C2-O2
3	B	802	GOL	O1-C1-C2-C3
3	B	802	GOL	C1-C2-C3-O3
2	A	701	PEG	O2-C3-C4-O4
3	B	802	GOL	O2-C2-C3-O3
2	A	701	PEG	C1-C2-O2-C3
2	B	801	PEG	O2-C3-C4-O4
2	B	801	PEG	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	601/620 (96%)	0.12	29 (4%)	30	39	16, 38, 67, 93	0
1	B	601/620 (96%)	0.24	35 (5%)	23	31	19, 42, 64, 83	0
1	C	582/620 (93%)	0.37	42 (7%)	15	21	20, 42, 79, 95	0
All	All	1784/1860 (95%)	0.24	106 (5%)	22	30	16, 41, 70, 95	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	430	ALA	5.0
1	A	242	TYR	5.0
1	A	483	ASP	4.6
1	C	512	GLU	4.6
1	C	534	TYR	4.5
1	C	570	SER	4.4
1	C	98	HIS	4.3
1	B	483	ASP	4.3
1	C	607	ALA	4.3
1	B	430	ALA	4.1
1	C	535	VAL	4.0
1	B	417	PHE	3.9
1	C	87	VAL	3.9
1	C	483	ASP	3.9
1	B	169	ALA	3.8
1	B	534	TYR	3.7
1	C	206	LEU	3.7
1	C	189	GLY	3.7
1	B	596	GLU	3.7
1	C	516	ASP	3.6
1	B	285	GLN	3.6
1	C	431	LEU	3.6
1	A	488	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	3.4
1	C	242	TYR	3.4
1	C	568	GLY	3.4
1	B	583	LEU	3.3
1	B	490	ASP	3.3
1	C	569	PHE	3.2
1	C	544	PHE	3.2
1	C	574	TRP	3.2
1	C	527	ASP	3.1
1	A	431	LEU	3.0
1	C	99	MET	3.0
1	A	9	GLY	2.9
1	B	290	GLY	2.9
1	A	172	ILE	2.9
1	B	125	GLU	2.9
1	C	530	ASP	2.8
1	B	289	LEU	2.8
1	C	317	MET	2.8
1	C	188	ALA	2.8
1	B	172	ILE	2.7
1	A	211	GLU	2.7
1	A	289	LEU	2.7
1	A	519	VAL	2.7
1	C	89	TRP	2.6
1	A	430	ALA	2.6
1	A	596	GLU	2.6
1	C	609	LEU	2.5
1	C	169	ALA	2.5
1	B	489	GLY	2.5
1	B	594	ASP	2.5
1	B	325	VAL	2.5
1	A	531	TYR	2.5
1	C	211	GLU	2.5
1	B	211	GLU	2.5
1	B	284	GLU	2.5
1	B	99	MET	2.4
1	B	324	TYR	2.4
1	B	122	VAL	2.4
1	A	617	TYR	2.4
1	B	605	ILE	2.4
1	C	508	TYR	2.4
1	A	535	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	513	LYS	2.4
1	A	99	MET	2.4
1	A	513	LYS	2.4
1	B	212	ASP	2.4
1	B	429	PRO	2.4
1	B	291	VAL	2.3
1	C	509	VAL	2.3
1	C	531	TYR	2.3
1	C	567	LEU	2.3
1	C	583	LEU	2.3
1	A	124	TYR	2.2
1	C	540	TYR	2.2
1	C	290	GLY	2.2
1	C	573	GLU	2.2
1	A	490	ASP	2.2
1	C	572	GLU	2.2
1	C	208	GLU	2.2
1	A	212	ASP	2.2
1	A	611	GLU	2.1
1	B	288	VAL	2.1
1	A	489	GLY	2.1
1	C	518	LEU	2.1
1	A	168	TYR	2.1
1	B	531	TYR	2.1
1	B	446	ALA	2.1
1	A	516	ASP	2.1
1	B	227	HIS	2.1
1	A	10	GLU	2.1
1	C	100	ASN	2.1
1	B	615	GLN	2.1
1	A	245	LEU	2.1
1	B	148	LYS	2.1
1	B	519	VAL	2.1
1	B	618	ASP	2.0
1	B	238	GLN	2.0
1	A	491	LYS	2.0
1	C	417	PHE	2.0
1	B	9	GLY	2.0
1	A	506	VAL	2.0
1	A	166	LEU	2.0
1	C	215	ASP	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 monosaccharides 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(\AA^2)	Q<0.9
2	PEG	A	701	7/7	0.83	0.45	27,35,57,61	0
3	GOL	B	802	6/6	0.86	0.13	41,55,56,68	0
2	PEG	B	801	7/7	0.87	0.28	43,47,53,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.