



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:20 PM UTC

PDB ID : 7CWX / pdb_00007cwx
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 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

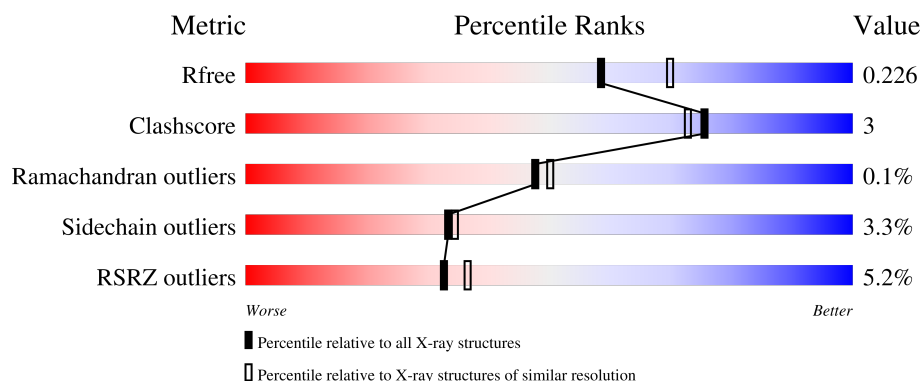
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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	4% 87% 10% .
1	B	620	2% 89% 8% ..
1	C	620	9% 84% 9% 6%

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.

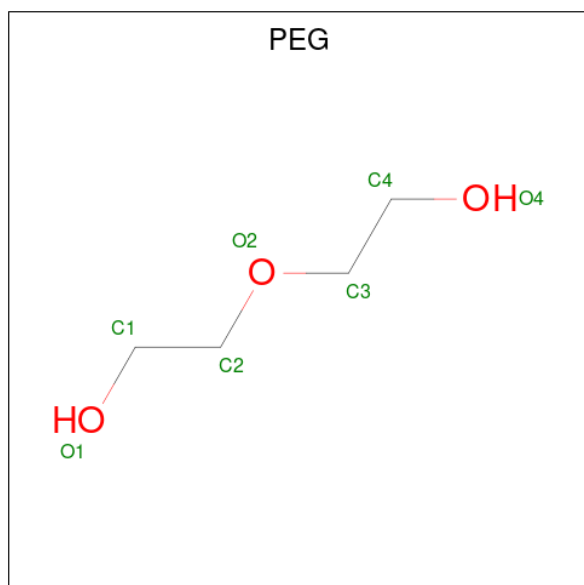
- Molecule 1 is a protein called Decarboxylase.

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:

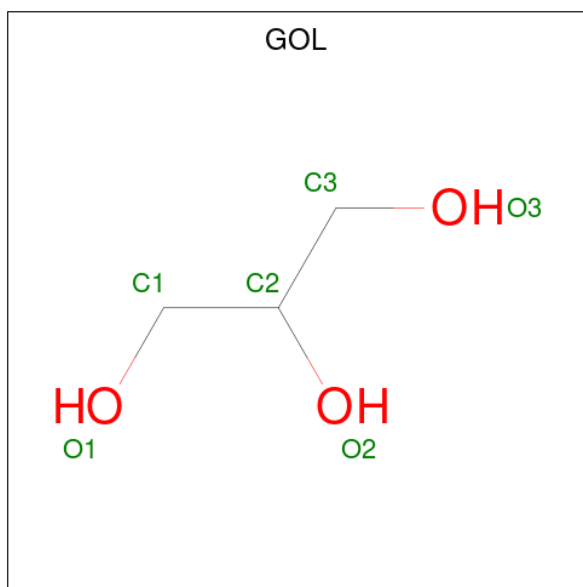
Chain	Residue	Modelled	Actual	Comment	Reference
A	62	LYS	GLU	conflict	UNP Q8KXD2
B	62	LYS	GLU	conflict	UNP Q8KXD2
C	62	LYS	GLU	conflict	UNP Q8KXD2

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

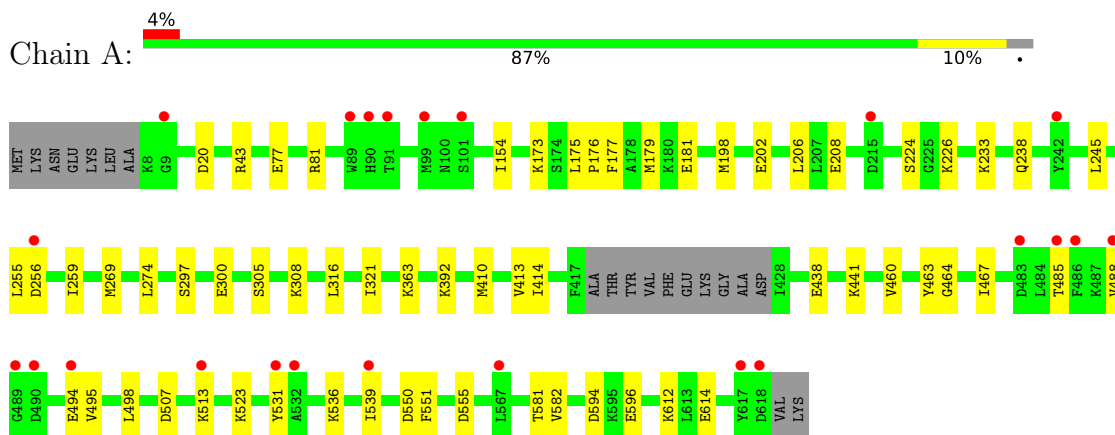
- Molecule 4 is water.

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		

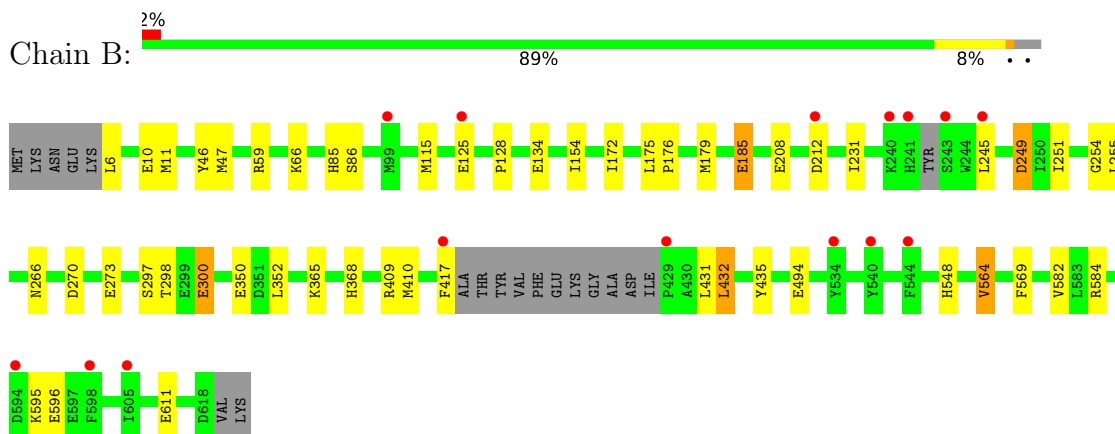
3 Residue-property plots

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.

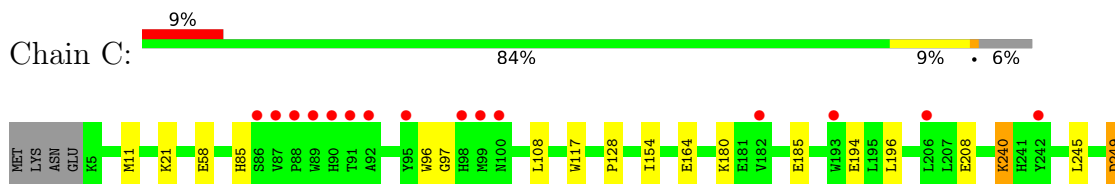
• Molecule 1: Decarboxylase

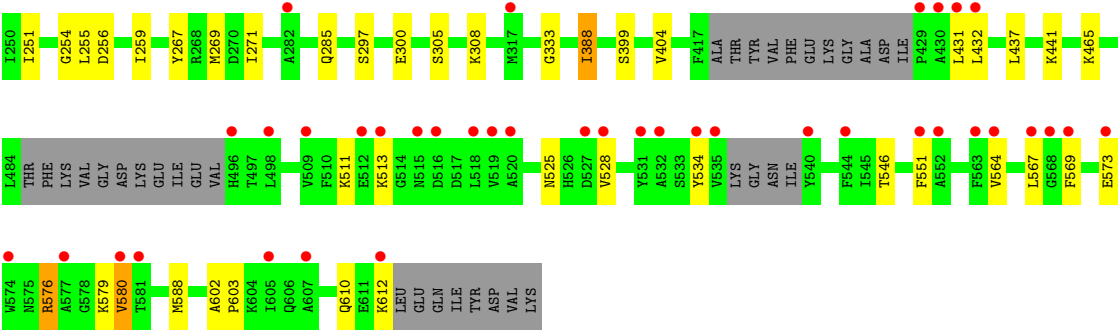


• Molecule 1: Decarboxylase



• 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 0.200 , 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 , 42.4	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	0.57	0/4906	0.78	1/6652 (0.0%)
1	B	0.76	2/4900 (0.0%)	1.03	5/6641 (0.1%)
1	C	0.79	0/4740	1.06	5/6424 (0.1%)
All	All	0.71	2/14546 (0.0%)	0.96	11/19717 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	MET	C-O	8.77	1.28	1.23
1	B	266	ASN	C-N	8.04	1.44	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ASP	CA-CB-CG	7.00	119.60	112.60
1	B	432	LEU	N-CA-C	-6.75	104.00	111.82
1	C	249	ASP	CA-CB-CG	6.69	119.29	112.60
1	C	285	GLN	CB-CA-C	5.73	120.02	111.89
1	B	254	GLY	CA-C-O	-5.71	118.29	122.23
1	C	432	LEU	N-CA-C	-5.54	105.78	112.54
1	C	249	ASP	CB-CA-C	5.39	119.35	110.88
1	B	249	ASP	CB-CA-C	5.34	119.26	110.88
1	A	43	ARG	CB-CG-CD	5.24	123.36	111.30
1	C	254	GLY	CA-C-O	-5.15	118.68	122.23
1	B	266	ASN	N-CA-C	-5.11	106.64	112.92

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	36	0
1	B	4784	0	4624	26	0
1	C	4627	0	4466	30	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	84	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 (84) 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:B:176:PRO:HA	1:B:179:MET:HE3	1.73	0.70
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:B:172:ILE:HD11	1:B:410:MET:HE3	1.83	0.60
1:A:77:GLU:OE2	1:A:81:ARG:HD2	2.02	0.59
1:A:269:MET:HE3	1:A:274:LEU:HD22	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:198:MET:HE1	1:A:206:LEU:HD12	1.94	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
1:C:610:GLN:C	1:C:612:LYS:H	2.20	0.47
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
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: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:B:115:MET:HE2	1:C:108:LEU:HD23	1.98	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:A:550:ASP:OD1	1:A:581:THR:OG1	2.27	0.44
1:C:240:LYS:HB3	1:C:240:LYS:HE2	1.58	0.44
1:A:507:ASP:HB3	1:A:582:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:SER:HG	1:B:300:GLU:HG2	1.83	0.42
1:C:297:SER:HG	1:C: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:A:198:MET:HE3	1:A:202:GLU:OE2	2.19	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:10:GLU:O	1:B:11:MET:C	2.62	0.41
1:B:134:GLU:HG3	1:B:154:ILE:HD12	2.02	0.41
1:C:588:MET:HB3	1:C:588:MET:HE2	1.76	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	595/620 (96%)	577 (97%)	18 (3%)	0	100	100
1	C	574/620 (93%)	551 (96%)	22 (4%)	1 (0%)	43	44
All	All	1766/1860 (95%)	1705 (96%)	60 (3%)	1 (0%)	48	50

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%)	504 (99%)	5 (1%)	68	75
1	B	509/525 (97%)	488 (96%)	21 (4%)	27	26
1	C	491/525 (94%)	467 (95%)	24 (5%)	22	19
All	All	1509/1575 (96%)	1459 (97%)	50 (3%)	33	34

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	GLU
1	A	392	LYS
1	A	485	THR
1	A	539	ILE
1	A	596	GLU
1	B	59	ARG
1	B	66	LYS
1	B	185	GLU
1	B	212	ASP
1	B	231	ILE
1	B	249	ASP
1	B	251	ILE
1	B	298	THR

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Mol	Chain	Res	Type
1	B	300	GLU
1	B	350	GLU
1	B	365	LYS
1	B	431	LEU
1	B	432	LEU
1	B	494	GLU
1	B	548	HIS
1	B	564	VAL
1	B	582	VAL
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	185	GLU
1	C	194	GLU
1	C	196	LEU
1	C	208	GLU
1	C	240	LYS
1	C	249	ASP
1	C	251	ILE
1	C	256	ASP
1	C	259	ILE
1	C	269	MET
1	C	271	ILE
1	C	388	ILE
1	C	399	SER
1	C	404	VAL
1	C	431	LEU
1	C	511	LYS
1	C	513	LYS
1	C	567	LEU
1	C	573	GLU
1	C	576	ARG
1	C	579	LYS
1	C	580	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS

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Mol	Chain	Res	Type
1	A	100	ASN
1	A	476	HIS
1	A	500	HIS
1	A	526	HIS
1	B	345	ASN
1	B	476	HIS
1	B	526	HIS
1	B	548	HIS
1	B	615	GLN
1	C	14	ASN
1	C	98	HIS
1	C	257	GLN
1	C	353	GLN
1	C	368	HIS
1	C	548	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](#)

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](#)

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	1.12	0	5,5,5	1.39	1 (20%)
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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	GOL	C3-C2-C1	-2.14	103.94	111.80

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
3	B	802	GOL	O1-C1-C2-C3
3	B	802	GOL	C1-C2-C3-O3
2	A	701	PEG	O1-C1-C2-O2
3	B	802	GOL	O2-C2-C3-O3
2	A	701	PEG	O2-C3-C4-O4
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%)	0.18	23 (3%)	44 49	16, 38, 67, 93	0
1	B	601/620 (96%)	0.31	15 (2%)	58 62	19, 42, 64, 83	0
1	C	582/620 (93%)	0.53	54 (9%)	14 16	20, 42, 79, 95	0
All	All	1784/1860 (95%)	0.34	92 (5%)	33 36	16, 41, 70, 95	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	HIS	4.4
1	B	417	PHE	4.3
1	C	431	LEU	4.2
1	C	535	VAL	4.2
1	C	607	ALA	4.1
1	C	87	VAL	3.9
1	C	531	TYR	3.9
1	C	544	PHE	3.5
1	B	243	SER	3.5
1	C	518	LEU	3.5
1	C	430	ALA	3.4
1	A	90	HIS	3.4
1	C	429	PRO	3.3
1	C	513	LYS	3.2
1	B	605	ILE	3.2
1	C	534	TYR	3.2
1	C	516	ASP	3.1
1	C	242	TYR	3.1
1	A	488	VAL	3.1
1	C	519	VAL	3.0
1	C	574	TRP	3.0
1	C	528	VAL	3.0
1	B	540	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	95	TYR	3.0
1	C	89	TRP	3.0
1	C	540	TYR	2.9
1	C	86	SER	2.9
1	A	9	GLY	2.9
1	B	125	GLU	2.9
1	C	612	LYS	2.8
1	A	618	ASP	2.7
1	C	605	ILE	2.7
1	B	544	PHE	2.7
1	B	598	PHE	2.7
1	C	580	VAL	2.7
1	A	490	ASP	2.7
1	C	432	LEU	2.7
1	C	520	ALA	2.6
1	C	569	PHE	2.6
1	C	498	LEU	2.6
1	C	496	HIS	2.6
1	C	91	THR	2.6
1	A	513	LYS	2.6
1	A	215	ASP	2.6
1	C	563	PHE	2.6
1	A	99	MET	2.6
1	C	182	VAL	2.5
1	B	241	HIS	2.5
1	C	90	HIS	2.5
1	C	551	PHE	2.5
1	C	317	MET	2.5
1	A	242	TYR	2.5
1	C	515	ASN	2.5
1	A	485	THR	2.4
1	C	581	THR	2.4
1	C	568	GLY	2.4
1	A	539	ILE	2.4
1	C	512	GLU	2.4
1	C	99	MET	2.4
1	C	282	ALA	2.3
1	C	100	ASN	2.3
1	C	527	ASP	2.3
1	A	494	GLU	2.3
1	C	564	VAL	2.3
1	B	429	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	256	ASP	2.3
1	B	594	ASP	2.3
1	C	577	ALA	2.3
1	B	245	LEU	2.3
1	A	617	TYR	2.3
1	A	101	SER	2.2
1	A	483	ASP	2.2
1	A	489	GLY	2.2
1	A	532	ALA	2.2
1	C	567	LEU	2.2
1	A	89	TRP	2.2
1	A	531	TYR	2.2
1	B	534	TYR	2.2
1	C	532	ALA	2.1
1	C	573	GLU	2.1
1	C	88	PRO	2.1
1	C	206	LEU	2.1
1	B	240	LYS	2.1
1	A	486	PHE	2.1
1	C	193	TRP	2.1
1	C	552	ALA	2.1
1	C	509	VAL	2.0
1	B	99	MET	2.0
1	C	92	ALA	2.0
1	A	567	LEU	2.0
1	B	212	ASP	2.0
1	A	91	THR	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 [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
3	GOL	B	802	6/6	0.73	0.15	41,55,56,68	0
2	PEG	A	701	7/7	0.77	0.25	27,35,57,61	0
2	PEG	B	801	7/7	0.81	0.11	43,47,53,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.